PSPManalysis

A package for numerical analysis of physiologically structured population models

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This software package is distributed in the hope that it will be useful for the analysis of physiologically structured population models (PSPMs) or life history models in general. If you are not familiar with PSPMs there are many sources you can check, in particular the original book by Metz & Diekmann (1986), but a more gentle introduction is provided in De Roos (1997).

An earlier version of this software has been used to produce the many bifurcation graphs of equilibria in structured population models that appear in De Roos & Persson (2013). The approach is also shortly discussed in the Technical Appendices of that Monograph. The basic layer of the software has hence been tested quite extensively. The current version is built on top of that basic layer to make the implementation of a particular PSPM easier and to make the software package accessible from R, Matlab or Octave. The software can also be used from the command-line of any Unix-based system (Linux or Mac OS) without the overhead of R, Matlab or Octave. This manual focuses on the use of the software package from R or Matlab (its use from Octave should be the same).

The package is free software and released under the GNU General Public License without any warranty or even the implied warranty of merchantability or fitness for a particular purpose (the official statement of the GPL). If you are using the software for publications, you are kindly asked to credit this software package by a reference to this documentation and the website that hosts the software package, as these are currently the only sources to be referred to.

In case you encounter any problem with the software package, please first verify the problem is not in your own model-specific file, but indeed is a bug in the general software layer. If you are convinced it is a bug in my programming, send me an email with as accurate a description of the problem as possible. Do not not forget to include your model-specific file and details about the invocation of the scripts that caused the problems.

Any comments and feedback, both on the code and on the current manual is appreciated and will be considered carefully. In particular concrete comments, for example, explicit suggestions for textual changes in the manual and/or corrections of the mistakes (they are definitely there!) will be highly valued and acknowledged.

Enjoy!

André de Roos
Introduction

This software package implements numerical procedures for the analysis of physiologically structured population models (PSPMs). PSPMs represent a class of models that consistently translate continuous-time models of individual life history to the population level. The formulation of such models is discussed extensively in [Metz & Diekmann, 1986] and [De Roos, 1997] and is presented here only as far as needed for the use of the software.

The software allows for four different types of analyses of PSPMs:

- **Demographic analysis**: For linear PSPMs that do not account for density dependence or population feedback on the life history of individual organisms, the long-term population growth rate can be calculated. If the dynamics of such a linear PSPM would be simulated over time in the long run the population would grow exponentially or decline to zero with this population growth rate. The software also automatically calculates the sensitivity of this population growth rate with respect to all model parameters. Furthermore, the software calculates the stable population distribution, which characterises the composition of the population during its exponential growth phase, and the reproductive value of the individuals in this stable population state as a function of their individual state.

- **Equilibrium analysis**: Equilibrium states can be computed for non-linear PSPMs that do account for density dependence or feedback of the population on the life history of individual organisms. These equilibrium states are computed as a function of a single model parameter, resulting in a parameterised curve of equilibrium states. Two types of special points can be detected in these equilibrium curves: limit points, also called saddle-node bifurcation points, and branching points or transcritical bifurcation points. Furthermore, the software allows for the computation of these two types of bifurcation points as a function of two model parameters.

- **Analysis of evolutionary fixed points**: During the computation of equilibrium curves of a non-linear PSM the software also can check whether an evolutionary singular point as defined by Adaptive Dynamics or ESS-theory ([Dieckmann, 1997]; [Metz et al., 1996]) is encountered. These singular points are subsequently classified as either a convergent stable strategy (CSS), an evolutionary branching point (EBP) or an evolutionary repellor (ERP) ([Geritz et al., 1998]). The software can also compute the value of a detected evolutionary singular point as a function of a second model parameter and can, starting from a detected evolutionary singular point, compute the pairwise invasibility plot ([Dieckmann, 1997]; [Metz et al., 1996]).
• **Evolutionary dynamics simulation**: The dynamics of life history trait values, which in the model occur as parameters, can be simulated over evolutionary time scales, using the canonical equation for adaptive dynamics as explained in [Dieckmann & Law (1996)](#). These evolutionary dynamic simulations are based on the assumption that the system approaches an ecological equilibrium in between mutation events, which change the value of the life history trait. The evolutionary rate of change is proportional to the selection gradient in the ecological equilibrium and the population birth rate.

The software package consists of a collection of routines implemented in C with frontends that allows the software to be used from either R, Matlab or Octave. The implementation of the elements of the PSPM under study, however, have to be programmed in C, using the template files provided with the package. These design decisions have been inspired by preliminary tests of the computational efficiency. I would have preferred to use either R or Matlab instead of C for the implementation of the user-defined ingredients of the PSPM under study, but this would increase the execution time by roughly 2 orders of magnitude. Computations would then have been excruciatingly slow, which (hopefully) justifies the added difficulty of using C.

The basic methodology to numerically compute the equilibrium of a PSPM has been presented in [Kirkilionis et al. (2001)](#) and [Diekmann et al. (2003)](#), while [De Roos (2008)](#) presented the modification of the latter approach to compute the demographic characteristics of a linear PSPM. For the interested reader this manual provides a brief sketch of this computational approach in chapter [16](#).
2.1 Prerequisites

The package uses the R CMD SHLIB command in R to compile C files into a shared library that can be loaded for computations. This implies that a functioning C compiler should be available, which is standard when using R on Linux systems. Newer versions of Mac OS X do not automatically include a compiler with the basic distribution and hence require installation of the command-line tools of Xcode, the development environment on Mac OS X. On Windows systems the Rtools package has to be installed to be able to compile the C files. The package is tested while using Rstudio as an environment to process R commands, although any other way to process R commands should work as well.

2.2 Package installation and testing

- Unpack the downloaded compressed file PSPManalysis.zip. This will create a directory PSPManalysis, which you can move to a location of your choice in your file system.
- Start Rstudio, change to the directory PSPManalysis and execute the command `source("PSPManalysis.R")`. This script defines the variables and functions that are necessary for further computations.
- Change to the directory Tests, which is a subdirectory of PSPManalysis. Execute the R script `alldemotests.R` using the command `source("alldemotests.R")`, which subsequently calls the R scripts Medfly_demo.R and KlanjsekDEB_demo.R and prints or plots the results in various ways. These scripts tests the working of the demographic analysis of the software package.
- Subsequently execute the R script `allequitests` using the command `source("allequitests.R")`, which runs the scripts PNAS2002equi_demo.R, Indet_growth_demo.R and KooijmanDEB_demo.R. These scripts perform equilibrium computations of 3 different PSPMs and illustrate the detection of saddle-node and transcritical bifurcations in equilibrium curves and the continuation of these bifurcation points as a function of 2 model parameters (PNAS2002equi_demo.R). The script Indet_growth_demo.R illustrates the detection of an evolutionary singular point and its continuation as a function of a model parameter, the construction of the pairwise invasibility plot starting from the detected evolutionary singular point, as well as the simulation of evolutionary dynamics in 2 life history parameters.
For demographic analysis of PSPMs use the problem file Medly.h as a template to implement the specific ingredients of the PSPM that you want to analyse, following the steps discussed in chapter 4. For equilibrium computations use the problem file PNAS2002.h as a template to implement the specific ingredients of the PSPM that you want to analyse, following the steps discussed in chapter 7.
Demographic analysis of linear PSPMs
Model formulation and ingredients

The core of a linear PSPM consists of a model of the individual life history that is based on the following assumptions:

- Individuals are characterised by their *individual* or *i-state*, which is a (finite) set of physiological characteristics (traits such as age, size, sex, energy reserves):
  \[ \chi = (\chi_1, \ldots, \chi_k) \in \Omega \subset \mathbb{R}^k \]

- Individuals are born with an *i-state* \( \chi_b \) that is one of a finite set of possible states at birth:
  \[ \chi_b \in \{ \phi_1, \ldots, \phi_m \} \]
  with each potential state at birth \( \phi_j \) a valid *i-state*:
  \[ \phi_j = (\phi_{j1}, \ldots, \phi_{jk}) \in \Omega \subset \mathbb{R}^k \]

- Development follows a deterministic process that is continuous in time:
  \[ \frac{d\chi}{da} = g(\chi, \chi_b) \]
  The development rate \( g(\chi, \chi_b) \) is a function of the individual state and the individual’s state at birth

- Reproduction is modeled by a per-capita offspring production rate (or fecundity) \( \beta(\chi, \chi_b) \), dependent on the individual state and the individual’s state at birth

- Mortality is modeled by a per-capita death rate \( \mu(\chi, \chi_b) \), dependent on the individual state and the individual’s state at birth

All assumptions above are characteristic for the general class of PSPMs. The most restrictive of these assumptions concerns the deterministic development process. Biologically, this assumption implies that all individuals that are born with the same state at birth will remain identical throughout their life and will hence not diverge in their *i-state* characteristics. Reproduction and mortality on the other hand are at an individual level considered as stochastic processes, which translate to per-capita rate functions at the population level, given that it is assumed that the number of individuals is large (technically speaking the number of individuals for every possible *i-state*).
Implementation of an example model

The steps needed for the implementation of a particular PSPM will be discussed using a simple model for the life history of the Mediterranean fruitfly, which is also discussed in De Roos (2008). The individual life history in this model is only age-dependent with both age-dependent birth and mortality rates. The PSPM for this model can be described by the following partial differential equation (PDE) for the population age-distribution \( n(t, a) \):

\[
\frac{\partial n}{\partial t} + \frac{\partial n}{\partial a} = -\mu(a) n(t, a)
\]

\[
n(t, 0) = \int_{A_j}^{\infty} \beta(a) n(t, a) \, da
\]

\[
\beta(a) = \beta_0 e^{-\beta_1 (a-A_j)}, \quad \text{if } a > A_j
\]

\[
\mu(a) = \mu_0 e^{\mu_1 a}
\]

The first, partial differential equation above describes the changes in the population age-distribution \( n(t, a) \) through aging (\( \partial n/\partial a \)) and mortality, which is modeled by the mortality rate \( \mu(a) \). The second equation, representing the boundary condition for the partial differential equation, describes the total population reproduction rate \( n(t, 0) \), which equals the cumulative fecundity of all individuals older than \( A_j \), the age at maturation. The mortality rate \( \mu(a) \) is an exponentially increasing function of age, whereas the fecundity \( \beta(a) \) is highest for just maturing individuals (\( a = A_j \)) and decreases exponentially with age afterward.

The implementation of this model, which I will refer to as the Medfly model, for analysis with the software package requires the specification of 10 pieces of C-code arranged in two different sections:

- **Section 1**: Problem dimensions, numerical settings and model parameters
- **Section 2**: Definition of the individual life history functions, such as development (growth), fecundity and mortality.

The pieces of C-code are discussed in detail in the next 2 sections with 10 subsections. The code can be found in the file `Medfly.h` in the directory `Tests`. To implement your own model you only need a basic understanding of C, which programming language I will
CHAPTER 4. IMPLEMENTATION OF AN EXAMPLE MODEL

not further discuss here. It is advisable to use one of the example models in the directory Tests as a basis for the implementation, for example, by opening the file Medfly.h in Matlab’s built-in editor and saving it with a different name. The extension of your model-specific file should however remain .h.

The software allows for the analysis of models with multiple structured populations, each of which consists of individuals that are characterised by a finite number of individual state variables. The number of state variables characterising an individual should, however, be the same for each of the structured populations in the model. Furthermore, at birth individuals may have one of a finite number of states-at-birth. To distinguish between populations, between individual state variables and between different states-at-birth, in the following the index \( p \) will consistently refer to the index of the structured population in the model. Because the dimension setting \( \text{POPULATION\_NR} \) is used to specify the number of populations in the model (see the next section), \( p \) should have values in the range 0, 1, \ldots, \( \text{POPULATION\_NR}-1 \). Similarly, the index \( i \) will consistently refer to the index of a particular individual state variable, which should always take values in the range 0, 1, \ldots, \( \text{I\_STATE\_DIM}-1 \), given that the dimension setting \( \text{I\_STATE\_DIM} \) determines the number of individual state variables (see the next section).

As listed in chapter 3, individuals are assumed to be born with an \( i\)-state \( \chi_b \) that is one of a finite set of possible states-at-birth, each of which is a valid \( i\)-state:

\[
\chi_b \in \{\phi_1, \ldots, \phi_m\}, \quad \phi_j = (\phi_j1, \ldots, \phi_jk) \in \Omega \subset \mathbb{R}^k
\]

Given that individual age is the only \( i\)-state variable in the Medfly model, all individuals have the same state at birth and hence \( m = 1 \). The option to specify multiple states-at-birth is hence not relevant for the example model discussed in this implementation chapter. This might hold more generally; most if not all physiologically structured population models that have been reported on in the literature so far are characterised by such a unique state-at-birth for all individuals. Nonetheless, the option to define multiple states-at-birth opens up some interesting research possibilities, which are discussed further in chapter 13.

Since models involving multiple states-at-birth are not very common, information that relates to this option will be distinguished in the text by setting them apart in paragraphs like this one. The index \( j \) will be used to refer to the index of a particular state-at-birth in the set \( \{\phi_1, \ldots, \phi_m\} \). The number \( m \) of possible states-at-birth is set dynamically in the model file (see section 4.2.1).

4.1 Problem dimensions, numerical settings and model parameters

4.1.1 Definition of problem dimensions and optional numerical settings

The code box below defines the different dimensions of the model and the numerical settings to be used in the computations.
4.1. PROBLEM DIMENSIONS, NUMERICAL SETTINGS AND MODEL PARAMETERS

Code box 4.1: Definition of dimensions and numerical settings

```
// Dimension settings: Required
#define POPULATION_NR 1 // Structured consumer population
#define STAGES 2 // Juvenile & adult
#define I_STATE_DIM 1 // See below
#define PARAMETER_NR 5

// Numerical settings: Optional (default values adopted otherwise)
#define MIN_SURVIVAL 1.0E-9 // Survival at which individual is considered dead
#define MAX_AGE 100000 // Give some absolute maximum for individual age
#define DYTOL 1.0E-7 // Variable tolerance
#define RHSTOL 1.0E-8 // Function tolerance
```

The software can simultaneously compute the population growth of more than a single population. At the start of the problem file the variable POPULATION_NR has to be defined equal to the number of structured populations accounted for in the model. For the Medfly example this is obviously equal to 1 (line 2 in the code box above).

The variable STAGES has to be defined equal to the number of life stages that can be distinguished in the individual life history (line 3 in the code box above). While integrating the ODEs for the individual life history numerical problems may occur when the right hand side of the ODEs changes abruptly in value at a certain threshold value of the individual state, as a consequence of discontinuities in the development rate, the mortality rate or the fecundity. Each of such thresholds in the individual life history should be distinguished as a stage boundary. In the Medfly model the fecundity $\beta(a)$ changes from 0 just before $a = A_J$ to $\beta_0$ at $a = A_J$ and $\beta_0 \exp(-\beta_1(a-A_J))$ at larger ages. At $a = A_J$ $\beta(a)$ thus exhibits a discontinuity, which separates the juvenile and the adult stage from each other. The variable STAGES is therefore set equal to 2.

The variable I_STATE_DIM (line 4 in the code box above) defines the dimension of the individual state. As only age characterises the individuals in the Medfly model, this variable is defined equal to 1.

The last required parameter that has to be specified is the number of parameters in the model (set in line 5 in the code box above). In the Medfly model this equals 5 ($\beta_0$, $\beta_1$, $A_J$, $\mu_0$ and $\mu_1$).

The remaining definitions in the code box are all optional and can be left away. A list of all possible variables that can be changed by a definition in this code section is provided in chapter [15]. The variable MIN_SURVIVAL determines the threshold of the survival probability below which an individual is considered dead. The integration over the individual life history stops whenever the survival probability falls below this threshold value. In the code above (line 8) the minimum survival is set to $10^{-9}$, which is in fact the default value and is hence superfluous. Note that the value of MIN_SURVIVAL can not be set equal to 0. As an alternative to using 0 MIN_SURVIVAL can be set to a very small value like $10^{-100}$.

The variable MAX_AGE (line 9 in the code box above) can be used as an alternative to determine the end of an individual life and to stop the integration over the individual life history. In the Medfly model there is no maximum individual age and hence the variable is set to a very high value (100000), which the individuals will never reach, because before that age their survival probability has already dropped below its threshold value ($10^{-9}$).
The remaining two quantities $\text{DYTOL}$ and $\text{RHSTOL}$ determine whether a solution has been found. In general, both demographic analysis as well as equilibrium analysis of PSPMs boils down to solving a system of nonlinear equations that can be represented as $G(y) = 0$ for a set of unknowns $y$ in an iterative manner. The subsequent estimates of the solution in the Newton iterations can be labeled as $y_p$ and $y_{p+1}$. A solution is now considered to be located if both of the following conditions hold:

$$
||y_{p+1} - y_p|| < \epsilon_y \\
||G(y_{p+1})|| < \epsilon_G
$$

where $||.||$ refers to the Euclidean norm. $\text{DYTOL}$ and $\text{RHSTOL}$ are the quantities $\epsilon_y$ and $\epsilon_G$, respectively. Increasing (decreasing) their value leads to easier (harder) acceptance of a set of unknowns as a solution to the system of equations $G(y) = 0$. The definition of these two accuracies in the code box is in fact superfluous as they are defined equal to their default values (see chapter [15]).

### 4.1.2 Definition of parameter names and values

The code box below assigns each of the model parameters a meaningful name and a default value.

**Code box 4.2: Definition of parameter names and values**

```c
// Descriptive names of parameters in parameter array (at least two parameters are required)
char *parameternames[PARAMETER_NR] =
{ "Beta0", "Beta1", "AJ", "Mu0", "Mu1"};

// Default values of all parameters
double parameter[PARAMETER_NR] =
{47.0, 0.04, 11.0, 0.00095, 0.0581};
```

Model parameter values are stored by the program in the vector variable `parameter`. The lines 2-3 above assign each of the elements this vector a more meaningful, model-specific name. These name strings can not be used in the remaining parts of the model implementation, they only serve to make the output files produced by the program more readable. These output files contain a small header text indicating among other details which parameter values were used for the computation of the results contained in the output file. In this report the parameter names are listed together with their value. To adapt the above code to a different model, the code on line 2 of the code box above should remain the same, only change line 3 as needed (possibly extending it over multiple lines in case there are many parameters).

The default values to use for the model parameters are specified by the declaration of the vector `parameter[PARAMETR_NR]` on line 6-7 of the previous code box. The values should be specified as a comma-separated array of values within braces (don’t forget the closing semi-colon at the end of the statement!). To adapt the above code to a different model, the code on line 6 of the code box above should remain the same, only change line 7 as needed (possibly extending it over multiple lines in case there are many parameters).

### 4.1.3 Definition of aliases to simplify implementation

The code box below defines aliases for program variables used in the C-implementation of the model, such that they are more easily identified with the model ingredients. Defining
these aliases is optional but strongly advised as it makes model implementation more straightforward.

**Code box 4.3: Definition of aliases**

```c
// Aliases definitions for all istate variables
#define AGE istate[0][0]

// Aliases definitions for all parameters
#define BETA0 parameter[ 0] // Default: 47.0
#define BETA1 parameter[ 1] // Default: 0.04
#define MU0 parameter[ 3] // Default: 0.00095
#define MU1 parameter[ 4] // Default: 0.0581
```

The developmental rates in individual state, fecundity and mortality in any model depend on the individual state itself, on the individual’s state at birth and on model parameters. The value of the individual state variables at a particular age are always referred to with the program variable `istate[p][i]`, where the index `p` refers to the number of the population and the index `i` refers to the number of the individual state variables. Notice that in C array indices run from 0 (as opposed to 1 like in Matlab)! Similarly, the value of the individual’s state variables at birth are always referred to with the program variable `birthstate[p][i]`. In case there are multiple populations and/or more than a single individual state variable, it is up to the user to keep track of which index pertains to which population or individual state variable. In the Medfly model there is only a single population and a single individual state variable, while the state at birth is rather irrelevant as it equals age 0. Therefore, `istate[0][0]` is the only program quantity to give a more meaningful name (line 2 in the code box above).

As discussed in the previous section all model parameters are contained in a vector named `parameter` in the code. Which element of this vector represents which model-specific parameter is up to the user. To prevent mixing up the interpretation of the different vector elements and hence to prevent mistakes, it is strongly advised to define meaningful, model-specific aliases for each of the elements of the vector `parameter` as is illustrated in lines 5-9 in the code box above. It is best to avoid completely the direct use of the program variable `parameter` in any part of the model specification and only use the models-specific aliases.

### 4.2 Definition of the individual life history

#### 4.2.1 Specifying the number of possible states-at-birth

The first routine to be implemented for a particular life history model defines for every population in the model the number of possible states-at-birth that an individual can be born with (i.e. the value of the size `m` of the set `\{\phi_1, \ldots, \phi_m\}`).
**CHAPTER 4. IMPLEMENTATION OF AN EXAMPLE MODEL**

**Code box 4.4: Specification of the number of possible states-at-birth**

```c
/*
 * Specify the number of states at birth for the individuals in all structured
 * populations in the problem in the vector BirthStates[].
 */
void SetBirthStates(int BirthStates[POPULATION_NR], double E[])
{
    BirthStates[0] = 1;
    return;
}
```

For each population with index $p$ the variable $\text{BirthStates}[p]$ has to be set to the number of possible states at birth. Because individual age is the only $i$-state variable the Medfly model, the state-at-birth is unique and hence $\text{BirthStates}[0]$ is set to 1.

Note that different populations may have different numbers of states-at-birth. $\text{BirthStates}[p]$ hence does not need to be the same for all $p$.

**4.2.2 Specifying the value of all possible states-at-birth**

The next routine to implement defines for every possible state-at-birth with index $j$ the actual value of the different individual state variables at birth $\phi_j = (\phi_{j1}, \ldots, \phi_{jk})$:

**Code box 4.5: Specification of the value of all possible states-at-birth**

```c
/*
 * Specify all the possible states at birth for all individuals in all
 * structured populations in the problem. BirthStateNr represents the index of
 * the state of birth to be specified. Each state at birth should be a single,
 * constant value for each i-state variable.
 *
 * Notice that the first index of the variable 'istate[]' refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */
void StateAtBirth(double *istate[POPULATION_NR], int BirthStateNr, double E[])
{
    AGE = 0.0;
    return;
}
```

For every population ($p = 0, 1, \ldots, \text{POPULATION_NR}-1$) the value of each individual state variable $\text{istate}[p][i]$ ($i = 0, 1, \ldots, \text{I_STATE_DIM}-1$) has to be assigned a unique value, from which individual development will start at age 0. As shown in the example of the Medfly model, if the life history depends on the age of the individual, age should be explicitly included as one of the individual state variables. The program does not automatically include individual age in its characterisation of the individual state, even though integration over the entire life history (as a function of age) is carried out. For the Medfly model age is the only individual state variables and set to 0 at birth.
This routine will be called as many times as there are possible states-at-birth. The variable \( \text{BirthStateNr} \) indicates the index \( j \) of the state-at-birth in the set \( \{ \phi_1, \ldots, \phi_m \} \) for which the values have to be set in the current invocation of the routine. The routine will thus be called with \( \text{BirthStateNr} \) set equal to a value in \( 0, 1, \ldots, m - 1 \) (Remember the starting index 0 in \( \mathbb{C} \)). If there are multiple states-at-birth (\( \text{BirthStates}[p] > 1 \)) the definition of the values of the \( i \)-state variables has to depend explicitly on the index \( \text{BirthStateNr} \) to make the states-at-birth different from each other. Furthermore, if the problem involves multiple structured populations the number of possible states-at-birth can be different for each of them, which might lead to a situation that the routine above is called with a value of the index \( \text{BirthStateNr} \) that is larger than the maximum number of states-at-birth for a particular population (\( \text{BirthStateNr} \geq \text{BirthStates}[p] \)). The program safely ignores such inappropriate state-at-birth specifications.

### 4.2.3 Definition of boundaries between discrete stages

The next routine determines the boundaries between consecutive stages in the individual life history.

**Code box 4.6: Definition of discrete stage boundaries**

```c
/*
 * Specify the threshold determining the end point of each discrete life
 * stage in individual life history as function of the i-state variables and
 * the individual's state at birth for all populations in every life stage.
 * Notice that the first index of the variable 'istate[]' refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void IntervalLimit(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
                   double *birthstate[POPULATION_NR], int BirthStateNr, double E[],
                   double limit[POPULATION_NR])
{
    if (lifestage[0] == 0)
        limit[0] = AGE - AJ;
    return;
}
```

In this routine the variable \( \text{limit}[p] \) has to be defined, which has as many elements as there are populations (\( p = 0 \ldots \text{POPULATION_NR}-1 \)). The life stage that the individual is in at the moment this routine is called, is determined by the variable \( \text{lifestage}[p] \), which has a value of 0 if the individual is in the first life stage and a value of \( \text{STAGES}-1 \) if it is in the last life stage. The element \( \text{limit}[p] \) should now indicate when the current life stage as given in \( \text{lifestage}[p] \) ends. In particular, the program considers the current life stage to end when \( \text{limit}[p] \) turns from negative to positive. For the end of the last life stage the death of old age, either by reaching the maximum age \( \text{MAX_AGE} \) or by reaching the minimum survival threshold \( \text{MIN_SURVIVAL} \), does not have to be specified separately,
the program takes care of that automatically. In the Medfly model therefore only the end
of the larval stage has to be specified, as expressed in lines 16-17 of the code box above.

The threshold value that has to be stored and returned to the program in \texttt{limit[p]} will depend on the individual state variables, possibly on the individual’s state-at-birth and will be different for individuals in different life stages. For this reason, the routine \texttt{IntervalLimit()} has as arguments \texttt{lifestage[]}, specifying the life stage that the individual is currently in, \texttt{istate[][]}, the individual state, and \texttt{birthstate[][]}, the individual’s state-at-birth.

Like the previous routine, this routine will be called as many times as there are possible states-at-birth, because the state-at-birth may influence the threshold between consecutive life stages. The same holds for the routines discussed in sections 4.2.4-4.2.7 below, which define changes in the \textit{i-state} variables, the fecundity and the mortality of individuals, respectively. In essence, individuals with different states-at-birth are treated as constituting subpopulations within the same structured population.

Because of the possible dependence on the state-at-birth the variables \texttt{birthstate[][]} and \texttt{BirthStateNr} are passed as arguments to this routine and the ones discussed in sections 4.2.4-4.2.7. These arguments contain the values of the \textit{i-state} variables and the index in the set \{\textit{φ}_1, \ldots, \textit{φ}_m\}, respectively, for which the routine is invoked and for which the threshold between consecutive life stages has to be evaluated.

If the problem involves multiple structured populations and the number of possible states-at-birth differs among them, the routine above may be called with a value of the index \texttt{BirthStateNr} that is larger than the maximum number of states-at-birth for a particular population (\texttt{BirthStateNr ≥ BirthStates[p]}). Although this circumstance may seem confusing, the user does not have to worry about it, as the program is designed to safely ignore such assignments of thresholds between consecutive life stages, changes in the \textit{i-state} variables, fecundity and mortality of individuals for states-at-birth with index \texttt{BirthStateNr ≥ BirthStates[p]} that are inappropriate for the structured population with index \texttt{p}.

Notice that the function header shown in code box 4.6 also contains an array \texttt{E[]} as a variable. This array will contain the values of the environment variables during equilibrium computations of PSPMs (see chapters 6 to 8). In demographic analysis of PSPMs this variable is non-functional and is best ignored, using it in a statement inside the routine may even cause the program to crash. The only reason for the presence of this variable in the function header is to keep the function declaration the same for both demographic and equilibrium analysis computations. In principle, the same model-specific file can hence be used for both types of analysis. The variable \texttt{E[]} will for the same reasons also be part of the headers of the next 4 routines.

Tip: The more advanced user who wants to perform both demographic and equilibrium analysis using the same model-specific file should notice that the array of environment variables \texttt{E[]} can in principle be used inside all the routines, if the dimension \texttt{ENVIRON_DIM} determining the number of environment variables has been set (see code box 7.1 on page 39 for details). The appropriate value to use for the environment variables should be assigned
4.2. DEFINITION OF THE INDIVIDUAL LIFE HISTORY

to the elements \( E[e] \) in the routine \texttt{StateAtBirth()} (see the next code box 4.5), after which it will keep the same value throughout all the subsequent routines.

4.2.4 Specification of continuous individual state development

Code box 4.7: Specification of continuous individual state development

```c
#include <stdio.h>

void Development(int lifestage[POPULATION_NR], double *istate[POPULATION_NR], double *birthstate[POPULATION_NR], int BirthStateNr, double E[], double development[POPULATION_NR][I_STATE_DIM])
{
    development[0][0] = 1.0;
    return;
}
```

This routine specifies the right-hand side of the ODE:

\[
\frac{d\chi}{da} = g(\chi, \chi_b)
\]

that determines the continuous development of the individual state variables during the life history. In the Medfly model the specification is obviously trivial. More generally, the value of \( \text{development}[p][i] \) determines for each structured population \( p \) the development in the individual state variable \( i \). Notice that these development rates may differ in different life stages, for example growth in body size may be different for juveniles and adults in case adults invest a lot of energy into reproduction. The development rates should then be specified dependent on the current life stage the individual is in. This current life stage at the moment the routine is evaluated is contained in the variable \( \text{lifestage}[p] \). The development rate may furthermore depend on the individual state variables and possibly on the individual’s state-at-birth, which is the reason for \( \text{istate}[] [] \), the individual state, and \( \text{birthstate}[] [] \), the individual’s state-at-birth, as arguments to this routine.

\textbf{⇒} Refer to the remarks in section 4.2.3 concerning the dependence on the individual’s state-at-birth.

4.2.5 Specification of discrete individual state changes at stage transitions

Even though not listed among the basic assumptions of the PSPM in the beginning of this chapter, it is permissible to have discrete changes or jumps in the individual state variables at the transition between two consecutive life stages. If these occur, they should be programmed in the following routine.
CHAPTER 4. IMPLEMENTATION OF AN EXAMPLE MODEL

Code box 4.8: Specification of discrete individual state changes

```c
/*
 * Specify the possible discrete changes (jumps) in the individual state
 * variables when ENTERING the stage specified by 'lifestage[]'.
 * Notice that the first index of the variable 'istate[][]' refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void DiscreteChanges(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
                     double *birthstate[POPULATION_NR], int BirthStateNr, double E[[]])
{
    return;
}
```

This routine is not relevant in case of the Medfly model and hence its contents are empty (apart for the necessary return; statement).

This routine is called whenever a transition between two consecutive life stages is reached during the integration over the individual life history. It should be noted that the value of the variable lifestage[p] indicates the life stage that is entered, that is, following the current stage boundary. This routine will hence never be called with a value of one of the elements lifestage[p] equal to 0. The discrete changes in the individual state variables have to be implemented by assigning new values to the variables istate[p][i]. These assignments may as before depend on the life stage that is entered, as specified by the variable lifestage[], the (old values) of the individual state variables, contained in the argument istate[][], and possibly on the individual’s state-at-birth, specified in the argument birthstate[]. If no assignment of a value to istate[p][i] is implemented, that particular individual state variable will keep its current value.

Refer also to the remarks in section 4.2.3 concerning the dependence on the individual’s state-at-birth.

4.2.6 Specification of fecundity

The following routine specifies the fecundity as a function of the individual state. The code fragment below implements the function \( \beta(a) = \beta_0 e^{-\beta_1(a-A)} \) for the Medfly model. It provides a good example of how to assign a different value for a particular life history rate dependent on the life stage that an individual is in. The same approach can also be used in the other routines specifying the life history rates of individuals.
4.2. DEFINITION OF THE INDIVIDUAL LIFE HISTORY

Code box 4.9: Specification of fecundity

```c
/*
 * Specify the fecundity of individuals as a function of the i-state
 * variables and the individual’s state at birth for all populations in every
 * life stage.
 *
 * The number of offspring produced has to be specified for every possible
 * state at birth in the variable ‘fecundity[]’'. The first index of this
 * variable refers to the number of the structured population, the second
 * index refers to the number of the birth state.
 *
 * Notice that the first index of the variable ‘istate[]’ refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void Fecundity(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
               double *birthstate[POPULATION_NR], int BirthStateNr, double E[],
               double *fecundity[POPULATION_NR])
{
  if (lifestage[0] == 1) // Only for adults
  {
    fecundity[0][0] = BETA0*exp(-BETA1*(AGE - AJ));
  }
  else
    fecundity[0][0] = 0;
  return;
}
```

In this routine not only the fecundity (i.e. the number of offspring produced per unit time) has to be specified, but also the state-at-birth of the produced offspring. Therefore, this routine has to assign values to the matrix `fecundity[p][j]`, which determines for the population with index `p` the number of offspring produced per unit time with state-at-birth with index `j` in the set \{\(\phi_1, \ldots, \phi_m\}\}. This fecundity will certainly depend on the life stage that the individual is in (only adults reproduce), which is contained in the argument `lifestage[]`, and on the individual state variables, i.e. the values of the argument `istate[][]`, but possibly also on the individual’s state-at-birth, the values and index of which are specified by the arguments `birthstate[][]` and `BirthStateNr`, respectively.

In the most common case of a unique state-at-birth and a single structured population, like in the Medfly model, the only valid indices are \(p = 0\) and \(j = 0\) and hence only the variable `fecundity[0][0]` has to be assigned.

For more detailed remarks about models with multiple states-at-birth consult section 4.2.3.

4.2.7 Specification of mortality

The last routine specifies the mortality as a function of the individual state.
CHAPTER 4. IMPLEMENTATION OF AN EXAMPLE MODEL

Code box 4.10: Specification of mortality

```c
/* Specify the mortality of individuals as a function of the i-state variables and the individual’s state at birth for all populations in every life stage.

* Notice that the first index of the variable ‘istate[]' refers to the number of the structured population, the second index refers to the number of the individual state variable. The interpretation of the latter is up to the user.
*/

void Mortality(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
               double *birthstate[POPULATION_NR], int BirthStateNr, double E[],
               double mortality[POPULATION_NR])
{
    mortality[0] = MU0*exp(MU1*AGE);
    return;
}
```

For each population the corresponding element of the array mortality[p] should be assigned the mortality rate, possibly dependent on the life stage the individual is in at the moment this routine is called (given in argument lifestage[]), the current i-state of the individual (given in argument istate[][]) and the individual’s state-at-birth (current values and index in the set \{ϕ₁,…,ϕₘ\} given by birthstate[][] and BirthStateNr, respectively).

In the Medfly model the mortality is not influenced by the life stage specifically and is only age-dependent. The line 16 in the code box above implements the function \( \mu(a) = \mu₀e^{μ₁a} \).

Refer to the remarks in section 4.2.3 concerning the dependence on the individual’s state-at-birth.
Model analysis in R

To carry out the analysis in R the first step is to load the script file `PSPManalysis.R` using the command `source("PSPManalysis.R")`. This defines all functions that are required for demographic, equilibrium and evolutionary analysis and a global variable that holds the directory name of of the PSPManalysis package. Compared to the use of this software in Matlab be aware that in R arrays (referred to as vectors in R) are defined using the concatenation function `c()` and strings are specified surrounded by double quotes (""") as opposed to single quotes (').

5.1 Executing the PSPMdemo function

Once the model has been implemented, you can proceed carrying out its analysis, which in the simplest approach is performed by calling the function `PSPMdemo` with the name of the file specifying the PSPM passed as a string argument. It is unnecessary to include the extension .h as part of the file name, the `PSPMdemo` function will strip the .h extension away if it is included. Therefore, the following two invocations of `PSPMdemo` are identical:

\[
\text{Command box 5.A: PSPMdemo call for a single parameter value}
\]

\[
> \text{PSPMdemo("Medfly")}
\]

and

\[
> \text{PSPMdemo("Medfly.h")}
\]

These two calls of the `PSPMdemo`-function will give the same output as the following invocation of the function with the two optional arguments `clean=TRUE` and `force=TRUE`:

\[
\text{Command box 5.A: PSPMdemo call for a single parameter value}
\]

\[
> \text{PSPMdemo("Medfly", clean=TRUE, force=TRUE)}
\]

\[
\text{Building executable /Users/andre/programs/PSPM analysis/Tests/Medflydemo.so ...}
\]

\[
<\text{compilation output suppressed in this box...}>
\]

\[
\text{Executing : PSPMdemo("Medfly", NULL, NULL, NULL)}
\]

\[
\text{Parameter values :}
\]
The `PSPMdemo` function first compiles the model-specific file using R command `R CMD SHLIB` into a dynamically loadable library file, which can subsequently be executed. The output of this compilation step is system specific and hence suppressed in the command box above. The compilation step is only carried out when the executable (on Mac OS X and Linux systems called `Medflydemo.so`) does not exist, or when the model-specific has been changed since the last compilation of the executable. Furthermore, the compilation step is forced by the invocation of `PSPMdemo` with the additional argument `force=TRUE` as in the command box shown above.

When the `PSPMdemo` function is invoked in the way shown above the output of the computation is only printed to the console, the function does not return any variables or results (as is clear from the boxed material above). Apart from printing the exact command-line that has been used to start the computation, the values of the parameters are printed using the meaningful, model-specific names, as set in the code box 4.2 on page 14. Notice that 3 additional but optional arguments to the function `PSPMdemo` are reported as being set to `NULL`, meaning they were not defined.

The numerical output generated by the model is printed as a single line of numbers. The first column of this output contains the computed population growth rate. The second column contains the generation time in the stable population state, which corresponds to the average age at reproduction in the exponentially growing population and is defined as:

\[
\int_0^\infty a e^{-ra} \beta(\chi(a)) F(a) da
\]

in which \(r\) represents the population growth rate, \(\beta(\chi(a))\) the fecundity of an individual with individual state \(\chi(a)\) at age \(a\) and \(F(a)\) the probability that an individual survived up to age \(a\). The following columns show the sensitivity of the population growth rate with respect to the model parameters in the order as they are defined in code box 4.2. For the Medfly model these are the sensitivities to the 5 model parameters that are printed directly above.

The second method to invoke the `PSPMdemo` function is with an additional arguments to calculate the population growth rate as a function of one of the model parameters for a range of values of this parameter. This can be achieved by passing as an additional argument to the function a vector of 5 elements of the following form:

\[c(\text{index}, \text{starting value}, \text{step size}, \text{minimum value}, \text{maximum value})\]

The first element indicates the index of the parameter in the array `parameter` (see code box 4.3) to vary, the second element of the array indicates its starting value from which to compute the curve of the population growth rate as a function of the parameter, the third value indicates the step size in the parameter along this curve (which can be either positive or negative), while the final two elements of the array indicate the minimum and maximum value of the parameter. The computation of the curve of the population growth
rate as a function of the model parameter stops, whenever the minimum or maximum parameter value is reached.

The following R code illustrates this use of the PSPMdemo function for the Medfly model by computing the population growth rate as a function of parameter[2], which is the value of $A_j$, starting at the initial and default value of $A_j = 11$ and computing the growth rate for increasing values of the parameter with step size 0.1, while limiting the computation to the interval $11 \leq A_j \leq 20$.

**Command box 5.B: PSPMdemo call to compute a curve over a parameter range**

```r
> output <- PSPMdemo("Medfly", c(2, 11, 0.1, 11, 20), c(47, 0.04, 11, 0.00095, 0.0581), c('isort', '0'),
+ clean=TRUE, force=TRUE, debug=FALSE)

Building executable /Users/andre/programs/PSPM analysis/Tests/Medflydemo.so ...

$curvedesc
[1] "# Executing : PSPMdemo('Medfly', c(2, 11, 0.1, 11, 20), c(47, 0.04, 11, 0.00095, 0.0581), c('isort', '0'))"
[2] 
[3] # Parameter values :
[4] 
[5] # Beta0 : 47 Beta1 : 0.04 AJ : 11
[6]
[7] # Mu0 : 0.00095 Mu1 : 0.0581
[8] 
[9] # Index of bifurcation parameter #1 : 2
[10] 
[12] 
$curvepoints
V1 V2 V3 V4 V5 V6 V7 V8
[1,] 11.0 0.4190566 13.16726 0.0016158600 -0.1645937 -0.03198198 -1.526360 -0.01132532
[2,] 11.1 0.4158843 13.28218 0.0016018800 -0.1642926 -0.03146749 -1.532324 -0.01148047
[3,] 11.2 0.4127627 13.39705 0.0015881500 -0.1639943 -0.03096572 -1.538315 -0.01163686
[4,] 19.8 0.2538800 23.15013 0.0009190646 -0.1447124 -0.11127611 -2.172537 -0.03082490
[5,] 19.9 0.2527722 23.26222 0.0009146362 -0.1445347 -0.11027447 -2.181510 -0.03112948
[6,] 20.0 0.2516744 23.37427 0.0009102513 -0.1443576 -0.10928690 -2.190525 -0.03143628
```

Some of the intermediate lines of output generated by R in this case are suppressed for brevity. When the PSPMdemo function is invoked in this way to compute parameter dependence, it generates a single list as output (assigned to the variable output in the command box above), which contains two elements, called curvedesc and curvepoints. The variable `output$curvedesc` contains the description of the executed calculation, which is the textual information that is also printed to the R console at the end of calculations. In fact, the PSPMdemo function prints its report on the calculations by execution of the statement `cat(output$curvedesc, sep='\n')`.

The output variable `output$curvepoints` is a two-dimensional array containing columns of computed output with as a first column the value of the parameter, the second column the value of the population growth rate for that particular parameter value and the third column the generation time (the average age at reproduction) in the stable population.
during the exponential growth phase. The subsequent columns represent the sensitivities of the population growth rate to all model parameters, as discussed before. The output of `output$curvepoints` in the box above shows that the data indeed start at \( A_j = 11 \) and that the computation is terminated when a value of \( A_j \) is reached that exceeds the maximum parameter value specified. The data contained in the output variable can subsequently be used for plotting or for further calculations.

### 5.2 Output files generated by the PSPMdemo function

The `PSPMdemo` function and module generates 2 output files when the function is only performing a single population growth rate calculation and 3 output files when the population growth rate is computed as a function of a model parameter. The name of these files is always of the form `<Modelname>-PGR-<NNNN>.<ext>`, in which `<Modelname>` is the same as the name of the file specifying the model excluding its .h extension, `<NNNN>` is a 4-digit number that is unique for the current computation and `<ext>` is the extension, which can be either .err, .csb or .out. Hence, the invocation of the `PSPMdemo` function for the Medfly model, as shown in R command box 5.A, generates the output files `Medfly-PGR-0000.err` and `Medfly-PGR-0000.csb`, while the invocation of the `PSPMdemo` function for the Medfly model, as shown in R command box 5.B, generates three output files: `Medfly-PGR-0001.err`, `Medfly-PGR-0001.csb` and `Medfly-PGR-0001.out`. For the 4-digit number `<NNNN>` in the file name, the program always finds the lowest positive value that is not in use yet. However, whenever the `PSPMdemo` function is invoked with the (optional) argument `clean=TRUE`, as is the case in R command box 5.B, the `PSPMdemo` function deletes all output files that have been generated for the particular model studied (all files called `<Modelname>-PGR-<NNNN>.err`, `<Modelname>-PGR-<NNNN>.csb` and `<Modelname>-PGR-<NNNN>.out`, and hence the 4-digit file identification number will restart at 0000 again.

The file called `<Modelname>-PGR-<NNNN>.err` contains information about the numerical progress of the computation. It reports details on the steps take during the Newton iteration, the convergence to the solution, as well as information about the steps taken along the curve that is being computed. This file can be informative in case the computation of a particular curve stops for unknown reasons, but is otherwise of little use.

The file called `<Modelname>-PGR-<NNNN>.out` contains the same information as is contained in the output variables `output$curvedesc` and `output$curvepoints` returned by the `PSPMdemo` function (see R command box 5.B). The first lines of this file all start with a # sign and contain the information about the run performed, which is also contained in `output$curvedesc` and can be listed by the statement `cat(output$curvedesc, sep='\n')` (see R command box 5.B). Following this descriptive header the file contains columns with computational results that are also contained in the variable `output$curvepoints` (see R command box 5.B), that is, the parameter values, population growth rates, generation times and sensitivities of the population growth rate to all model parameters. R command box 5.B provides an example of the type of output generated by the computational module.

The last output file generated during the population growth rate has a name of the form `<Modelname>-PGR-<NNNN>.csb` and contains information on the stable population distribution for every parameter value for which the population growth rate is computed. This is a binary file, the content of which can be accessed from R using the function
csbread. For example, the file contents of the file Medfly-PGR-0000.csb generated by the computation in R command box 5.B can be listed by:

```r
> csbread("Medfly-PGR-0000.csb")
States in file Medfly-PGR-0000.csb:
1: State-1.100000E+01
2: State-1.110000E+01
3: State-1.120000E+01
...output lines suppressed in this box...
89: State-1.980000E+01
90: State-1.990000E+01
91: State-2.000000E+01
```

Invoking the function csbread with only the file name as argument provides a listing of all the population state stored in the file, one for each of the parameter value for which the population growth rate has been computed. The contents each of these population states can be listed by providing as a second argument to the function csbread either the index of the particular population state in the file or a string with its descriptive name. Therefore, the commands `csbread("Medfly-PGR-0000.csb", 3)` and `csbread("Medfly-PGR-0000.csb", "State-1.120000E+01")` are equivalent, producing the following output:

```r
> csbread("Medfly-PGR-0000.csb", 3)
$BifPars
[1] 11.2
$Parameters
[1] 47.00000 0.04000 11.20000 0.00095 0.05810
$PGR
[1] 0.4127627
$Pop00_BirthStates
Istate00
[1,] 0
$Pop00
StableDist Istate00 ReproVal
[1,] 1.0000000e+00 0.0000000 1.000000
[2,] 8.1299059e-01 0.5004307 1.230034
[3,] 6.6093670e-01 1.0008614 1.513004
...output lines suppressed in this box...
[98,] 1.5566999e-09 46.5417781 8.421419
[99,] 1.2390337e-09 49.0422089 4.603061
[100,] 1.0000000e-09 49.5413326 0.000000
```

This population state, with index 3 and descriptive name State_1_120000E01, pertains to the parameter value $A_j = 11.2$ as its name suggests. The state is returned by the function csbread as a list, which can hence be assigned to a variable in R with the command `state<-csbread("Medfly-PGR-0000.csb", 3)`. The first element of this list (called $BifPars$) contains the value of the bifurcation parameter for this particular state. The second element, an array called $Parameters$, contains the values of all the model parameters for which the population growth rate has been computed, while the third member of the list contains the computed population growth rate. In the case of the Medfly model this is a single scalar value, but if the population growth rate is computed for more than one population at a time, the population growth rate values are making up an array as well. The two subsequent elements characterise the stable population distribution, of which the first (called $Pop00_BirthStates$) specifies the state at birth of the individuals. The other (called $Pop00$) is a two-dimensional array containing in the first column the density profile of the stable population, in the second column the individual state variable and the reproductive value of the individuals in the last column, as shown in the box above.
In the Medfly model individuals are only characterised by their age and hence their is only a single column with individual state variables. If individuals are characterised by more than a single individual state variable the values of these follow in additional columns of the two-dimensional array $\text{Pop00}$. The last column of this array always contains the reproductive value of an individual. For an explanation of the reproductive value and its computation I refer to [De Roos (2008)](http://example.com).

### 5.3 Possible arguments of the PSPMdemo function

As shown in R command box [5.A](http://example.com) at least one argument has to be passed to the `PSPMdemo` function, the base name of the file with the model specification, that is without its `.h` extension. It is the only obligatory argument, all other arguments that can be passed to the `PSPMdemo` function are optional. If the model name is the only argument, the function computes the population growth rate for the default parameter set defined in the `.h` file (see box [5.A](http://example.com)).

The optional second argument to the `PSPMdemo` function is used to compute the population growth rate over a range of a particular model parameter, as shown in and discussed following R command box [5.B](http://example.com).

The optional third argument of the `PSPMdemo` function is a 1-dimensional array of model parameter values. When used, this array should have the same length as the number of parameters in the model (`PARAMETER_NR`). When of this length the values will replace the default values of the parameters that are listed in the model specification file (see code box [4.2](http://example.com) for an example). If the array used for this third argument is not of the correct length `PARAMETER_NR`, it will simply be ignored.

The optional fourth argument of the `PSPMdemo` function is a vector containing possible options that modify the behaviour of the computational module. A useful option is the "test" option, which can be passed to the computational module by using the argument `c("test")` as fourth argument to the `PSPMdemo` function. This invokes the computational module in testing mode, which implies that only a single integration of the individual life history is carried out and no iteration to locate the population growth rate is performed. In testing mode the computational module reports on the dynamics of the individual state variables, the survival and the expected number of offspring produced by an individual during its different life stage as well as over its entire life. Testing mode is very useful to discover whether or not the model implementation gives sensible results or not.

The other possible element of the option vector that modifies the behaviour of the computational module is the "isort" option, which can be passed to the computational module by using for example `c("isort", "1")` as fourth argument to the `PSPMdemo` function (as shown in box [5.B](http://example.com) above). This option modifies the population state output that is stored in the output file, which when using the package in R is a binary file with a name of the form `<Modelname>-PGR-<NNNN>.csb` (see above). By default the computational module reports the information about the stable population state distribution and the reproductive value for 100 equidistant values of the first individual state variable. More specifically, the range of the first individual state variable that is covered during the entire life of an individual until the moment that it is considered dead (i.e. the maximum age or the minimum survival threshold has been reached, see section [4.1.1](http://example.com)) is subdivided into 100 equidistant intervals and the population density function, individual state variables and reproductive value are computed at each of these 100 nodal values of the first state variable. By using the option "isort" the default choice to use the first individual state
variable for this subdivision can be changed to the second, third, and so on. Notice though, that the obligatory index value that has to be passed together with the use of the "isort" option follows the C-convention of ordering arrays starting at 0 (as opposed to R where array indices start at 1). Therefore, passing c("isort", "0") as option array to the PSPMdemo function is the same as the default behaviour: the first individual state variable is used for the subdivision and ordering of the population state distribution, while passing c("isort", "1") would use the second individual state variable for this purpose. Also notice that the default number of subdivisions of the individual state variable and hence the number of nodal values for which the population state distribution is reported can be changed by including a statement of the form

```c
#define COHORT_NR 200
```

among the definitions of the numerical settings in the model specification (see code box 4.2 in section 4.1.1 and chapter 15).

If necessary the options "test" and "isort" can be combined, for example, as

```
c("isort", "1","test")
```

Or equivalently,

```
c("isort", "1","test")
```

Four other optional arguments can be passed to the PSPMdemo function: cvode, clean, force and debug. These are all boolean arguments that hence have to be passed to the PSPMdemo function as `<option name>=TRUE` or `<option name>=FALSE`, the latter being the default value of all options (Specifying these options as argument is hence only useful when setting them equal to TRUE). Unlike the previous arguments, which all modify the computations to be performed, these options modify the behaviour of the PSPMdemo function itself, in particular the compilation of the model specific file into a dynamic library module that can be executed from R. Also unlike all the previous arguments that can be passed, these arguments can be passed in any order and at any position, the PSPMdemo function will filter these 4 optional arguments from the argument list before passing the filtered argument list to the computational routine.

- **Option clean**: When `clean=TRUE` is passed as argument, this argument instructs the PSPMdemo function to delete all result files that have been generated during previous calculations with the model, i.e. as a result of previous calls to PSPMdemo. These result files have names of the form `<Modelname>-<Type>-PGR.err`, `<Modelname>-PGR-<NNNN>.csb` and `<Modelname>-PGR-<NNNN>.out`, in which `<Modelname>` refers to the name of the model (i.e. Medfly in the example model presented in previous sections) and `<NNNN>` is a unique number that distinguishes consecutive computations of the same type of curve with the same model.

- **Option force**: When `force=TRUE` is passed as argument, it instructs the PSPMdemo function to force re-compilation of the model specific file into a dynamic library module that can be executed by R. This option will usually not be needed by normal users, as the PSPMdemo function automatically recompiles the computational module when the model specific file with an .h extension is more recently changed than the compiled dynamic library file. However, if for some unclear reason this automatic recompilation fails, the `force` option can be used to initiate re-compilation.
• Option debug: When debug=TRUE is passed as argument, it instructs the PSPMdemo function to turn on debugging flags while compiling the model specific file into a dynamic library module. This option can be useful to detect programming mistakes in the model-specific file that are otherwise hard to track down. The downside is that depending on the version of R that is used, turning on debugging flags during compilation may generate a lot of output, including warnings about standard files of the operating system that are perfectly correct. It is hence not so easy to spot among all these messages the warnings that relate to the model-specific code that has been implemented.

• Option cvode: Passing cvode=TRUE as argument to the PSPMdemo function is currently only relevant for users of Unix-based systems (Mac OS and Linux) as it has not been tested on Windows installations. By default the computational module uses the Dormand-Prince method (DOPRI5: Hairer et al. [1993]) for the integration of the ordinary differential equations describing the life history of individuals (see chapter 16 for details about these ordinary differential equations). An implementation of the DOPRI5-method is provided with the package in a separate program file (dopri5.c). An alternative integration method, called CVODE, is provided by the Sundials (SUite of Nonlinear and DIfferential/ALgebraic equation Solvers) collection of nonlinear and differential/algebraic equation solvers (see http://www.llnl.gov/CASC/sundials for details). If the appropriate Sundials libraries are installed on your system, the use of the option cvode in the call to PSPMdemo will instruct the function to use the Sundials solver instead of the default DOPRI5 solver for the integration of the ordinary differential equations. In particular for long-lasting integrations, that is when the maximum age reached by individuals is large, using the CVODE-method can significantly speed up the computations.

A full summary of all possible arguments of the PSPMdemo function is given in the R command box 5.C.
5.3. POSSIBLE ARGUMENTS OF THE PSPMDEMO FUNCTION

**Command box 5.C: PSPMdemo help page**

PSPMdemo: Performs demographic analysis of a structured population model.

Syntax:
```r
code <- PSPMdemo(modelname = NULL, curvepars = NULL, parameters = NULL, options = NULL,
cvode = FALSE, clean = FALSE, force = FALSE, debug = FALSE)
```

Arguments:
- **modelname**: (string, required)
  Basename of the file with model specification. The file should have extension `.h`. For example, the model "Medfly" is specified in the file "Medfly.h".
- **curvepars**: (row vector, optional, can be left equal to its default NULL)
  Vector of length 5, specifying:
  - `curvepars[1]`: the index of the parameter to vary
  - `curvepars[2]`: the initial value of the parameter
  - `curvepars[4]`: lower threshold, below which value of the parameter the computation stops
  - `curvepars[5]`: upper threshold, above which value of the parameter the computation stops
- **parameters**: (row vector, optional, can be left equal to its default NULL)
  Vector of length `PARAMETER_NR` (set in the model program file), specifying the values for the model parameters to use in the computation. Vectors of other lengths, including an empty vector will be ignored.
- **options**: (row vector of strings, optional, can be left equal to its default NULL)
  Vector with pairs of strings, consisting of an option name and a value (for example `c("isort", "i")` or single options (i.e. `c("test")`). Possible option names and their values are:
  - `'isort'`, `<index>`: Index of i-state variable to use as ruling variable for sorting the structured populations
  - `'test'`: Perform only a single integration over the life history, reporting dynamics of survival, R0, i-state and interaction variables
- **cvode**: (Boolean, optional argument)
  Specify `cvode = TRUE` as argument to use the CVODE integrator from the Sundials collection of nonlinear and differential/algebraic equation solvers (see http://www.llnl.gov/CASC/sundials for details) Only available on Unix-based systems when Sundials has been installed.
- **clean**: (Boolean, optional argument)
  Specify `clean = TRUE` as argument to remove all the result files of the model before the computation
- **force**: (Boolean, optional argument)
  Specify `force = TRUE` as argument to force a rebuilding of the model before the computation
- **debug**: (Boolean, optional argument)
  Specify `debug = TRUE` as argument to compile the model in verbose mode and with debugging flag set

Output:
- The output is a list containing the following elements:
  - **curvepoints**: Matrix with output for all computed points along the curve
  - **curvevec**: Column vector with strings, summarizing the numerical details of the computed curve (i.e., initial point, parameter values, numerical settings used).
Equilibrium analysis of nonlinear PSPM
Model formulation and ingredients

The core of a nonlinear PSPM consists of a model of the individual life history that is based on the following assumptions:

- Individuals are characterised by their *individual* or *i-state*, which is a (finite) set of physiological characteristics (traits such as age, size, sex, energy reserves):
  \[ \chi = (\chi_1, \ldots, \chi_k) \in \Omega \subset \mathbb{R}^k \]

- Individuals are born with an *i-state* \( \chi_b \) that is one of a finite set of possible states at birth:
  \[ \chi_b \in \{\phi_1, \ldots, \phi_m\} \]
  with each potential state at birth \( \phi_j \) a valid *i-state*:
  \[ \phi_j = (\phi_{j1}, \ldots, \phi_{jk}) \in \Omega \subset \mathbb{R}^k \]

- Individuals are assumed to live in an environment characterised by a (finite) set of *environment variables*:
  \[ E = (E_1, \ldots, E_n) \in \mathbb{R}^n \]
  Environment variables can include independent quantities like resource density and density of predators, but also density-dependent measures like total number of individuals or biomass in the population

- Individual and environmental state variables determine, possibly together with the individual’s state-at-birth, the individual life history (development, reproduction, mortality)

- Development follows a deterministic process that is continuous in time:
  \[ \frac{d\chi}{da} = g(\chi, \chi_b, E) \]

- Reproduction is a function \( \beta(\chi, \chi_b, E) \) of the individual state, the individual’s state-at-birth and its environment
• Mortality is a function $\mu(\chi, \chi_b, E)$ of the individual state, the individual’s state-at-birth and its environment

• Individuals have an impact $\gamma(\chi, \chi_b, E)$ on their environment

• Environment variables may follow autonomous dynamics in absence of individuals:

$$ \frac{dE_i}{dt} = G(E) $$

or be a density-dependent function of the population:

$$ E_i(t) = \int_{\Omega} \gamma_i(\chi, \chi_b, E) n(t, \chi) d\chi $$

Most of the above assumptions are characteristic for the entire class of non-linear PSPMs. The most restrictive of these assumptions concerns the deterministic development process. Biologically, this assumption implies that all individuals that are born with the same state at birth will remain identical throughout their life and will hence not diverge in their $i$-state characteristics. Reproduction and mortality on the other hand are at an individual level considered as stochastic processes, which translate to per-capita rate functions at the population level, given that it is assumed that the number of individuals is large (technically speaking the number of individuals for every possible $i$-state).
Implementation of an example model

The steps needed for the implementation of a particular nonlinear PSPM will be discussed using a simple, tritrophic model for the basic resource, a size-structured consumer population and an unstructured predator population, which is discussed in [De Roos & Persson (2002)]. The individual life history of the consumer in this model is dependent on the individual body length $\ell$, the resource density $R$ and the predator density $P$. The PSPM for this can be described by the following set of ordinary and partial differential equations for the resource density $R$, the consumer size (i.e. length) distribution $c(t, \ell)$ and the predator density $P$:

\[
\frac{dR}{dt} = \rho (R_{\text{max}} - R) - \int_{\ell_b}^{\ell_m} I(\ell, R) c(t, \ell) d\ell \\
\frac{\partial c(t, \ell)}{\partial t} + \frac{\partial g(\ell, R) c(t, \ell)}{\partial \ell} = -\mu(\ell, P) c(t, \ell) \\
g(\ell, R) c(t, \ell_b) = \int_{\ell_j}^{\ell_m} \beta(\ell, R) c(t, \ell) d\ell \\
\frac{dP}{dt} = \left( \epsilon \frac{aB}{1 + T_h B} - \delta \right) P \\
B = \int_{\ell_b}^{\ell_v} \omega \ell^3 c(t, \ell) d\ell
\]

In this model the resource follows semi-chemostat dynamics in the absence of consumers. Consumers forage on the resource following the length-dependent function $I(\ell, R)$, defined as:

\[I(\ell, R) = I_m \ell^2 \frac{R}{R_h + R}\]

Consumers grow in length from their size at birth $\ell_b$ to their absolute maximum size $\ell_m$ with a growth rate $g(\ell, R)$ and produce offspring at a rate $\beta(\ell, R)$, which rates both depend on the consumer length itself and the current resource density:

\[g(\ell, R) = \gamma \left( \ell_m \frac{R}{R_h + R} - \ell \right)\]

\[\beta(\ell, R) = \begin{cases} 
0 & \text{if } \ell < \ell_j \\
\frac{\ell_m \ell^2}{R_h + R} & \text{otherwise}
\end{cases}\]
Consumers experience a mortality rate \( \mu(\ell, P) \) dependent on their own length and the current predator density:

\[
\mu(\ell, P) = \begin{cases} 
\mu_b + \frac{aP}{1 + T_h B} & \text{if } \ell < \ell_v \\
\mu_b & \text{otherwise}
\end{cases}
\]

From these equations it can be inferred that predators forage only on consumers with a length between the length at birth \( \ell_b \) and \( \ell_v \). Larger consumers are invulnerable to predation. The quantity \( B \) represents the biomass of consumers in this vulnerable size range, which biomass governs the growth rate of the predator population following a type II functional response.

The implementation of this model for analysis with the software package requires the specification of 12 pieces of C-code arranged in three different sections:

- **Section 1:** Problem dimensions, numerical settings and model parameters
- **Section 2:** Definition of the individual life history functions, such as development (growth), fecundity and mortality.
- **Section 3:** Definition of the individual feedback on the environment and the equilibrium conditions for environment variables.

The pieces of C-code are discussed in detail in the next 3 sections with 12 subsections. The code can be found in the file `PNAS2002.h` in the directory `Tests`. For ease of writing I will in the following sections often refer to this model as the PNAS model. The first 2 sections with C-code, specifying model constants and the individual life history, are to a considerable extent similar to the corresponding sections with code snippets discussed in the previous chapter on demographic analysis. Some of the text presented in that chapter is therefore repeated here for those readers that skipped the previous chapter.

The software allows for the analysis of models with multiple structured populations, each of which consists of individuals that are characterised by a finite number of individual state variables. The number of state variables characterising an individual should, however, be the same for each of the structured populations in the model. Furthermore, at birth individuals may have one of a finite number of states-at-birth. To distinguish between populations, between individual state variables and between different states-at-birth, in the following sections the index \( p \) will consistently refer to the index of the structured population in the model. Because the dimension setting \texttt{POPULATION_NR} is used to specify the number of populations in the model (see the next section), \( p \) should have values in the range \( 0, 1, \ldots, \texttt{POPULATION_NR} - 1 \). Similarly, the index \( i \) will consistently refer to the index of a particular individual state variable, which should always take values in the range \( 0, 1, \ldots, \texttt{I_STATE_DIM} - 1 \), given that the dimension setting \texttt{I_STATE_DIM} determines the number of individual state variables (see the next section).

\[\Rightarrow\] As listed in chapter 6, individuals are assumed to be born with an \textit{i-state} \( \chi_b \) that is one of a finite set of possible states-at-birth, each of which is a valid \textit{i-state}:

\[
\chi_b \in \{ \phi_1, \ldots, \phi_m \}, \quad \phi_j = (\phi_{j1}, \ldots, \phi_{jk}) \in \Omega \subset \mathbb{R}^k
\]
Given that in the PNAS model all individuals are born with age 0 and length \( \ell = \ell_b \), all individuals have the same state at birth and hence \( m = 1 \). The option
to specify multiple states-at-birth is hence not relevant for the example model
discussed in this implementation chapter. This might hold more generally;
mmost if not all physiologically structured population models that have been
reported on in the literature so far are characterised by such a unique state-
at-birth for all individuals. Nonetheless, the option to define multiple states-
at-birth opens up some interesting research possibilities, which are discussed
further in chapter \[13\].

Since models involving multiple states-at-birth are not very common, information
that relates to this option will be distinguished in the text by setting
them apart in paragraphs like this one. The index \( j \) will be used to refer to the
index of a particular state-at-birth in the set \( \{ \phi_1, \ldots, \phi_m \} \). The number \( m \) of
possible states-at-birth is set dynamically in the model file (see section \[7.2.1\]).

### 7.1 Problem dimensions, numerical settings and model parameters

#### 7.1.1 Definition of problem dimensions and numerical settings.

The code box below defines the different dimensions of the model and the numerical
settings to be used in the computations. These definitions, using \#define\-statement
interpreted by the C\-precompiler, have to appear at the very beginning of the model-
specific file for the code to compile correctly.

The software can handle problems with multiple structured populations. Therefore, the
variable \( \text{POPULATION\_NR} \) has to be defined equal to the number of structured populations
accounted for in the model. For the PNAS example this is obviously equal to 1 (line 2 in
the code box below).

**Code box 7.1: Definition of dimensions and numerical settings**

```c
// Dimension settings: Required
#define POPULATION_NR 1
#define STAGES 3
#define I_STATE_DIM 2
#define ENVIRON_DIM 3
#define INTERACT_DIM 4
#define PARAMETER_NR 16

// Numerical settings: Optional (default values adopted otherwise)
#define MIN_SURVIVAL 1.0E-9 // Survival at which individual is considered dead
#define MAX_AGE 100000 // Give some absolute maximum for individual age
#define DYTOL 1.0E-7 // Variable tolerance
#define RHSTOL 1.0E-6 // Function tolerance
#define ALLOWNEGATIVE 0 // Negative solution values allowed?
#define COHORT_NR 100 // Number of cohorts in state output
```

The variable \( \text{STAGES} \) has to be defined equal to the number of life stages that can be
distinguished in the individual life history (line 3 in the code box above). While integrating
the ODEs for the individual life history numerical problems may occur when the right hand side of the ODEs changes abruptly in value at a certain threshold value of the individual state, as a consequence of discontinuities in the development rate, the mortality rate or the fecundity. Each of such thresholds in the life history should be distinguished as a stage boundary. In the PNAS model the mortality changes discontinuously at \( \ell = \ell_v \), while the fecundity changes discontinuously at \( \ell = \ell_j \). Three life stages can hence be distinguished: vulnerable juveniles, invulnerable juveniles and adults, and the changes in the life history rates are indeed abrupt at the transition boundaries between these stages. The variable \textit{STAGES} is therefore set equal to 3.

The variable \textit{I\_STATE\_DIM} (line 4 in the code box above) defines the dimension of the individual state. For the PNAS model this is defined equal to 2 to account for both individual age and individual length.

The variable \textit{ENVIRON\_DIM} is required in nonlinear PSPM, whereas it is optional for demographic analysis of linear PSPMs. It represents the number of environment variables that determine the life history of an individual. In the PNAS model the growth and fecundity of individual consumers are functions of the resource density \( R \), whereas the mortality is a function of the predator density \( P \) and the biomass of vulnerable consumers \( B \). The latter only influences the mortality of the vulnerable consumers, because it determines the value of the predator functional response. \textit{ENVIRON\_DIM} hence equals 3 in the PNAS model.

The variable \textit{INTERACT\_DIM} defines the number of functions that represent the impact of an individual on its environment. In the PNAS model this feedback of an individual consumer on its environment consists of its grazing rate \( I(\ell, R) \) and the biomass-length relation \( \omega \ell^3 \) determining the biomass of vulnerable consumers, as it represents food for predators. Therefore, the variable \textit{INTERACT\_DIM} should be at least set equal to 2. However, all interaction functions are also saved to the output file generated during a computation. The interaction functions can hence be conveniently used to produce arbitrary output quantities of the form

\[
\int_{\Omega} h(\chi, \chi_b, E) \tilde{n}(\chi) \, d\chi
\]

where \( h(\chi, \chi_b, E) \) is an interaction (weighing) function that can depend on the values of the individual state \( \chi \), the state-at-birth of individuals \( \chi_b \) and the values of the environment variables \( E \), and \( \tilde{n}(\chi) \) is the stable population distribution in equilibrium. Such quantities can therefore represent the total population density in equilibrium (when \( h(\chi, \chi_b, E) = 1 \)), the total population biomass (when \( h(\chi, \chi_b, E) \) equals the biomass of an individual with individual state \( \chi \) and state-at-birth \( \chi_b \)) or the total population birth rate in equilibrium (when \( h(\chi, \chi_b, E) \) is the fecundity of an individual with individual state \( \chi \) and state-at-birth \( \chi_b \)). In the PNAS model I want in addition to the biomass of vulnerable consumers, also the biomass of non-vulnerable juvenile consumers and the biomass of adult consumers as output of the model and hence have set the variable \textit{INTERACT\_DIM} equal to 4.

The last required parameter that has to be specified is the number of parameters in the model (set in line 7 in the code box above). In the PNAS model this equals 16 (\( \rho, R_{\text{max}}, \ell_b, \ell_v, \ell_j, \ell_m, \omega, I_{\text{max}}, R_h, \gamma, r_m, \mu_b, a, T_h, \epsilon \) and \( \delta \)).

The remaining definitions in the code box are all optional and can be left away. A list of all possible variables that can be changed by a definition in this code section is
7.1. PROBLEM DIMENSIONS, NUMERICAL SETTINGS AND MODEL PARAMETERS

The variable \texttt{MIN\_SURVIVAL} determines the threshold of the survival probability below which an individual is considered dead. The integration over the individual life history stops whenever the survival probability falls below this threshold value. In code box 7.1 (line 10) the minimum survival is set to $10^{-9}$, which is in fact the default value and is hence superfluous. Note that the value of \texttt{MIN\_SURVIVAL} can \emph{not} be set equal to 0. As an alternative to using 0 \texttt{MIN\_SURVIVAL} can be set to a very small value like $10^{-100}$.

The variable \texttt{MAX\_AGE} (line 11 in code box 7.1) can be used as an alternative to determine the end of an individual life and to stop the integration over the individual life history. In the PNAS model there is no maximum individual age and hence the variable is set to a very high value (100000), which the individuals will never reach, because before that age their survival probability has already dropped below its threshold value ($10^{-9}$).

The two quantities \texttt{DYTOL} and \texttt{RHSTOL} determine whether a solution has been found. In general, both demographic analysis as well as equilibrium analysis of PSPMs boils down to solving a system of nonlinear equations that can be represented as $G(y) = 0$ for a set of unknowns $y$ in iterative manner. The subsequent estimates of the solution in the Newton iterations can be labeled as $y_p$ and $y_{p+1}$. A solution is now considered to be located if both of the following conditions hold:

$$
\|y_{p+1} - y_p\| < \epsilon_y
$$
$$
\|G(y_{p+1})\| < \epsilon_G
$$

where $\|\|$ refers to the Euclidean norm. \texttt{DYTOL} and \texttt{RHSTOL} are the quantities $\epsilon_y$ and $\epsilon_G$, respectively. Increasing (decreasing) their value leads to easier (harder) acceptance of a set of unknowns as a solution to the system of equations $G(y) = 0$. The definition of these two accuracies in the code box is in fact superfluous as they are defined equal to their default values (see chapter [15]).

The quantity \texttt{ALLOWNEGATIVE} is a flag that can only have a value of 0 or 1 and determines whether or not computations should stop when one of the variables to solve for reaches a negative value. In most population models negative solution values are biologically not relevant and \texttt{ALLOWNEGATIVE} is hence set to 0 by default. Line 16 in code box 7.1 is only included to illustrate the use of \texttt{ALLOWNEGATIVE} and does not change the value of this variable from its default value. Most likely, setting \texttt{ALLOWNEGATIVE} equal to 1 as opposed to 0 will only be useful in specific cases.

The last quantity \texttt{COHORT\_NR} defines the number of cohorts making up the equilibrium population output. During computations of the equilibrium a number of output files will be generated (see section [12.4]), one of which is a Matlab file containing the population equilibrium state for each parameter that the equilibrium values are computed for. \texttt{COHORT\_NR} specifies how many cohorts should be used to represent these equilibrium population states. Larger values will generate more detailed representations of the equilibrium population state at the expense of larger file sizes.

7.1.2 Definition of parameter names and values

The code box below assigns each of the model parameters a meaningful name and a default value.
CHAPTER 7. IMPLEMENTATION OF AN EXAMPLE MODEL

Code box 7.2: Definition of parameter names and values

```c
// Descriptive names of parameters in parameter array (at least two parameters are required)
char *parameternames[PARAMETER_NR] = 
    { "Rho", "Rmax", "Lb", "Lv", "Lj", "Lm", "Beta", "Imax", "Rh", "Gamma", "Rm", "Mub",
    "A", "Th", "Epsilon", "Delta"};

// Default values of all parameters
double parameter[PARAMETER_NR] = 
    { 0.1, 3.0E-4, 7.0, 27.0, 110.0, 300.0, 9.0E-6, 1.0E-4, 1.5E-5, 0.006, 0.003, 0.01,
      5000.0, 0.1, 0.5, 0.01};
```

Model parameter values are stored by the program in the vector variable `parameter`. The lines 2-4 above assign each of the elements this vector a more meaningful, model-specific name. These name strings can not be used in the remaining parts of the model implementation, they only serve to make the output files produced by the program more readable. These output files contain a small header text indicating among other details which parameter values were used for the computation of the results contained in the output file (see section 12.4). In the output file parameters are referred to with their names as defined in the array of strings `parameternames[k]`. To adapt the above code to a different model, the code on line 2 of the code box above should remain the same, only change lines 3-4 as needed (possibly extending it over more lines in case there are many parameters).

The default values to use for the model parameters are specified by the declaration of the vector `parameter[PARAMETER_NR]` on line 7-9 of the previous code box. The values should be specified as a comma-separated array of values within braces (don’t forget the closing semi-colon at the end of the statement that is required in the C-language!). To adapt the above code to a different model, the code on line 7 of the code box above should remain the same, only change lines 8-9 as needed (possibly extending it over more lines in case there are many parameters).

7.1.3 Definition of aliases to simplify implementation

The following code box defines aliases for program variables used in the C-implementation of the model, such that they are more easily identified with the model ingredients. Defining these aliases is optional but strongly advised as it makes model implementation more straightforward.

The life history functions in any model depend on the individual state itself, on the environment variables and on model parameters. The value of the individual state variables at a particular age are always referred to with the program variable `istate[p][i]`, where the index `p` refers to the number of the population and the index `i` refers to the number of the individual state variables. Notice that in C array indices run from 0 (as opposed to 1 like in Matlab)! Similarly, the value of the individuals state variables at birth are always referred to with the program variable `birthstate[p][i]`. In case there are multiple populations and/or more than a single individual state variable, it is up to the user to keep track of which index pertains to which population or individual state variable. In the PNAS model the two individual state variables are age and length, which are identified with the first and second element of the individual state vector, `istate[0][0]` and `istate[0][1]`, respectively (line 2-3 in the code box below).
7.1. PROBLEM DIMENSIONS, NUMERICAL SETTINGS AND MODEL PARAMETERS

Code box 7.3: Definition of aliases

```c
// Aliases definitions for all istate variables
#define AGE istate[0][0]
#define LENGTH istate[0][1]

// Aliases definitions for all environment variables
#define R E[0]
#define P E[1]
#define B E[2]

// Aliases definitions for all parameters
#define RHO parameter[0] // Default: 0.1
#define RMAX parameter[1] // Default: 3.0E-4
#define IMAX parameter[7] // Default: 1.0E-4
#define RH parameter[8] // Default: 1.5E-5
#define GAMMA parameter[9] // Default: 0.006
#define RM parameter[10] // Default: 0.003
#define MUB parameter[11] // Default: 0.01
#define A parameter[12] // Default: 5000.0
#define TH parameter[13] // Default: 0.1
#define EPSILON parameter[14] // Default: 0.5
#define DELTA parameter[15] // Default: 0.01
```

The value of the environment variables are contained in an array $E[e]$ with $e$ an index in the range $0 \ldots$ ENVIRON_DIM-1. Again, it is up to the user to keep track of which index pertains to which environmental state variable. The use of aliases is really beneficial for this purpose. As defined in code box 7.1 three environment variables are identified in the PNAS model: the resource density, the density of predators and the biomass of juvenile consumers that are vulnerable to predation. Lines 6-8 in code box 7.3 identifies these with the first, second and third element of the array $E[e]$, respectively, and introduces the aliases $R$, $P$ and $B$ for these quantities. All code shown below will make use of these aliases as opposed to their real names in the program ($E[0]$, $E[1]$ and $E[2]$).

Similar arguments as given above for the individual state variables contained in the array $istate[p][i]$ and the environment variables contained in the array $E[e]$ hold for the model parameters. All model parameters are contained in a vector named $parameter[k]$ in the code (see the previous section) with $k$ an index in the range $0 \ldots$ PARAMETER_NR-1. Which element of this vector represents which model-specific parameter is up to the user. To prevent mixing up the interpretation of the different vector elements and hence to prevent mistakes, it is strongly advised to define meaningful, model-specific aliases for each of the elements of the vector $parameter[k]$ as is illustrated in lines 11-32 in the code box above. It is best to avoid completely the direct use of the program variable $parameter[k]$ in any part of the model specification and only use the models-specific aliases.
7.2 Definition of the individual life history

7.2.1 Specifying the number of possible states-at-birth

The first routine to be implemented for a particular life history model defines for every population in the model the number of possible states-at-birth that an individual can be born with (i.e. the value of the size \( m \) of the set \( \{\phi_1, \ldots, \phi_m\} \)).

Code box 7.4: Specification of the number of possible states-at-birth

```c
/*
 * Specify the number of states at birth for the individuals in all structured
 * populations in the problem in the vector BirthStates[].
 */

void SetBirthStates(int BirthStates[POPULATION_NR], double E[])
{
    BirthStates[0] = 1;
    return;
}
```

For each population with index \( p \) the variable \( \text{BirthStates}[p] \) has to be set to the number of possible states at birth. Because in the PNAS model all individuals are born with age 0 and length \( \ell = \ell_b \), all individuals have the same, unique state at birth and hence \( \text{BirthStates}[0] \) is set to 1.

⇒ Note that different populations may have different numbers of states-at-birth. \( \text{BirthStates}[p] \) hence does not need to be the same for all \( p \).

7.2.2 Specifying the value of all possible states-at-birth

The next routine to implement defines for every possible state-at-birth with index \( j \) the actual value of the different individual state variables at birth \( \phi_j = (\phi_{j1}, \ldots, \phi_{jk}) \).

Code box 7.5: Specifying the value of all possible states-at-birth

```c
/*
 * Specify all the possible states at birth for all individuals in all
 * structured populations in the problem. BirthStateNr represents the index of
 * the state of birth to be specified. Each state at birth should be a single,
 * constant value for each i-state variable.
 *
 * Notice that the first index of the variable 'istate[]' refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void StateAtBirth(double *istate[POPULATION_NR], int BirthStateNr, double E[])
{
    AGE = 0.0;
    LENGTH = LB;
    return;
}
```

For every population \( (p = 0, 1, \ldots, \text{POPULATION_NR}-1) \) the value of each individual state variable \( \text{istate}[p][i] \) \( (i = 0, 1, \ldots, \text{I_STATE_DIM}-1) \) has to be assigned a unique value,
from which individual development will start at age 0. Notice that the program does not automatically include individual age in its characterisation of the individual state, even though integration over the entire life history (as a function of age) is carried out. For the PNAS model age at birth is (obviously) set to 0, while the length at birth is given by the parameter $\ell_b$ (line 15 and 16, respectively in the code box below).

This routine will be called as many times as there are possible states-at-birth. The variable $\text{BirthStateNr}$ indicates the index $j$ of the state-at-birth in the set $\{\phi_1, \ldots, \phi_m\}$ for which the values have to be set in the current invocation of the routine. The routine will thus be called with $\text{BirthStateNr}$ set equal to a value in $0, 1, \ldots, m - 1$ (Remember the starting index 0 in C!). If there are multiple states-at-birth ($\text{BirthStates[p]} > 1$) the definition of the values of the $i$-state variables has to depend explicitly on the index $\text{BirthStateNr}$ to make the states-at-birth different from each other. Furthermore, if the problem involves multiple structured populations the number of possible states-at-birth can be different for each of them, which might lead to a situation that the routine above is called with a value of the index $\text{BirthStateNr}$ that is larger than the maximum number of states-at-birth for a particular population ($\text{BirthStateNr} \geq \text{BirthStates[p]}$). The program safely ignores such inappropriate state-at-birth specifications.

7.2.3 Definition of boundaries between discrete stages

The next routine determines the boundaries between consecutive stages in the individual life history:

**Code box 7.6: Definition of discrete stage boundaries**

```c
/*
 * Specify the threshold determining the end point of each discrete life
 * stage in individual life history as function of the i-state variables and
 * the individual's state at birth for all populations in every life stage.
 * Notice that the first index of the variable 'istate[][]' refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void IntervalLimit(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
                   double *birthstate[POPULATION_NR], int BirthStateNr, double E[],
                   double limit[POPULATION_NR])
{
    switch (lifestage[0])
    {
        case 0:
            limit[0] = LENGTH - LV;
            break;
        case 1:
            limit[0] = LENGTH - LJ;
            break;
    }
    return;
}
```
In this routine the variable \( \text{limit}[p] \) has to be defined, which has as many elements as there are populations \((p = 0 \ldots \text{POPULATION_NR}-1)\). The life stage that the individual is in at the moment this routine is called, is determined by the variable \( \text{lifestage}[p] \), which has a value of 0 if the individual is in the first life stage and a value of \( \text{STAGES}-1 \) if it is in the last life stage. The element \( \text{limit}[p] \) should now indicate when the current life stage as given in \( \text{lifestage}[p] \) ends. In particular, the program considers the current life stage to end when \( \text{limit}[p] \) turns from negative to positive. For the end of the last life stage the death of old age, either by reaching the maximum age \( \text{MAX_AGE} \) or by reaching the minimum survival threshold \( \text{MIN_SURVIVAL} \), does not have to be specified separately, the program takes care of that automatically.

The threshold value that has to be stored and returned to the program in \( \text{limit}[p] \) will depend on the individual state variables, possibly on the individuals state-at-birth and will be different for individuals in different life stages. For this reason, the routine \( \text{IntervalLimit()} \) has as arguments \( \text{lifestage}[\cdot] \), specifying the life stage that the individual is currently in, \( \text{istate}[\cdot][\cdot] \), the individual state, \( \text{birthstate}[\cdot][\cdot] \) and \( \text{BirthStateNr} \), the value and index of the individual’s state-at-birth, respectively. The threshold value marking the end of a particular stage may, however, in addition depend on the value of the environment variables \((\text{E}[\cdot])\).

In the PNAS model there is a discontinuous change at the length threshold \( \ell = \ell_v \) when individuals turn from vulnerable to completely invulnerable to predation. The value that indicates the end of the first life stage (when \( \text{lifestage}[p] = 0 \)) is hence set to \( \ell - \ell_v \) (line 18-20 in the code box above). Furthermore, individuals mature at \( \ell = \ell_j \), which changes their fecundity discontinuously from a 0 value just before maturation to a positive value just after maturation. The value that indicates the end of the second (juvenile) stage (when \( \text{lifestage}[p] = 1 \)) is hence set to \( \ell - \ell_j \) (line 21-23 in the code box above).

Like the previous routine, this routine will be called as many times as there are possible states-at-birth, because the state-at-birth may influence the threshold between consecutive life stages. The same holds for the routines discussed in sections 7.2.4, 7.2.7, and 7.3.1 below, which define changes in the \( i\)-state variables, the fecundity and the mortality of individuals and their impact on the environment, respectively. In essence, individuals with different states-at-birth are treated as subpopulations within the same structured population.

Because of the possible dependence on the state-at-birth the variables \( \text{birthstate}[\cdot][\cdot] \) and \( \text{BirthStateNr} \) are passed as arguments to this routine and the once discussed in sections 7.2.4, 7.2.7, and 7.3.1. These arguments contain the values of the \( i\)-state variables and the index in the set \( \{\phi_1, \ldots, \phi_m\} \), respectively, for which the routine is invoked and for which the threshold between consecutive life stages has to be evaluated.
If the problem involves multiple structured populations and the number of possible states-at-birth differs among them, the routine above may be called with a value of the index \( \text{BirthStateNr} \) that is larger than the maximum number of states-at-birth for a particular population \( \text{BirthStateNr} \geq \text{BirthStates}[p] \). Although this circumstance may seem confusing, the user does not have to worry about it, as the program is designed to safely ignore such assignments of thresholds between consecutive life stages, changes in the \( i \)-state variables, fecundity, mortality and impact on the environment of individuals for states-at-birth with index \( \text{BirthStateNr} \geq \text{BirthStates}[p] \) that are inappropriate for the structured population with index \( p \).

### 7.2.4 Specification of continuous individual state development

This routine specifies the right-hand side of the ODE:

\[
\frac{d\chi}{da} = g(\chi, \chi_b, E)
\]

that determines the continuous development of the individual state variables during the life history as a function of the state variables themselves, the individual’s state-at-birth and the environment variables.

**Code box 7.7: Specification of continuous individual state development**

```c
/*
* Specify the development of individuals as a function of the i-state
* variables and the individual's state at birth for all populations in every
* life stage.
* Notice that the first index of the variables 'istate[][]' and 'development[][]'
* refers to the number of the structured population, the second index refers
* to the number of the individual state variable. The interpretation of the
* latter is up to the user.
*/

void Development(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
                  double *birthstate[POPULATION_NR], int BirthStateNr,
                  double E[],
                  double development[POPULATION_NR][I_STATE_DIM])
{
  development[0][0] = 1.0;
  development[0][1] = GAMMA*(LM*R/(R + RH) - LENGTH);
  return;
}
```

For each individual state variable \( i \) of every structured population \( p \) that is part of the individual state \( \text{istate}[p][i] \), its rate of development during the life history has to be specified in \( \text{development}[p][i] \). Notice that these development rates may differ in different life stages, for example growth in body size may be different for juveniles and adults in case adults invest a lot of energy into reproduction. The development rates should then be specified dependent on the current life stage the individual is in. This current life stage at the moment the routine is evaluated is contained in the variable \( \text{lifestage}[p] \). The development rate may furthermore depend on the individual state variables, on the individuals state-at-birth and on the value of the environment variables, which is the reason
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for istate[], the individual state, birthstate[], and BirthStateNr, the value and index of the individual's state-at-birth, respectively, and E[], the environment variables, as arguments to this routine.

In the PNAS model the first individual state variable corresponds to the individual age, which obviously has a rate of development equal to 1. The rate of development in individual length, the second individual state variable, follows the von Bertalanffy growth function, as specified by the function \( g(\ell, R) \) (refer to the model formulation at the start of this chapter).

Refer to the remarks in section 7.2.3 concerning the dependence on the individual's state-at-birth.

7.2.5 Specification of discrete individual state changes at stage transitions

Even though not listed among the basic assumptions of the PSPM in the beginning of this chapter, it is permissible to have discrete changes or jumps in the individual state variables at the transition between two consecutive life stages. If these occur, they should be programmed in the following routine.

Code box 7.8: Specification of discrete individual state changes

```c
/*
 * Specify the possible discrete changes (jumps) in the individual state
 * variables when ENTERING the stage specified by 'lifestage[]'.
 * Notice that the first index of the variable 'istate[]' refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void DiscreteChanges(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
                     double *birthstate[POPULATION_NR], int BirthStateNr, double E[])
{
    return;
}
```

This routine is not relevant in case of the PNAS model and hence its contents are empty (apart for the necessary return; statement).

This routine is called whenever a transition between two consecutive life stages is reached during the integration over the individual life history. It should be noted that the value of the variable lifestage[\( p \)] indicates the life stage that is entered, that is, following the current stage boundary. This routine will hence never be called with a value of one of the elements lifestage[\( p \)] equal to 0. The discrete changes in the individual state variables have to be implemented by assigning new values to the variables istate[\( p \)] [\( i \)].

These assignments may as before depend on the life stage that is entered, as specified by the variable lifestage[], the (old values) of the individual state variables, contained in the argument istate[], the individuals state-at-birth, determined by the arguments birthstate[] and BirthStateNr, and on the environment variables E[]. If no assignment of a value to istate[\( p \)] [\( i \)] is implemented, that particular individual state variable will keep its current value.
7.2. DEFINITION OF THE INDIVIDUAL LIFE HISTORY

Refer to the remarks in section 7.2.3 concerning the dependence on the individual’s state-at-birth.

7.2.6 Specification of fecundity

The following routine specifies the fecundity as a function of the individual state.

**Code box 7.9: Specification of fecundity**

```c
/*
* Specify the fecundity of individuals as a function of the i-state
* variables and the individual's state at birth for all populations in every
* life stage.
* The number of offspring produced has to be specified for every possible
* state at birth in the variable 'fecundity[][]'. The first index of this
* variable refers to the number of the structured population, the second
* index refers to the number of the birth state.
* Notice that the first index of the variable 'istate[]' refers to the
* number of the structured population, the second index refers to the
* number of the individual state variable. The interpretation of the latter
* is up to the user.
*/

void Fecundity(int lifestage[], double *istate[], double *birthstate[], int BirthStateNr, double E[], double *fecundity[])
{
    fecundity[0][0] = 0.0;
    if (lifestage[0] == 2)
        fecundity[0][0] = RM*R/(R + RH)*LENGTH*LENGTH;
    return;
}
```

In this routine not only the fecundity (i.e. the number of offspring produced per unit time) has to be specified, but also the state-at-birth of the produced offspring. Therefore, this routine has to assign values to the matrix `fecundity[p][j]`, which determines for the population with index `p` the number of offspring produced per unit time with state-at-birth with index `j` in the set `{φ₁, ..., φₘ}`. This fecundity will certainly depend on the life stage that the individual is in (only adults reproduce), which is contained in the argument `lifestage[]`, and on the individual state variables, i.e. the values of the argument `istate[]`, but possibly also on the individual’s state-at-birth, the values and index of which are specified by the arguments `birthstate[]` and `BirthStateNr`, respectively, and on the value of environment variables, provided by the argument `E[]`, at the moment this routine is called.

In the most common case of a unique state-at-birth and a single structured population, like in the PNAS model, the only valid indices are `p = 0` and `j = 0` and hence only the variable `fecundity[0][0]` has to be assigned. The code fragment above implements a non-zero fecundity for individuals in the third life stage (`lifestage[0] == 2`), which corresponds to the adult individuals with `ℓ > ℓ_j`. The implemented expression corresponds to the function \( \beta(ℓ, R) = r_m R / (R_0 + R) ℓ^2 \) as assumed in the PNAS model (see chapter 7).

The code provides a good example of how to assign a different value for a particular life
history rate dependent on the life stage that an individual is in. The same approach can also be used in the other routines specifying the life history rates of individuals.

For more detailed remarks about models with multiple states-at-birth consult section 7.2.3

### 7.2.7 Specification of mortality

The following routine specifies the mortality as a function of the individual state.

**Code box 7.10: Specification of mortality**

```c
/*
 * Specify the mortality of individuals as a function of the i-state variables and the individual's state at birth for all populations in every life stage.
 * Notice that the first index of the variable 'istate[]' refers to the number of the structured population, the second index refers to the number of the individual state variable. The interpretation of the latter is up to the user.
*/
void Mortality(int lifestage[POPULATION_NR], double *istate[POPULATION_NR], double *birthstate[POPULATION_NR], int BirthStateNr, double E[], double mortality[POPULATION_NR])
{
    if (lifestage[0] == 0)
        mortality[0] = MUB + A*P/(1+A*TH*B);
    else
        mortality[0] = MUB;
    return;
}
```

For each population the corresponding element of the array `mortality[p]` should be assigned the mortality rate, possibly dependent on the life stage the individual is in at the moment this routine is called (given in argument `lifestage[]`), the current `i-state` of the individual (given in argument `istate[][]`), the individual’s state-at-birth (values and index in the set `{φ₁,...,φₘ}` given by `birthstate[][]` and `BirthStateNr`, respectively) and the value of environment variables (`E[]`).

In the PNAS model all individuals experience a background mortality rate $\mu_b$, while small juvenile individuals, which are in the first distinguished life stage (`lifestage[0] == 0`), experience on top of the background mortality a predation mortality equal to $aP/(1+T_hB)$ as expressed by the function $\mu(\ell, P)$ in chapter 7.

Refer to the remarks in section 7.2.3 concerning the dependence on the individual’s state-at-birth.
7.3 Feedback on and equilibrium condition of the environment

7.3.1 Specification of feedback impact on the environment

In this routine the functions should be programmed that represent the influence of individuals in the structured populations on their environment. These functions may represent effects like grazing rates or availability as food for higher trophic levels.

Code box 7.11: Specification of feedback impact on the environment

```c
/*
 * For all the integrals (measures) that occur in interactions of the
 * structured populations with their environments and for all the integrals
 * that should be computed for output purposes (e.g. total juvenile or adult
 * biomass), specify appropriate weighing function dependent on the i-state
 * variables, the individual’s state at birth, the environment variables and
 * the current life stage of the individuals. These weighing functions should
 * be specified for all structured populations in the problem. The number of
 * weighing functions is the same for all of them.
 * Notice that the first index of the variables ‘istate[]’ and ‘impact[]’
 * refers to the number of the structured population, the second index of the
 * variable ‘istate[]’ refers to the number of the individual state variable,
 * while the second index of the variable ‘impact[]’ refers to the number of
 * the interaction variable. The interpretation of these second indices is up
 * to the user.
 */

void Impact(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
            double *birthstate[POPULATION_NR], int BirthStateNr, double E[],
            double impact[POPULATION_NR][INTERACT_DIM])
{
    impact[0][0] = IMAX*R/(R + RH)*LENGTH*LENGTH;
    switch (lifestage[0])
    {
    case 0:
        impact[0][1] = OMEGA*LENGTH*LENGTH*LENGTH;
        impact[0][2] = 0;
        impact[0][3] = 0;
        break;
    case 1:
        impact[0][1] = 0;
        impact[0][2] = OMEGA*LENGTH*LENGTH*LENGTH;
        impact[0][3] = 0;
        break;
    case 2:
        impact[0][1] = 0;
        impact[0][2] = 0;
        impact[0][3] = OMEGA*LENGTH*LENGTH*LENGTH;
        break;
    }
    return;
}
```

As explained in section 7.1.1 interaction functions are of the form

\[
\int_{\Omega} h(\chi, \chi_b, E) \tilde{n}(\chi) \, d\chi
\]

where \(h(\chi, \chi_b, E)\) is an interaction (weighing) function that can depend on the values of the individual state \(\chi\), the state-at-birth of individuals \(\chi_b\) and the values of the environment variables \(E\), and \(\tilde{n}(\chi)\) is the stable population distribution in equilibrium.
Such quantities can therefore represent the total population density in equilibrium (when $h(\chi, \chi_b, E) = 1$), the total population biomass (when $h(\chi, \chi_b, E)$ equals the biomass of an individual with individual state $\chi$ and state-at-birth $\chi_b$) or the total population birth rate in equilibrium (when $h(\chi, \chi_b, E)$ is the fecundity of an individual with individual state $\chi$ and state-at-birth $\chi_b$). These interaction variables, in fact, determine the equilibrium of the model, because the nonlinearities that make an equilibrium possible arise through the impact of an individual on its environment.

As also explained in section 7.1.1 all interaction functions are saved to the output file when an equilibrium has been computed. Interaction functions are hence not only used to compute the density-dependent feedback in the model, but also to obtain model output quantities of the form shown above.

In the PNAS model this feedback of an individual consumer on its environment consists of its grazing rate $I(\ell, R)$ and the biomass-length relation $\omega_3$ determining the biomass of vulnerable consumers, as it represents food for predators. The grazing rate of an individual consumer in the PNAS model is independent of the life stage it is in. As is shown in line 23 of the code box above, this impact is assigned to the first interaction variable (the one with index 0). Line 25-42 of the code box 7.11 show that biomass of juvenile consumers that are vulnerable to predation is assigned to the second interaction variable (lines 27-31), whereas the biomass of the invulnerable juvenile and adult consumers is assigned to the third (lines 32-36) and fourth (lines 37-41) interaction variable. These last two interaction variables are obviously not needed for the specification of the equilibrium, but are only included as additional output.

It should be pointed out that the routine in code box 7.11 should only specify the impact of an individual on its environment, given its current life stage (function argument lifestage[]), its individual state (argument istate[]), its state-at-birth (values and index in the set $\{\phi_1, \ldots, \phi_m\}$ given by birthstate[] and BirthStateNr, respectively) and the value of environment variables ($E[]$). In other words, the routine should only specify the weighing function $h(\chi, \chi_b, E)$. The program automatically translates this individual-level impact function to the feedback of the total population on its environment, as explained in the next section.

Refer to the remarks in section 7.2.3 concerning the dependence on the individual’s state-at-birth.

7.3.2 Specification of equilibrium conditions of the environment

The last routine has to specify the equilibrium conditions of the environment, dependent on the values of the environment variables itself and/or the values of the population feedback functions. As explained in chapter 6 environment variables can be of different types. As shown in the code box 7.12 below 3 different types of environment variables are distinguished that are referred to with the keywords PERCAPITARATE, GENERALODE and POPULATIONINTEGRAL, respectively.

The first type of environment variable, indicated with the keyword PERCAPITARATE, is one that follows dynamics described by an ordinary differential equation (ODE) and in addition can potentially be 0 in equilibrium. The ODE describing the dynamics of such an environment variable $E_i(t)$ is then of the general form:

$$\frac{dE_i}{dt} = G(E, I) E_i$$
in which $E$ is the vector of environment variables, $I$ is the vector of population feedback functions on the environment and $G(E, I)$ is a bounded function. More formally, $G(E, I)$ should satisfy $-\infty < -C \leq G(E, I) \leq C < \infty$ for some positive real value $C$, such that the value $E_i = 0$ (the zero equilibrium, also referred to as the trivial or boundary equilibrium) indeed represents a regular equilibrium value of the ODE above. The function $G(E, I)$ then represents the per-capita rate of change of $E_i$ and any non-zero (non-trivial or internal) equilibrium of $E_i$ fulfills the condition $G(E, I) = 0$. To handle more easily the continuation of zero equilibrium values for this type of environment variables and to be able to detect transcritical bifurcation points (also referred to as branching points) between an equilibrium curve with $E_i = 0$ and a curve with $E_i \neq 0$, this type of environment variable has to be labeled as PERCAPITARATE in the program (see code box 7.12 below) and its equilibrium condition has to be specified by the per capita growth rate $G(E, I)$.

The second type of environment variable, indicated with the keyword GENERALODE, is one that follows dynamics described by an ordinary differential equation (ODE), but $E_i = 0$ is not a potential equilibrium value for this environment variable. The ODE describing the dynamics of such an environment variable $E_i(t)$ is then of the general form:

$$\frac{dE_i}{dt} = G(E, I)$$

in which $E$ is the vector of environment variables, $I$ is the vector of population feedback functions on the environment and $G(E, I) \neq 0$ when $E_i = 0$. Such an environment variable can never have a zero equilibrium value and transcritical bifurcation points between an equilibrium curve with $E_i = 0$ and a curve with $E_i \neq 0$ do not occur either. All equilibrium values of $E_i$ satisfy the condition $G(E, I) = 0$. This type of environment variable has to be labeled as GENERALODE in the program (see code box 7.12 below) and its equilibrium condition has to be specified by the function $G(E, I)$.

The last type of environment variable are variables that represent measures (weighted integrals) of the population distribution itself. More formally, environment variables that can be expressed as:

$$E_i(t) = I_i(t) \quad \text{with} \quad I_i(t) = \int_{\Omega} \gamma_i(\chi, \chi_b, E) \, n(t, \chi) \, d\chi$$

in which the function $\gamma_i(\chi, \chi_b, E)$ is some arbitrary weighing function and $I_i$ is one of the functions representing the feedback of a population on its environment. This type of environment variable represents a direct density-dependent effect of the population on the life history of the individuals. Examples of the weighing functions include $\gamma_i(\chi, \chi_b, E) = 1$, in which case $E_i$ would represent the total population density in numbers, or $\gamma_i(\chi, \chi_b, E) = \chi_i$ with $\chi_i$ referring to the mass of an individual organism, in which case $E_i$ would represent the total population biomass. Obviously, the value of $E_i$ equals 0 in case of a zero-valued or trivial equilibrium state for the population distribution $n(t, \chi)$. This type of environment variable has to be labeled as POPULATIONINTEGRAL in the program (see code box 7.12 below) and its equilibrium condition has to be specified by identifying it with the appropriate feedback function $I_i$. 
CHAPTER 7. IMPLEMENTATION OF AN EXAMPLE MODEL

Code box 7.12: Specification of equilibrium condition of the environment

```c
/*
* Specify the type of each of the environment variables by setting
* the entries in EnvironmentType[ENVIRON_DIM] to PERCAPITARATE, GENERALODE
* or POPULATIONINTEGRAL based on the classification below:
*   * Set an entry to PERCAPITARATE if the dynamics of E[j] follow an ODE and 0
*     is a possible equilibrium state of E[j]. The ODE is then of the form
*     dE[j]/dt = P(E,I)*E[j], with P(E,I) the per capita growth rate of E[j].
* Specify the equilibrium condition as condition[j] = P(E,I), do not include
*   the multiplication with E[j] to allow for detecting and continuing the
*   transcritical bifurcation between the trivial and non-trivial equilibrium.
*   * Set an entry to GENERALODE if the dynamics of E[j] follow an ODE and 0 is
*     NOT an equilibrium state of E. The ODE then has a form dE[j]/dt = G(E,I).
* Specify the equilibrium condition as condition[j] = G(E,I).
*   * Set an entry to POPULATIONINTEGRAL if E[j] is a (weighted) integral of the
*     population distribution, representing for example the total population
*     biomass. E[j] then can be expressed as E[j] = I[p][i]. Specify the
*     equilibrium condition in this case as condition[j] = I[p][i].
* Notice that the first index of the variable 'I[[]]' refers to the
* number of the structured population, the second index refers to the
* number of the interaction variable. The interpretation of the latter
* is up to the user. Also notice that the variable 'condition[j]' should
* specify the equilibrium condition of environment variable 'E[j]'.
*/

const int EnvironmentType[ENVIRON_DIM] = {GENERALODE, PERCAPITARATE, POPULATIONINTEGRAL};

void EnvEqui(double E[], double I[POPULATION_NR][INTERACT_DIM],
              double condition[ENVIRON_DIM])
{
    condition[0] = RH0*(RMAX - R) - I[0][0];
    condition[1] = EPSILON*A*I[0][1]/(1+A*TH*I[0][1]) - DELTA;
    condition[2] = I[0][1];
    return;
}
```

In the code box above, the array EnvironmentType[ENVIRON_DIM] has to define for each environment variable separately its type (PERCAPITARATE, GENERALODE or POPULATIONINTEGRAL). This array hence has as many elements as there are environment variables. Secondly, in the routine that follows the specification of EnvironmentType[ENVIRON_DIM] the equilibrium conditions have to be implemented as a function of the values of the environment variables itself E[] and the value of the population feedbacks functions I[[]]. These latter two arrays are passed as arguments to the routine EnvEqui, while the equilibrium conditions have to be specified in the array condition[]. Notice that the ordering of the elements in the arrays condition[] and E[] are the same, meaning for example that the equilibrium condition for the second environment variable E[1] has to be returned in condition[1].

Notice that the feedback functions I[[]] are the population-level representations of the individual-level impact functions impact[[]] as they are defined in code box [7.11]. In case of a unique state-at-birth the expected life history is the same for all individuals in the population and hence not dependent on a state-at-birth $\chi_b$. In this case, such an expected impact of an individual during its entire life on its environment is given by an integral of the form:

$$\Gamma = \int_0^\infty \gamma(\chi(a), E) F(a) da$$
in which \( \gamma(\chi(a), E) \) quantifies the impact dependent on the individual state and the environment variables, \( \chi(a) \) is the individual state at age \( a \) and \( \mathcal{F}(a) \) represents the probability that the individual survives until age \( a \), which is defined as:

\[
\mathcal{F}(a) = \exp \left( - \int_0^a \mu(\chi(a), E) \, da \right)
\]

with \( \mu(\chi(a), E) \) the individual’s instantaneous mortality rate. The population-level impact on the environment now simply equals the product of the total population birth rate in equilibrium \( \bar{b} \) and the individual-level impact:

\[
\bar{I} = \bar{b} \Gamma
\]

The elements of \( I[][] \) and \( \text{impact}[][] \) therefore correspond one-to-one, such that for example in the PNAS model, in which \( \text{impact}[0][0] \) is defined as the individual feeding rate on the resource, the quantity \( I[0][0] \) equals the grazing rate of the entire population on the resource.

In the PNAS model, the first environment variable represents the resource density, which follows semi-chemostat growth in the absence of consumers. As a consequence, the resource \( R \) does NOT have an equilibrium value \( \bar{R} = 0 \). The type of the first environment variable is therefore set to \( \text{GENERALODE} \) and its equilibrium condition is specified in line 34 of the code box above as \( \text{RHO} \ast (\text{RMAX} - R) - \text{I}[0][0] \). The first term in this line of C-code implements the semi-chemostat dynamics in the absence of consumers and the quantity \( \text{I}[0][0] \) represents the grazing rate by the total population of consumers as mentioned above.

The second environment variable represents the predator density, the dynamics of which is described by the ODE

\[
\frac{dP}{dt} = \left( \epsilon \frac{aB}{1 + T_h B} - \delta \right) P
\]

Because \( P = 0 \) is a regular fixed point of this ODE, the type of the second environment variable is set to \( \text{PERCAPITARATE} \) on line 29 of code box 7.12 above, while its per capita growth rate \( \epsilon aB/(1 + T_h B) - \delta \) is used to define its equilibrium condition on line 35. Notice in this respect that the population feedback quantity \( \text{I}[0][1] \) represents \( B \), the total biomass of small juvenile consumers that are vulnerable to predation, which is calculated from the individual-level impact quantity \( \text{impact}[0][1] \) defined on lines 27-31 in code box 7.11.

Finally, the third environment variable in the PNAS model is the total biomass of small juvenile consumers \( B \), which exerts a direct density-dependent effect on the mortality rate of small juvenile consumer individuals themselves, as it influences the predator functional response. The type of the third environment variable is therefore set to \( \text{POPULATIONINTEGRAL} \) on line 29 of code box 7.12 above. On line 36 of code box 7.12 the equilibrium condition of this third environment variable is specified by identifying it with the population feedback quantity \( \text{I}[0][1] \), which the program computes on the basis of the individual-level impact quantity \( \text{impact}[0][1] \) that represents the biomass of an individual consumer that is in the first life stage, where it is vulnerable to predation (lines 27-31 in code box 7.11).
In case of multiple states-at-birth, individuals with different states-at-birth may have different impacts on their environment. The expected impact of an individual during its entire life on its environment is then given by an integral of the form:

$$
\Gamma_j = \int_0^\infty \gamma(\chi(a, \phi_j), \phi_j, E) \mathcal{F}_j(a) \, da
$$

in which $\gamma(\chi(a, \phi_j), \phi_j, E)$ quantifies the impact of an individual that is born with state $\phi_j$ state dependent on its individual state at age $a$, $\chi(a, \phi_j)$, its state-at-birth $\phi_j$ and the environment variables. $\mathcal{F}_j(a)$ now represents the probability that an individual born with state-at-birth $\phi_j$ survives until age $a$, which is defined as:

$$
\mathcal{F}_j(a) = \exp \left( - \int_0^a \mu(\chi(a, \phi_j), \phi_j, E) \, da \right)
$$

with $\mu(\chi(a, \phi_j), \phi_j, E)$ the individual’s instantaneous mortality rate.

If the possible states-at-birth are given by the set $\{\phi_1, \ldots, \phi_m\}$, the individual-level impact is an $m$-dimensional vector $\Gamma = (\Gamma_1, \ldots, \Gamma_m)$. The population-level impact on the environment in this case equals the dot product of this vector $\Gamma$ with the $m$-dimensional vector $\vec{b}$, representing the equilibrium distribution of produced offspring over the possible states-at-birth $\{\phi_1, \ldots, \phi_m\}$ (refer to Diekmann et al., 2003 for details).

The program automatically computes the equilibrium distribution of produced offspring over the possible states-at-birth and uses it to compute the population-level impacts contained in $\mathbf{I}$ from the individual-level impacts that have been specified in $\mathbf{impact}$. 
Model analysis in R

To carry out the analysis in R the first step is to load the script file `PSPManalysis.R` using the command `source("PSPManalysis.R")`. This defines all functions that are required for demographic, equilibrium and evolutionary analysis and a global variable that holds the directory name of the PSPManalysis package. Compared to the use of this software in Matlab be aware that in R arrays (referred to as vectors in R) are defined using the concatenation function `c()` and strings are specified surrounded by double quotes (") as opposed to single quotes (').

8.1 Computation of curves and detections of bifurcation points

The software package allows to carry out 6 different types of computations of equilibria, corresponding to 6 different types of curves. These different types of computations are uniquely labeled with a 2- or 3-letter abbreviation code.

"EQ": This is the basic type of computation and hence the one that one usually starts out with. In this computational mode the software calculates the equilibrium of the PSPM as a function of a particular parameter over a range of values of that parameter. This type of computation hence yields a type of curve that I will refer to as “equilibrium curve” (as opposed to the more general “bifurcation curve”).

During the computation of an equilibrium curve the software will detect 4 types of special points or bifurcation points:

- **Branching point**: A branching or transcritical bifurcation point is a point where two different equilibrium curves intersect. Generically, such a bifurcation occurs in a PSPM at a parameter value that represents the invasion or extinction threshold of a structured population and the two equilibrium curves are characterised by a zero (trivial) and non-zero (non-trivial) equilibrium value for a particular structured population, respectively. The program will report the occurrence of a branching point as "BP #N", where N is the number of the structured population, for which the switch from a zero to non-zero equilibrium value occurs.

- **Environment branching point**: A branching or transcritical bifurcation point can also occur for an environment variable. The two equilibrium curves are then characterised by a zero (trivial) and non-zero (non-trivial) equilibrium...
CHAPTER 8. MODEL ANALYSIS IN R

value for a particular environment variable as opposed to a structured population. From the point of view of bifurcation theory, branching points that involve a zero and non-zero value of a structured population are the same as branching points that involve a zero and non-zero environment variable. The two types are only distinguished by the software, because they are computed differently. The program will report the occurrence of a branching point as "BPE #N", where N is the number of the environment variable, for which the switch from a zero to non-zero equilibrium value occurs. Notice that environment branching points can only be detected for environment variables that are of the type PERCAPITARATE (see section 7.3.2 above).

- **Limit point**: At a limit point a saddle-node bifurcation occurs, in which 2 different equilibria in the model, an unstable saddle and a stable node, disappear at a particular threshold value of a parameter. At this parameter value the equilibrium curve reaches an extremum in the parameter values and hence bends back on itself. The program will report the occurrence of a limit point as "LP".

- **Evolutionary fixed point**: The equilibrium condition for a structured population model can be expressed as:
  \[ R_0(p, E(p)) = 1 \]
  in which \( p \) is one of the model parameters. The quantity \( R_0(p, E(p)) \) refers to the expected number of offspring that an individual of the structured population will produce during its lifetime, in an environment that is characterised by the environment variables \( E(p) \). The parameter \( p \) may directly influence the value of \( R_0(p, E(p)) \) but also indirectly, because it may have an impact on the equilibrium values of the environment variables. The software uses the condition above to compute the equilibrium of a PSPM (see also chapter 16).
  In an evolutionary setting, in which mutations in the parameter \( p \) can occur and selection acts to increase or decrease the parameter \( p \) over evolutionary time, higher values of \( p \) are selected for if \( \partial R_0/\partial p > 0 \), while lower values of \( p \) are selected for if \( \partial R_0/\partial p \) is negative. Any parameter value where \( \partial R_0/\partial p = 0 \) is a fixed point of the evolutionary process, as for this parameter value the selection gradient for the parameter \( p \) is 0 (Metz et al., 1996; Geritz et al., 1998; Diekmann et al., 2003). The software will detect these evolutionary fixed points. In addition, the software will compute the second-order partial derivatives of \( R_0 \) to classify the evolutionary fixed point as a convergent stable strategy (CSS), an evolutionary repellor (ERP) or an evolutionary branching point (EBP) (Geritz et al., 1998).
  It should be noted that evolutionary fixed points are normal equilibrium points of the dynamics system, as opposed to special bifurcation points, since the (ecological) dynamics of the model do not change at the critical parameter value. However, from an evolutionary perspective these points are special. They moreover play a key role in the theory of Adaptive Dynamics (Metz et al., 1996; Geritz et al., 1998; Diekmann et al., 2003). It is for this reason that the software reports them as special points.

The remaining 5 types of computations that the software can carry out all involve one of the special, bifurcation points that the software detects during the computation of an
equilibrium curve. During the computation of the following curves always 2 model parameters are varied, hence these computations are referred to as *two-parameter bifurcations*, as opposed to the *one-parameter bifurcation* of an equilibrium curve.

"BP": In this computational mode the software computes the location of a branching point of a structured population as a function of 2 model parameters. The resulting line can hence be interpreted as the invasion or extinction boundary of the structured population. This computation should start from an initial point close to a (detected) branching point.

"BPE": Similarly, in this computational mode the software computes the location of an environment branching point as a function of 2 model parameters. The resulting line can hence be interpreted as the boundary separating a parameter region with a zero equilibrium value for the environment variable from a region with a non-zero equilibrium value of the environment value. This computation should start from an initial point close to a (detected) environment branching point.

"LP": In this computational mode the software computes the location of a limit point as a function of 2 model parameters. The resulting line can hence be interpreted as the boundary separating a parameter region with (at least) two equilibrium states from a parameter region where these two specific equilibrium states do not occur. This computation should start from an initial point close to a (detected) limit point.

"ESS": The value of a particular parameter for which an evolutionary fixed point occurs is generically referred to as an ESS parameter value. In this computational mode the software computes the location of such an ESS parameter value as a function of the bifurcation parameter. This computational mode can hence be used to investigate how the evolutionary optimal value of one model parameter depends on the value of a second parameter. Curves of this type correspond to the evolutionary isocline of the ESS parameter as a function of the bifurcation parameter. "ESS" computations are, however, not limited to a single parameter having its ESS value, the program can also compute curves of equilibria, in which multiple model parameters are at their ESS value. The bifurcation parameter, which parameterises the curve, is not one of these ESS parameters. This computation should start from an initial point close to a (detected) evolutionary fixed point.

"PIP": This computation also starts from an initial point close to a (detected) evolutionary fixed point. In the theory of adaptive dynamics that focuses on evolutionary analysis the pairwise invasibility plot or PIP plays an important role (Dieckmann [1997], Metz *et al.* [1996]). The PIP is a two-dimensional plot, spanned by the parameter value of a resident type on the *x*-axis and the parameter value of a mutant type on the *y*-axis. The plot indicates for which parameter values the mutant type has a positive (negative) growth rate and hence can (can not) invade in the equilibrium as set by the resident type. In the computational mode "PIP" the software computes the boundary between the parameter regions, for which the mutant has a positive and a negative growth rate.

### 8.2 Arguments of the *PSPMequi* function

Once the model has been implemented, you can proceed carrying out its analysis with the *R*-function *PSPMequi*. The syntax for calling *PSPMequi* is shown in the *R* command box below, which lists all possible arguments to the function as well as their default values.
CHAPTER 8. MODEL ANALYSIS IN R

Command box 8.A: General syntax of a PSPMequi call

```r
> output <- PSPMequi(modelname = NULL, biftype = NULL, startpoint = NULL, stepsize = NULL, parbnds = NULL,
  parameters = NULL, options = NULL, cvode = FALSE, clean = FALSE, force = FALSE, debug = FALSE)
```

The first 5 arguments of the function PSPMequi are needed for the software to function properly and are hence obligatory. The last 6 arguments are optional. The last 4 arguments are boolean arguments which have to be defined as either `TRUE` or `FALSE`, for example by passing as argument to the function PSPMequi the argument `clean = TRUE`.

A full summary of all arguments of PSPMequi is given in the R command box [8.H](#).

The 7 obligatory arguments to the PSPMequi function are the following:

1. The first argument to the R-function PSPMequi is the name of the file specifying the PSPM, passed as a string argument. It is unnecessary to include the extension `.h` as part of the file name, the R-function will strip the `.h` extension away if it is included. The R-command to analyze the PNAS model that will be used as illustrations below will therefore all take "PNAS2002" as their first argument.

2. The second argument to the PSPMequi function determines which type of computation should be carried out for the particular model. These types of computation are discussed in section [8.1](#) above. This string argument should hence be either "BP", "BPE", "EQ", "LP", "ESS" or "PIP".

3. The third argument is the initial point of the computation. This initial point should be close to a solution point for the selected computation, that is, close to an equilibrium point, a branching point, an environment branching or a limit point for an "EQ", "BP", "BPE" and a "LP" computation, respectively. For either a "ESS" or a "PIP" computation the initial point should be close to an evolutionary fixed point. The initial point should be a (row) vector with the proper dimension. For equilibrium computations (type "EQ") this vector in general consists of the initial value of the model parameter to vary, the estimated equilibrium values for all the environment variables and the estimated values of the birth rate for all the structured populations in the model, in the following order:

   \[ c(<\text{parameter}>,<\text{environment variables}>,<\text{population birth rates}>) \]

However, environment variables that have been explicitly specified with the program option "envZE" as having a zero equilibrium value and birth rates of populations that have been explicitly specified with the program option "popZE" to be in a zero equilibrium state (see the description of these options under point 7 below), should be omitted from this vector of initial values.

For all two-parameter types of bifurcation computations ("BP", "BPE", "LP", "ESS" and "PIP") the value of the second model parameter should be appended as last element to the vector of initial values, which therefore has the format:

\[ c(<\text{parameter}>,<\text{environment variables}>,<\text{population birth rates}>,<\text{parameter 2}>) \]

For "ESS" computations with multiple parameters having their ESS value this vector has to be extended with the initial estimate of the ESS value for each of these model parameters.
Also for these computations holds that environment variables that have been explicitly specified with the program option "envZE" as having a zero equilibrium value and birth rates of populations that have been explicitly specified with the program option "popZE" to be in a zero equilibrium state (see the description of these options under point 7 below), should be omitted from this vector of initial values. In addition, in case of a continuation of a branching point, either for a structured population model (type "BP") or for an environment variable (type "BPE"), the zero value for the birth rate of the structured population or the environment variable (specified with the program options "popBP" and "envBP", respectively; see below), for which the branching point occurs, should also be omitted from the vector of initial values.

4. The fourth argument to the \texttt{PSPMequi} function determines the step size along the computed curve. The absolute spacing between subsequent solution points computed on the curve is difficult to predict, as it is determined by both the step size and how quickly the different variables change along the curve. The step size can be either positive or negative, while step sizes of smaller absolute value will lead to the computation of solution points that are more closely spaced together.

5. The fifth argument to the \texttt{PSPMequi} function determines which of the model parameters should be varied during the computation and at which parameter values the computations should stop. This information should be specified by a (row) vector, which for every parameter to be varied specifies a triplet of values including the index of the parameter, its minimum and its maximum value at which the computation should stop. For equilibrium computations (type \texttt{"EQ"}) the vector should hence have the following format:

\[
c(\langle index\ 1\rangle,\langle minimum\ 1\rangle,\langle maximum\ 1\rangle)
\]

The first element of the vector indicates the index of the parameter in the array \texttt{parameter} (see code box 7.3) to vary, while the final two elements of the array indicate the minimum and maximum value of the parameter. The computation of the equilibrium curve as a function of the model parameter stops, whenever the minimum or maximum parameter value is reached.

For all two-parameter type of computations ("BP", "BPE", "LP", "ESS" and "PIP") the vector should be extended with the index of the second parameter to vary in the computation as well as the minimum and the maximum value of this parameter, at which to stop the curve computation. The vector with parameter information has therefore in this case the format:

\[
c(\langle index\ 1\rangle,\langle minimum\ 1\rangle,\langle maximum\ 1\rangle,\langle index\ 2\rangle,\langle minimum\ 2\rangle,\langle maximum\ 2\rangle)
\]

For \texttt{"ESS"} computations with multiple parameters having their ESS value this vector has to be extended with a triplet of values for each of these model parameters with the triplet specifying the index of the particular ESS parameter as well as its minimum and the maximum value. The number of triplets should correspond with the number of initial estimates for the ESS values of parameters as specified in the third argument to the function.
6. The sixth, optional argument of the `PSPMequi` function is a (row) vector of model parameter values. When used, this array should have the same length as the number of parameters in the model (`PARAMETER_NR`). When of this length the values will replace the default values of the parameters that are listed in the model specification file (see code box 7.2 for an example). If the array used for this sixth argument is not of the correct length `PARAMETER_NR` or when it is not specified at all, it will simply be ignored.

7. The seventh, optional argument of the `PSPMequi` function is a (row) vector of string elements, containing possible options that modify the behaviour of the computational module. Most of the options require a value and hence occur as a pair of option name and option value. Only the "test" option (see below) occurs on its own. Options can be specified in any order, but the option value should always immediately follow after the option name. All option values refer to indices of either environment variables, structured populations or individual state variables. Notice, that this index value follows the C-convention of ordering arrays starting at 0 (as opposed to R where array indices start at 1). Multiple options can be included into the vector like:

\[
c("\text{name 1"},"\text{value 1"},"\text{name 2"},"\text{value 2"},"\text{name 3"},"\text{value 3")}
\]

Possible options are:

- Option pair `c("envBP", "i")`: This option pair is only relevant for continuations of a branching points or transcritical bifurcation in an environment variable (curve type "BPE"). The option value "i" determines the index of the environment variables, of which to continue the transcritical bifurcation as a function of 2 parameters. Notice that this computation can only be carried out for environment variables that are of the type `PERCAPITARATE` (see section 7.3.2 above).

- Option pair `c("popBP", "i")`: This option pair is only relevant for continuations of branching points or transcritical bifurcations of a structured population (curve type "BP"). The option value "i" determines the index of the population, of which to continue the transcritical bifurcation as a function of 2 parameters.

- Option pair `c("popEVO", "i")`: This option pair is only relevant for continuations of evolutionary fixed points (curve type "ESS") and the construction of pairwise invasibility plots (curve type "PIP"). The option value "i" determines the index of the population, in which the evolutionary singularity occurs that should be computed as a function of 2 parameters.

- Option pair `c("envZE", "i")`: This option pair can be specified several times as part of the option vector of strings. Including this option instructs the computational module to set the value of the environment variable with index "i" equal to 0 during the computations of the fixed point problem that determines the curve. In addition, the equilibrium condition for this environment variable (as, for example, specified in code box 7.12) is ignored and hence not included as condition to hold in the particular equilibrium point. Notice that this can only occur for environment variables that are of the type `PERCAPITARATE` or
8.2. ARGUMENTS OF THE PSPMEQUI FUNCTION

POPULATIONINTEGRAL (see section 7.3.2 above). Forcing an environment variable to have a zero equilibrium value as opposed to specifying a value of 0 for it as part of the initial point of the computation, allows for the proper detection and handling of branching or transcritical bifurcation points in this environment variable. Omitting this option for an environment variable, but providing instead a value of 0 as part of the initial point of the computation, may lead to the proper computation of an equilibrium curve, in which the environment variable has a 0 value, but may also lead to numerous, spurious messages about branching points in this variable.

- Option pair c("popZE", "i"): This option pair can be specified several times as part of the option vector. Including this option forces the computational module to assume that the structured population with index "i" in the model is in a zero equilibrium state for the curve that has to be computed. This is the only way to compute an equilibrium curve with a zero equilibrium state for a particular parameter. Even if a value of 0 would be specified for the birth rate of a population as part of the initial point of the computation, the software would compute the equilibrium curve with a non-zero (non-trivial) equilibrium state for this population. Notice that if a structured population is forced to be in a zero equilibrium state by using the "popZE" option, a zero equilibrium state should also be enforced for all the environment variables that represent integrals over this population distribution (that are hence of the type POPULATIONINTEGRAL).

- Option pair c("isort", "i"): This option modifies the output of the equilibrium state of the populations that are stored in an output file with a name of the form <Modelname>-<Type>-<NNNN>.csb (see below). By default the computational module reports the information about the stable population state distributions by subdividing the axis of the first state variable (the one with index "0") in 100 subintervals of equal length and reporting the statistics for the cohort of individuals within each subinterval. By using the option "isort" the default choice to use the first individual state variable for this subdivision can be changed to the second, third, and so on. Therefore, passing c("isort", "0") as option vector to the PSPMequi function is the same as the default behaviour: the first individual state variable is used for the subdivision and ordering of the population state distribution, while passing c("isort", "1") would use the second individual state variable for this purpose. Also notice that the number of subdivisions of the individual state variable can be redefined by assigning the dimension COHORT_NR a value different from 100 (see code box 7.2 in section 7.1.1 as well as chapter 15).

- Option c("test"): The last possible option that can be passed to the PSPMequi function as part of the option vector is the "test" option. This invokes the computational module in testing mode, which implies that only a single integration of the individual life history is carried out and no iteration to locate a fixed point of a set of equations is performed. In testing mode the computational module reports on the dynamics of the individual state variables, the survival, the cumulative impact on the environment and the expected number of offspring produced by an individual during its different life stage as well
as over its entire life. Testing mode is very useful to discover whether or not the model implementation gives sensible results or not.

Four other optional arguments can be passed to the `PSPMequi` function: `cvode`, `clean`, `force` and `debug`. These are all boolean arguments that hence have to be passed to the `PSPMequi` function as `<option name>=TRUE` or `<option name>=FALSE`, the latter being the default value of all options (Specifying these options as argument is hence only useful when setting them equal to TRUE). Unlike the previous arguments, which all modify the computations to be performed, these options modify the behaviour of the `PSPMequi` function itself, in particular the compilation of the model specific file into a dynamic library module that can be executed from R. Also unlike all the previous arguments that can be passed, these arguments can be passed in any order and at any position, the `PSPMequi` function will filter these 4 optional arguments from the argument list before passing the filtered argument list to the computational routine.

- **Option clean**: When `clean=TRUE` is passed as argument, this argument instructs the `PSPMequi` function to delete all result files that have been generated during previous calculations with the model, i.e. as a result of previous calls to `PSPMequi`. These result files have names of the form `<Modelname>-<Type>-<NNNN>.bif`, `<Modelname>-<Type>-<NNNN>.err`, `<Modelname>-<Type>-<NNNN>.csb` and `<Modelname>-<Type>-<NNNN>.out`, in which `<Modelname>` refers to the name of the model (i.e. `PNAS2002` in the example model presented in previous sections), `<Type>` refers to the type of continuation that has been performed, i.e. either `BP`, `BPE`, `EQ`, `ESS`, `LP` or `PIP`, and `<NNNN>` is a unique number that distinguishes consecutive computations of the same type of curve with the same model.

- **Option force**: When `force=TRUE` is passed as argument, it instructs the `PSPMequi` function to force re-compilation of the model specific file into a dynamic library module that can be executed by R. This option will usually not be needed by normal users, as the `PSPMequi` function automatically recompiles the computational module when the model specific file with an `.h` extension is more recently changed than the compiled dynamic library file. However, if for some unclear reason this automatic recompilation fails, the `force` option can be used to initiate re-compilation.

- **Option debug**: When `debug=TRUE` is passed as argument, it instructs the `PSPMequi` function to turn on debugging flags while compiling the model specific file into a dynamic library module. This option can be useful to detect programming mistakes in the model-specific file that are otherwise hard to track down. The downside is that depending on the version of R that is used, turning on debugging flags during compilation may generate a lot of output, including warnings about standard files of the operating system that are perfectly correct. It is hence not so easy to spot among all these messages the warnings that relate to the model-specific code that has been implemented.

- **Option cvode**: Passing `cvode=TRUE` as argument to the `PSPMequi` function is currently only relevant for users of Unix-based systems (Mac OS and Linux) as it has not been tested on Windows installations. By default the computational module uses the Dormand-Prince method (DOPRI5; Hairer et al. 1993) for the integration of the ordinary differential equations describing the life history of individuals (see chapter 16 for details about these ordinary differential equations). An implementation of the DOPRI5-method is provided with the package in a separate program file (`dopri5.c`). An alternative integration method, called CVODE, is
8.3 OUTPUT VARIABLES OF THE PSPMEQUI FUNCTION

provided by the Sundials (SUite of Nonlinear and DiFFerential/Algebraic equation Solvers) collection of nonlinear and differential/algebraic equation solvers (see http://www.llnl.gov/CASC/sundials for details). If the appropriate Sundials libraries are installed on your system, the use of the option cvode in the call to PSPMequi will instruct the function to use the Sundials solver instead of the default DOPRI5 solver for the integration of the ordinary differential equations. In particular for long-lasting integrations, that is when the maximum age reached by individuals is large, using the CVODE-method can significantly speed up the computations.

8.3 Output variables of the PSPMequi function

When calling the PSPMequi function it first compiles the model-specific file called <Model>.h using the R command R CMD SHLIB into a dynamically loadable library file, which can subsequently be executed. This compilation step is only carried out when the dynamically loadable library file (called <Model>equi.so on my system on Mac OS X and Linux systems) does not exist, or when the model-specific file has been changed since the last compilation of the executable. Furthermore, the compilation step is forced by the invocation of PSPMequi with the additional argument force=TRUE as discussed in the previous section. For example, for the PNAS model, the implementation of which is specified in the file PNAS2002.h, the dynamically loadable library file is called PNAS2002equi.so (on other operating systems this file may be called PNAS2002equi.dll). Following successful compilation the PSPMequi function executes the compiled, computational module with the arguments passed to it.

The computational module generates on execution a single list object as output with up to 4 member elements (see the help page on PSPMequi in command box 8.H). The first element of the output list, output$curvepoints, contains the numerical information of the points along the computed curve (assuming that the list is assigned to a variable called output). This variable output$curvepoints is a matrix, in which each row represents one solution point along the curve. The columns contain the value of the parameter(s) that have been varied, the equilibrium value of all environment variables, the equilibrium value for the birth rate of all structured populations in the problem, the equilibrium value of all interaction variables defined in the routine Impact() (see code box 7.11), the per capita growth rate of all environment variables for which this is relevant (those of the type PERCAPITARATE, see section 7.3.2), for each of the structured populations the expected number of offspring produced by an individual during its lifetime ($R_0$), for the structured population with index popEVO (if this index is defined via de option vector) the derivative of its $R_0$ value with respect to the bifurcation parameter and finally the norm of the right-hand side of the system of equations that is solved. The latter quantity (referred to as RHS norm) measures how close the computed solution point is to the true solution. The derivative of the $R_0$ value for a structured population with respect to the bifurcation parameter can be used as an indicator for evolutionary change: positive and negative values of this derivative indicate that there is selection for larger and smaller values of the bifurcation parameter, respectively.

The column layout just described pertains to computations of equilibrium curves. For other types of computed curves the number of columns in the output variable output$curvepoints is different. For all curves that depend on two parameters (curve types "BP", "BPE", "LP" and "PIP") the value of the second parameter is inserted as an
additional column after all equilibrium values for the birth rates of the structured populations. For "ESS" curves additional columns are inserted after all these equilibrium birth rate values for each of the parameters that is forced to its evolutionary stationary value along the curve. In addition, preceding the final column with the RHS norm additional columns are added for the second-order partial derivatives of \( R_0 \) of the structured population with index popEVO with respect to the resident and mutant value of each of the evolutionary parameters, respectively (see chapters 9 to 11 for more details). These partial derivatives characterise the evolutionary fixed point as a convergent stable strategy (CSS), an evolutionary repellor (ERP) or an evolutionary branching point (EBP).

When the PSPMequi function finishes, it prints textual information about the computation that has been carried out. This text also contains a header line indicating which column of the output contains which particular value (see the section 8.4 below).

The second member element of the output list, `output$curvedesc`, (see command box 8.H), which is always produced by the computational module irrespective of the type of curve computation that is carried out, contains the description of the executed calculation, which includes the command-line that is used for the invocation of the computational routine, the values of all parameters used for the current computation and a header line indicating the meaning of all the output variables produced by the computational module. This textual information is also printed to the \( R \) console at the end of calculations. In fact, the PSPMequi function prints its report on the calculations by execution of the statement `cat(output$curvedesc, sep='\n')`. More details about the content of the description variable `output$curvedesc` is provided in the section below discussing the example of a model analysis using the PSPMequi function.

The third and fourth member elements of the output list are only non-empty for computations of equilibrium curves (type "EQ"). The third output variable `output$bifpoints` (see command box 8.H) contains the same type of information as the first output variable `output$curvepoints`, but now only for the detected bifurcation points along the computed curve. Finally, the fourth and last output variable `output$biftypes` (see command box 8.H) is a vector with string values that indicate the type of bifurcation point detected. These strings can be, for example, "BP #0", "BPE #0", "LP" or "CSS #0". Each element in the vector `output$biftypes` characterises the corresponding row in the output variable `output$bifpoints`.

### 8.4 An example session using the PSPMequi function

To illustrate the use of the PSPMequi function I will discuss the analysis of the PNAS model, presented in chapter 7. The statements below are taken from the R-script `PNAS2002equi_demo.R`, which executes in addition to the statements represented here, \( R \) commands to visualize the computed results in graphs. It is therefore recommended to run the `PNAS2002equi_demo.R` script at the same time as reading the explanation in this section.

Starting the analysis of a PSPM from some random initial values to search for the equilibrium values of environment variables and population birth rates is often not a very successful strategy. Most likely, the initial point will be too far off a solution point, which might cause the software not to converge to the solution. A better alternative is to start with a trivial equilibrium of the model, the value of which is known on beforehand. For example, it is biologically realistic to assume that at very high mortality or at very low
food conditions a population is extinct. Such an extinct state is often easily characterised and hence provides a useful starting point.

The analysis of the PNAS model is therefore started from the trivial equilibrium, which is stable for very low values of the resource productivity $R_{\text{max}}$. In this equilibrium only the resource density has a non-zero value equal to its maximum $\tilde{R} = R_{\text{max}}$, while both the consumer and the predator equilibrium are in a zero equilibrium state. For this reason, the PSPMequi function is invoked with the option vector c("popZE", "0", "envZE", "1", "envZE", "2"), which enforces this zero equilibrium state for the structured population with index 0 (the consumer), the environment variable with index 1 (the predator) and the environment variable with index 2 (the biomass of small consumers that are vulnerable to predation). The latter is obviously in a zero equilibrium state, because the variable represents an integral over the population distribution of the consumer. More generally, if a structured population is assumed to be in a zero equilibrium state by using the "popZE" option, a zero equilibrium state should also be enforced for all the environment variables that represent integrals over this population distribution (that are hence of the type POPULATIONINTEGRAL). Because consumer and predator are assumed to be in a zero equilibrium state the initial point for the call to the PSPMequi function shown in the box 8.B below consists of only 2 elements, $R_{\text{max}}$ and the initial guess for $\tilde{R}$, which are both taken equal to $1 \cdot 10^{-6}$. The parameter with index 1, which corresponds to $R_{\text{max}}$, is the one to be varied in positive direction with step size $0.5$ over the range $0$ to $4.0 \cdot 10^{-4}$.

The sixth argument in the call to the PSPMequi function shown below is left undefined by specifying it as NULL. This argument represents the parameter values to be used for the computation. Because a vector is not specified, the argument is ignored and the default parameter values, as specified in code box 7.2, are used. This sixth argument will also be left undefined in all further calls to the PSPMequi function discussed below and will therefore from hereon be ignored.

**Command box 8.B: Starting PSPM analysis from a trivial equilibrium**

```r
> output1 <- PSPMequi("PNAS2002", "EQ", c(1.0E-06, 1.0E-06), 0.5, c(1, 0, 4E-4), NULL,  
+ c("popZE", "0", "envZE", "1", "envZE", "2"), clean=TRUE, force=TRUE);

Building executable PNAS2002equi.so ...

# Executing : PSPMequi("PNAS2002", "EQ", c(1E-06, 1E-06), 0.5, c(1, 0, 0.0004), NULL, c("popZE", '0', 'envZE', '1', 'envZE', '2'))
# Parameter values :
# Rho : 0.1 Rmax : 1E-06 Lb : 7
# Lo : 07 Lj : 110 Lm : 300
# Beta : 9E-06 Imax : 0.0001 Kh : 1.5E-05
# Gamma : 0.006 Rn : 0.003 Mub : 0.01
# A : 6000 Th : 0.1 Epsilon : 0.5
# Delta : 0.01
# Index of bifurcation parameter #1 : 1
```

After the specific call shown, the \texttt{PSPMequi} function first cleans all previous output file (notice the option \texttt{clean=TRUE}) and subsequently compiles the computational module using the R command \texttt{R CMD SHLIB} into a dynamically loadable library file (notice the somewhat superfluous option \texttt{force=TRUE}). Subsequently, the compiled module is executed with the obligatory arguments that the \texttt{PSPMequi} function passes on. The computational module computes the particular equilibrium curve over the required range of the parameter with index 1 (representing $R_{max}$; see code box 7.2). At the end of the computation the \texttt{PSPMequi} function prints a textual summary of the computation that has been executed. This is summary is in fact the content of the second element of the output list of the function, \texttt{output1$curvedesc}, which is printed to the R console using the statement \texttt{cat(output1$curvedesc, sep='\n')}.

Apart from printing the exact command-line that has been used to start the computation, the values of the parameters are printed using the meaningful, model-specific names, as set in the code box 7.2 on page 42. Furthermore, a header line is printed with a short description of each of the columns in the output matrix \texttt{output1$curvepoints}. As shown in the box above, executing the command \texttt{output1$curvepoints} shows the value of the various columns in this output matrix.

Most importantly, halfway during the computation of the trivial equilibrium the software reports that a branching point has been located, indicated with "BP #0". This branching or transcritical bifurcation point corresponds to the invasion threshold of the consumer. The exact data about the branching point are returned as the third member element of the output list, \texttt{output1$bifpoints}. Displaying \texttt{output1$bifpoints} reveals that it has the same layout as the output matrix \texttt{output1$curvepoints}, but only contains a single row with data for the branching point. Notice that the value of $R_0$, the expected number of offspring produced by an individual consumer during its lifetime, is exactly equal to 1 in this branching point (as it should be), whereas it is smaller and larger than 1 for lower and higher values of $R_{max}$, respectively. The corresponding element of the fourth output variable, assigned to the member element \texttt{output1$biftypes} of the output list, contains the descriptive string "BP #0" that is also printed to the console on detection of the branching point.

In addition to executing the call to the \texttt{PSPMequi} function shown in box 8.B, the \texttt{PNAS2002equi_demo.R} script also uses the output variables \texttt{output1$curvepoints}, \texttt{output1$bifpoints} and \texttt{output1$biftypes} to generate a plot of the computed results.

The next step in the analysis of the PNAS model starts from the detected transcritical bifurcation point that is stored in \texttt{output1$bifpoints}. Starting from that point the
8.4. AN EXAMPLE SESSION USING THE PSPMequi FUNCTION

call to **PSPMequi** shown in the next R command box computes the equilibrium curve with a non-zero equilibrium state of the consumer, while the predator is still assumed to have a zero equilibrium value. Because the absence of the predator ensures that the third environment variable, representing the total biomass of small consumers that the predator forages on, does not influence the equilibrium state, this third environment variable is also ignored. The **PSPMequi** function is therefore called with the option array `c("envZE","1","envZE","2")`. As before, the curve is computed as a function of the parameter with index 1, which corresponds to `Rmax`, with step size 0.2 over the range of `Rmax` values between 0 and 4.0 \( \times 10^{-4} \). As initial point of the computation the `Rmax`-value and the equilibrium values of the resource density and the population birth rate in the bifurcation point are used, which correspond to the first, second and fifth element in `output1$bifpoints` (although `output1$bifpoints[5]` is of course equal to 0).

**Command box 8.C:** Computation of the consumer-resource equilibrium

```r
> output2 <- PSPMequi("PNAS2002", "EQ", output1$bifpoints[c(1,2,5)],0.2, c(1,0,4E-4),NULL,c("envZE","1","envZE","2"))
```

Dynamic library file PNAS2002equi.so is up-to-date

<table>
<thead>
<tr>
<th>V1</th>
<th>V2</th>
<th>V3</th>
<th>V4</th>
<th>V5</th>
<th>V6</th>
<th>V7</th>
<th>...</th>
<th>V10</th>
<th>V11</th>
<th>V12</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0002536023</td>
<td>8.856903e-06</td>
<td>0</td>
<td>0</td>
<td>2.333335e-06</td>
<td>2.447454e-05</td>
<td>4.008016e-06</td>
<td>...</td>
<td>-9.538660e-11</td>
<td>5.628762e-09</td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>0.1</td>
<td>8.856903e-06</td>
<td>0</td>
<td>0</td>
<td>2.333335e-06</td>
<td>2.447454e-05</td>
<td>4.008016e-06</td>
<td>...</td>
<td>-9.538660e-11</td>
<td>5.628762e-09</td>
</tr>
<tr>
<td>8.856903e-06</td>
<td>8.856903e-06</td>
<td>0</td>
<td>0</td>
<td>0.000000e+00</td>
<td>0.000000e+00</td>
<td>0</td>
<td>...</td>
<td>-1.000000e-02</td>
<td>1.4.93640e-08</td>
<td></td>
</tr>
</tbody>
</table>
```

As in the previous R command box a number of output lines and columns have been suppressed to fit the page width of this manual. Please consult the listing in your R console for the complete output of the commands executed.

The layout of the output and the output variables of the call to **PSPMequi** shown in box 8.C is similar to the output as discussed following R command box 8.B. The data of the computation are stored in the output list `output2`. The data of the computed equilibrium points are stored in the element `output2$curvepoints`. Halfway during the computation of the equilibrium the software reports that a branching point has been located for the environment variable with index 1, indicated with "BPE #1". This branching or transcritical bifurcation point corresponds to the invasion threshold of the predator.
For $R_{\text{max}}$-values above this threshold the predator can invade the equilibrium of the consumer population, but it fails to invade for lower $R_{\text{max}}$-values. The exact data about this branching point are contained in `output2$bifpoints`. Displaying `output2$bifpoints` reveals that it has the same layout as the output matrix `output2$curvepoints`, but only contains a single row with data for the branching point. Notice that the population growth rate of the predator, shown in column 10 labeled `pcgE[1]` of the output, is equal to 0 at the detected branching point (as it should be), whereas it is smaller and larger than 0 for lower and higher values of $R_{\text{max}}$, respectively. The last element of the output list, `output2$biftypes`, contains the descriptive string "BPE #1" that is also printed to the console on detection of the branching point.

As before, the `PNAS2002equi_demo.R` script also uses `output2$curvepoints`, `output2$bifpoints` and `output2$biftypes` to plot the computed results of the call to the PSPMequi function shown in box 8.C as additional curves in the graphs that it had generated previously.

The final step in this part of the analysis of the PNAS model starts from the detected transcritical bifurcation point of environment variable 1, representing the predator population, which is stored in the output variable `output2$bifpoints`. Starting from that point the call to PSPMequi shown in the next R command box computes the equilibrium curve with a non-zero equilibrium state of the consumer and predator. All environment variables influence this equilibrium state, hence the PSPMequi function is called without specifying any options. As before, the curve is computed as a function of the parameter with index 1, which corresponds to $R_{\text{max}}$, with step size -0.1 over the range of $R_{\text{max}}$ values between 0 and 4.0 $\cdot 10^{-4}$. The choice of a negative step size is arrived at by trial and error. Choosing a positive step size to start the continuation from this point would have quickly shown that the equilibrium predator density would turn negative, whereas this equilibrium density increases from 0 to positive values with a negative step size. The transcritical bifurcation in this invasion point of the predator is hence subcritical.

As initial point of the computation the data of the branching point contained in `output2$bifpoints` are used. This initial point should contain appropriate values for the bifurcation parameter $R_{\text{max}}$, the equilibrium values of the resource density, the predator density and the biomass density of small, vulnerable consumers as well as the population birth rate in the bifurcation point. Normally, appropriate starting values for these variables are to be found in the first 5 elements of the vector `output2$bifpoints`. Inspection of `output2$bifpoints[1:5]`, however, shows that both `output2$bifpoints[3]` and `output2$bifpoints[4]` are equal to 0:

```
> output2$bifpoints[1:5]
[1] 2.536023e-04 8.856903e-06 0.000000e+00 0.000000e+00 2.333335e-06
```

Obviously, `output2$bifpoints[3]` is equal to 0 as it represents the zero equilibrium value of the predator in the consumer-resource equilibrium curve that is computed with the call to PSPMequi shown in R command box 8.C. Given that the next computation starts from the invasion threshold of the predator the value of 0 for the initial predator density is correct. The value of `output2$bifpoints[4]`, however, representing the total biomass density of consumers vulnerable to predation is also 0, because it was produced by a call to PSPMequi with the option `c("envZE", "2")`, which forces this environment variable to equal 0. Since this is not appropriate as estimate for the environment variable in an equilibrium with predator, consumer and resource present, the value of the interaction
8.4. AN EXAMPLE SESSION USING THE PSPMEQUI FUNCTION

variable $I[0][1]$ (column 7 in `output2$bifpoints`) is used instead as initial estimate, which corresponds to the population integral representing the total biomass of small consumers that are vulnerable to predation (see code box 7.11 and 7.12). Hence, the vector `output2$bifpoints[c(1,2,3,7,5)]` is used as initial point for the computation shown in the next box:

**Command box 8.D: Computing the predator-consumer-resource equilibrium**

```r
> output3 <- PSPMequi("PNAS2002", "EQ", output2$bifpoints[c(1,2,3,7,5)], -0.1, c(1,0,0.0004), NULL, NULL)
```

Dynamic library file `PNAS2002equi.so` is up-to-date

```
2.53602314E-04 8.85690312E-06 0.00000000E+00 4.00801596E-06 2.33335406E-06
2.53602314E-04 8.85690312E-06 0.00000000E+00 4.00801596E-06 2.33335406E-06
2.53602314E-04 8.85690312E-06 0.00000000E+00 4.00801596E-06 2.33335406E-06
```

In the output shown in the box above a large number of output lines have been suppressed and even more intermediate columns then in the previous `R` output box have been deleted, because the page width does not allow them to be shown completely. Consult the listing in your `R` console for the complete output of the commands executed. Otherwise the layout of the output and the output variables of the call to `PSPMequi` shown in box 8.D is the same as in `R` command box 8.C. The data of all computed equilibrium points making up the curve are contained in `output3$curvepoints` and the description of the computed curve in the variable `output3$curvedesc`. Issuing the command `cat(output3$curvedesc, sep="\n")` would lead to the textual output with information about the computation that is also produced by the `PSPMequi` function when finishing.

This last call to the `PSPMequi` function illustrates the detection of the last type of bifurcation that can occur in the dynamics of the PSPM, the saddle-node bifurcation. Starting from the predator invasion threshold the curve representing the predator-consumer-resource equilibrium first bends toward lower values of $R_{max}$ reaching a minimum at $R_{max} = 8.8476 \times 10^{-5}$. The curve subsequently turns toward higher values of $R_{max}$ again. The saddle-node bifurcation or limit point occurs at this minimum value of $R_{max} = 8.8476 \times 10^{-5}$. The data pertaining to this limit point is contained in the variable `output3$bifpoints[c(1,2,3,7,5)]`.
CHAPTER 8. MODEL ANALYSIS IN R

The limit point is the minimum value of $R_{\text{max}}$ for which a predator-consumer-resource equilibrium occurs. It is hence also referred to as the predator persistence boundary.

The PNAS2002equi_demo.R script uses output3$curvepoints, output3$bifpoints and output3$biftypes to draw the additional curves representing the predator-consumer-resource equilibrium in the bifurcation graphs that already showed the curves resulting from the previous 2 call to PSPMequi (see R command box 8.B and 8.C).

The following 3 calls to PSPMequi that are executed by the PNAS2002equi_demo.R script, illustrated in R command box 8.E, 8.F and 8.G, compute the location of the 3 detected bifurcation points, the branching point representing the invasion threshold of the consumer, the branching point of environment variable 2 representing the invasion threshold of the predator and the limit point representing the persistence threshold of the predator, as a function of two parameters: the value of $R_{\text{max}}$ and the value of the consumer background mortality $\mu_b$. These calls hence all use as 4th argument to the function the vector c(1,0,4.0E-4,11,0,0.1) indicating that the parameters with index 1 and 11 are to be varied (see code box 7.3) within the ranges 0 to 4.0-10^{-4} and 0 to 0.1, respectively.

Computing the consumer invasion boundary as a function of $R_{\text{max}}$ and $\mu_b$ starts from the data on the branching point stored in the output variable output1$bifpoints, which was detected during the computation of the trivial equilibrium without any consumers and predators (see R command box 8.B). The first two elements of this vector represent the value of $R_{\text{max}}$ and the equilibrium resource density at the consumer invasion boundary. To complete the specification of the initial point of the computation the default value of consumer background mortality (0.01) is added. Hence, the initial point of the computation is c(output3$bifpoints[1:2],0.01). The type of the computation, which is the second argument to the PSPMequi function, is now specified as "BP" as opposed to the value "EQ" that was used in all previous calls to PSPMequi.

At the consumer invasion boundary, the environment variables with index 1 and 2, representing the predator density and the total biomass density of small consumers vulnerable to predation, respectively, are both 0. The last argument of the call to PSPMequi shown in R command box 8.E hence equals the vector c("envZE","1","envZE","2","popBP","0"), which in addition to the zero equilibrium value for the environment variables also instructs the computational module that the transcritical bifurcation point that is computed occurs in the population with index 0.

Command box 8.E: Computing the consumer invasion boundary

```r
> output4 <- PSPMequi("PNAS2002","BP",c(output1$bifpoints[1:2],0.01),0.05,c(1,0,4.0E-4,11,0,0.1),NULL,
  c("envZE","1","envZE","2","popBP","0"))

Dynamic library file PNAS2002equi.so is up-to-date

Parameter values :
  # Rho : 0.1 Rmax : 8.8569E-06 Lb : 7
  # Le : 27 Lj : 110 Ln : 300
  # Beta : 5E-06 Imax : 0.0001 Kb : 1.5E-05
```
### 8.4. AN EXAMPLE SESSION USING THE PSPMEQUI FUNCTION

#### 8.4.1. Gamma, Rm, Mub, A, Th, Epsilon, Delta

- Gamma : 0.006
- Rm : 0.003
- Mub : 0.01
- A : 5000
- Th : 0.1
- Epsilon : 0.5
- Delta : 0.01

#### 8.4.2. Index of bifurcation parameter #1: 1
- Index of bifurcation parameter #2: 11
- Index of structured population with transcritical bifurcation: 0

#### 8.4.3. Columns in output4$curvedesc

<table>
<thead>
<tr>
<th>V1</th>
<th>V2</th>
<th>V3</th>
<th>V4</th>
<th>V5</th>
<th>V6</th>
<th>V7</th>
<th>V8</th>
<th>V9</th>
<th>..</th>
<th>V13</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,]</td>
<td>8.856903e-06</td>
<td>8.856903e-06</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>..</td>
<td>4.920353e-08</td>
</tr>
<tr>
<td>(2,]</td>
<td>8.884831e-06</td>
<td>8.884831e-06</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>..</td>
<td>1.327406e-08</td>
</tr>
<tr>
<td>(3,]</td>
<td>8.913583e-06</td>
<td>8.913583e-06</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>..</td>
<td>1.515673e-08</td>
</tr>
<tr>
<td>(511,)</td>
<td>3.945989e-04</td>
<td>3.945989e-04</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>..</td>
<td>9.558855e-10</td>
</tr>
<tr>
<td>(512,)</td>
<td>3.981262e-04</td>
<td>3.981262e-04</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>..</td>
<td>9.616150e-10</td>
</tr>
<tr>
<td>(513,)</td>
<td>4.016538e-04</td>
<td>4.016538e-04</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>..</td>
<td>9.642264e-10</td>
</tr>
</tbody>
</table>

#### 8.4.4. Computing the predator invasion boundary

- Rmax (first column) on the x-axis and \( \mu_b \) (sixth column) on the y-axis, showing the regions parameter space for which persistence of the consumer population is and is not possible.

- Computing the predator invasion boundary as a function of \( R_{max} \) and \( \mu_b \) starts from the data on the branching point stored in the output variable output2$bifpoints, which was detected during the computation of the consumer-resource equilibrium without any predators (see R command box 8.C). The first two elements of this vector represent the value of \( R_{max} \) and the equilibrium resource density at the predator invasion boundary, while the fifth element of output2$bifpoints represents the birth rate of the structured consumer population in this equilibrium (see the listing of output2$bifpoints in R command box 8.C). To complete the specification of the initial point of the computation the default value of consumer background mortality (0.01) is added. Hence, the initial point of the computation is c(output2$bifpoints[c(1,2,5)],0.01). The type of the computation, which is the second argument to the PSPMequi function, is now specified as "BPE", indicating that a transcritical bifurcation curve in an environment variable is to be computed as a function of 2 model parameters.

- The environment variables with index 2, representing the total biomass density of small consumers vulnerable to predation does not affect the predator invasion boundary, as it only influences the predation mortality of small consumers (see code box 7.10). This environment variable can hence be assumed to equal 0 and its equilibrium condition can be ignored by passing the appropriate option pair to the PSPMequi function. Furthermore, the option vector should instruct the computational module to compute the...
transcritical bifurcation curve for the environment variable with index 1. The last argument of the call to PSPMequi shown in R command box [L] therefore equals the vector c("envBP","1","envZE","2"). Notice that compared to the previous call to PSPMequi, this option array does not contain any specific instructions concerning the structured consumer population.

Command box 8.F: Computing the predator invasion boundary

```r
> output5 <- PSPMequi("PNAS2002","BPE",c(output2$bifpoints[c(1,2,5)],0.01), 0.1,c(1,0,4E-4,11,0,0.1),NULL,
4 2 c("envZE","2","envBP","1"))
```

Dynamic library file PNAS2002equi.so is up-to-date

```
2.53602314E-04 8.85690312E-06 2.33333540E-06 1.00000000E-02
2.44422274E-04 8.88032498E-06 2.35250524E-06 1.02628274E-02
2.35413020E-04 8.90710825E-06 2.37324896E-06 1.05420330E-02
2.44422274E-04 8.88032498E-06 2.35250524E-06 1.02628274E-02
2.35413020E-04 8.90710825E-06 2.37324896E-06 1.05420330E-02
```

(Once again, consult your R console for a complete listing of the output of the commands shown above as parts of this output is deleted for the sake of brevity and layout).

The R command box above shows that the output of the PSPMequi function has in this case a similar layout as when computing the consumer invasion boundary (R command box 8.E). The data about the points making up the computed curve are contained in output5$curvepoints, whereas output5$curvedesc contains the description of the computations. These are the only two elements of the output list for computations involving two variable parameters, as was the case for the continuation of the "BP" curve. The PNAS2002equi_demo.R script again uses the first and sixth column of output5$curvepoints to create a graph with $R_{max}$ (first column) on the $x$-axis and $\mu_b$ (sixth column) on the $y$-axis, showing the regions of parameter space for which invasion of the consumer-resource equilibrium by the predator is possible or not.

The final analysis step to be performed is to compute the location of the limit point in the predator-consumer-resource equilibrium curve as a function of $R_{max}$ and $\mu_b$. This computation starts from the data on the limit point stored in the output variable output3$bifpoints, which was detected during the computation of the predator-consumer-resource equilibrium (see R command box 8.D). The first five elements of this vector represent the value of $R_{max}$, the equilibrium resource density, the equilibrium
8.4. AN EXAMPLE SESSION USING THE PSPMEQUI FUNCTION

predator density, the equilibrium biomass density of small consumers vulnerable to predation and the equilibrium birth rate of the consumer population. To complete the specification of the initial point of the computation the default value of consumer background mortality (0.01) is added. Hence, the initial point of the computation is specified as `c(output3$bifpoints[1:5],0.01)`. The type of the computation, which is the second argument to the PSPMequi function, is now specified as "LP", indicating that a saddle-node bifurcation curve is to be computed as a function of 2 model parameters.

For this computation the option vector is left undefined (`NULL`), because all variables influence the location of the limit point and hence none of the quantities are characterised by a zero equilibrium state.

Command box 8.G: Computing the predator persistence boundary

```r
> output6 <- PSPMequi("PNAS2002","LP",c(output3$bifpoints[1:5],0.01),0.05,c(1,0,4E-4,11,0,0.1),NULL,NULL)

Dynamic library file PNAS2002equi.so is up-to-date

2

4

8.84988526E-05 1.31478259E-05 3.80697042E-05 4.00801603E-06 5.17387205E-05 1.00133536E-02

6

8.86520738E-05 1.31876853E-05 3.79221368E-05 4.00801603E-06 5.13061665E-05 1.01309246E-02

8

8.88161578E-05 1.32276419E-05 3.77736423E-05 4.00801603E-06 5.08694956E-05 1.02496461E-02

10

8.89812207E-05 1.32686671E-05 3.76151471E-05 4.00801603E-06 5.04244896E-05 1.03683875E-02

12

8.91442326E-05 1.33096923E-05 3.74566518E-05 4.00801603E-06 5.00895129E-05 1.04871289E-02

14

# Executing : PSPMequi("PNAS2002","LP",c(8.84989E-05,1.32327E-05,3.8454E-05,4.00802E-06,5.25658E-05,0.01),0.05,
c(1,0,0.0004,11,0,0.1),NULL,NULL)

# Parameter values :

# Rho : 0.1 Rmax : 8.84989E-05 Lb : 7
# Lv : 27 Lj : 110 Lm : 300
# Beta : 9E-06 Imax : 0.0001 Rh : 1.5E-05
# Gamma : 0.006 R : 0.003 Rh : 0.006
# A : 5000 Th : 0.1 Epsilon : 0.5
# Delta : 0.01

> output6$curvepoints

V1 V2 V3 V4 V5 V6 V7 V8 .. V13
[1,] 8.849885e-05 1.314783e-05 3.806970e-05 4.008016e-06 5.173872e-05 1.001335e-02
[2,] 8.865207e-05 1.318769e-05 3.792214e-05 4.008016e-06 5.130617e-05 1.013092e-02
[3,] 8.881616e-05 1.322764e-05 3.777364e-05 4.008016e-06 5.086949e-05 1.024965e-02
[4,] 8.898122e-05 1.326867e-05 3.761515e-05 4.008016e-06 5.042449e-05 1.036839e-02
[5,] 8.914423e-05 1.330969e-05 3.745665e-05 4.008016e-06 5.008951e-05 1.048713e-02

# Index of bifurcation parameter #1 : 1
# Index of bifurcation parameter #2 : 11


> output6$curvedesc

V1 V2 V3 V4 V5 V6 V7 V8 .. V13
[1,] 8.849885e-05 1.314783e-05 3.806970e-05 4.008016e-06 5.173872e-05 1.001335e-02
[2,] 8.865207e-05 1.318769e-05 3.792214e-05 4.008016e-06 5.130617e-05 1.013092e-02
[3,] 8.881616e-05 1.322764e-05 3.777364e-05 4.008016e-06 5.086949e-05 1.024965e-02
[4,] 8.898122e-05 1.326867e-05 3.761515e-05 4.008016e-06 5.042449e-05 1.036839e-02
[5,] 8.914423e-05 1.330969e-05 3.745665e-05 4.008016e-06 5.008951e-05 1.048713e-02

(Once again, consult your R console for a complete listing of the output of the commands shown above as parts of this output is deleted for the sake of brevity and layout).

The output of the PSPMequi function in this last call has a similar layout as in the previous two calls to compute consumer and predator invasion boundary (R command box 8.E and 8.F). The data about the points making up the computed curve are stored in `output6$curvepoints`, whereas the description of the computations is stored in `output6$curvedesc`. These are, as before, the only two elements of the output list `output6`. The PNAS2002equi_demo.R script again uses the first and and the sixth column of `output6$curvepoints` to create a graph with $R_{max}$ (first column) on the x-axis and $\mu_b$ (sixth column) on the y-axis, showing the regions of parameter space for which a predator-consumer-resource equilibrium occurs or not and hence for which predators can persist.
8.5 Output files generated by the PSPMequi function

The computational module that is produced by the PSPMequi function generates 4 output files in case of a one-parameter bifurcation (continuation type "EQ") and 3 output files in other cases (continuation types "BP", "BPE", "LP", "ESS" and "PIP"). The name of these files is always of the form <Modelname>-<Type>-<NNNN>.<ext>, in which <Modelname> is the same as the name of the file specifying the model excluding its .h extension, <Type> refers to the type of the continuation performed (either EQ, BP, BPE, LP, ESS or PIP) and <NNNN> is a 4-digit number that is unique for the current computation and .<ext> is the extension, which can be either .bif, .err, .csb or .out. The unique number distinguishes the same types of curve computations for the same model from each other. The number is obtained by considering for a specific type of continuation ("BP", "BPE" , "EQ", "LP", "ESS" or "PIP") increasing values of <NNNN> (i.e., 0000, 0001, 0002 and so forth) and testing whether result files with the particular index are already present. The program uses the first value of <NNNN> that is not in use.

Hence, the call of the PSPMequi function for the PNAS model, as shown in R command box [8.B], generates the output files PNAS2002-EQ-0000.bif, PNAS2002-EQ-0000.err, PNAS2002-EQ-0000.out and PNAS2002-EQ-0000.csb, the following call as shown in R command box [8.C] generates the output files PNAS2002-EQ-0001.bif, PNAS2002-EQ-0001.err, PNAS2002-EQ-0001.out and PNAS2002-EQ-0001.csb, while the last computation of an equilibrium curve, as shown in R command box [8.D], generates the output files PNAS2002-EQ-0002.bif, PNAS2002-EQ-0002.err, PNAS2002-EQ-0002.out and PNAS2002-EQ-0002.csb. The computations of the consumer invasion, predator invasion and predator persistence boundary (see R command box [8.E, 8.F and 8.G]) each generate only 3 output files, called PNAS2002-<Type>-0000.err, PNAS2002-<Type>-0000.out and PNAS2002-<Type>-0000.csb with <Type> equal to BP, BPE and LP in case of the consumer invasion, the predator invasion and the predator persistence boundary, respectively.

The file called <Modelname>-<Type>-<NNNN>.err that is generated during the computations of curves contains information about the numerical progress of the computations. It reports details on the steps taken during the Newton iteration, the convergence to the solution, as well as information about the steps taken along the curve that is being computed. This file can be informative in case the computation of a particular curve stops for unknown reasons, but is otherwise of little use.

The output file called <Modelname>-<Type>-<NNNN>.out contains the same information as in the member elements curvepoints and curvedesc of the output list returned by the PSPMequi function (see R command box [8.H]). The first lines of this file all start with a # sign and contain the information about the run performed, which is also contained in curvedesc and can be listed by the statement cat(output$curvedesc,sep="\n"). Following this descriptive header the file contains columns with computational results that are also contained in the variable curvepoints (see, for example, R command box [8.C]). In fact, the first two output elements curvepoints and curvedesc are generated by reading the contents of the file <Modelname>-<Type>-<NNNN>.out from disk after the computations have ended, storing all lines that start with a # sign into curvedesc, while storing the information on all other lines into the data matrix curvepoints.

Similarly, the output file called <Modelname>-<Type>-<NNNN>.bif, which is only generated during the computation of an equilibrium curve (type "EQ"), contains the same information as is contained in the last two elements of the output list, called bifpoints.
and `biftypes`, returned by the `PSPMequi` function (see R command box 8.H). Each row in the file `<Modelname>-<Type>-<NNNN>.bif` pertains to a single detected bifurcation point. A row starts with the numerical data that characterises the bifurcation point, which are exactly the same columns of data as stored in the file `<Modelname>-<Type>-<NNNN>.out`. Appended to the numerical data is a string of the form *** `<Type>` ***, where `<Type>` can be, for example, BP #0, BP #0, LP or CSS #0. The numerical data that form the first part of each row are stored by the `PSPMequi` function into the list element `bifpoints`, which hence has as many columns as there are in the output list element `curvepoints` and as many rows as there bifurcation points occurring in the computed equilibrium curve. The strings representing the type of bifurcation point are stored by the `PSPMequi` function into `biftypes`, which hence has as many elements as there are bifurcation points.

The file called `<Modelname>-<Type>-<NNNN>.csb` contains for every curve point that has been computed information on the parameters, for which the point has been computed, the equilibrium values of all environment variables and the stable distribution of all structured populations in the model. This is a binary file, the content of which can be accessed from R using the function `csbread`. For example, the file `PNAS2002-EQ-0002.csb` is generated by the invocation of the `PSPMequi` function for the PNAS model shown in R command box 8.D. Its contents can be listed by:

```r
> csbread("PNAS2002-EQ-0002.csb")
States in file PNAS2002-EQ-0002.csb:
  1: State-2.536023E-04
  2: State-2.525758E-04
  3: State-2.515530E-04
  ...output lines suppressed in this box...
  437: State-3.989129E-04
  438: State-3.970218E-04
  439: State-4.042258E-04
```

(The first time you invoke the function `csbread` you might see some output generated by the compilation of the dynamic library module that contains the function `csbread`). The population state called `State_4.042258E-04` pertains to the parameter value $R_{\text{max}} = 4.042258 \cdot 10^{-4}$ as its name suggests. Its contents can be read into the workspace by issuing the command `csbread("PNAS2002-EQ-0002.csb",439)` or `csbread("PNAS2002-EQ-0002.csb","State-4.042258E-04")`.

Loading this state into the R workspace reveals it to be a list containing various arrays of numbers, as shown in the following box:
The first element of the list (called \$BifPars) representing the population state State-4.042258E-04 is the value of the bifurcation parameter(s) for this particular state. The second element, an array called \$Parameters (not completely displayed in the box above because of space restrictions), contains the values of all the model parameters characterising this particular equilibrium state, while the third member of the list contains the equilibrium values of all environment variables. The two subsequent arrays in the list characterise the stable population distribution, of which the first (called \$Pop00_BirthStates) specifies the state at birth of the individuals. The other (called \$Pop00) is a two-dimensional array characterising the population distribution in equilibrium with the first column \$Pop00[,1] representing the density profile of the equilibrium population and the subsequent columns \$Pop00[,2] and \$Pop00[,3] representing the average values of the individual state variables with index 0 and 1 in the model (corresponding to individual age and length in the PNAS model), as shown in the \texttt{R} command box above. If individuals are characterised by more than two individual state variables, the values of these follow in additional columns of the two-dimensional array \$Pop00. The \texttt{R} command box above also illustrates that the dimension of the array \$Pop00 indicates that the population is represented by 100 cohorts of individuals (see chapter [15] for the option to change this number). The number of individuals in cohort $i$ is given by the array element \$Pop00$[i,1], while the average value of the individual state variable with index 0 and 1 (average age and average length in the PNAS model) are given by \$Pop00$[i,2] and \$Pop00$[i,3], respectively.
8.5. OUTPUT FILES GENERATED BY THE PSPMEQUI FUNCTION

Command box 8.H: PSPMequi help page

PSPMequi: Computes a bifurcation curve for a structured population model

Syntax:

```r
output <- PSPMequi(modelname = NULL, biftype = NULL, startpoint = NULL, stepsize = NULL, parbnds = NULL,
parameters = NULL, options = NULL, cvode = FALSE, clean = FALSE, force = FALSE, debug = FALSE)
```

Arguments:

- **modelname**: (string, required)
  Basename of the file with model specification. The file should have extension `.h`. For example, the model "PNAS2002" is specified in the file "PNAS2002.h"

- **biftype**: (string, required)
  Type of bifurcation to compute: "BP", "BPE", "EQ", "LP", "ESS" or "PIP"

- **startpoint**: (row vector, required)
  The initial point from which to start the continuation of the curve

- **stepsize**: (double value, required)
  Value of the step size in the first bifurcation parameter

- **parbnds**: (row vector of length n*3, required)
  Vector of length n*3 with n=1 for EQ continuation, n=2 for "BP", "BPE", "LP" and "PIP" continuation and n>=2 for "ESS" continuation. Each triple specifies:
  - `parbnds[1]`: the index of the first bifurcation parameter
  - `parbnds[2]`: lower threshold, below which value of the first bifurcation parameter the computation stops
  - `parbnds[3]`: upper threshold, above which value of the first bifurcation parameter the computation stops

  In case of two-parameter bifurcations:
  - `parbnds[5]`: lower threshold, below which value of the second bifurcation parameter the computation stops
  - `parbnds[6]`: upper threshold, above which value of the second bifurcation parameter the computation stops

- **parameters**: (row vector, optional, can be left equal to its default NULL)
  Vector of length PARAMETER_NR (set in the model program file), specifying the values for the model parameters to use in the computation. Vectors of other lengths, including an empty vector will be ignored.

- **options**: (row vector of strings, optional, can be left equal to its default NULL)
  Vector with pairs of strings, consisting of an option name and a value (for example `c("popBP", "1")`) or single options (i.e. `c("test")`). Possible option names and their values are:
  - "envBP", "<index>": Index of environment variable, of which to continue the transcritical bifurcation
  - "popBP", "<index>": Index of structured population, of which to continue the transcritical bifurcation
  - "popEVO", "<index>": Index of structured population, for which to perform ESS or PIP continuation
  - "envZE", "<index>": Index of environment variable in trivial equilibrium (can be used multiple times)
  - "popZE", "<index>": Index of structured population in trivial equilibrium (can be used multiple times)
  - "isort", "<index>": Index of i-state variable to use as ruling variable for sorting the structured populations
  - "test": Perform only a single integration over the life history, reporting dynamics of survival, R0, i-state and interaction variables

- **cvode**: (Boolean, optional argument)
  Specify `cvode = TRUE` as argument to use the CVODE integrator from the Sundials collection of nonlinear and differential/algebraic equation solvers (see http://www.llnl.gov/CASC/sundials for details)
  Only available on Unix-based systems when Sundials has been installed

- **clean**: (Boolean, optional argument)
  Specify `clean = TRUE` as argument to remove all the result files of the model before the computation

- **force**: (Boolean, optional argument)
  Specify `force = TRUE` as argument to force a rebuilding of the model before the computation

- **debug**: (Boolean, optional argument)
  Specify `debug = TRUE` as argument to compile the model in verbose mode and with debugging flag set
Output:
The output is a list containing the following elements:

- `curvepoints`: Matrix with output for all computed points along the curve.
- `curvedesc`: Column vector with strings, summarizing the numerical details of the computed curve (i.e., initial point, parameter values, numerical settings used).
- `bifpoints`: Matrix with the located bifurcation points along the curve.
- `biftypes`: Column vector of strings, containing a description of the type of bifurcation for each of the located bifurcation points.
Analysis of evolutionary fixed points of non-linear PSPMs
Theoretical and computational background

The analysis evolutionary fixed points of non-linear PSPMs focuses on the question how the value of a particular model parameter would change if mutations would generate variability in this parameter value and selection would act on this variability. Adaptive dynamics ([Metz et al. 1996] [Geritz et al. 1998]) constitutes an approach to answer such questions, while carefully taking into account the feedback of populations on their environment. The central function in the theory of adaptive dynamics is the long-term population growth of a mutant type in an environment that is completely dominated and hence determined by a resident population. This quantity is usually referred to with the symbol $s_x(y)$, in which $x$ refers to the type of the resident population and $y$ refers to the type of the mutant. Not surprisingly, when the mutant is identical to the resident it has a population growth rate 0, since the resident is assumed to persist indefinitely (Notice that this does no require the population to be in equilibrium). Therefore:

$$s_x(y)|_{y=x} = 0$$

Furthermore, the partial derivative $\frac{\partial s_x(y)}{\partial y}$ equals the selection gradient, indicating whether a mutation-selection process will lead to larger or smaller values of the trait $x$. If

$$\frac{\partial s_x(y)}{\partial y} \bigg|_{y=x} > 0$$  (9.1)

a mutant with a trait value $y$ larger than the resident trait value $x$ will have a positive long-term growth rate and hence will be able to invade, while the opposite holds for when the partial derivative is negative. An evolutionary singular point, which will be indicated with $x^*$, now occurs where

$$\frac{\partial s_x(y)}{\partial y} \bigg|_{y=x^*} = 0$$

Furthermore, The second-order partial derivatives

$$\frac{\partial^2 s_x(y)}{\partial x^2} \bigg|_{y=x^*} \quad \text{and} \quad \frac{\partial^2 s_x(y)}{\partial y^2} \bigg|_{y=x^*}$$

determine whether the evolutionary singular point is a convergent stable strategy (CSS), an evolutionary repeller (ERP) or an evolutionary branching point (EBP) ([Geritz et al. 1998]).
In the bifurcation analysis of PSPMs the equilibrium of a structured population is determined by the condition

\[ R_0 - 1 = 0 \]

in which \( R_0 \) is the expected number of offspring produced by a single individual of the structured population during its entire life. \( R_0 \) is not the same as the long-term population growth rate, but the condition \( R_0 - 1 \) is sign-equivalent with the population growth rate: the sign of \( R_0 - 1 \) and the population growth rate are always the same and when \( R_0 - 1 \) equals 0, the population growth rate is 0 as well. According to the theory of adaptive dynamics (Metz et al. [1996]; Geritz et al. [1998]) the function \( R_0 - 1 \) can therefore be used for the analysis of evolutionary fixed points of PSPMs.

In the context of the PSPMs the traits \( x \) and \( y \) will refer to the resident and mutant value, respectively, of one of the model parameters. The value of such a parameter will influence the expected number of offspring produced by a single individual of the structured population during its entire life, \( R_0 \), if the parameter represents a life history characteristic. On the other hand, \( R_0 \) is also influenced by the environment in which the individual lives. A key element of PSPMs is that this environment itself is influenced by the structured population to such an extent that the equilibrium value of the environment is determined by the population. The equilibrium value of the environment is hence also a function of the model parameters and we can write the equilibrium condition of the structured population more appropriately as:

\[ R_0(y, \hat{E}(x))|_{y=x} - 1 = 0 \]

\( x \) in this condition refers to the value of one of the model parameters in the PSPM of the resident type of individual that dominates the structured population and hence determines the equilibrium value of the environment variables \( \hat{E}(x) \), whereas \( y \) refers to the value of that same parameter for a mutant type, which invades the population at low density. The partial derivatives of the function \( R_0(y, \hat{E}(x)) - 1 \) can therefore be used to classify a computed equilibrium in a PSPM as an evolutionary fixed point and determine whether it is a convergent stable strategy (CSS), an evolutionary repellor (ERP) or an evolutionary branching point (EBP) (Geritz et al. [1998]). Since the constant 1 in this function is irrelevant for the partial derivatives, the quantities of interest are:

\[ R_{0x} := \frac{\partial R_0(y, \hat{E}(x))}{\partial y}|_{y=x^*} \]

\[ R_{0xx} := \frac{\partial^2 R_0(y, \hat{E}(x))}{\partial x^2}|_{y=x^*} \]

\[ R_{0yy} := \frac{\partial^2 R_0(y, \hat{E}(x))}{\partial y^2}|_{y=x^*} \]

During an equilibrium computation with the PSPMequi script the program can check for every computed equilibrium point the value of \( R_{0x} \). This test is, however, only performed when the option ‘popEVO’ is set to a valid value, that is in the range 0 to \texttt{POPULATION\_NR-1}. The value of this option identifies the index of the structured population, for which to carry out the evolutionary fixed point analysis. As default the option
'popEVO' is not defined and the test of the evolutionary properties of the equilibrium is skipped, as was the case in the model analyzed in chapter 8. When the software detects a sign change in this quantity, it attempts to locate the exact position of the evolutionary fixed point by solving for the equilibrium of the PSPM with the additional condition $R_{0x} = 0$. When successful the software computes the second-order partial derivatives $R_{0xx}$ and $R_{0yy}$ to classify the evolutionary fixed point. The computation of these partial derivatives is done entirely numerically using a central-differencing approach. Unless it fails to compute one of the partial derivatives properly, the software will report whether a convergent stable strategy (CSS), an evolutionary repellor (ERP) or an evolutionary branching point (EBP) has been detected.

Once an evolutionary fixed point is detected, the software allows for 2 further steps of analysis of the evolutionary fixed point. The first type of analysis that can be carried out is that the evolutionary fixed point can be computed for a range of values of a second model parameter. More precisely, the condition $R_{0x} = 0$ is added as supplementary condition to the system of equations determining the equilibrium of the PSPM and because of this additional condition one more unknown quantity, the value of a second model parameter, has to be solved for. This type of computations is referred to with the acronym 'ESS'. They yield curves that show the evolutionary stable value of the evolutionary parameter as a function of the first bifurcation parameter.

The software is in fact sufficiently general to allow for continuation of curves with multiple model parameters having their evolutionary stationary value. These curves are all indicated with the acronym 'ESS'. For each evolutionary parameter the corresponding condition $R_{0x} = 0$ is added to the system of equations to solve. For each parameter at its evolutionary stationary value the vector of initial estimates of a solution point (the third argument to the function PSPMequi) should contain a value close this evolutionary stationary value, whereas the index of the parameter in the model and its allowable minimum and maximum value are defined by the triplet in the fifth argument to the function PSPMequi (see section 8.2). As discussed in section 8.2 this fifth argument to the function PSPMequi should for 'ESS' computations contain at least 2 triplets, one for the (first) bifurcation parameter and one for the model parameter that is fixed at its evolutionary stationary value, but it can be extended with more triplets in case the 'ESS' curve is characterised by multiple parameters at their evolutionary stationary value. The number of triplets for evolutionary parameters should match the number of initial estimates for these parameters in the third argument to the function PSPMequi. The current version of the software computes for each parameter at its evolutionary stationary value the second-order partial derivatives $R_{0xx}$ and $R_{0yy}$ and writes these second-order derivatives to the output file. Notice, however, that these derivatives only provide a classification of the evolutionary stationary point in terms of convergent stable, evolutionary repellor or evolutionary branching point in the case of a single evolutionary parameter, as the classification of multidimensional evolutionary fixed point involves more complex computations of derivatives (see Leimar, 2005).

The second type of analysis that can be performed is the computation of the pairwise invasibility plot (or PIP; for an explanation see Geritz et al. (1998)) starting from the evolutionary fixed point. This type of computation is indicated with the acronym 'PIP' and is carried out by supplementing the system of equations determining the equilibrium of the PSPM with the condition $R_0(y, \bar{E}(x)) = 1$. Because of this extension, one more unknown variable has to be solved for, which in this case is the mutant value of the model parameter $y$. The first and second bifurcation parameter in this case have the
same index in the array of parameter values, but the first bifurcation parameter refers to
the resident value $x$ of this parameter, while the second bifurcation parameter refers to
the mutant value $y$. The result of such a computation is a curve in the parameter space
spanned by $x$ and $y$, where the growth rate of a mutant with parameter value $y$ in an
equilibrium environment determined by a resident population with parameter value $x$ has
a zero population growth rate. PIPs are plots of such curves and these plots can be used
for inferring various evolutionary consequences (Geritz et al. 1998).

While performing computations of the type ‘ESS’ and ‘PIP’ the software continuously
computes the value of the second order partial derivatives $R_{0xx}$ and $R_{0yy}$ and writes these
values to the output file (with extension .out). Inspection of the output file can hence also
indicate whether an evolutionary fixed point changes its type, for example from CSS to
EBP or vice versa. Automatic detection and processing of such type changes is, however,
(currently) not implemented in the software.
An example model for the analysis of evolutionary fixed points

The analysis of evolutionary fixed points of PSPMs will be illustrated using a model for a size-structured consumer population feeding on a resource $R$. Individual consumers are assumed to be born at size $s_b$ and forage on the resource at a rate proportional to an allometric function of their size, $s^q$. They are furthermore assumed to have a linear functional response, such that their ingestion rate equals $\gamma(s, R) = I_{max} Rs^q$. Ingested energy is assimilated with a constant conversion efficiency $\sigma$. Maintenance costs are also assumed to follow an allometric relation of body size, $Ts^p$.

Juvenile individuals spend all their net energy production on growth in body size and hence have a somatic growth rate $\sigma \gamma(s, R) - Ts^p$. Above a body size threshold $s = s_j$, referred to as the maturation size, individuals decrease the fraction of their net-energy production that they invest in somatic growth and use the remainder for investments in reproduction. The function $\kappa(s)$ indicates the fraction of net-energy production invested in somatic growth. $\kappa(s)$ is a cubic function of size that decreases smoothly and continuously from a value of 1 at $s = s_j$ to a value 0 at $s = s_m$. The size threshold $s = s_m$ hence represents the maximum body size individual consumers can possibly reach. The energy invested into reproduction is converted into offspring with size $s = s_b$. No further conversion losses are assumed to occur during somatic growth and reproduction, the conversion efficiency $\sigma$ is assumed to include all such losses. The somatic growth rate hence equals $g(s, R) = \kappa(s)(\sigma \gamma(s, R) - Ts^p)$, while the fecundity is given by $\beta(s, R) = (1 - \kappa(s))(\sigma \gamma(s, R) - Ts^p)/s_b$. Consumers experience a constant, size-independent mortality. Finally, in the absence of consumers the resource follows semi-chemostat dynamics with turn-over rate $\delta$ and maximum resource density $R_{max}$.

The model dynamics can now be described by the following system of partial and ordinary differential equations for the resource density $R$ and the consumer size distribution $n(t, s)$:

$$\frac{\partial n(t, s)}{\partial t} + \frac{\partial (g(s, R)n(t, s))}{\partial s} = -\mu n(t, s)$$

$$g(s_b, R) \ n(t, s_b) = \int_{s_b}^{s_m} \beta(s, R) \ n(t, s) \ ds$$

$$\frac{dR}{dt} = \delta (R_{max} - R) - \int_{s_b}^{s_m} \gamma(s, R) n(t, s) \ ds$$
As discussed above the individual life history functions representing food ingestion, somatic growth, fecundity and the fraction of net-energy production allocated to somatic growth are given by:

\[
\gamma(s, R) = I_{max} R s^q
\]
\[
g(s, R) = \kappa(s) (\sigma \gamma(s, R) - T s^p)
\]
\[
\beta(s, R) = \frac{(1 - \kappa(s)) (\sigma \gamma(s, R) - T s^p)}{s_b}
\]
\[
\kappa(s) = \begin{cases} 
1 & \text{if } s \leq s_j \\
1 - 3 \left( \frac{s - s_j}{s_m - s_j} \right)^2 + 2 \left( \frac{s - s_j}{s_m - s_j} \right)^3 & \text{otherwise}
\end{cases}
\]

The evolutionary fixed point analysis will focus on the parameter \( q \), the allometric scaling exponent of ingestion rate with body size \( s \). Default values of the other parameters are: \( \delta = 0.1 \), \( R_{max} = 2.0 \), \( I_{max} = 1.0 \), \( T = 0.1 \), \( p = 1.0 \), \( s_b = 0.05 \), \( s_j = 1.0 \), \( s_m = 2.0 \) and \( \sigma = 0.5 \). The background mortality experienced by consumers is assumed to equal \( \mu = 0.01 \).

The model is implemented in the model-specific file `Indet_growth.h` that you can find in the `Tests` directory. The implementation of the model follows the guidelines as presented for the PNAS model in chapter 7 and will therefore not be discussed in detail. The reader is encouraged to inspect the file `Indet_growth.h` and work out the translation of the mathematical formulation given above into the necessary C-code elements required for analysis.
Model analysis in R

The analysis using R can be performed by executing the R script `Indet_growth_demo.R`, which is to be found together with the model-specific file `Indet_growth.h` in the Tests directory. Below 3 commands will be discussed that are executed by the `Indet_growth_demo.R` script and that illustrate the possibilities to use the software for evolutionary fixed point analysis. The `Indet_growth_demo.R` script furthermore performs some plotting of the output data generated by the computational module.

The analysis starts out by computing the equilibrium of the consumer-resource model as a function of the parameter \( q \), the allometric scaling exponent of ingestion with body size \( s \). This parameter has index 6 in the parameter array defined in the model-specific file `Indet_growth.h` (see line 50–80 in that file). The computation starts from an equilibrium point at \( q = 1 \), computing the equilibrium for decreasing values of \( q \) in the range \( 0.5 \leq q \leq 2.0 \). Hence, the fourth and fifth argument of the `PSPMequi` function, which specify the step size along the equilibrium curve and the index of the bifurcation parameter plus the limits to its range for the computation, respectively, are taken equal to \(-0.1\) and \( c(6,0.5,2.0) \).

The initial point for the computations is a rather crude estimate of the equilibrium state for \( q = 1 \), for which parameter value all rates are linear in body mass \( s \). Per unit biomass the net-production rate of new biomass, either through somatic growth or through fecundity, then equals \( \sigma I_{\text{max}} R - T \), while the loss rate per unit biomass equals the mortality rate \( \mu \). Equating these two rates to each other, yields the equilibrium resource density \( \tilde{R} = (T + \mu)/(\sigma I_{\text{max}}) = 0.22 \). The initial estimate for the population birth rate in equilibrium is especially crude, as it is taken equal to 0. Despite that the initial point is not close to the equilibrium solution for \( q = 1 \) the computations easily converge as can be seen in the R command box below.

Furthermore, the computations are carried out with the default parameter values, such that the 6th argument of the function `PSPMequi` is left undefined (NULL). The last argument of the function `PSPMequi` is the option vector, in which the option "popEVO" is set equal to "0". Defining this option not only instructs the program to assess whether or not a computed equilibrium is an evolutionary fixed point, but also identifies the structured population with index 0 as the population for which to carry out the evolutionary analysis (obviously, as it is the only population in this problem).
Command box 11.A: Detection of an evolutionary fixed point

```r
> output1 <- PSPMequi("Indet_growth","EQ",c(1.0,0.22,0),-0.1,c(6,0.5,2),NULL,c("popEVO","0"))

Building executable Indet_growth_equi.so ...

<...compilation output lines suppressed in this box...>

    1.00000000E+00 2.20000000E-01 3.55373787E-02
    9.98043762E-01 2.19653632E-01 3.45381701E-02
    9.96005285E-01 2.19313094E-01 3.35389579E-02
    <...output lines suppressed in this box...>
    9.44570226E-01 2.15621677E-01 1.85536239E-02
    9.38034889E-01 2.15593014E-01 1.75557539E-02
    <...output lines suppressed in this box...>
    5.18672354E-01 2.40531837E-01 7.04499110E-03
    5.09283848E-01 2.41208401E-01 7.01122421E-03

# Executing : PSPMequi("Indet_growth", "EQ", c(1, 0.22, 0), -0.1, c(6, 0.5, 2), NULL, c('popEVO', '0'))

# Parameter values :
# Delta : 0.1 Rmax : 2 Sb : 0.05
# Sj : 1 Sigma : 0.5 T : 0.1
# q : 1 Mu : 0.01

# Index of bifurcation parameter #1 : 6
# 1:q 2:E[0] 3:b[0] 4:I[0][0] 5:I[0][1] 6:I[0][2] 7:R0[0] 8:R0_x[6] 9:RHS norm

> output1$curvepoints
V1  V2  V3  V4  V5  V6  V7  V8  V9
[1,] 1.0000000 0.2200000 0.03553738 0.1780000 0.53230236 0.2767885 1.0000000 -4.144555e+01 9.579106e-09
[2,] 0.9980438 0.2196536 0.03453817 0.1780346 0.52939068 0.2798577 1.0000000 -3.894615e+01 3.294274e-08
[3,] 0.9960053 0.2193131 0.03353896 0.1780687 0.52628792 0.2831152 1.0000000 -3.648053e+01 3.052791e-08
[4,] 0.9445702 0.2156217 0.01855362 0.1784378 0.43178150 0.3792995 1.0000000 -2.091709e+00 1.618872e-08
[5,] 0.9382634 0.2155930 0.01758857 0.1784407 0.41943590 0.3916582 1.0000000 -9.063882e-11 7.983139e-09
[6,] 0.9380349 0.2155930 0.01755575 0.1784407 0.41899094 0.3921031 1.0000000 7.059485e-02 8.044140e-09
[7,] 0.5186724 0.2405318 0.00704499 0.1759468 0.10149399 0.6982643 1.0000000 6.421252e+00 1.465988e-09
[8,] 0.5092838 0.2412084 0.00701122 0.1758792 0.09943055 0.7000202 1.0000000 6.322922e+00 2.255060e-09
[9,] 0.4998558 0.2418902 0.00697869 0.1758110 0.09742641 0.7017144 1.0000000 6.227017e+00 1.991225e-09

> output1$bifpoints
V1   V2   V3   V4   V5   V6   V7   V8   V9
[1,] 0.9382634 0.215593 0.01758857 0.1784407 0.4194359 0.3916582 1.0000000 -9.063882e-11 7.983139e-09

> output1$biftypes
[1] "CSS #0"
```

As can be seen in the command box above an evolutionary fixed point is detected at \( q^* = 0.938266 \). On the basis of the second-order partial derivatives, which are not reported explicitly by the program during this computation, the fixed point is classified as a convergent stable strategy. It occurs (self-evidently in this model) in the structured population with index 0. The output element `output1$biftypes` therefore consists of the single string "CSS #0".

Because the program is instructed to assess the evolutionary properties of the computed equilibrium points, the output matrix `output1$curvepoints` produced by the call to `PSPMequi`, has an additional column of output compared to the columns of output discussed in chapter 8 labeled `R0_x[0]` (column 8). This is the derivative of the \( R_0 \) value, the expected number of offspring produced by an individual during its entire life, with respect to the bifurcation parameter \( q \) for the population with index 0. Inspection of this column shows that this derivative is negative for \( q \)-values larger than \( q^* \) and positive for \( q \)-values smaller than this evolutionary fixed point value. This implies that for \( q > q^* \) a mutation-selection process will select for smaller values of the trait \( q \), while larger \( q \)-values will be selected for when \( q < q^* \). The evolutionary fixed point \( q^* \) is therefore convergent. The R script `Indet_growth_demo.R` illustrates this computation by plotting the equilibrium resource density and the equilibrium consumer biomass as a function of the parameter \( q \). At the CSS the equilibrium resource density reaches a minimum value.
In the next step of the analysis the detected evolutionary fixed point is used as starting point for a computation of its value as a function of a second model parameter, \( p \), the allometric scaling exponent of the maintenance rate with body size. The acronym of this type of computation is "ESS", which is supplied as the second argument to the `PSPMequi` function in the next R command box. Such "ESS" computations always use a parameter that is not defined to have its evolutionary stationary value as (first) bifurcation parameter. The evolutionary parameters are added as additional variables to the problem, which are following all values for the environmental variable(s) and population birth rate(s). Since the default parameter value for \( p \) is 1.0, the initial point of the "ESS" computation below is specified as \( c(1.0, output1$bifpoints[c(2,3,1)]) \), given that the second, third and first element of the array `bdata1` represent the equilibrium resource density, equilibrium birth rate and the evolutionary stationary value \( q \)-value in the evolutionary fixed point, respectively.

The fifth argument to the function `PSPMequi`, specifying the indices and range limits of the variable parameters in the computation, now has to contain as first triplet the index, minimum and maximum value of the bifurcation parameter \( p \) in the problem, while the second triplet specifies the index, minimum and maximum value of the parameter \( q \), which is assumed to have its evolutionary stationary value. The parameter \( p \) has index 9 in the parameter array defined in the model-specific file `Indet_growth.h` (see line 50–80 in that file) and for the computation its value is restricted to the interval \( 0.5 \leq p \leq 2.0 \). The array \( c(9,0.5,2.0,6,0.5,2.0) \) is therefore passed as 5th argument to the `PSPMequi` function.

Lastly, as in the invocation of the function `PSPMequi` shown in command box 11.A the option vector that is supplied to the `PSPMequi` function as 7th argument equals `c("popEVO","0")` to indicate that the evolutionary computations should focus on the \( R_0 \) value of the structured population with index 0.

Command box 11.B: Continuation of an evolutionary fixed point

```r
> output2 <- PSPMequi("Indet_growth","ESS",c(1.0, output1$bifpoints[c(2,3,1)]),-0.1, c(9,0.5,2.0,6,0.5,2.0), NULL, c("popEVO","0"))
```

```
out... suppressed in this box...
6.8456601E-01 2.133161E-01 1.20092558E-02 5.0877277E-01 5.9357308E-01 2.132929E-01 1.19365247E-02 5.0187254E-01 5.3214939E-01 2.1326847E-01 1.1870112E-02 4.9497146E-01
# Executing : PSPMequi("Indet_growth","ESS",c(1,0.215593,0.0175886,0.938263),-0.1,c(9,0.5,2,6,0.5,2),NULL,c("popEVO","0"))
# Parameter values :
Delta : 0.1 Rmax : 2 Sb : 0.05
Sj : 1 Sm : 2 Imax : 1
q : 0.938263 Sigma : 0.5 T : 0.1
p : 1 Mu : 0.01
Index of bifurcation parameter #1 : 9
Index of parameter #1 at ESS value : 6
Index of structured population for evolutionary analysis : 0
# 1:p 2:E[ 0] 3:b[ 0] 4:q 5:I[ 0][ 0] 6:I[ 0][ 1] .. 8:R0[ 0] 9:R0_x[ 9] 10:R0_yy[ 0] 11:RHS norm
> output2$curvepoints
```

```
V1 V2 V3 V4 V5 V6 .. V8 V9 V10 V11 V12
[1,] 1.0000000 0.2155930 0.0175886 0.9382634 0.1784407 0.4194359 .. 1 -0.8414241 0.0045934060 -0.004593000 7.18910e-10
[2,] 0.9521122 0.2152702 0.01683441 0.8934149 0.1784730 0.4127882 .. 1 -0.8367670 0.004258623 -0.004258500 6.769479e-09
[3,] 0.9505941 0.2149607 0.01650101 0.8898855 0.1785039 0.4058301 .. 1 -0.8310503 0.004152570 -0.004152500 6.244702e-09
[4,] 0.5456805 0.2135176 0.01200593 0.5087723 0.1786692 0.3653016 .. 1 -0.8236482 0.0046733900 -0.004673400 6.764797e-09
[5,] 0.5393873 0.2129209 0.01185522 0.5017725 0.1787077 0.3541999 .. 1 -0.8202615 0.0043816040 -0.004381600 6.44701e-10
```
(Notice that some of the intermediate columns of output have been suppressed in the R command box above to keep the displayed output within the page width).

The most important quantities to observe in the output above are the columns in the data matrix `output2$curvepoints` labelled `R0_xx` and `R0_yy`, which represent the second-order partial derivatives of the $R_0$ value with respect to the resident and mutant value of the parameter $q$, respectively. As discussed in chapter 9 these second-order partial derivatives classify the evolutionary fixed point as a convergent stable strategy, an evolutionary repellor or an evolutionary branching point (see Geritz et al. (1998) for details). The output shown above indicates that the evolutionary fixed point remains a convergent stable strategy over the entire range of parameters for which the curve is computed, because $R0_{xx}$ is always larger than $R0_{yy}$.

The graphical illustration produced by the R script `Indet_growth_demo.R` for this computation consists of the curve of the evolutionary fixed point value of $q$ (column 4 in the data matrix `output2$curvepoints`) as a function of the bifurcation parameter $p$ (column 1 in the data matrix `output2$curvepoints`).

Notice that the quantities $R0_{xx}$ and $R0_{yy}$ are only relevant in the 1-dimensional case, that is if only a single life history is assumed to adopt its evolutionary stationary value in the ESS continuation. In the multi-dimensional case, when computing curves of evolutionary stationary points with multiple life history traits evolving, the situation is more complicated. During such multi-dimensional ESS continuations, the program does not report the quantities $R0_{xx}$ and $R0_{yy}$, but instead provides as output the dominant eigenvalues of the Jacobian and Hessian matrices of the canonical equation, as well as the quantity $z^T C_{01} z$, which determines whether or not evolutionary branching can occur at an evolutionary stationary state that is attracting, but not evolutionary stable. In this expression $z$ is the dominant eigenvector of the Hessian matrix and $C_{01} = J - H$, the matrix with cross-derivatives of the canonical equation with respect to the mutant and the resident traits. For more details, see Leimar (2005) and Geritz et al. (2015).

The last step in the analysis of the evolutionary fixed point is to construct the pairwise invasibility plot or PIP, starting from the detected evolutionary fixed point. The type of computation is now specified as "PIP". The third argument in the call to the function `PSPMequi`, representing the starting point of the computation, equals `c(output1$bifpoints[,c(1,2,3,1)])`, which array contains in addition to the resident value of the parameter $q$, the equilibrium resource density and the equilibrium population birth rate the mutant value of the parameter $q$. In the detected evolutionary fixed point this mutant parameter value equals the resident value. Because the resident and mutant parameter are two values of the same model parameter the two triplets that make up the fifth argument to the function `PSPMequi` are identical. This argument hence equals `c(6,0.5,2.0,6,0.5,2.0)`. The function is moreover called twice, once with a positive step size of 0.1 and once with a negative step size of -0.1, to compute the boundary in the PIP that radiates out from the evolutionary fixed point in two directions.

**Command box 11.C: Construction of a pairwise invasibility plot**

```r
> output3 <- PSPMequi("Indet_growth","PIP",c(output1$bifpoints[,c(1,2,3,1)]),0.1,c(6,0.5,2.0,6,0.5,2.0),NULL,c("popEVO","0"))
```

Dynamic library file `Indet_growthequi.so` is up-to-date

9.38263361E-01 2.15592978E-01 1.75885671E-02 9.38263361E-01
9.44757579E-01 2.15623452E-01 1.85841380E-02 9.31442039E-01
9.50520866E-01 2.15706603E-01 1.95802172E-02 9.24768482E-01
9.56324464E-01 2.15779791E-01 2.05763871E-02 9.18115283E-01
The commands and output in the box above do not need further explanation, except that the first and the fourth column are the value of the resident and the mutant value of the parameter $q$, respectively. From the 8th and 9th column it can be verified that both the resident and the mutant type indeed attain $R_0 = 1$ in the equilibrium states computed. The R script `Indet_growth_demo.R` uses the first and fourth output columns, corresponding to the two bifurcation parameters, from the data matrices `output3$curvepoints` and `output4$curvepoints` that result from the first and second call to the function `PSPMequi` in the command box above to construct the pairwise invasibility plot (PIP).
independent structured populations that compete for the same resource. Using this im-
plementation with two populations, the boundary in the pairwise invasibility plot that
separates parameter regions with a positive and negative population growth rate of the
mutant type, corresponds to the transcritical bifurcation curve (or invasion boundary) of
the mutant population into the resident population. The R script `Indet_growth_demo.R`
computes this transcritical bifurcation curve by taking the last computed equilibrium
point from the data matrix `output4$curvepoints` and using it as initial point for the
following command:

```
> output5 <- PSPMequi("Indet_growth_resmut","BP",tail(output4$curvepoints,n=1)[,c(1,2,3,4)],0.1,c(0.5,0.5,2.0,12,0.5,2.0),NULL,
c("popBP","1"))
```

The plot that is subsequently generated by the `Indet_growth_demo.R` script confirms the
correctness of the curve.
Simulating evolutionary dynamics

12.1 Theoretical background

In the context of adaptive dynamics the change over evolutionary time in a set of life history traits, characterising the individuals of a population, can be described by the so-called canonical equation (Dieckmann & Law, 1996). This canonical equation specifies a system of ordinary differential equation for the values of a trait vector \( \mathbf{x} = (x_1, \ldots, x_n) \), assuming that the population size is large (infinite) and that evolution is limited by small mutation steps in the trait values. More specifically,

\[
\frac{d\mathbf{x}}{dt} = n_e(\mathbf{x}) \theta \Sigma \frac{\partial s_{\mathbf{x}}(\mathbf{y})}{\partial \mathbf{y}} \bigg|_{\mathbf{y}=\mathbf{x}} \tag{12.1}
\]

Here, \( n_e(\mathbf{x}) \) is the effective population size, \( \theta \) the mutation probability per birth event, \( \Sigma \) the \( n \)-dimensional mutational variance–covariance matrix summarising the distribution of mutations around the resident type \( \mathbf{x} \) and \( \partial s_{\mathbf{x}}(\mathbf{y})/\partial \mathbf{y} \) is the selection gradient (see also equation (9.1)). As discussed in section 9 the selection gradient is sign–equivalent with the derivative of \( R_0 \):

\[
\frac{\partial R_0(\mathbf{y}, \tilde{E}(\mathbf{x}))}{\partial \mathbf{y}} \bigg|_{\mathbf{y}=\mathbf{x}} \tag{12.2}
\]

This partial derivative of \( R_0 \) with respect to life history parameters is the quantity that is used to analyse evolutionary fixed points of PSPMs, as explained in chapters 9, 11. Furthermore, we can assume that the effective population size \( n_e(\mathbf{x}) \) is proportional to the birth rate of a structured population, \( \tilde{b}(\mathbf{x}) \), for a given value of the trait vector. In other words, the evolutionary dynamics of the values of the life history parameters can be assumed to be proportional to the product of the population birth rate and the partial derivative of \( R_0 \):

\[
\frac{d\mathbf{x}}{dt} \propto \tilde{b}(\mathbf{x}) \Sigma \frac{\partial R_0(\mathbf{y}, \tilde{E}(\mathbf{x}))}{\partial \mathbf{y}} \bigg|_{\mathbf{y}=\mathbf{x}} \tag{12.3}
\]

Given that the software package routinely computes both \( \tilde{b}(\mathbf{x}) \) as well as \( \partial R_0(\mathbf{y}, \tilde{E}(\mathbf{x}))/\partial \mathbf{y} \) while analysing evolutionary fixed points in PSPMs, it is easy to understand that simulating the dynamics of the life history trait values over evolutionary time is a straightforward extension.
Hence, the **PSPManalysis** package contains in addition to the **PSPMdemo** and **PSPMequi** functions a function called **PSPMevodyn** to simulate the change in an arbitrary number of life history parameters over evolutionary time. As a starting point the function takes an ecological equilibrium state for a particular set of parameters and computes both the partial derivative of \( R_0 \) with respect to the evolving parameters and the value of the population birth rate \( \tilde{b} \) in equilibrium. Given these 2 quantities, it computes the value of the right-hand side of expression (12.3) that is proportional to the evolutionary rate of change in the life history parameters as determined by the canonical equation. Unless explicitly specified, the function assumes that the mutational variance-covariance matrix \( \Sigma \) equals the identity matrix. Finally, it uses the computed value of the evolutionary rate of change to derive new values for the evolving parameters using the Euler method for numerical integration of ordinary differential equations.

### 12.2 Simulating evolutionary dynamics in R

The use of the **PSPMevodyn** function will be illustrated with the same model as described in chapter [10](#) and analysed in chapter [11](#). In fact, the R script `Indet_growth_demo.R`, that is to be found together with the model-specific file `Indet_growth.h` in the Tests directory and that was already discussed in the previous chapter, performs at the end 2 computations of trait dynamics over evolutionary time. The `Indet_growth_demo.R` script furthermore performs some plotting of the output data generated by these computations.

The general call to the **PSPMevodyn** function is shown in the command box below.

**Command box 12.A: General syntax of a PSPMevodyn call**

```r
> output <- PSPMevodyn(modelname = NULL, startpoint = NULL, curvepars = NULL, evopars = NULL, covars = NULL, parameters = NULL, options = NULL, cvode = FALSE, clean = FALSE, force = FALSE, debug = FALSE)
```

The obligatory and optional arguments to the **PSPMevodyn** function are the following:

1. The first, obligatory argument to the function **PSPMevodyn** is the name of the file specifying the PSPM, passed as a string argument. It is unnecessary to include the extension `.h` as part of the file name, the `.h` extension will be stripped away if it is included. The R-commands to analyse the model specified in `Indet_growth.h` that will be used for the illustration below will therefore all take "**Indet_growth**" as their first argument.

2. The second, obligatory argument is the initial point of the computation. This initial point should be close to an equilibrium point of the ecological dynamics. The initial point should be a (row) vector with the proper dimension, including as first elements the estimated equilibrium values for all the environment variables and the estimated values of the birth rate for all the structured populations in the model, followed by initial values for all parameters that are allowed to evolve over evolutionary time:

\[
c(\text{<environment variables>}, \text{<population birth rates>}, \text{<parameter 1>}, \text{<parameter 2>}, \ldots)
\]

However, environment variables that have been explicitly specified with the program option "**envZE**" as having a zero equilibrium value and birth rates of populations that have been explicitly specified with the program option "**popZE**" to be in a zero
equilibrium state (see the description of these options under point 7 below), should be omitted from this vector of initial values.

3. The third, obligatory argument to the \texttt{PSPMevodyn} function is a row vector consisting of 2 elements: (1) the maximum step size in evolutionary time during the integration of the canonical equation and (2) the maximum evolutionary time at which to stop the integration of the canonical equation.

4. The fourth, obligatory argument to the \texttt{PSPMevodyn} function determines which of the model parameters are allowed to evolve and at which limits further evolution of these parameter is prohibited. This information should be specified by a (row) vector, which for every evolving parameter should include a triplet of values specifying the index of the parameter, its minimum and its maximum value at which its evolution should stop. Therefore, in case of a single evolving parameter, the row vector is of the form:

\[
c(\langle \text{index 1} \rangle, \langle \text{minimum 1} \rangle, \langle \text{maximum 1} \rangle)
\]

The first element of the vector indicates the index of the parameter in the array \texttt{parameter} to vary, while the final two elements of the array indicate the minimum and maximum value of the parameter. When two parameters are allowed to evolve, the row vector is of the form:

\[
c(\langle \text{index 1} \rangle, \langle \text{minimum 1} \rangle, \langle \text{maximum 1} \rangle, \langle \text{index 2} \rangle, \langle \text{minimum 2} \rangle, \langle \text{maximum 2} \rangle)
\]

With multiple evolving parameters the vector has to be extended with a triplet of values for each of these model parameters with the triplet specifying the index of the particular parameter as well as its minimum and the maximum value. The number of triplets should correspond with the number of initial values for the evolving parameters as specified in the second argument to the function. The integration of the canonical equation is halted before reaching the maximum integration time specified in the third argument to the function, whenever all evolving parameter have reached either their minimum or their maximum limit.

5. The fifth, optional argument of the \texttt{PSPMevodyn} function specifies the variance–covariance matrix $\Sigma$ (see equation (12.1)). This argument can be specified as an $n \times n$ matrix or as a vector of length $n \cdot n$, where $n$ equals the number of evolving parameters. The element $(i, j)$ of the matrix (or equivalently the element $(i \cdot n + j)$ of the vector) should indicate how the selection gradient in trait $j$ changes the value of trait $i$ through genetic coupling. If the vector is not specified the matrix $\Sigma$ is taken equal to the identity matrix.

6. The sixth, optional argument of the \texttt{PSPMevodyn} function is a (row) vector of model parameter values. When used, this array should have the same length as the number of parameters in the model (\texttt{PARAMETER\_NR}). When of this length the values will replace the default values of the parameters that are listed in the model specification file. If the array used for this sixth argument is not of the correct length \texttt{PARAMETER\_NR} or when it is not specified at all, it will simply be ignored.

7. The seventh, optional argument of the \texttt{PSPMevodyn} function is a (row) vector of string elements, containing possible options that modify the behaviour of the com-
putational module. Most of the options require a value and hence occur as a pair of option name and option value. Only the "test" option (see below) occurs on its own. Options can be specified in any order, but the option value should always immediately follow after the option name. All option values refer to indices of either environment variables, structured populations or individual state variables. Notice, that this index value follows the C-convention of ordering arrays starting at 0 (as opposed to R where array indices start at 1). Multiple options can be included into the vector like:

\[ c("name 1", "value 1", "name 2", "value 2", "name 3", "value 3") \]

Possible options are:

- **Option pair** `c("popEVO", "i")`: This option pair specifies the index of the structured population, whose life history parameters are evolving. If not specified, this index defaults to 0.

- **Option pair** `c("envZE", "i")`: This option pair can be specified several times as part of the option vector of strings. Including this option instructs the computational module to set the value of the environment variable with index "i" equal to 0 during the computations of the fixed point problem that determines the selection gradient in the evolving parameters. In addition, the equilibrium condition for this environment variable (as, for example, specified in code box 7.12) is ignored and hence not included as condition to hold in the particular equilibrium point. Notice that this can only occur for environment variables that are of the type PERCAPITARATE or POPULATIONINTEGRAL (see section 7.3.2 above).

- **Option pair** `c("popZE", "i")`: This option pair can be specified several times as part of the option vector. Including this option forces the computational module to assume that the structured population with index "i" in the model is in a zero equilibrium state. This is the only way to compute an equilibrium with a zero equilibrium state for a particular population. Even if a value of 0 would be specified for the birth rate of a population as part of the initial point of the computation, the software would compute the equilibrium curve with a non-zero (non-trivial) equilibrium state for this population. Notice that if a structured population is forced to be in a zero equilibrium state by using the "popZE" option, a zero equilibrium state should also be enforced for all the environment variables that represent integrals over this population distribution (that are hence of the type POPULATIONINTEGRAL).

- **Option pair** `c("isort", "i")`: This option modifies the output of the equilibrium state of the populations that are stored in an output file with a name of the form `<Modelname>-EVODYN-<NNNN>.csb` (see below). By default the computational module reports the information about the stable population state distributions by subdividing the axis of the first state variable (the one with index "0") in 100 subintervals of equal length and reporting the statistics for the cohort of individuals within each subinterval. By using the option "isort" the default choice to use the first individual state variable for this subdivision can be changed to the second, third, and so on. Therefore, passing
Option `c("isort", "0")` as option vector to the \texttt{PSPMevodyn} function is the same as the default behaviour: the first individual state variable is used for the subdivision and ordering of the population state distribution, while passing `c("isort", "1")` would use the second individual state variable for this purpose. Also notice that the number of subdivisions of the individual state variable can be redefined by assigning the dimension \texttt{COHORT_NR} a value different from 100 (see chapter [15]).

- **Option \texttt{c("test")}:** The last possible option that can be passed to the \texttt{PSPMevodyn} function as part of the option vector is the \"test\" option. This invokes the computational module in testing mode, which implies that only a single integration of the individual life history is carried out and no iteration to locate a fixed point of a set of equations is performed. In testing mode the computational module reports on the dynamics of the individual state variables, the survival, the cumulative impact on the environment and the expected number of offspring produced by an individual during its different life stage as well as over its entire life. Testing mode is very useful to discover whether or not the model implementation gives sensible results or not.

Four other optional arguments can be passed to the \texttt{PSPMevodyn} function: \texttt{cvode}, \texttt{clean}, \texttt{force} and \texttt{debug}. These are all boolean arguments that hence have to be passed to the \texttt{PSPMevodyn} function as `<option name>=TRUE` or `<option name>=FALSE`, the latter being the default value of all options (Specifying these options as argument is hence only useful when setting them equal to \texttt{TRUE}). Unlike the previous arguments, which all modify the computations to be performed, these options modify the behaviour of the \texttt{PSPMevodyn} function itself, in particular the compilation of the model specific file into a dynamic library module that can be executed from \texttt{R}. Also unlike all the previous arguments that can be passed, these arguments can be passed in any order and at any position, the \texttt{PSPMevodyn} function will filter these 4 optional arguments from the argument list before passing the filtered argument list to the computational routine.

- **Option clean:** When \texttt{clean=TRUE} is passed as argument, this argument instructs the \texttt{PSPMevodyn} function to delete all result files that have been generated during previous calculations with the model, i.e. as a result of previous calls to \texttt{PSPMdemo}, \texttt{PSPMequi} or \texttt{PSPMevodyn}. These result files have names of the form \texttt{<Modelname>-<Type>-<NNNN>.err}, \texttt{<Modelname>-<Type>-<NNNN>.csb} and \texttt{<Modelname>-<Type>-<NNNN>.out}, in which \texttt{<Modelname>} refers to the name of the model, \texttt{<Type>} refers to the type of computation that has been performed, which in the case of \texttt{PSPMevodyn} equals \texttt{EVODYN}, and \texttt{<NNNN>} is a unique number that distinguishes consecutive computations of the same type of curve with the same model.

- **Option force:** When \texttt{force=TRUE} is passed as argument, it instructs the \texttt{PSPMevodyn} function to force re-compilation of the model specific file into a dynamic library module that can be executed by \texttt{R}. This option will usually not be needed by normal users, as the \texttt{PSPMevodyn} function automatically recompiles the computational module when the model specific file with an .\texttt{h} extension is more recently changed than the compiled dynamic library file. However, if for some unclear reason this automatic recompilation fails, the \texttt{force} option can be used to initiate re-compilation.

- **Option debug:** When \texttt{debug=TRUE} is passed as argument, it instructs the
The computational module generates on execution a single list object as output with 2 member elements (see the help page on `PSPMevodyn` in R command box 12.D). The first element of the output list, `output$curvepoints`, contains the numerical information of the points along the computed curve. This variable `output$curvepoints` is a matrix, in which each row represents one solution point along the curve. The columns contain the evolutionary time value, the equilibrium value of all environment variables, the equilibrium value for the birth rate of all structured populations in the problem, the current value of the evolving parameter(s), the equilibrium value of all interaction variables defined in the routine `Impact()`, the per capita growth rate of all environment variables for which this is relevant (those of the type `PERCAPITARATE`), for each of the structured populations the expected number of offspring produced by an individual during its lifetime ($R_0$) and finally the norm of the right-hand side of the system of equations that is solved to obtain the ecological equilibrium. The latter quantity (referred to as RHS norm) measures how close the computed equilibrium point is to the true solution.

The second member element of the output list, `output$curvedesc`, (see box 12.D) contains the description of the executed calculation, which includes the command-line that is used for the invocation of the computational routine, the values of all parameters used for the current computation and a header line indicating the meaning of all the output variables produced by the computational module. This textual information is also printed to the R console at the end of calculations. In fact, the `PSPMevodyn` function prints its report on the calculations by execution of the statement \texttt{cat(output$curvedesc, sep='\n')}.
12.3 An example session using the PSPMevodyn function

The R script `Indet_growth_demo.R` illustrates the use of the PSPMevodyn function by simulating the evolutionary dynamics in the parameter $q$, the scaling power in the model implemented in `Indet_growth.h` that relates the resource ingestion rate to individual body size (see chapter 10). The particular call to the PSPMevodyn function is shown in the following R command box:

**Command box 12.B: Simulating evolutionary dynamics in a single parameter**

```r
> output1 <- PSPMevodyn("Indet_growth", c(0.22, 0.03554, 1.0), c(0.05, 10), c(6, 0.5, 1.5), options=c("popEVO", "0"))
```

Starting from an (approximate) equilibrium resource density of 0.22 and an (approximate) equilibrium birth rate value of 0.03554 for an initial parameter value $q = 1.0$ the evolutionary dynamics is simulated from $t = 0$ (this starting time is always taken equal to 0) till $t = 2.681562$. The simulation stops at this time point, because the evolution in $q$ has converged to a fixed value and $q$ is not going to change any further. This final value of $q$ hence represents a stable and attracting evolutionary state (CSS). In general, the computation will be stopped whenever all evolving parameters have stabilised at a constant value.

The starting point of the computation is contained in the second argument to the function `PSPMevodyn`, as shown above, whereas the first argument defines the basename of the file with the model implementation "Indet_growth". The third argument to the function `PSPMevodyn` sets the maximum evolutionary time step to 0.05 and the maximum time at which to stop the evolutionary simulation to 10.0, but the latter is never reached because of the convergence to an evolutionarily constant $q$ value. The fourth argument to the function `PSPMevodyn` contains a single triplet of values, given that only a single parameter is allowed to evolve, defining the index of the parameter $q$ in the parameter array as defined in `Indet_growth.h` and its minimum and maximum value at which to stop the computations. The fifth and sixth argument are left undefined, which implies that the variance–covariance matrix $\Sigma$ (refer to equation (12.1)) defaults to the identity matrix.
and default values are used for all non-evolving model parameters. These default values are defined in the file `Indet_growth.h`. The final argument to the function `PSPMevodyn`, the option vector, defines the index of the structured population, in which the evolutionary dynamics takes place, equal to 0, but as discussed before, specifying this option is superfluous as the option "popEVO" is equal to 0 by default.

During the computations the program reports the current value of the evolutionary time, the ecological equilibrium values of the resource density and the population birth rate and the current value of the evolving parameter $q$. In the R command box above the values of the computed points along the evolutionary trajectory are saved in the output list element `output1$curvepoints`, the contents of which are inspected after the `PSPMevodyn` function finishes and it has printed out the textual information about the computation. The demonstration script `Indet_growth_demo.R` uses the data contained in the first and the fourth column of `output1$curvepoints` to plot the time course of evolutionary change in the parameter $q$.

In the following R command box, a similar trajectory of the evolutionary dynamics is computed starting from the same ecological equilibrium, but now both the parameter $q$ and the parameter $p$, which relates the maintenance costs to individual body size (see chapter 10), are allowed to evolve. To that end, the starting point of the computation is extended with an initial value for the parameter $p$ (1.0) and the fourth argument of the `PSPMevodyn` function is extended with a triplet of values that indicate the index of the parameter $p$ in the parameter array as defined in `Indet_growth.h` and its minimum and maximum value at which to stop the computations. In addition, the maximum integration time at which to stop the evolutionary computations is increased to 100. Otherwise, the command line of this computation is identical to the one shown in R command box 12.B.

Command box 12.C: Simulating evolutionary dynamics in two parameters

```r
> output2 <- PSPMevodyn("Indet_growth",c(0.22,0.03554,1,1),c(0.05,100),c(6,0.5,1.5,9,0.5,1.5),options=c("popEVO","0"))
```

The output in the command box above shows that again the evolutionary dynamics are halted before the maximum time (100) is reached. As soon as an evolving parameter (here the parameter $q$) drops below its minimum value or exceeds its maximum value, as
specified in the fourth argument to the function `PSPMevodyn`, it is stopped from evolving further, which in the case of the computation shown above leads to convergence to a constant value of the second evolving life history parameter $p$. This convergence ultimately halts the computation. The computation is therefore in this case stopped because no further evolution occurs, but computations will also stop whenever all evolving parameters have reached either their minimum or their maximum limit.

### 12.4 Output files generated by the `PSPMevodyn` function

The computational module that is produced by the `PSPMevodyn` function generates 3 output files. The name of these files is always of the form `<Modelname>-EVODYN-<NNNN>.<ext>`, in which `<Modelname>` is the same as the name of the file specifying the model excluding its `.h` extension, `<NNNN>` is a 4-digit number that is unique for the current computation and `<ext>` is the extension, which can be either `.err`, `.csb` or `.out`. The unique number distinguishes the same types of curve computations for the same model from each other. The number is obtained by considering increasing values of `<NNNN>` (i.e., 0000, 0001, 0002 and so forth) and testing whether result files with the particular index are already present. The program uses the first value of `<NNNN>` that is not in use.

The file called `<Modelname>-EVODYN-<NNNN>.err` that is generated during the computations contains information about the numerical progress of the computations. It reports details on the steps taken during the Newton iteration, the convergence to the solution, as well as information about the steps taken along the curve that is being computed. This file can be informative in case the computation of a particular curve stops for unknown reasons, but is otherwise of little use.

The output file called `<Modelname>-EVODYN-<NNNN>.out` holds the same information as is contained in the two elements of the output list returned by the `PSPMevodyn` function, `output$curvepoints` and `output$curvedesc` (see box 12.D). The first lines of this file all start with a `#` sign and contain the information about the run performed, which is also contained in `output$curvedesc` and can be listed by the statement `cat(output$curvedesc, sep='\n')`. Following this descriptive header the file contains columns with computational results that are also contained in the variable `output$curvepoints` (see, for example, R command box 12.B). In fact, the two elements of the output list, `output$curvepoints` and `output$curvedesc`, are generated by reading the contents of the file `<Modelname>-EVODYN-<NNNN>.out` from disk after the computations have ended, storing all lines that start with a `#` sign into a single string variable `output$curvedesc`, while storing the information on all other lines into the data matrix `output$curvepoints`.

The file called `<Modelname>-EVODYN-<NNNN>.csb` contains for every curve point that has been computed information on the parameters, for which the point has been computed, the equilibrium values of all environment variables and the stable distribution of all structured populations in the model. This is a binary file, the content of which can be accessed from R using the function `csbread`. For example, the file `Indet_growth-EVODYN-0000.csb` is generated by the invocation of the `PSPMevodyn` function in R command box 12.B. Its contents can be listed by:
(The first time you invoke the function \texttt{csbread} you might see some output generated by the compilation of the dynamic library module that contains the function \texttt{csbread}). The structure called \texttt{State-1.500000E-02} contains the population state in the ecological equilibrium that occurred at time point $t = 0.015$ during the simulation of evolutionary dynamics, as its name suggests. Its contents can be read into the workspace by issuing the command \texttt{csbread("Indet\_growth-EVODYN-0000.csb",3)} or \texttt{csbread("Indet\_growth-EVODYN-0000.csb","State-1.500000E-02")}.

Loading this state into the R workspace reveals it to be a list containing various arrays of numbers, as shown in the following box:

\begin{verbatim}
> popstate <- csbread("Indet\_growth-EVODYN-0000.csb","State-1.500000E-02")
> popstate

$EvoTime
 [1] 0.015

$EvoPars
 [1] 0.9874089

$Parameters
 [1] 0.1000000 2.0000000 0.0500000 1.0000000 2.0000000 1.0000000 0.9874089 0.5000000 0.1000000
 [11] 0.0100000

$Environment
 [1] 0.2180892

$Pop00\_BirthStates
 Istate00 Istate01
 [1,] 0 0.05

$Pop00

Density Istate00 Istate01
 [1,] 5.571417e-01 10.00401 0.05718031
 [2,] 4.528618e-01 30.72728 0.07462823
 [3,] 3.680999e-01 51.45054 0.09665210
 [4,] 5.571417e-01 10.00401 0.05718031
 [5,] 4.528618e-01 30.72728 0.07462823
 [6,] 3.680999e-01 51.45054 0.09665210
 [7,] 5.571417e-01 10.00401 0.05718031
 [8,] 4.528618e-01 30.72728 0.07462823
 [9,] 3.680999e-01 51.45054 0.09665210
 [10,] 5.571417e-01 10.00401 0.05718031
 [11,] 4.528618e-01 30.72728 0.07462823
 [12,] 3.680999e-01 51.45054 0.09665210

$Pop00\_BirthStates
 Istate00 Istate01
 [1,] 0 0.05

$Pop00

Density Istate00 Istate01
 [1,] 5.571417e-01 10.00401 0.05718031
 [2,] 4.528618e-01 30.72728 0.07462823
 [3,] 3.680999e-01 51.45054 0.09665210
 [4,] 5.571417e-01 10.00401 0.05718031
 [5,] 4.528618e-01 30.72728 0.07462823
 [6,] 3.680999e-01 51.45054 0.09665210
 [7,] 5.571417e-01 10.00401 0.05718031
 [8,] 4.528618e-01 30.72728 0.07462823
 [9,] 3.680999e-01 51.45054 0.09665210
 [10,] 5.571417e-01 10.00401 0.05718031

The first element of the list (called \texttt{$EvoTime$}) representing the population state \texttt{State-1.500000E-02} is the value of the evolutionary time $t$ at which the current population state occurs. The second element, an array called \texttt{$EvoPars$}, contains the values at evolutionary time $t$ of all the evolving model parameters. The third element, an array called \texttt{$Parameters$}, contains the values of all the model parameters for which the population state has been computed, while the fourth member of the list contains the equilibrium values of all environment variables. The two subsequent arrays in the list characterise the stable population distribution, of which the first (called \texttt{$Pop00\_BirthStates$}) specifies the state at birth of the individuals. The other (called \texttt{$Pop00$}) is a two-dimensional array characterising the population distribution in equilibrium with the first column \texttt{$Pop00[1,]$} representing the density profile of the equilibrium population and the subsequent columns \texttt{$Pop00[2,]$} and \texttt{$Pop00[3,]$} representing the average values of the
individual state variables with index 0 and 1 (corresponding to individual age and body size in the model implemented in `Indet_growth.h`), as shown in the \texttt{R} command box above. If individuals are characterised by more than two individual state variables, the values of these follow in additional columns of the two-dimensional array \$Pop00. The \texttt{R} command box above also illustrates that the dimension of the array \$Pop00 indicates that the population is represented by 100 cohorts of individuals (see chapter \ref{chapter15} for the option to change this number). The number of individuals in cohort $i$ is given by the array element \$Pop00[\texttt{i,1}], while the average value of the individual state variable with index 0 and 1 (average age and average length in the PNAS model) are given by \$Pop00[\texttt{i,2}] and \$Pop00[\texttt{i,3}] respectively.
PSPMevodyn help page

PSPMevodyn: Computes the evolutionary dynamics for a structured population model using the canonical equation

Syntax:

```
output <- PSPMevodyn(modelname = NULL, startpoint = NULL, curvepars = NULL, evopars = NULL, covars = NULL, parameters = NULL, options = NULL, cvode = FALSE, clean = FALSE, force = FALSE, debug = FALSE)
```

Arguments:

- `modelname`: (string, required)
  Basename of the file with model specification. The file should have extension ".h". For example, the model "PNAS2002" is specified in the file "PNAS2002.h"

- `startpoint`: (row vector, required)
  The initial point from which to start the simulation of the dynamics over evolutionary time, including the initial values of the evolving parameters

- `curvepars`: (row vector of length 2, required)
  Vector of length 2 specifying:
  - `curvepars[1]`: the maximum step size in evolutionary time during the integration of the canonical equation
  - `curvepars[2]`: the maximum evolutionary time at which to stop the integration of the canonical equation

- `evopars`: (row vector of length n*3, required)
  Vector of length n*3 specifying:
  - `evopars[2]`: lower threshold, below which value of the first evolution parameter the computation stops
  - `evopars[3]`: upper threshold, above which value of the first evolution parameter the computation stops
  ......
  - `evopars[n*3-2]`: the index of the last evolution parameter
  - `evopars[n*3-1]`: lower threshold, below which value of the last evolution parameter the computation stops
  - `evopars[n*3]`: upper threshold, above which value of the last evolution parameter the computation stops

- `covars`: (row vector or matrix, optional, can be left equal to its default NULL)
  Vector of length $N^2$ or $N \times N$ matrix, where $N$ is the number of evolving parameters. The vector or matrix elements specify the values of the covariance matrix in the selection gradients. Vectors of other lengths, including an empty vector will be ignored.

- `parameters`: (row vector, optional, can be left equal to its default NULL)
  Vector of length `PARAMETER_NR` (set in the model program file), specifying the values for the model parameters to use in the computation. Vectors of other lengths, including an empty vector will be ignored.

- `options`: (row vector of strings, optional, can be left equal to its default NULL)
  Vector with pairs of strings, consisting of an option name and a value (for example c("popEVO", "1")) or single options (i.e. c("test"). Possible option names and their values are:
  - "popEVO", "<index>": Index of structured population, for which to perform ESS or PIP continuation
  - "envZE", "<index>": Index of environment variable in trivial equilibrium (can be used multiple times)
  - "popZE", "<index>": Index of structured population in trivial equilibrium (can be used multiple times)
  - "isort", "<index>": Index of i-state variable to use as ruling variable for sorting the structured populations
  - "test" : Perform only a single integration over the life history, reporting dynamics of survival, $R_0$, i-state and interaction variables

- `cvode`: (Boolean, optional argument)
  Specify `cvode = TRUE` as argument to use the CVODE integrator from the Sundials collection of nonlinear and differential/algebraic equation solvers (see http://www.llnl.gov/CASC/sundials for details)
  Only available on Unix-based systems when Sundials has been installed

- `clean`: (Boolean, optional argument)
  Specify `clean = TRUE` as argument to remove all the result files of the model before the computation

- `force`: (Boolean, optional argument)
  Specify `force = TRUE` as argument to force a rebuilding of the model before the computation

- `debug`: (Boolean, optional argument)
  Specify `debug = TRUE` as argument to compile the model in verbose mode with debugging flag set
Output:

The output is a list containing the following elements:

- **curvepoints**: Matrix with output for all computed points along the curve.
- **curvedesc**: Column vector with strings, summarizing the numerical details of the computed curve (i.e., initial point, parameter values, numerical settings used).
Additional information
Multiple states at birth

The previous chapters focused mainly on models that assume that all newborn individuals have the same, unique state-at-birth. In the Medfly model, used in chapter 4 to discuss the implementation of a model for demographic analysis, individual age was the only *i-state* variable, which obviously equals 0 for all individuals at birth. In the PNAS model, used in chapter 7 to discuss the implementation of a model for equilibrium analysis, all individuals were assumed to be born with the same length at birth $\ell = \ell_b$. The directory Test contains, however, also 4 files (*Indet_growth_5bs.h*, *KlanjscekDEB2.h*, *Medfly_periodic.h* and *PNAS2002_5bs.h*) that implement models, in which individuals have different states-at-birth. These models will not be discussed extensively. Instead, the following sections will only briefly present some details about their implementation and usage, which are specific to the multiple states-at-birth.

The implementation of a model with multiple states-at-birth differs in at least 3 aspects from a model with a unique state-at-birth:

1. The number of possible states at birth has to be defined larger than 1.

2. The values of the *i-state* variables at birth have to be defined separately for the different states-at-birth.

3. Not only the number of offspring produced has to be specified, but also the state-at-birth of the offspring has to be specified.

4. In addition, the state-at-birth of an individual may influence the threshold value separating consecutive stages, the development and discrete changes in the individual state variables, the fecundity, the mortality and the impact of the individual on its environment (the latter only in case of equilibrium analysis of non-linear models). If this is the case, the values assigned in the routines *IntervalLimit()*, *Growth()*, *DiscreteChanges()*, *Fecundity()*, *Mortality()*, and possibly *Impact()* will be dependent on the state-at-birth as well.

This last aspect is, however, not absolutely necessary, whereas the aspects 1-3 mentioned above are.
CHAPTER 13. MULTIPLE STATES AT BIRTH

13.1 Demographic analysis with multiple states-at-birth

13.1.1 Two different offspring body sizes

The file _KlanjscekDEB2.h_ implements a model, in which the life history of the individuals is described by a dynamic energy budget (DEB) model. The model is a variant of the model implemented in the file _KlanjscekDEB.h_, which assumes that all individuals at birth have the same size at birth $V_b$. In contrast, the model implemented in the file _KlanjscekDEB2.h_ is based on an assumption that two types of offspring are produced: small offspring with a body size $0.7 \cdot V_b$ and large offspring with a body size $1.3 \cdot V_b$. Both models are discussed in detail in De Roos (2008), the model implemented in _KlanjscekDEB.h_ on page 5-7 and the model with two types of offspring (implemented in _KlanjscekDEB2.h_) on page 13-14 of De Roos (2008). The R script _KlanjscekDEB_demo.R_ carries out the demographic analysis for both models and graphs the results as a function of food density in the environment, which can be compared with Figure 2 in De Roos (2008).

As shown in the code box below, which contains a snippet from the model implemented in _KlanjscekDEB2.h_, the number of possible states-at-birth should be defined larger than 1 in the routine _SetBirthStates()_. In this particular model _BirthStates[0]_ is set equal to 2.

**Code box 13.1: Specification of the number of possible states-at-birth**

```c
/*
 * DEFINITION OF THE LIFE HISTORY MODELS FOLLOWS BELOW
 * Specify the number of states at birth for the individuals in all structured populations in the problem in the vector BirthStates[].
 */

void SetBirthStates(int BirthStates[POPULATION_NR], double E[])
{
    BirthStates[0] = 2;
    return;
}
```

The values of the _i-state_ variables in the different states-at-birth have to be defined separately. This means that in the routine _StateAtBirth()_ the assignment of the values to the variables _istate[][]_ has to be made conditional on the value of the index of the state-at-birth _BirthStateNr_. The model implemented in the file _KlanjscekDEB2.h_ has 2 states-at-birth \{\phi_1, \phi_2\}. In the code box below it is shown that the state-at-birth $\phi_1$ (with index _BirthStateNr = 0_) corresponds to the small-sized offspring with body size $0.7 \cdot V_b$, while the the state-at-birth $\phi_2$ (BirthStateNr = 1) corresponds to the large-sized offspring with body size $1.3 \cdot V_b$. 

[86x745]112
13.1. DEMOGRAPHIC ANALYSIS WITH MULTIPLE STATES-AT-BIRTH

Code box 13.2: Specifying the value of all possible states-at-birth

```c
/*
 * Specify all the possible states at birth for all individuals in all
 * structured populations in the problem. BirthStateNr represents the index of
 * the state of birth to be specified. Each state at birth should be a single,
 * constant value for each i-state variable.
 * Notice that the first index of the variable ‘istate[]’ refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void StateAtBirth(double *istate[POPULATION_NR], int BirthStateNr, double E[])
{
    if (BirthStateNr == 0)
    {
        AGE = 0.0;
        VOLUME = 0.7*VB;
        Q = 0.0;
        H = 0.0;
    }
    else
    {
        AGE = 0.0;
        VOLUME = 1.3*VB;
        Q = 0.0;
        H = 0.0;
    }
    return;
}
```

Finally, the last part of the code that has to be changed in case of multiple states-at-birth is the assignment of fecundity to different states-at-birth. The model implemented in the file KlanjscekDEB2.h assumes that individuals with a different state-at-birth differ in their offspring production. More specifically, individuals that are born with a small size \( V = 0.7 \cdot V_b \) are assumed to invest 2/3 of the energy that they have available for reproduction on producing small offspring (i.e. with \( V = 0.7 \cdot V_b \)) and 1/3 of the reproductive energy producing large-sized offspring with \( V = 1.3 \cdot V_b \). Vice versa, individuals that are born with a large body size \( V = 1.3 \cdot V_b \) are assumed to invest 2/3 of the energy that they have available for reproduction on producing large offspring (i.e. with \( V = 1.3 \cdot V_b \)) and 1/3 of the reproductive energy producing small-sized offspring with \( V = 0.7 \cdot V_b \). Parents bias their energetic investment into reproduction therefore toward producing offspring with the same size at birth as they were born with themselves. These different energetic investments into the two types of offspring are subsequently converted into a number of offspring by dividing them by the energy costs to produce a single offspring. For small- and large-sized offspring these costs are proportional to \( 0.7 \cdot V_b \) and \( 1.3 \cdot V_b \), respectively. For mothers born with a small size-at-birth this implies that the biased energetic investment in producing offspring with small sizes-at-birth is even more pronounced when considered in terms of number of offspring produced, whereas for mothers born with a large size-at-birth the bias is dampened by the conversion to number of offspring produced.

The size-at-birth of the offspring produced is therefore on average smaller in the model implemented in KlanjscekDEB2.h, compared to the model with a single state-at-birth, which is implemented in KlanjscekDEB.h. As a consequence, the number of offspring produced is larger, which is the most likely reason for the finding that the population
growth rate of the model with 2 states-at-birth is consistently larger than in case of a single state-at-birth (see the graphical output of the KlanjscekDEB_demo.R script).

**Code box 13.3: Specification of fecundity**

```c
/*
 * Specify the fecundity of individuals as a function of the i-state
 * variables and the individual’s state at birth for all populations in every
 * life stage.
 * The number of offspring produced has to be specified for every possible
 * state at birth in the variable ‘fecundity[]’ . The first index of this
 * variable refers to the number of the structured population, the second
 * index refers to the number of the birth state.
 * Notice that the first index of the variable ‘istate[]’ refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 */

void Fecundity(int lifestage[POPULATION_NR], double *istate[POPULATION_NR],
               double *birthstate[POPULATION_NR], int BirthStateNr, double E[],
               double *fecundity[POPULATION_NR])
{
    double Er;
    if (lifestage[0] == 1) // Only for adults
    {
        Er = (1-KAPPA)*EM*FOOD*G*(NU*pow(VOLUME, 2.0/3.0) + M*VOLUME)/(FOOD + G);
        fecundity[0][0] = fecundity[0][1] = max(Er - (1-KAPPA)*EM*M*G*VP,0);
        if (BirthStateNr == 0)
            fecundity[0][0] *= (2.0/3.0)*KAPPA_R/(EM*(KAPPA*G + FOOD)*0.7*VB);
            fecundity[0][1] *= (1.0/3.0)*KAPPA_R/(EM*(KAPPA*G + FOOD)*1.3*VB);
    } else
    {
        fecundity[0][0] *= (1.0/3.0)*KAPPA_R/(EM*(KAPPA*G + FOOD)*0.7*VB);
        fecundity[0][1] *= (2.0/3.0)*KAPPA_R/(EM*(KAPPA*G + FOOD)*1.3*VB);
    }
    return;
}
```

In case of multiple states at birth the structures in the output file containing the stable population states is more complex. Consider for example the computation with the file KlanjscekDEB2.h that is executed when running the test script alldemotests.R:

```r
> output2 <- PSMDemo("KlanjscekDEB2", c(0, 1.0, -0.02, 0.4, 1.0), clean=TRUE, force=TRUE)
Building executable KlanjscekDEB2demo.so ... 
...compilation output lines suppressed in this box...
1.00000000E+00 6.95608116E-01
9.80000000E-01 6.82539595E-01
9.60000000E-01 6.69183490E-01
...output lines suppressed in this box...
```
Obviously, this model contains more parameters and hence there are many more columns in the output representing sensitivities of the population growth rate with respect to model parameters. Loading the first structure from the the output file KlanjscekDEB2-PGR-0000.csb containing the stable population states and displaying its contents reveals the additional elements due to the multiple states at births:

The first additional element of the list representing the equilibrium population state is Pop00_StableBirthDist, which specifies the stable distribution of offspring produced with the 2 possible states at birth that are defined in the model. Each of the rows of the element Pop00_BirthStates of the structure specifies a different state at birth with its columns specifying the value of the 4 individual state variables in that particular state. For each state at birth, a stable population distribution for individuals born in that particular state is stored in two-dimensional arrays, called Pop00_Bstate00 and Pop00_Bstate01 respectively. As before, these two-dimensional arrays contain as the first and last column the stable population density and the reproductive value, respectively, while the intervening columns contain the values of the individual state variables.
13.1.2 Periodic environments

The file Medfly_periodic.h implements a variant of the Medfly model that is discussed in chapter 4 in which juvenile medflies are periodically exposed to a very high mortality rate that decays exponentially within a short time period. Such a scenario could, for example, reflect a periodic treatment of the population with an insecticide that affects all juvenile individuals equally, irrespective of their age. This model is discussed in detail in De Roos [2008, pp. 8-10] and will thus not be presented further here. The R script Medfly_periodic_demo.R can be used to obtain the results that are also shown in Figure 3 of De Roos [2008]. Notice, however, that this computation takes a long time (several hours) because the periodicity in the juvenile mortality makes it computationally very intensive.

The model implemented in the file Medfly_periodic.h illustrates that it is possible to carry out demographic analysis, i.e. calculation of the population growth rate as a function of a parameter and the sensitivity of the growth rate with respect to all model parameters, even in case of periodic environments. This does, however, not extend to equilibrium and evolutionary analysis, which are based on the assumption that the environment is in a constant, equilibrium state.

13.2 Equilibrium and evolutionary fixed point analysis with multiple states-at-birth

The two files PNAS2002_5bs.h and Indet_growth_5bs.h implement versions of the models implemented in the files PNAS2002.h and Indet_growth.h and discussed in chapters 6-8 and 9-11, respectively, but with 5 states-at-birth instead of the unique state-at-birth accounted for in the original models. The analysis of these model versions with multiple states-at-birth is largely similar to the analysis of the original models and will hence not be discussed further. The R scripts PNAS2002_5bs_demo.R and Indet_growth_5bs_demo.R carry out the same analysis steps as presented in detail in chapters 8 and 11 respectively, but for the model versions with 5 states-at-birth. Instead, in the following I will only discuss for the model implemented in PNAS2002_5bs.h the details, in which this implementation differs from the original model implemented in PNAS2002.h.

The following code box defines two macros, BIRTHSTATES and BIRTHSPREAD, which determine the number of different states-at-birth and the variation in size-at-birth between the smallest and the largest offspring body size. The number of states-at-birth is defined equal to 5 in the routine SetBirthStates(), as shown below:

Code box 13.4: Specification of the number of possible states-at-birth

```c
/*
 * DEFINITION OF THE LIFE HISTORY MODELS FOLLOWS BELOW
 * Specify the number of states at birth for the individuals in all structured
 * populations in the problem in the vector BirthStates[].
 */
#define BIRTHSTATES 5
#define BIRTHSPREAD 2.0
```
13.2. EQUILIBRIUM AND EVOLUTIONARY FIXED POINT ANALYSIS WITH MULTIPLE STATES-AT-BIRTH

```c
void SetBirthStates(int BirthStates[POPULATION_NR], double E[])
{
    BirthStates[0] = BIRTHSTATES;
    return;
}
```

Subsequently, the values of the different states-at-birth is set in the routine StateAtBirth(), dependent on the index BirthStateNr of the state-at-birth. The 5 states-at-birth in the model form a set \( \{ \phi_1, \phi_2, \phi_3, \phi_4, \phi_5 \} \). The code box below shows that the length-at-birth in these 5 different states equals \( \ell_b - \Delta / 2, \ell_b - \Delta / 4, \ell_b, \ell_b + \Delta / 4 \) and \( \ell_b + \Delta / 2 \), respectively, where \( \Delta \) is the difference in size-at-birth between the smallest and the largest offspring as given by the macro BIRTHSPREAD (Remember that indices in C start at 0 and that the values adopted by BirthStateNr hence run from 0 thru 4). Of course, for all states-at-birth the age of the individual is set to 0.

**Code box 13.5: Specifying the value of all possible states-at-birth**

```c
/*
 *===========================================================================
 * Specify all the possible states at birth for all individuals in all
 * structured populations in the problem. BirthStateNr represents the index of
 * the state of birth to be specified. Each state at birth should be a single,
 * constant value for each i-state variable.
 *
 * Notice that the first index of the variable 'istate[]' refers to the
 * number of the structured population, the second index refers to the
 * number of the individual state variable. The interpretation of the latter
 * is up to the user.
 *===========================================================================
 */

void StateAtBirth(double *istate[POPULATION_NR], int BirthStateNr, double E[])
{
    AGE = 0.0;
    LENGTH = LB + (((double)BirthStateNr)/((double)(BIRTHSTATES-1)) - 0.5)*BIRTHSPREAD;
    return;
}
```

The final routine that differs between the models with a unique state-at-birth and 5 states-at-birth is the routine specifying the fecundity of an individual, as this routine should not only specify the number of offspring produced, but also the state-at-birth of the offspring produced. The code box below shows that the model implemented in the file PNAS2002_5bs.h assumes that the distribution of the produced offspring is independent of the size-at-birth of the mother, since the variables fecundity[0][0] thru fecundity[0][4] are assigned the same values irrespective of the index BirthStateNr or the state-at-birth birthstate[]. All mothers produce 50% of their offspring with a length-at-birth equal to \( \ell_b \), 20% of their offspring each with a length-at-birth equal to \( \ell_b - \Delta / 4 \) and \( \ell_b + \Delta / 4 \) and 10% each with the most extreme lengths-at-birth of \( \ell_b - \Delta / 2 \) and \( \ell_b + \Delta / 2 \).

The R script PNAS2002_5bs_demo.R performs the same analysis steps for the PNAS2002 model with 5 states-at-birth, as carried out by the R script PNAS2002equi_demo.R for the original model. Executing this script shows that there are at most quantitative differences, if at all, between the results of the two models. A similar finding is obtained when comparing the results of the R script Indet_growth_5bs_demo.R that performs the
analysis of the model presented in chapter 10 but with 5 states-at-birth with the results of the original model, the analysis of which was discussed in chapter 11. In both cases the additional states-at-birth hence hardly affect model predictions.

**Code box 13.6: Specification of fecundity**

```c
/*
 * Specify the fecundity of individuals as a function of the i-state variables and the individual's state at birth for all populations in every life stage.
 * The number of offspring produced has to be specified for every possible state at birth in the variable 'fecundity[]'. The first index of this variable refers to the number of the structured population, the second index refers to the number of the birth state.
 * Notice that the first index of the variable 'istate[]' refers to the number of the structured population, the second index refers to the number of the individual state variable. The interpretation of the latter is up to the user.
 */

void Fecundity(int lifestage[POPULATION_NR], double *istate[POPULATION_NR], double *birthstate[POPULATION_NR], int BirthStateNr, double E[], double *fecundity[POPULATION_NR])
{
    double fec;
    fecundity[0][0] = 0.0;
    fecundity[0][1] = 0.0;
    fecundity[0][2] = 0.0;
    fecundity[0][3] = 0.0;
    fecundity[0][4] = 0.0;
    if (lifestage[0] == 2) {
        fec = RM*R/(R + RH)*LENGTH*LENGTH;
        fecundity[0][0] = 0.1*fec;
        fecundity[0][1] = 0.2*fec;
        fecundity[0][2] = 0.5*fec;
        fecundity[0][3] = 0.2*fec;
        fecundity[0][4] = 0.1*fec;
    }
    return;
}
```

### 13.3 Some other applications of multiple states-at-birth

The models with multiple states-at-birth discussed here only represent the basic type of application of this modeling feature. The option to account for multiple states-at-birth allows, however, for modeling a variety of scenarios. It goes too far to present this range of scenarios in detail and I will hence limit myself to pointing out a few examples.

As one example, multiple states-at-birth can be used to distinguish between the sexes in a population model. Two states-at-birth can then be defined, representing the male and female sex of an individual. An individual’s sex can influence its life history through for example development and mortality. If in addition the fecundity of the (female) individuals is modeled following a particular type of mating structure, it might be necessary in to define the total number of mature males and/or females in the population as environment variables.
As another example, multiple states-at-birth make it possible to account for population-genetic processes in a model. For example, 3 states-at-birth could be used to model the 2 homozygous and the single heterozygous genotypes in a one locus-two allele population model. Multiple alleles would be possible to account for as well at the expense of defining more states-at-birth. In this manner, the interplay between population-genetic processes and complex individual life histories could be analyzed for its population and even community consequences.
UNIX command-line usage

Even though in the previous chapters its use from a Matlab or Octave console was discussed, the software itself is a standard C-program. The programs can hence also be compiled outside Matlab and Octave and used from a command line in, for example, a bash shell under a Unix-based operating system (such as provided by the Terminal.app on Mac OS X). In this chapter I will shortly discuss how to compile and execute the programs within such an interactive bash shell. I will assume that the reader is familiar with the Unix operating system and command line use in bash shells.

The use of the program from a bash command line does not influence the model specification in the .h file. Hence, for details of the model implementation I refer to sections 4.1.1 to 4.2.7 for the implementation of a model, which is going to be investigated using demographic analysis, and to the sections 7.1.1 to 7.3.2 for a model that is to be investigated using bifurcation analysis.

14.1 The Makefile and compilation of a program

The distribution includes a Makefile that can be used to build the computational programs. The following box shows the top lines in this Makefile.

```
# Generic Makefile for the compilation of a continuation problem of the class
# of models that can be analyzed with the generic program files PSPMequi.c or
# PSPMdemo.c
#
# Possible targets to make:
# make <model>demo  (builds demographic executable from .h file)
# make <model>equi  (builds equilibrium executable from .h file)
# make clean        (cleans up all target programs)
# make cleanoutput  (cleans up all error and output files)
# make allclean     (combines previous two)
#
#==============================================================================
# Specify where the library modules are located.
#==============================================================================
MODDIR = $(HOME)/programs/PSPManalysis

#==============================================================================
# Specify whether or not to use the SUNDIALS library for ODE integration
#==============================================================================
SUNDIALS = 0
```

To adapt this Makefile to your system the definitions of MODDIR and SUNDIALS might have to be changed. The variable MODDIR should point at the directory in which the files PSPMequi.c and PSPMdemo.c are located.
Setting the variable \texttt{SUNDIALS} to the value of 1 selects the use of the CVODE integration method provided by the Sundials (\texttt{SU}ite of \texttt{N}onlinear and \texttt{D}ifferential/\texttt{A}lgebraic equation \texttt{S}olvers) collection of nonlinear and differential/algebraic equation solvers (see \url{http://www.llnl.gov/CASC/sundials} for details). By default the computational module uses the Dormand-Prince method (DOPRI5; Hairer \textit{et al.} (1993)) for the integration of the ordinary differential equations describing the life history of individuals (see chapter 16 for details about these ordinary differential equations). An implementation of the DOPRI5-method is provided with the package in a separate program file (\texttt{dopri5.c}). If the appropriate Sundials libraries are installed on your system, setting the variable \texttt{SUNDIALS} to the value of 1 enforces the use of the Sundials solver instead of the default DOPRI5 solver for the integration of the ordinary differential equations. In particular for long-lasting integrations, that is when the maximum age reached by individuals is large, using the CVODE-method can significantly speed up the computations.

Further adaptations to the Makefile are most likely not needed. Note, however, that a number of libraries have to be installed for the programs to compile successfully. In particular, the Makefile assumes that the Lapack, Cblas and Atlas libraries are installed, as it uses the linking options \texttt{-llapack -lcblas -latlas -lm} during the final link step of the programs. Furthermore, if the variable \texttt{SUNDIALS} is set to the value of 1, the options \texttt{-lsundials_nvecserial -lsundials_cvode} are prepended to the default options.

Successful compilation requires that the libraries invoked by these linking options are installed on your operating system and can be found by the compiler.

The Makefile defines a number of targets as is also visible from the command box above. Executing the command \texttt{make <model>demo} will build a program for demographic analysis of the model that is specified in the file \texttt{<model>.h}. Hence, building the program for the Medfly model discussed as an example in chapters 3 to 5 can be done by executing \texttt{make Medflydemo}.

Similarly, executing the command \texttt{make <model>equi} will build a program for bifurcation analysis of the model that is specified in the file \texttt{<model>.h}. Hence, building the program for the PNAS model discussed as an example in chapters 6 to 8 can be done by executing \texttt{make PNAS2002equi}.

The remaining targets defined by the Makefile are all cleaning targets. The command \texttt{make clean} will clean up all files in the current directory that have been produced during compilation steps. In particular, this step will scan the directory for all the \texttt{.h} files in it and will remove all the existing \texttt{<model>demo} and \texttt{<model>equi} programs, as well as the object modules that were produced during intermediate compilation steps of these programs.

Executing the command \texttt{make cleanoutput} will delete all files that have been produced by running either a demographic analysis program or a bifurcation analysis program. In particular, this step will scan the directory for all files with a name \texttt{<model>.h}, which will all be considered to be model-specific include files. For each of these files \texttt{<model>.h} it will delete all files in the current directory that start with \texttt{<model>} and have an extension of \texttt{.bif, .err, .mat, .csb} or \texttt{.out}. This will remove all output files generated by the computation modules, whether they have been executed from the Matlab command line or from the bash command line.

Finally, the command \texttt{make allclean} combines the previous two cleaning steps into one.
14.2 Executing a compiled program

After building a program for demographic analysis, its use from the command-line follows a similar approach as its execution from Matlab, only the syntax is different because all options, initial values for the computation, the step size in the bifurcation parameter and the limits to the parameter range have to be passed as command-line arguments. The syntax can be inspected by executing the compiled program with a single argument `-?`, which prints out a help message:

**Command box 14.A: Command-line syntax for demographic analysis**

```plaintext
 ~/programs/PSPManalysis/Tests: Medflydemo -?
 Usage: Medflydemo [-par1 <index> <initial value> <step> <min. par.1> <max. par.1>] [-isort <index>] [-test]
 Aim: Computation of the population growth rate and its parameter sensitivities for (multiple) structured populations possibly as a function of a model parameter
 Possible options are:
 -par1 <index>: Index of the parameter, as a function of which to compute the population growth rate
   If this option is used <initial value>, <step>, <min. par.1> and <max. par.1> specify the initial value, stepsize value, minimum and maximum value of this parameter.
   If not specified, a single computation of the population growth rate and parameter sensitivities is carried out for the current parameter values.
 -isort <index>: Index of i-state variable to use as ruling variable for sorting the structured populations.
 -test : Perform only a single integration over the life history, reporting dynamics of survival, R0 and i-state variables.
```

The help message in the box above shows that executing the computations from the command-line takes the same options as when executing the module from Matlab as explained in chapter 5. I will hence not discuss in detail the structure of the command-line, as the help message shown above in combination with the explanation about the demographic analysis program in chapter 5 should suffice to infer the correct use of the program.

As an example the box below shows how to execute the demographic analysis from the command-line without any further parameters. This example corresponds to the call to the PSPMdemo function shown in Matlab command box 5.A. Comparing the output below with that in box 5.A shows that the two are identical. For further explanations I therefore refer to the explanation of the use of the computational program from Matlab in chapter 5.

**Command box 14.B: Demographic analysis call for a single parameter value**

```plaintext
 ~/programs/PSPManalysis/Tests: Medflydemo
 # Executing : Medflydemo
 # Parameter values : 
 # Beta0 : 47 Beta1 : 0.04 AJ : 11
 # Mu0 : 0.00095 Mu1 : 0.0581
 # 0:PGR[ 0] 1:Tc[ 0] 2:S[ 0][ 0] 3:S[ 0][ 1] 4:S[ 0][ 2] 5:S[ 0][ 3] 6:S[ 0][ 4]
 # 0.419057 13.167260 0.001616 -0.164595 -0.031982 -1.526368 -0.011325
```

In a similar vein, the output of an execution of the program to compute the population growth rate over a range of parameters is the same as in Matlab command box 5.B as shown in the following box:
CHAPTER 14. UNIX COMMAND-LINE USAGE

Command box 14.C: Demographic analysis call for a parameter range

```
 chapters/PSPManalysis/Tests: Medflydemo -par1 2 11 0.1 11 20
```

Notice that the placement of the options and their subsequent values like `-par1 2` on the command-line is arbitrary, but that the initial value, step size and minimum and maximum parameter value should be specified in this specific order.

Executing a compiled program for bifurcation analysis from the bash command-line (with or without an option `-?`) also prints out a help message that reveals the syntax to be used for such programs, as shown in the following box:

```
chapters/PSPManalysis/Tests: PNAS2002equi
```

The help message becomes more specific once the type of computation that has to be carried out is specified, as illustrated in the code box below:

```
chapters/PSPManalysis/Tests: PNAS2002equi BPE
```

The values for `-par1`, `-par2`, `-envBP` and `-popBP` have to be set on the command-line and otherwise default to 0
The values for `-envZE` and `-popZE` can only be set on the command-line and otherwise are undefined
The help message in the boxes above show that executing the computations from the command-line is quite similar to executing the module from Matlab as explained in section 8.2. I will hence not discuss in detail the structure of the command-line, the meaning of the options and the required input variables for the program as the help message shown above in combination with the explanation about the bifurcation analysis program in section 8.2 should suffice to infer the correct use of the program. One thing to notice, though, is that in all calls to a bifurcation analysis program the option -par1 <index> has to be specified. If this option is not specified on the command-line the program exists with an appropriate error message. The placement of the options and their subsequent values on the command-line is again arbitrary, but all other input quantities, such as the initial values of all variables, the step size along the curve and minimum and maximum parameter values should be specified in the specific order as shown in the help message.

As an example the box below shows how to execute the same calculation for the PNAS model as illustrated in Matlab command box 8.B.

**Command box 14.D: Command-line example of a bifurcation analysis program**

```
~/programs/PSPManalysis/Tests: PNAS2002equi -par1 1 -popZE 0 -envZE 1 -envZE 2 EQ 1.0E-06 1.0E-06 0.5 0 4E-4

1.00000E-06 1.00000E-06
1.03536E-06 1.03536E-06
1.07071E-06 1.07071E-06
1.00000E-06 1.00000E-06
9.18697E-06 9.18697E-06
8.85690E-06 8.85690E-06 **** BP #0 ****
9.54052E-06 9.54052E-06
3.33749E-04 3.33749E-04
3.69104E-04 3.69104E-04
4.04460E-04 4.04460E-04
```

The output in the box above is identical to the output shown in box 8.B. For further details I therefore refer to the explanation of the use of the computational program from Matlab in sections 8.2 and 8.4.

Furthermore, in the directory Tests of the package a shell script allequitests.sh is provided that illustrates a large number of computations using command-line execution. Executing . allequitests.sh from the command line not only tests that the package functions correctly, but also illustrates how to use the program for different types of computations and with a variety of options.

### 14.3 Output files

When executing a compiled program from the command line the same output files are produced as discussed in sections 5.2 and 12.4 except for the files with an extension .mat that are Matlab-specific files. Instead, the information about the stable population states are written to a binary file with extension .csb. Hence, the call to the program Medflydemo as shown in command box 14.C generates the output files Medfly-PGR-0001.err, Medfly-PGR-0001.out and Medfly-PGR-0001.csb, as opposed to the files Medfly-PGR-0001.err, Medfly-PGR-0001.out and Medfly-PGR-0001.mat produced by the corresponding Matlab command in command box 5.B (the numeric identifier 0001 results because the Medfly program was first executed without parameters, which produces output files with identifier 0000). Similarly, the call to the program PNAS2002equi in box 14.D above produces output files PNAS2002-EQ-0000.bif, PNAS2002-EQ-0000.err, PNAS2002-EQ-0000.out
and PNAS2002-EQ-0000.csb, as opposed to the files PNAS2002-EQ-0000.bif, PNAS2002-EQ-0000.err, PNAS2002-EQ-0000.out and PNAS2002-EQ-0000.mat produced by the corresponding Matlab command in command box. The files with extensions .bif, .err and .out will not be discussed further here. Refer to the sections 5.2 and 12.4 for details about their contents. The files with extension .csb, which from hereon will be referred to as CSB file, are binary files with a specific structure. The format of these files is inherited from the software package called ‘EBTtool’ that I developed to perform numerical integrations of PSPMs and which is freely available from my webpage: http://staff.fnwi.uva.nl/a.m.deroos/EBT/Software/index.html. The EBTtool program contains a graphical interface that allows you to graphically inspect the population states stored in the CSB file, browse through the various states in a file and also output the population states to a text file. It hence provides an easy approach for graphical investigation of the stable population states at different values of the bifurcation parameter.

For those users that do not want to install the EBTtool program, however, a utility program is included, called csb2txt.c that will read the binary CSB file and translate it to plain text. The source file csb2txt.c can be found in the same directory as where the files PSPM demo.c and PSPM equi.c are located. This source file can be compiled into an executable program by issuing the command make csb2txt in the directory with the source file csb2txt.c. The compilation should not pose any major problems as the program is written in fairly standard C.

Executing the csb2txt program by itself generates a help message that explains its usage as shown below:

```
/*programs/PSPManalysis: csb2txt

Usage: csb2txt [-f "printf() format string"] <CSB filename> [parameter value]
```

When the program is called with the name of a CSB file (with or without the extension .csb does not matter), it will write the information in the entire CSB file to the terminal (unless of course this output is piped into an output file). Alternatively, the name of the CSB file can be followed by a particular parameter value, in which case the program searches in the CSB file for the population state that is closest to the specified value and writes this single population state to the terminal.

Hence, the stable population distribution for the third population state (for parameter value 11.1908) stored in Medfly-PGR-0001.csb, which results from the calculations illustrated in box above, can be inspected with the following call to the csb2txt program:

```
/*programs/PSPManalysis/Tests: ../csb2txt Medfly-PGR-0001 1.12000E+01

# Population growth rates for parameter value 11.2
1.0000000000 0.4127626846
# State of population #0 for parameter value 11.2
1.0000000000 0.0000000000 1.0000000000
0.8129899031 0.5004188126 1.2300275762
0.6609431768 1.0008376252 1.5129893689
<...output suppressed in this box...>
1.000000E-09 49.5413326488 0.0000000000
```

A large number of intermediate lines are suppressed in the output of the command, as it would take up too much space. The population distribution displayed is, however, identical to the population distribution that is presented as an example in section 5.2 when discussing the contents of the Medfly-PGR-0001.mat file. The first line of output specifies the value of the bifurcation parameter as the first entry on the line and the calculated population growth rate value as the second entry. The following 3 columns represent the stable population density, the corresponding age as well as the reproductive value of the individuals at that age, respectively.

Similarly, the last population state stored in the file PNAS2002-EQ-0000.csb can be inspected by executing the following command, which uses the last parameter value of the computations 4.04758E-04 for selecting the state:

```
"/programs/PSPManalysis/Tests:../csb2txt PNAS2002-EQ-0000 4.04460E-04
2
# Environment variables for parameter value 0.00040446
0.0004044597 0.0004044597 0.0000000000 0.0000000000
4
# State of population W for parameter value 0.00040446
0.0000000000 10.046106826 23.276732599
0.0000000000 30.727264609 54.874389369
8
0.0000000000 51.650423862 81.88632000
<...output suppressed in this box.>
10
0.0000000000 2020.161796457 289.2703746568
0.0000000000 2040.884027837 289.270564476
12
0.0000000000 2061.6073286205 289.2707132173
```

As before, a large number of intermediate lines are suppressed in the output of the command for brevity.

The layout of the stable population distribution is always the same, irrespective of the type of bifurcation computation that has been carried out. The first line of the output contains the value of the bifurcation parameter as first entry and the equilibrium values of all environment variables as subsequent entries. After an empty line, the stable population distribution is printed. Each line of this distribution corresponds to a cohort of individuals with the first entry on a line specifying the number of individuals in that cohort and the subsequent entries on the line the average values of the individual state variables of the individuals in the cohort, in the order as adopted in the model specification file. Hence, for the PNAS model the second and third entry on a row specifies the average age and length, respectively, of the individuals in a cohort (see code box 7.3). The example of the stable population distribution shown in the box above is of course rather special, because the computations pertain to a curve with a zero equilibrium state of the structured consumer population. For this reason, the cohort density in the first entry on each row is consistently 0. This would, however, be different in the more general case of an equilibrium curve with a non-zero equilibrium state of the consumer.
Optional numerical settings

The values of the following options, modifying the numerical program settings, can be changed by means of `#define` statements in the model-specific file as illustrated in the code boxes 4.1 and 7.1.
<table>
<thead>
<tr>
<th>Setting name</th>
<th>Default value</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIN_SURVIVAL</td>
<td>$10^{-9}$</td>
<td>Minimum survival probability at which an individual is considered dead</td>
</tr>
<tr>
<td>MAX_AGE</td>
<td>$10^6$</td>
<td>Absolute maximum age after which an individual is considered dead</td>
</tr>
<tr>
<td>DYTOL</td>
<td>$10^{-7}$</td>
<td>Variable tolerance. The Newton iteration has converged when the norm of the right-hand side of the equations is less than $\text{RHSTOL}$ and the norm of the consecutive adjustments to the solution vector of unknowns is less than $\text{DYTOL}$</td>
</tr>
<tr>
<td>RHSTOL</td>
<td>$10^{-8}$</td>
<td>Right-hand side tolerance. The Newton iteration has converged when the norm of the right-hand side of the equations is less than $\text{RHSTOL}$ and the norm of the consecutive adjustments to the solution vector of unknowns is less than $\text{DYTOL}$</td>
</tr>
<tr>
<td>ALLOWNEGATIVE</td>
<td>0</td>
<td>If equal to 1 negative solution values are permissible, otherwise the program stops when a component of the solution vector becomes negative</td>
</tr>
<tr>
<td>FULLSTATEOUTPUT</td>
<td>2</td>
<td>If equal to 0 no output of the complete population state is produced. If equal to 1, output of the population state is produced, either in a Matlab file with .mat extension or in a binary file with .csb extension, with individuals originating from different states-at-birth weighted according to the stable distribution of produced offspring over states-at-birth and lumped into cohorts. If equal to 2, output of the population state is produced and individuals originating from different states-at-birth are stored as separate subpopulations.</td>
</tr>
<tr>
<td>COHORT_NR</td>
<td>100</td>
<td>Sets the number of cohorts in the output of the population state</td>
</tr>
<tr>
<td>Setting name</td>
<td>Default value</td>
<td>Interpretation</td>
</tr>
<tr>
<td>-------------------------</td>
<td>---------------</td>
<td>--------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>ODESOLVE_INIT_STEP</td>
<td>0.1</td>
<td>Initial step size in the numerical integration of the ODEs</td>
</tr>
<tr>
<td>ODESOLVE_MIN_STEP</td>
<td>$10^{-8}$</td>
<td>Smallest possible step size in the numerical integration of the ODEs</td>
</tr>
<tr>
<td>ODESOLVE_MAX_STEP</td>
<td>10.0</td>
<td>Largest possible step size in the numerical integration of the ODEs</td>
</tr>
<tr>
<td>ODESOLVE_FIXED_STEP</td>
<td>-</td>
<td>If defined, determines a value $\Delta t$, which forces the ODE integration method to include all time values $t = n\Delta t$ with $n = 0, 1, \ldots$ among its integration time steps in addition to possibly intervening time values enforced by the adaptive step size mechanism.</td>
</tr>
<tr>
<td>ODESOLVE_ABS_ERR</td>
<td>$10^{-10}$</td>
<td>Absolute error in the numerical integration of the ODEs</td>
</tr>
<tr>
<td>ODESOLVE_REL_ERR</td>
<td>$10^{-8}$</td>
<td>Relative error in the numerical integration of the ODEs</td>
</tr>
<tr>
<td>ODESOLVE_FUNC_TOL</td>
<td>$10^{-8}$</td>
<td>Threshold value determining whether a stopping event in the numerical integration routine has been detected</td>
</tr>
<tr>
<td>JACOBIAN_MIN_STEP</td>
<td>$10^{-7}$</td>
<td>Absolute minimum change in variable when computing Jacobian matrix</td>
</tr>
<tr>
<td>JACOBIAN_STEP</td>
<td>$10^{-4}$</td>
<td>Relative change in variable when computing Jacobian matrix</td>
</tr>
<tr>
<td>JACOBIAN_UPDATES</td>
<td>5</td>
<td>Number of Newton adjustments before the Jacobian matrix is computed anew</td>
</tr>
</tbody>
</table>
Analytical background

In this chapter I give a brief sketch of the computational approach, which is discussed in detail in Kirkilionis et al. (2001), Diekmann et al. (2003) and De Roos (2008). The description is far from complete, but only captures the basic idea of the computational machinery implemented in the package.

Consider the following generic model for the interaction of a size-structured consumer population foraging on an unstructured resource:

\[
\frac{\partial n(t,s)}{\partial t} + \frac{\partial (g(s,R)n(t,s))}{\partial s} = -\mu(s,R)n(t,s) \quad (16.1)
\]

\[
g(s_b,R)n(t,s_b) = \int_{s_b}^{s_m} \beta(s,R)n(t,s) \, ds \quad (16.2)
\]

\[
dRdt = G(R) - \int_{s_b}^{s_m} \gamma(s,R)n(t,s) \, ds \quad (16.3)
\]

In this model \(n(t,s)\) represents the size distribution of the consumer population at time \(t\) and \(R(t)\) is the resource density. The functions \(g(s,R)\), \(\beta(s,R)\) and \(\mu(s,R)\) represent the growth rate in size of an individual with size \(s\), its fecundity and its mortality rate, respectively. The function \(G(R)\) described the autonomous dynamics of the resource \(R\) in the absence of consumers.

The computational approach is based on the idea that this model can also be expressed as a system of integro-differential equations of the following form:

\[
b(t) = \int_0^\infty \beta(s(t,a,R(t)),R(t))F(t,a,R_t) \, b(t-a) \, da \quad (16.4)
\]

\[
dRdt = G(R(t)) - \int_0^\infty \gamma(s(t,a,R(t)),R(t))F(t,a,R_t) \, b(t-a) \, da \quad (16.5)
\]

in which \(b(t)\) is the population birth rate of the consumer population at time \(t\) and \(R_t\) represents the history of the resource density prior to time \(t\), i.e. the function \(R(\xi)\) with \(\xi \in (-\infty,t]\).

The function \(s(t,a,R_t)\) represents the body size of an individual consumer that is of age \(a\) at time \(t\) and has been exposed to the resource densities \(R_t\) since its birth. This body size is the integrated result of the growth rate \(g(s,R)\) that the individual has experienced.
since birth:

\[ s(t, a, R_t) = s^0 + \int_0^a g(s(t - \alpha, \alpha, R_{t-\alpha}), R(t - \alpha)) \, d\alpha \]  

(16.6)

The function \( F(t, a, R_t) \) represents the probability that an individual that is of age \( a \) at time \( t \) and has been exposed to the resource densities \( R_t \) since its birth is still alive. \( F(t, a, R_t) \) is related to the mortality rate \( \mu(s, R) \) following:

\[ F(t, a, R_t) = \exp\left( - \int_0^a \mu(s(t - \alpha, \alpha, R_{t-\alpha}), R(t - \alpha)) \, d\alpha \right) \]  

(16.7)

Figure 16.1 illustrates how the integro-differential equation system relates the birth rate in the past to the birth rate at time \( t \) through the intervening history of the resource density and the development of the consumers that have experienced this resource history.

16.1 The system of equations determining the population growth rate

For demographic analysis of a linear PSPM only the integral equation [16.4] is relevant. In linear PSPMs the individual life history is not influenced by any density dependence or
16.1. THE SYSTEM OF EQUATIONS DETERMINING THE POPULATION GROWTH RATE

by any dependence on environment variables. We can hence drop the dependence of the development rate, fecundity and mortality rate on environment variables and generalize the integral equation [16.4] for an arbitrary choice of the individual state to:

\[ b(t) = \int_0^\infty \beta(\chi(a)) \mathcal{F}(a) b(t - a) \, da \]

in which \( \chi(a) \) is the state that individuals reach at age \( a \) provided they were born with state \( \chi_b \). \( \chi(a) \) is formally given by:

\[ \chi(a) = \chi_b + \int_0^a g(\chi(\alpha)) \, d\alpha \]

and \( \mathcal{F}(a) \) is the probability of survival up to age \( a \):

\[ \mathcal{F}(a) = \exp \left( - \int_0^a \mu(\chi(\alpha)) \, d\alpha \right) \]

Assuming exponential growth of the population birth rate:

\[ b(t) = e^{ra}b(t - a) \]

leads to Lotka’s integral equation for the population growth rate \( r \):

\[ \int_0^\infty e^{-ra} \beta(\chi(a)) \mathcal{F}(a) \, da = 1 \] (16.8)

Define the function \( H(a, r) \) as the value of Lotka’s integral up to age \( a \):

\[ H(a, r) = \int_0^a e^{-ra} \beta(\chi(\alpha)) \mathcal{F}(\alpha) \, d\alpha \]

Equation [16.8] can then be expressed as:

\[ H(\infty, r) = 1 \] (16.9)

which is a non-linear equation for the population growth rate \( r \). This is the equation that is solved by the software package for the unknown quantity \( r \) using an iterative approach based on the Newton-Chord method. For more details of the Newton-Chord method I refer to Kuznetsov [1995], which source I have used to a large extent for the iterative calculation of the solution \( \tilde{r} \).

The central idea of the computational approach relates to the evaluation of the function \( H(\infty, r) \), which is computed by solving an ordinary differential equation. To derive this ODE differentiate \( \mathcal{F}(a) \) with respect to \( a \) using the chain rule:

\[ \frac{d}{da} \mathcal{F}(a) = -\exp \left( - \int_0^a \mu(\chi(\alpha)) \, d\alpha \right) \frac{d}{da} \left( \int_0^a \mu(\chi(\alpha)) \, d\alpha \right) \]

Applying Leibniz rule for differentiation of an integral:

\[ \frac{d}{d\theta} \left( \int_{a(\theta)}^{b(\theta)} f(\chi, \theta) \, d\chi \right) = \int_{a(\theta)}^{b(\theta)} f_\theta(\chi, \theta) \, d\chi + f(b(\theta), \theta)b'(\theta) - f(a(\theta), \theta)a'(\theta) \]
then leads to:

\[
\frac{dF}{da} = -\mu(\chi(a)) F(a), \quad F(0) = 1
\]

Similarly, differentiate \(H(a,r)\) with respect to \(a\) and applying Leibniz rule yields:

\[
\frac{dH}{da} = e^{-ra} \beta(\chi(a)) F(a), \quad H(0) = 0
\]

The value of \(H(\infty, r)\) can hence be calculated by (numerical) integration of the ODEs:

\[
\begin{aligned}
\frac{d\chi}{da} &= g(\chi), \quad \chi(0) = \chi_b \\
\frac{dF}{da} &= -\mu(\chi(a)) F(a), \quad F(0) = 1 \\
\frac{dH}{da} &= e^{-ra} \beta(\chi(a)) F(a), \quad H(0) = 0
\end{aligned}
\]

In practice numerical integration of these ODEs is carried out up to \(a = A_{\text{max}}\) with \(A_{\text{max}}\) either a fixed value or by \(F(A_{\text{max}}) = \epsilon\) with \(\epsilon\) a very small value (i.e. \(\epsilon = 10^{-9}\)). Whenever an evaluation of the function \(H(\infty, r)\) is required in the Newton iterations of equation \(16.9\) this system of ODEs has to be integrated numerically. Once, a solution \(\tilde{r}\) has been found, the sensitivities of this solution with respect to the model parameters are calculated using numerical differentiation.

16.2 The system of equations determining an equilibrium

The idea discussed above for the demographic analysis of a linear PSPM extends to the computation of an equilibrium of a nonlinear PSPM. In such a nonlinear PSPM the fecundity and the development and mortality rates of individuals does depend on their environment, but in equilibrium this environment is necessarily constant: \(\tilde{E}\). Therefore, Lotka's integral equation should determine as before the population growth rate \(r\):

\[
\int_0^\infty e^{-ra} \beta(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}) \, da = 1
\]

(Note that all parts of life history now depend on \(E\). \(\chi\) and \(F\) do because of \(g(\chi, E)\) and \(\mu(\chi, E)\)). However, \(r\) should equal 0 for equilibrium of the structured population:

\[
\int_0^\infty \beta(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}) \, da = 1
\]

In addition, the autonomous dynamics of the environment should be balanced by the impact of the population:

\[
G(\tilde{E}) = \tilde{b} \int_0^\infty \gamma(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}) \, da
\]

The survival rate \(F(a, \tilde{E})\) and the value of the cumulative reproduction integral:

\[
H(a, \tilde{E}) = \int_0^a \beta(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}) \, da
\]
can be computed as before by solving the corresponding ODEs. To compute the impact of the population on the environment, define the function $I(a, \tilde{E})$ as:

$$I(a, \tilde{E}) = \int_0^a \gamma(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}) \, da$$

$I(a, \tilde{E})$ represents the cumulative, expected impact that a single individual exerts on its environment until age $a$. Differentiating $I(a, \tilde{E})$ with respect to $a$ yields after applying Leibniz rule:

$$\frac{dI}{da} = \gamma(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}), \quad I(0) = 0$$

The equilibrium of a nonlinear structured population model is therefore determined by the system of equations:

$$H(\infty, \tilde{E}) = 1$$

$$\tilde{b} I(\infty, \tilde{E}) = G(\tilde{E})$$

which has to be solved (numerically and iteratively) for the unknowns $\tilde{E}$ and $\tilde{b}$. These equations are solved by the software package for the unknown quantities using the Newton-Chord method as discussed before. Whenever the functions $H(\infty, \tilde{E})$ and $I(\infty, \tilde{E})$ have to be evaluated in this iterative procedure, the following system of ODEs is integrated numerically:

$$\begin{cases}
\frac{d\chi}{da} = g(\chi(a, \tilde{E}), \tilde{E}), & \chi(0, \tilde{E}) = \chi_b \\
\frac{dF}{da} = -\mu(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}), & F(0, \tilde{E}) = 1 \\
\frac{dH}{da} = \beta(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}), & H(0, \tilde{E}) = 0 \\
\frac{dI}{da} = \gamma(\chi(a, \tilde{E}), \tilde{E}) F(a, \tilde{E}), & I(0, \tilde{E}) = 0
\end{cases}$$

### 16.3 Curve continuation and detection of bifurcation points

The package uses the Newton-Chord method with Broyden updating of the Jacobian matrix to solve for the root of the nonlinear system of equations that determines the population growth rate of linear PSPMs or the equilibrium of nonlinear PSPMs. In addition, pseudo-arclength continuation is used to compute a curve of either the population growth rate or the equilibrium as a function of a single parameter. The numerical details about the Newton-Chord method as well as the pseudo-arclength continuation will not be discussed here. For details I refer to the appropriate sections in [Kuznetsov (1995)](Kuznetsov1995), which has been used as the basis for the implementations in the package. Both the Newton-Chord method as well as the pseudo-arclength continuation method make extensive use of partial derivatives of the system of equations with respect to variables and parameters. These partial derivatives, which for example make up the Jacobian matrix of the system of equations, are always computed numerically using a central-differencing approach.

The partial derivatives also play a role in the detection of bifurcation points, as explained in chapter 9. For example, the evolutionary analysis of PSPM using Adaptive Dynamics
(AD) centers around the analysis of $s_x(y)$, which is the population growth rate of a mutant with trait $y$ in an environment that is completely determined by a resident population with trait $x$ (Geritz et al., 1998). An evolutionary fixed point occurs at $x = x^*$ where
\[
\frac{\partial s_x(y)|_{x,y=x^*}}{\partial y} = 0
\]

The evolutionary fixed point can be classified as a convergent stable strategy (CSS), an evolutionary repellor (ERP) or evolutionary branching point (EBP) based on the value of (Geritz et al., 1998):
\[
\frac{\partial^2 s_x(y)|_{x,y=x^*}}{\partial y^2} \quad \text{and} \quad \frac{\partial^2 s_x(y)|_{x,y=x^*}}{\partial x^2}
\]

Because the equilibrium conditions for a structured model
\[
\int_0^\infty \beta(\chi(a, \hat{E}), \hat{E}) F(a, \hat{E}) \, da - 1 = R_0 - 1 = 0
\]
is sign-equivalent with $s_x(y)$ AD analysis can be performed using $R_0$ and its (partial) derivatives with respect to resident and mutant traits $x$ and $y$, respectively (Geritz et al., 1998). Hence, the detection of evolutionary fixed points, their classification as convergent stable strategies, repellors or branching points, as well as the continuation of these evolutionary singularities as a function of two parameters, which is discussed in chapters 9 to 11 relies on the computation of these partial derivatives, which are computed numerically as pointed out above.
Bibliography


