Accelerated Variational Infinite Mixture Models

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Abstract

Infinite mixture models, such as the Dirichlet process mixture, are promising candidates for clustering applications where the number of clusters is unknown a priori. Due to computational considerations these models are unfortunately unsuitable for large scale data-mining applications. We propose a class of deterministic accelerated infinite mixture models that can routinely handle millions of data-cases. The speedup is achieved by incorporating kd-trees into a variational Bayesian algorithm for infinite mixture models in the stick breaking representation. Besides kd-trees, this algorithm is also different from Blei and Jordan (2005) in the way we handle truncation: we only assume that the variational distributions are fixed at their priors after a certain truncation level. Experiments show that speedups relative to the standard variational algorithm can be significant.

1 Introduction

Evidenced by three recent workshops[1], nonparametric Bayesian methods are gaining popularity in the machine learning community. In each of these workshops computational efficiency was mentioned as an important direction for future research. In this paper we propose computational speedups for infinite mixture models, aka Dirichlet process mixtures [1, 2, 3, 4, 5], with the purpose of improving their applicability in modern day data-mining problems where millions of data-cases are no exception.

Our approach is related to, and complements, the variational mean-field algorithm of Blei and Jordan [5] for infinite mixture models in the stick-breaking representation. In this approach, the intractable posterior of an infinite mixture is approximated with a fully factorized variational model

[1] http://aluminum.cse.buffalo.edu:8079/npbayes/nipsws05/topics
http://www.cs.toronto.edu/~beal/npbayes/
http://www2.informatik.hu-berlin.de/~bickel/npb-workshop.html

that is optimized to minimize the KL distance to the posterior. In [5] the variational model boils down to a finite mixture (truncated infinite mixture), in which case all update equations involve finite sums. The downside of their algorithm, however, is that there may exist an optimal *finite* truncation level for the mixture that may be difficult to locate (see Section 3).

In this paper we propose an alternative variational mean-field algorithm, called VIM (for Variational Infinite Mixtures), in which the variational model itself is infinite. To deal with the infinitely many parameters of the model, we entertain an infinite pool of components with *tied* variational distributions, and release components when this improves (significantly) the KL bound. Releasing is most effectively done by splitting a component in two children and updating them to convergence. Our approach essentially resolves the issue in [5] of searching for an optimal truncation level (see Section 4).

Additionally, a significant contribution is that we incorporate kd-trees into the VIM algorithm as a way to speed up convergence [6, 7]. A kd-tree structure recursively partitions the data space into a number of nodes, where each node contains a subset of the data-cases. Following [7], for a given tree expansion we tie together the responsibility over mixture components of all data-cases contained in each outer node of the tree. By caching certain sufficient statistics in each node of the kd-tree we then achieve computational gains, while the variational approximation becomes a function of the depth of the tree at which one operates (see Section 6).

The resulting Fast-VIM algorithm provides an elegant way to trade off computational resources against accuracy. We can always release new components from the pool and split kd-tree nodes as long as we have computational resources left. Our setup guarantees that this will always (at least in theory) improve the KL bound (in practice local optima may force us to reject certain splits, see Section 7). As we empirically demonstrate in Section 8, a kd-tree can offer significant speedups, allowing our algorithm to handle millions of data-cases. As a result, Fast-VIM is the first algorithm entertaining an infinite number of clusters that is practical for modern day data-mining applications.

2 The Infinite Mixture Model in the Stick-Breaking Representation

According to the stick-breaking representation, an infinite mixture model (Dirichlet process mixture) can be viewed as possessing an infinite number of components that are ordered according to non-increasing mixing weights [3]. In particular, the generative model of an infinite mixture assumes:

- An infinite collection of components $H = \{\eta_i\}_{i=1}^{\infty}$ that are independently drawn from a prior $p_\eta(\eta_i|\lambda)$ with hyperparameters λ.
- An infinite collection of 'stick lengths' $V = \{v_i\}_{i=1}^{\infty}$, $v_i \in [0,1]$, $\forall i$, that are independently drawn from a prior $p_v(v_i|\alpha)$ with hyperparameters α. They define the mixing weights $\{\pi_i\}_{i=1}^{\infty}$ as
$$\pi_i(V) = v_i \prod_{j=1}^{i-1}(1-v_j), \qquad \text{for} \quad i = 1, \ldots, \infty. \tag{1}$$
- An observation model $p_x(x|\eta)$ that generates a datum x from component η.

Given a dataset $X = \{x_n\}_{n=1}^{N}$, each data-case x_n is assumed to be independently generated by first drawing a component label $z_n = k \in \{1, \ldots, \infty\}$ from the infinite mixture with probability π_k, and then drawing x_n from the corresponding observation model $p_x(x_n|\eta_k)$. We will denote the set of all labels by $Z = \{z_n\}_{n=1}^{N}$.

Let $W = \{H, V, Z\}$ be the set of all latent variables of the infinite mixture and $\theta = \{\lambda, \alpha\}$ the hyperparameters. Given the above, the joint density of the infinite mixture reads
$$p(W, X|\theta) = \Big[\prod_{i=1}^{\infty} p_v(v_i|\alpha)\, p_\eta(\eta_i|\lambda)\Big] \prod_{n=1}^{N} p_z(z_n|V) p_x(x_n|\eta_{z_n}) \tag{2}$$
where $p_z(z_n = i|V) = \pi_i(V)$ from (1). In clustering problems we are mainly interested in the posterior of data labels $p(z_n|X, \theta)$, and in the predictive density
$$p(x|X, \theta) = \int_{H,V} p(x|H, V) \int_Z p(W|X, \theta) dH dV dZ, \tag{3}$$

which are both intractable since $p(W|X,\theta)$ cannot be computed analytically.

3 Variational Inference in Infinite Mixtures

To approximate the intractable posterior $p(W|X,\theta)$ we can use a factorized parametric family of distributions $q(W;\phi)$ defined as

$$q(W;\phi) = \prod_{i=1}^{\infty} q_{v_i}(v_i;\phi_i^v)\; q_{\eta_i}(\eta_i;\phi_i^\eta) \prod_{n=1}^{N} q_{z_n}(z_n) \tag{4}$$

where $q_{v_i}(v_i;\phi_i^v)$ and $q_{\eta_i}(\eta_i;\phi_i^\eta)$ are parametric models with parameters ϕ_i^v and ϕ_i^η (one parameter per i), and $q_{z_n}(z_n)$ are discrete distributions over the infinite labels (one distribution per n).

Variational inference consists in finding parameters ϕ_i^v, ϕ_i^η and distributions q_{z_n} (collectively denoted by ϕ) that minimize the Kullback-Leibler divergence $\mathrm{D}[q(W;\phi)||p(W|X,\theta)]$ between the true posterior and the variational approximation, or equivalently that minimize the free energy $F(\phi) = E_q[\log q(W;\phi)] - E_q[\log p(W,X|\theta)]$. Using (2) and (4), the free energy reads

$$F = \sum_{i=1}^{\infty} E_{q_{v_i}}\left[\log \frac{q_{v_i}(v_i;\phi_i^v)}{p_v(v_i|\alpha)}\right] + E_{q_{\eta_i}}\left[\log \frac{q_{\eta_i}(\eta_i;\phi_i^\eta)}{p_\eta(\eta_i|\lambda)}\right] + \sum_{n=1}^{N} E_q\left[\log \frac{q_{z_n}(z_n)}{p_z(z_n|V)p_x(x_n|\eta_{z_n})}\right]. \tag{5}$$

Clearly, minimizing F over infinitely many parameters is infeasible. In [5] the variational mixture is explicitly truncated at level T by setting $q_{v_T}(v_T = 1) = 1$ and $q_{z_n}(z_n > T) = 0$. In this setup, data-cases assign zero responsibility to components with index higher than the truncation level T, and therefore only components of the mixture up to T need to be considered. Variational inference involves minimizing F over T parameters $\{\phi_i^v, \phi_i^\eta\}_{i=1}^T$ and N distributions $\{q_{z_n}(z_n)\}_{n=1}^N$. Since each distribution $q_{z_n}(z_n)$ has zero support for $z_n > T$, the variational update equations are straightforward as they involve only finite sums [5].

However, explicitly truncating the variational mixture as above has the undesirable property that the variational family with truncation level T is not contained within the variational family with truncation level $T+1$, i.e., the families are not nested.[2] The result is that there may be an optimal *finite* truncation level T for q, that contradicts the intuition that the more components we allow in q the better the approximation should be (reaching its best when $T = \infty$). Moreover, locating a near-optimal truncation level may be difficult since F as a function of T may exhibit local minima (see Fig. 4 in [5]).

4 Variational Inference with an Infinite Variational Model

Here we propose a slightly different variational model for q that allows families over T to be nested. In our setup, q is given by (4) where we *tie* together all models after some level T. In particular, we impose the condition that for all components with index $i > T$ the variational distributions for the stick-lengths $q_{v_i}(v_i)$ and the variational distributions for the components $q_{\eta_i}(\eta_i)$ are equal to their corresponding priors, i.e., $q_{v_i}(v_i;\phi_i^v) = p_v(v_i|\alpha)$ and $q_{\eta_i}(\eta_i;\phi_i^\eta) = p_\eta(\eta_i|\lambda)$. As in Section 3, we need to minimize F over T parameters $\{\phi_i^v, \phi_i^\eta\}_{i=1}^T$ and N distributions $\{q_{z_n}(z_n)\}_{n=1}^N$. However, contrary to Section 3, data-cases may now assign *nonzero* responsibility to components beyond level T, and therefore each $q_{z_n}(z_n)$ must now have infinite support (which requires computing infinite sums in the various quantities of interest). An important implication of our setup is that the variational families are now nested w.r.t. T (since for $i > T$, $q_{v_i}(v_i)$ and $q_{\eta_i}(\eta_i)$ can always revert to their priors), and as a result it is guaranteed that as we increase T there exist solutions that decrease F. This is an important result because it allows for optimization with adaptive T starting from $T = 1$ (see Section 7).

From the last term of (5) we directly see that the $q_{z_n}(z_n)$ that minimizes F is given by

$$q_{z_n}(z_n = i) = \frac{\exp(S_{n,i})}{\sum_{j=1}^{\infty} \exp(S_{n,j})} \tag{6}$$

[2] We thank David Blei for pointing this out.

where

$$S_{n,i} = E_{qV}[\log p_z(z_n = i|V)] + E_{q_{\eta_i}}[\log p_x(x_n|\eta_i)]. \tag{7}$$

Minimization of F over ϕ_i^v and ϕ_i^η can be carried out by direct differentiation of (5) for particular choices of models for q_{v_i} and q_{η_i} (see Section 5). Using q_{z_n} from (6), and the parameter tying assumption $q_{v_i} = p_v$ and $q_{\eta_i} = p_\eta$ for $i > T$, the free energy (5) reads

$$F = \sum_{i=1}^{T} E_{q_{v_i}}\left[\log \frac{q_{v_i}(v_i;\phi_i^v)}{p_v(v_i|\alpha)}\right] + E_{q_{\eta_i}}\left[\log \frac{q_{\eta_i}(\eta_i;\phi_i^\eta)}{p_\eta(\eta_i|\lambda)}\right] - \sum_{n=1}^{N} \log \sum_{i=1}^{\infty} \exp(S_{n,i}). \tag{8}$$

Evaluation of F requires computing the infinite sum $\sum_{i=1}^{\infty} \exp(S_{n,i})$ in (8). The difficult part is $\sum_{i=T+1}^{\infty} \exp(S_{n,i})$. Under the parameter tying assumption for $i > T$, most terms of $S_{n,i}$ in (7) factor out of the infinite sum as constants (since they do not depend on i) except for the term $\sum_{j=T+1}^{i-1} E_{p_v}[\log(1-v)] = (i-1-T)E_{p_v}[\log(1-v)]$. From the above, the infinite sum can be shown to be

$$\sum_{i=T+1}^{\infty} \exp(S_{n,i}) = \frac{S_{n,T+1}}{1 - \exp\left(E_{p_v}[\log(1-v)]\right)}. \tag{9}$$

Using the variational $q(W)$ as an approximation to the true posterior $p(W|X,\theta)$, the required posterior over data labels can be approximated by $p(z_n|X,\theta) \approx q_{z_n}(z_n)$. Although $q_{z_n}(z_n)$ has infinite support, in practice it suffices to use the individual $q_{z_n}(z_n = i)$ for the finite part $i \leq T$, and the cumulative $q_{z_n}(z_n > T)$ for the infinite part. Finally, using the parameter tying assumption for $i > T$, and the identity $\sum_{i=1}^{\infty} \pi_i(V) = 1$, the predictive density (3) can be approximated by

$$p(x|X,\theta) \approx \sum_{i=1}^{T} E_{q_V}[\pi_i(V)] E_{q_{\eta_i}}[p_x(x|\eta_i)] + \Big[1 - \sum_{i=1}^{T} E_{p_v}[\pi_i(V)]\Big] E_{p_\eta}[p_x(x|\eta)]. \tag{10}$$

Note that all quantities of interest, such as the free energy (5) and the predictive distribution (10), can be computed analytically even though they involve infinite sums.

5 Solutions for the exponential family

The results in the previous section apply independently of the choice of models for the infinite mixtures. In this section we provide analytical solutions for models in the exponential family. In particular we assume that $p_v(v_i|\alpha) = \text{Beta}(\alpha_1, \alpha_2)$ and $q_{v_i}(v_i;\phi_i^v) = \text{Beta}(\phi_{i,1}^v, \phi_{i,2}^v)$, and that $p_x(x|\eta)$, $p_\eta(\eta|\lambda)$, and $q_{\eta_i}(\eta_i;\phi_i^\eta)$ are given by

$$p_x(x|\eta) = h(x)\exp\{\eta^T x - a(\eta)\} \tag{11}$$

$$p_\eta(\eta|\lambda) = h(\eta)\exp\{\lambda_1\eta + \lambda_2(-a(\eta)) - a(\lambda)\} \tag{12}$$

$$q_{\eta_i}(\eta_i;\phi_i^\eta) = h(\eta_i)\exp\{\phi_{i,1}^\eta\eta_i + \phi_{i,2}^\eta(-a(\eta_i)) - a(\phi_i^\eta)\}. \tag{13}$$

In this case, the probabilities $q_{z_n}(z_n = i)$ are given by (6) with $S_{n,i}$ computed from (7) using

$$E_{q_{v_i}}[\log v_i] = \Psi(\phi_{i,1}^v) - \Psi(\phi_{i,1}^v + \phi_{i,2}^v) \tag{14}$$

$$E_{q_{v_j}}[\log(1-v_j)] = \Psi(\phi_{i,2}^v) - \Psi(\phi_{i,1}^v + \phi_{i,2}^v) \tag{15}$$

$$E_{q_{\eta_i}}[\log p_x(x_n|\eta_i)] = E_{q_{\eta_i}}[\eta_i]^T x_n - E_{q_{\eta_i}}[a(\eta_i)] \tag{16}$$

where $\Psi(\cdot)$ is the digamma function. The optimal parameters ϕ^v, ϕ^η can be found to be

$$\phi_{i,1}^v = \alpha_1 + \sum_{n=1}^{N} q_{z_n}(z_n = i) \qquad \phi_{i,2}^v = \alpha_2 + \sum_{n=1}^{N}\sum_{j=i+1}^{\infty} q_{z_n}(z_n = j) \tag{17}$$

$$\phi_{i,1}^\eta = \lambda_1 + \sum_{n=1}^{N} q_{z_n}(z_n = i)x_n \qquad \phi_{i,2}^\eta = \lambda_2 + \sum_{n=1}^{N} q_{z_n}(z_n = i). \tag{18}$$

The update equations are identical to those in [5] except that we have used $\text{Beta}(\alpha_1, \alpha_2)$ instead of $\text{Beta}(1, \alpha)$, and that $\phi_{i,2}^v$ involves the infinite sum $\sum_{j=i+1}^{\infty} q_{z_n}(z_n = j)$ which can be computed using (6) and (9). In [5] the corresponding sum is finite since $q_{z_n}(z_n)$ is truncated at T.

Note that the variational VB algorithm operates in a space where component labels are distinguishable, i.e., if we permute the labels the total probability of the data changes. Since the prior probabilities of the components are size ordered, the optimal ordering of the component labels in the variational posterior is also size ordered. Hence, we have incorporated a reordering step after each optimization step in our final algorithm (which is also different from [5].)

6 Accelerating inference using a kd-tree

In this section we show that we can achieve accelerated inference for large datasets when we store the data in a kd-tree [8] and cache data sufficient statistics in each node of the kd-tree [6]. A kd-tree is a binary tree in which the root node contains all points, and each child node contains a subset of the data points contained in its father node, where points are separated by a (typically axis-aligned) hyperplane. Each point in the set is contained in exactly one node, and the set of outer nodes (or 'boxes') of a given expansion of the kd-tree form a partition of the data set.

Suppose the kd-tree containing our data X is expanded to some level. Following [7], to achieve accelerated update equations we constrain all x_n in box A to share the same $q_{z_n}(z_n) \equiv q_{z_A}(z_A)$. We can then show that, under this constraint, the $q_{z_A}(z_A)$ that minimizes F is given by

$$q_{z_A}(z_A = i) = \frac{\exp(S_{A,i})}{\sum_{j=1}^{\infty} \exp(S_{A,j})} \tag{19}$$

where $S_{A,i}$ is computed as in (7) using (14)–(16) with (16) replaced by $E_{q_{\eta_i}}[\eta_i]^T \langle x \rangle_A - E_{q_{\eta_i}}[a(\eta_i)]$, and $\langle x \rangle_A$ denotes average over all data x_n contained in box A. Similarly, if $|n_A|$ is the number of data in box A, the optimal parameters can be shown to be

$$\phi^v_{i,1} = \alpha_1 + \sum_A |n_A| q_{z_A}(z_A = i) \qquad \phi^v_{i,2} = \alpha_2 + \sum_A |n_A| \sum_{j=i+1}^{\infty} q_{z_A}(z_A = j) \tag{20}$$

$$\phi^\eta_{i,1} = \lambda_1 + \sum_A |n_A| q_{z_A}(z_A = i) \langle x \rangle_A \qquad \phi^\eta_{i,2} = \lambda_2 + \sum_A |n_A| q_{z_A}(z_A = i). \tag{21}$$

Finally, using $q_{z_A}(z_A)$ from (19) the free energy (5) reads

$$F = \sum_{i=1}^{T} E_{q_{v_i}}\left[\log \frac{q_{v_i}(v_i; \phi^v_i)}{p_v(v_i|\alpha)}\right] + E_{q_{\eta_i}}\left[\log \frac{q_{\eta_i}(\eta_i; \phi^\eta_i)}{p_\eta(\eta_i|\lambda)}\right] - \sum_A |n_A| \log \sum_{i=1}^{\infty} \exp(S_{A,i}). \tag{22}$$

The infinite sums in (20) and (22) can be computed from (9) with $S_{n,T+1}$ replaced by $S_{A,T+1}$. Note that the cost of each update cycle is $O(T|A|)$, which can be a significant improvement over the $O(TN)$ cost when not using a kd-tree. (The cost of building the kd-tree is $O(N \log N)$ but this is amortized by multiple optimization steps.)

Note that by refining the tree (expanding outer nodes) the free energy F cannot increase. This allows us to control the trade-off between computational resources and approximation: we can always choose to descend the tree until our computational resources run out, and the level of approximation will be directly tied to F (deeper levels will mean lower F).

7 The algorithm

The proposed framework provides a principled way to tradeoff accuracy with computation and hence it offers several options in the design of an algorithm. Below we show in pseudocode the algorithm that we used in our experiments (for infinite Gaussian mixtures). Input is a dataset $X = \{x_n\}_{n=1}^N$ that is already stored in a kd-tree structure. Output is a set of parameters $\{\phi^v_i, \phi^\eta_i\}_{i=1}^T$ and a value for T. From that we can compute responsibilities q_{z_n} using (6).

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1. Set $T = 1$. Expand the kd-tree to some initial level (e.g. four).
2. Sample a number of 'candidate' components c according to size $\sum_A |n_A| q_{z_A}(z_A = c)$, and split the component that leads to the maximal reduction of F_T. For each candidate c do:

(a) Expand one-level deeper the boxes of the kd-tree that assign to c the highest responsibility $q_{z_A}(z_A = c)$ among all components.

(b) Split c in two components, i and j, through the bisector of its principal component. Initialize the responsibilities $q_{z_A}(z_A = i)$ and $q_{z_A}(z_A = j)$.

(c) Update only $S_{A,i}$, ϕ_i^v, ϕ_i^η and $S_{A,j}$, ϕ_j^v, ϕ_j^η for the new components i and j, keeping all other parameters as well as the kd-tree expansion fixed.

3. Update $S_{A,t}, \phi_t^v, \phi_t^\eta$ for all $t \leq T+1$, while expanding the kd-tree and reordering components.

4. If $F_{T+1} > F_T - \epsilon$ then halt, else set $T := T+1$ and go to step 2.

In the above algorithm, the number of sampled candidate components in step 2 can be tuned according to the desired cost/accuracy tradeoff. In our experiments we used 10 candidate components. In step 2b we initialized the responsibilities by $q_{z_A}(z_A = i) = 1 = 1 - q_{z_A}(z_A = j)$ if $\langle x \rangle_A$ is closer to i than to j (according to distance to the expected first moment). In order to speed up the partial updates in step 2c, we additionally set $q_{z_A}(z_A = k) = 0$ for all $k \neq i, j$ (so all responsibility is shared between the two new components). In step 3 we reordered components every one cycle and expanded the kd-tree every three update cycles, controlling the expansion by the relative change of $q_{z_A}(z_A)$ between a box and its children (alternatively one can measure the change of F_{T+1}). Finally, in step 2c we monitored convergence of the partial updates through F_{T+1} which can be efficiently computed by adding/subtracting terms involving the new/old components.

8 Experimental results

In this section we demonstrate VIM, and its kd-tree extension Fast-VIM, on synthetic and real datasets. Throughout we assume Gaussian observation model $p_x(x|\eta)$, and a Gaussian-inverse Wishart for $p_\eta(\eta|\lambda)$ and $q_{\eta_i}(\eta_i; \phi_i^\eta)$.

Synthetic datasets. As argued in Section 4, an important advantage of VIM over the 'BJ' algorithm of [5] is that in VIM the variational families are nested over T, which ensures that the free energy is a monotone decreasing function of T and therefore allows for an adaptive T (starting with the trivial initialization $T = 1$). On the contrary, BJ optimizes the parameters for fixed T (and possibly minimizing the resulting free energy over different values of T), which requires a nontrivial initialization step for each T. Clearly, both the total runtime as well as the quality of the final solution of BJ depend largely on its initialization step, which makes the direct comparison of VIM with BJ difficult. Still, to get a feeling of the relative performance of VIM, Fast-VIM, and BJ, we applied all three algorithms on a synthetic dataset containing 1000 to 5000 data-cases sampled from 10 Gaussians in 16 dimensions, in which the free parameters of BJ were set exactly as described in [5] (20 initialization trials and $T = 20$). VIM and Fast-VIM were also executed until $T = 20$. In Fig. 1 we show the speedup factors and free energy ratios[3] among the three algorithms. Fast-VIM was approximately 23 times faster than BJ, and three times faster than VIM on 5000 data-cases. Moreover, Fast-VIM and VIM were always better than BJ in terms of free energy.

In the second synthetic set of experiments we compared the speedup of Fast-VIM over VIM. We sampled data from 10 Gaussians in dimension D with component separation[4] c. Using default number of data-cases $N = 10,000$, dimensionality $D = 16$, and separation $c = 2$, we varied each of them, one at a time. In Fig. 2 we show the speedup factor (left y-axis) and the free energy ratio (right y-axis) between the two algorithms. Note that the latter is always worse for Fast-VIM since it is an approximation to VIM (ratio closer to one means better approximation). Fig. 2-left illustrates that the speedup of Fast-VIM over VIM is at least linear in N, as expected from the update equations in Section 6. The speedup factor was approximately 154 for one million data-cases, while the free energy ratio was almost constant over N. Fig. 2-center shows an interesting dependence of speed on dimensionality, with $D = 64$ giving the largest speedup. The three plots in Fig. 2 are in agreement with similar plots in [6, 7].

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[3] Free energy ratio is defined as $1 + (F_A - F_B)/|F_B|$, where A and B are either Fast-VIM, VIM or BJ.

[4] Following [9], a Gaussian mixture is c-separated if for each pair (i, j) of components we have $||m_i - m_j||^2 \geq c^2 D \max(\lambda_i^{\max}, \lambda_j^{\max})$, where $\lambda^{\max}$ denotes the maximum eigenvalue of their covariance.

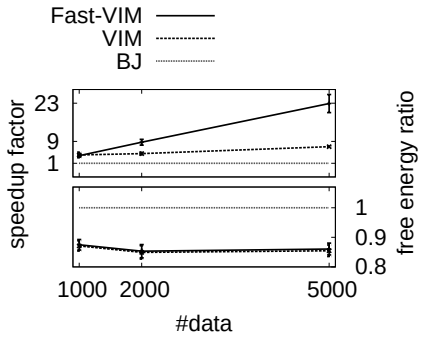


Figure 1: Relative runtimes and free energies of Fast-VIM, VIM, and BJ [5].

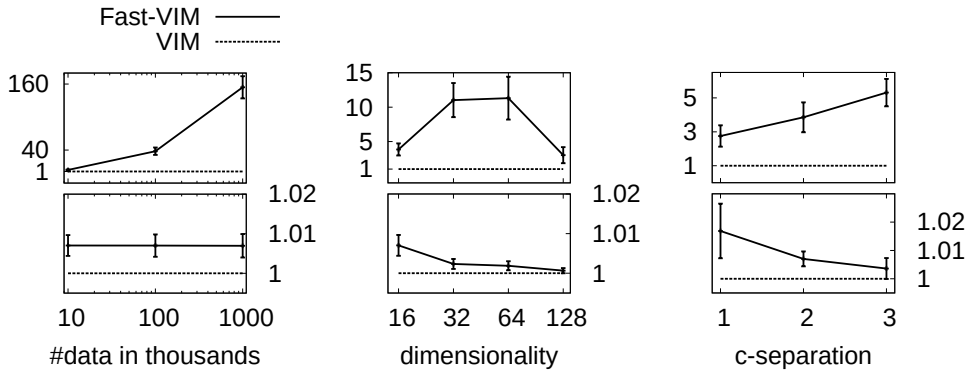
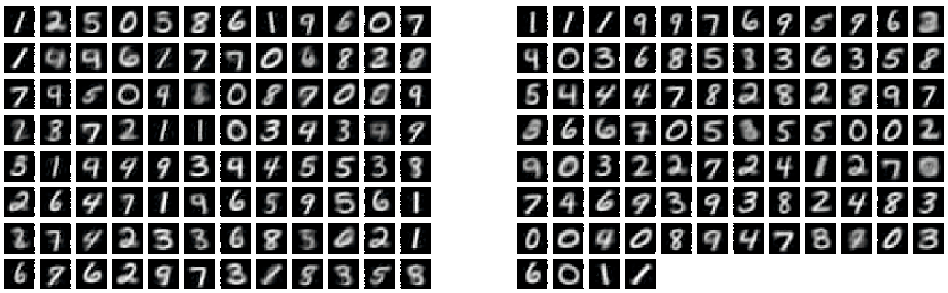


Figure 2: Speedup factors and free energy ratios between Fast-VIM and VIM. Top and bottom figures show speedups and free energy ratios, respectively.



Fast-VIM VIM

Figure 3: Clustering results of Fast-VIM and VIM, with a speedup of 21. The clusters are ordered according to size (from top left to bottom right).

Real datasets. In the first real data experiment we applied VIM and Fast-VIM for clustering image data. We used the MNIST dataset (`http://yann.lecun.com/exdb/mnist/`), which consists of $60,000$ images of the digits 0–9 in 784 dimensions (28 by 28 pixels). We first applied PCA to reduce the dimensionality of the data to 50. Fast-VIM found 96 clusters in $3,379$ seconds with free energy $F = 1.759 \times 10^7$, while VIM found 88 clusters in $72,037$ seconds with free energy 1.684×10^7. The speedup was 21, and the free energy ratio was 1.044. The mean images of the discovered components are illustrated in Fig. 3. The results of the two algorithms seem qualitatively similar, while Fast-VIM computed its results much faster than VIM.

In the second real data experiment we clustered documents from citeseer (`http://citeseer.ist.psu.edu`). The dataset has $30,696$ documents, with a vocabulary size of $32,473$ words. Each

		accelerated VIM					naive VIM					
cluster (in descending order)		a	b	c	d	e	A	B	C	D	E	F
the three most	1	81	73	35	49	76	81	73	35	76	49	73
frequent topics	2	102	174	50	92	4	102	40	50	4	92	174
	3	59	40	110	94	129	59	174	110	129	94	40

Table 1: The three most frequent topics in each clusters. Fast-VIM found five clusters, a–e, while VIM found six clusters, A–F.

cluster	the most frequent topic	words
a, A	81	economic, policy, countries, bank, growth, firm, public, trade, market, ...
b, B, F	73	traffic, packet, tcp, network, delay, rate, bandwidth, buffer, end, loss, ...
c, C	35	algebra, algebras, ring, algebraic, ideal, field, lie, group, theory, ...
d, E	49	motion, tracking, camera, image, images, scene, stereo, object, ...
e, D	76	grammar, semantic, parsing, syntactic, discourse, parser, linguistic, ...

Table 2: Words in the most frequent topic of each cluster.

document is represented by the counts of words in its abstract. We preprocessed the dataset by Latent Dirichlet Allocation with 200 topics[5] [5]. We subsequently transformed these topic-counts $y_{j,k}$ (count value of k'th topic in the j'th document) into $x_{j,k} = \log(1 + y_{i,j})$ to fit a normal distribution better. In this problem, the elapsed time of Fast-VIM and VIM were 335 seconds and 2,256 seconds, respectively, hence a speedup of 6.7. The free energy ratio was 1.040. Fast-VIM found five clusters, while VIM found six clusters. Table 1 shows the three most frequent topics in each cluster. Although the two algorithms found a different number of clusters, we can see that the clusters B and F found by VIM are similar clusters, whereas Fast-VIM did not distinguish between these two. Table 2 shows words included in these topics, showing that the documents are well-clustered.

9 Conclusions

We described VIM, a variational mean-field algorithm for infinite mixtures, and its fast extension Fast-VIM that utilizes kd-trees to achieve speedups. Our contribution is two fold: First, we demonstrated that it's possible (and in fact very advantageous) to do variational inference in infinite mixtures using infinite variational models. Second, we showed how kd-trees can be employed in the framework offering significant speedups, thus extending related results for finite mixture models [6, 7]. Our approach complements and strengthens the variational framework of [5], and provides the first nonparametric Bayes approach to large-scale data mining.

Future work include extending this work to other models in the stick-breaking representation (e.g., priors of the form $p_{v_i}(v_i|a_i, b_i) = \text{Beta}(a_i, b_i)$), as well as alternative infinite mixture representations such as the Chinese restaurant process [5].

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