Small-Variance Asymptotics for Dirichlet Process Mixtures of SVMs

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Abstract

Infinite SVM (iSVM) is a Dirichlet process (DP) mixture of large-margin classifiers. Though flexible in learning nonlinear classifiers and discovering latent clustering structures, iSVM has a difficult inference task and existing methods could hinder its applicability to large-scale problems. This paper presents a small-variance asymptotic analysis to derive a simple and efficient algorithm, which monotonically optimizes a max-margin DP-means (M^2DPM) problem, an extension of DP-means for both predictive learning and descriptive clustering. Our analysis is built on Gibbs infinite SVMs, an alternative DP mixture of large-margin machines, which admits a partially collapsed Gibbs sampler without truncation by exploring data augmentation techniques. Experimental results show that M^2DPM runs much faster than similar algorithms without sacrificing prediction accuracies.

Introduction

Clustering is a fundamental task in descriptive unsupervised learning with many popular methods such as K-means and various Bayesian models. It also plays an important role in predictive supervised learning for discovering subgroup structures and improving time efficiency. For example, when learning SVM classifiers, it could be computationally expensive to directly solve a large optimization problem on all training data. To improve efficiency and/or disclose descriptive structures, practitioners have used clustering methods to partition the data into subgroups and learn a simple classifier within each cluster (Fu, Robles-Kelly, and Zhou 2010).

Recent work on DP mixtures of generalized linear models (Shahbaba and Neal 2009; Hannah, Blei, and Powell 2011) provides flexible solutions to jointly learn classifiers and perform clustering; meanwhile these methods automatically resolve the unknown number of clusters, thereby bypassing the model selection problem of K-means and parametric mixture models. Along this line, infinite SVM (iSVM) (Zhu, Chen, and Xing 2011), a DP mixture of large-margin machines, provides an alternative approach that enjoys the advantages of Bayesian nonparametrics to resolve the number of components as well as the discriminative property of large-margin machines. However, these nonparametric methods normally have difficult inference problems, for which both variational and Monte Carlo methods could be too expensive to be applied to large-scale applications.

Small-variance asymptotics (SVA) offers useful techniques to setup conceptual links between probabilistic and non-probabilistic models and derive new algorithms that can be simple and scalable. For instance, connections between probabilistic PCA (pPCA) and standard PCA can be made by letting the covariance of the likelihood in pPCA approach zero (Tipping and Bishop 1999); and similarly the K-means algorithm can be obtained from the EM algorithm for Gaussian mixtures when the covariances of Gaussian components go to zero. Recent progress has been made on deriving new computational methods. For example, DP-means is a deterministic extension to K-means by applying SVA analysis to the Gibbs sampling algorithm of DP mixtures (Kulis and Jordan 2012); and the work (Broderick, Kulis, and Jordan 2013) provides a generic SVA analysis on MAP estimates and presents an example of latent feature learning. However, SVA analysis has been exclusively performed in unsupervised learning, while little work has been done for supervised learning, which imposes new challenges and requires more careful analysis as shown later.

This paper presents an SVA analysis to DP mixtures of SVMs and derives simple and scalable algorithms that perform descriptive clustering and predictive classifier learning jointly. Technically, our analysis is built on Gibbs infinite SVMs (Gibbs-iSVM) which learns component-wise classifiers by exploring the ideas of Gibbs classifiers, a powerful paradigm in learning theory (Germain et al. 2009). For Gibbs-iSVM with the generic exponential family likelihood, we present a partially collapsed Gibbs sampler by exploring data augmentation (Tanner and Wong 1987;olson and Scott 2011; Zhu et al. 2014) techniques. Compared to the variational algorithm of iSVM, the Gibbs sampler does not require truncated mean-field assumptions, thus converging to the true posterior. However, some expectations in the Gibbs sampler are hard to compute in closed forms. To improve efficiency, we perform SVA analysis to the Gibbs sampler and derive a simple deterministic algorithm by scaling both the covariances of the likelihood and the regularization parameters appropriately, where scaling the regularization parameters is a key new feature for extend-
ing SVA analysis to supervised models. In addition, by expressing the Chinese Restaurant Process (CRP, a marginalized version of DP) prior as exchangeable partition probability functions (EPPF) (Blackwell and MacQueen 1973; Pitman 1995; Aldous 1985) and adopting the same set of scalings to the posterior directly, we obtain a max-margin DP-means (M^2DPM) optimization problem, an extension to the descriptive DP-means for both predictive learning and descriptive clustering. We prove that the deterministic algorithm monotonically optimizes the M^2DPM problem for local optimums. Experimental results on both synthetic and real datasets demonstrate the efficiency and effectiveness of the M^2DPM algorithm compared to other competitors.

Preliminaries

Exponential family distributions

An exponential family distribution can be characterized as follows (Barndorff-Nielsen 1978):

\[ p(x|\theta) = \exp(\langle x, \theta \rangle - \psi(\theta) - h(x)), \]

where \( \theta \) is the natural parameter and \( \psi(\theta) \) is the log-partition function. The mean and covariance of an exponential family are given by \( \nabla \psi(\theta) \) and \( \nabla^2 \psi(\theta) \) respectively. In the Bayesian setting, a convenient prior would be the conjugate prior (Agarwal and Daume 2010)

\[ p(\theta|\tau, \kappa) = \exp(\langle \theta, \tau \rangle - \kappa \psi(\theta) - m(\tau, \kappa)), \]

where \( \tau \) and \( \kappa \) are hyper-parameters.

Given a convex set \( S \subseteq \mathbb{R}^d \) and a differentiable, strictly convex function \( \varphi : S \rightarrow \mathbb{R} \), Bregman divergence (Bregman 1967) \( D_\varphi(x, y) \) is defined over pairs of points \( x, y \in S \) as

\[ D_\varphi(x, y) = \varphi(x) - \varphi(y) - \langle x - y, \nabla \varphi(y) \rangle. \]

In (Banerjee et al. 2005), a bijection between exponential family distributions and Bregman divergence was established. Specifically, we can use the mean parameter of an exponential family distribution to equivalently characterize the distribution and conjugate prior as:

\[ p(x|\mu) = \exp(-D_\varphi(x, \mu)) f_\varphi(x), \]

\[ p(\mu|\tau, \kappa) = \exp(-\kappa D_\varphi(\tau, \mu)) g_\varphi(\tau, \kappa), \]

where \( \varphi() \) is the Legendre-conjugate function of the log-partition function \( \psi() \) and \( f_\varphi(x) = \exp(\varphi(x) - h(x)) \). These representations can greatly simplify our small-variance analysis (Jiang, Kulis and Jordan 2012).

Infinite SVMs: a DP mixture of SVMs

A DP mixture (DPM) is a nonparametric Bayesian mixture model (Hjort et al. 2010), where the number of cluster components is unbounded. Given an instance \( x_i \in \mathbb{R}^d \) and its component assignment \( z_i \in \mathbb{N} \), we consider the general exponential family likelihood of the data instance:

\[ p(x_i|z_i, \mu_z) = \exp(-D_\varphi(x_i, \mu_z)) f_\varphi(x_i), \]

where \( \mu_z \) is the mean parameter of component \( k \). For priors, the cluster assignments \( z_{1:n} \) follow a CRP with the concentration parameter \( \alpha \), and the parameter of each component \( \mu_z \) follows a conjugate prior as in (4) with the hyper-parameters \( (\tau, \kappa) \).

Given a set of data \( X = \{x_i\}_{i=1}^n \), we can apply Bayes’ rule to obtain the posterior distribution \( p(z, \mu|X) \), which is equivalent to the solution of the convex problem:

\[ \min_{q(\theta, \mu) \in P} \text{KL}(q(\theta, \mu)||p_0(\theta, \mu)) - \mathbb{E}_q[\log p(X|z, \mu)], \]

where \( p_0 \) is the prior; \( p(X|z, \mu) = \prod_{i=1}^n p(x_i|z_i, \mu) \) is the likelihood; and \( P \) is a space of normalized distributions.

Infinite SVMs (iSVM) extends the unsupervised DPM for both predictive supervised learning and descriptive clustering. Let’s consider binary classification, where each instance is a pair of input features \( x_i \) and class label \( y_i \in \{-1, +1\} \). In iSVM, each cluster \( k \) is associated with a mean parameter \( \mu_k \) to characterize the likelihood of \( x \) and a classifier \( \eta_k \) to predict \( y \). For the common linear classifiers, the discriminant function is

\[ f(x_i; \eta, z_i) = \eta_{z_i}^\top x_i = \sum_{k=1}^\infty \delta_{z_i=k} \eta_k^\top x_i. \]

To resolve the uncertainty of \( \Theta := \{\mu, \eta, z\} \), characterized by a distribution \( q(\theta) \), iSVMs defines the averaging (or expected) discriminant function \( f(x_i; q) = \mathbb{E}_q[f(x_i; \eta, z_i)] \), and makes predictions using the rule \( \hat{y} = \text{sign} f(x_i; q) \). For this averaging classifier, we can measure its performance by using the hinge loss, \( \mathcal{L}(q, X) = \sum_{i=1}^n \max(0, 1 - y_i f(x_i; q)) \), where \( (x_i)_+ = \max(0, x) \), and \( l \geq 1 \) is the cost of a wrong prediction. The hinge loss is an upper bound of training error. Then, iSVM solves the regularized Bayesian inference (RegBayes) (Zhu, Chen, and Xing 2014) problem

\[ \min_{q(\theta) \in P} \mathcal{L}(q(\theta)) + 2c \cdot \mathcal{R}(q(\theta), X), \]

where \( \mathcal{L}(q(\theta)) = \text{KL}(q\|p_0) - \mathbb{E}_q[\log p(X|z, \eta)] \) is the objective of Bayesian inference for the DPM, and \( c \) is a positive regularization parameter balancing the two terms. For \( \eta \), a common Gaussian prior is \( \eta_k \sim \mathcal{N}(0, \nu^2 I_d) \). Variation methods have been developed for approximate inference in iSVM, with a truncated mean-field assumption for tractability (Zhu, Chen, and Xing 2011). Generally, it is hard to develop Monte Carlo methods for such Bayesian max-margin models, which may involve solving a dual problem still with mean-field assumptions (Jiang et al. 2012).

Gibbs Infinite SVMs

We present Gibbs iSVMs with the generic exponential family likelihood and develop a Gibbs sampler that grounds our small-variance asymptotic (SVA) analysis. Gibbs iSVMs is formulated as a DP mixture of Gibbs classifiers (Germain et al. 2009; Zhu et al. 2014; Zhang, Zhu, and Zhang 2014).

Learning with an expected hinge loss

For our DP mixtures, a Gibbs classifier randomly draws a sample \( (\eta, z) \) from the target posterior \( q(\theta) \), and makes predictions using the linear discriminant function (7) via the training rule \( \hat{y} = \text{sign} f(x_i; \eta, z_i) \). We measure the performance of this latent classifier using the hinge loss as a surrogate to the training error; \( \mathcal{R}'(q, z, X) = \sum_{i=1}^n l - y_i \eta_{z_i}^\top x_i \). To resolve the uncertainty, we take the expectation and define the expected hinge loss

\[ \mathcal{R}'(q, \Theta, X) = \mathbb{E}_q[\mathcal{R}'(q, \eta, z, X)]. \]
Then, Gibbs iSVMs solves the new RegBayes problem:

$$
\min_{\theta \in \mathcal{P}} \mathcal{L}(\theta) + 2c \cdot \mathcal{R}'(\theta, X).
$$

(10)

Note: by using Jensen’s inequality, we can show the relationship between the two hinge losses as: $\mathcal{R}'(q, X) \geq \mathcal{R}(q, X)$.

**Representation with data augmentation**

One nice property of Gibbs iSVMs is that we can develop a Gibbs sampler without making truncated mean-field approximations. This sampler will lead to a simple deterministic algorithm via our SVA analysis, as shown soon later. Specifically, we can express the solution to (10) as

$$
q(\theta) = \frac{p_0(\theta) \prod_{i=1}^{n} p(x_i|\mu, \phi(y_i|z_i, \eta))}{Z(D)}
$$

(11)

where $\phi(y_i|z_i, \eta) = \exp(\beta \eta_i^n D_i^j)$ is an unnormalized likelihood corresponding to the hinge loss, $\eta_i^n = l - y_i\eta_i^n x_i$, is the margin achieved by applying classifier $\eta_i^n$ on data $x_i$, and $Z(D)$ is the normalization factor. As in (Polson and Scott 2011), we can show that

$$
\phi(y_i|z_i, \eta) = \int_0^\infty \frac{1}{\sqrt{2\pi\omega_i}} \exp\left(-\frac{(\omega_i + c\eta_i^n)^2}{2\omega_i}\right) d\omega_i,
$$

(12)

where $\omega_i > 0$ is an augmented variable. Then, $q(\theta)$ can be written as a marginal of the complete distribution:

$$
q(\theta, \omega) = \frac{p_0(\theta) \prod_{i=1}^{n} p(x_i|\mu, \phi(y_i|z_i, \eta))Z(D)}{\omega_i}
$$

(13)

where $\phi(y_i, \omega|z_i, \eta) = \frac{1}{\sqrt{2\pi\omega_i}} \exp\left(-\frac{(\omega_i + c\eta_i^n)^2}{2\omega_i}\right)$ is the augmented (unnormalized) likelihood for the hinge loss.

**Partially collapsed Gibbs sampling**

With data augmentation, we develop a Gibbs sampler that iteratively samples $z$, $\mu$, $\eta$, and $\omega$ from the posterior (13); thus the samples of Gibbs iSVM by dropping the variables $\omega$. To improve the convergence rate, we also adopt a partially collapsed approach (van Dyk and Park 2008) when sampling $z$ by integrating out $\omega$. The Gibbs sampler iteratively samples from the following conditional distributions:

**For $\mu_k$:** the conditional distribution is $q(\mu_k|z) \propto p(\mu_k, \tau, \kappa) \prod_{i \in N_k} p(x_i|\mu_k)$, where $N_k := \{i : z_i = k\}$ is the set of indices assigned to cluster $k$. With the conjugate prior, $q(\mu_k|z)$ is still an exponential family distribution:

$$
q(\mu_k|z) \propto \exp\left(-\kappa D_\phi\left(\frac{\tau_k}{\kappa}, \mu_k\right)\right),
$$

(14)

where $\tau' = \tau + \sum_{i \in N_k} x_i$, $\kappa' = \kappa + n_k$ and $n_k = |N_k|$ is the number of data samples in cluster $k$.

**For $z_i$:** let $n_{-i,k}$ be the number of instances other than $x_i$ that belong to cluster $k$. Then, for cluster $k$ with $n_{-i,k} > 0$, the conditional probability of getting $z_i = k$ is

$$
q(z_i = k|z_{-i}, \eta) \propto p_0(z_i = k|z_{-i})p(x_i|\mu_k)\phi(y_i|z_i = k) \propto n_{-i,k} p(x_i|\mu_k)\phi(y_i|z_i = k, \eta).
$$

(15)

The probability of assigning $x_i$ to a new cluster is

$$
q(z_i = z_{\text{new}}|\alpha) \propto \alpha p(x_i) \int \phi(\eta|\eta)p_0(\eta) d\eta,
$$

(16)

where $p(x_i) = \int p(x_i|\mu)p_0(\mu)d\mu$ and $\phi(y_i|\eta) = \exp(-2c(l - y_i\eta x_i))$. Though $p(x_i)$ has closed forms because of conjugate priors, the integral $\int \phi(\eta|\eta)p_0(\eta)d\eta$ does not have a simple closed form due to the hinge loss term $\phi(y_i|\eta)$ and approximation is needed in practice.

**For $\eta$:** when the margin $\eta_i^n$ is fixed, the conditional distribution over the augmented variable $\omega_i$ is a generalized inverse Gaussian distribution (Devroye 1986). Consequently, $\omega_i^{-1}$ follows an inverse Gaussian distribution

$$
q(\omega_i^{-1}|z_i, \tau, \kappa) = IG\left(\omega_i^{-1}; \frac{1}{c\eta_i^n}, 1\right),
$$

(17)

where $IG(x; a, b) = \sqrt{\frac{b}{2\pi x}} \exp(-\frac{b(x-a)^2}{2ax})$ for $a > 0$ and $b > 0$. We can sample $\omega_i^{-1}$ from an inverse Gaussian distribution in $O(1)$ time (Michael, Schucany, and Haas 1976).

**For $\eta_k$:** the conditional distribution of $\eta_k$ is

$$
q(\eta_k|z, \tau, \kappa) \propto \exp\left(-\frac{\|\eta_k\|^2}{2\sigma^2} - \sum_{i \in N_k} \frac{(\omega_i + c\eta_i^n)^2}{2\omega_i}\right),
$$

(18)

a Gaussian distribution with covariance and mean: $\Lambda_k = \left(\frac{1}{\sigma^2} + c^2 \sum_{i \in N_k} \frac{\omega_i + c\eta_i^n}{\omega_i}\right)^{-1}$; $\Lambda_k = \Lambda_k (c \sum_{i \in N_k} \frac{\omega_i + c\eta_i^n}{\omega_i}, x_i)$.

**Small-Var...
For $\mu_k$: applying the scaling $\tilde{\theta}_k = \beta \theta_k$, and the fact in Eq. (19), the conditional in Eq. (14) now becomes:

$$q(\mu_k | z, \beta) \propto \exp \left( -\kappa'' D_\phi \left( \frac{\tau''}{\kappa''}, \mu_k \right) \right),$$

(21)

where $\kappa'' = \kappa + \beta n_k$ and $\tau'' = \tau + \beta \sum_{i \in N_k} x_i$. Similar as in (Jiang, Kulis, and Jordan 2012) we can show that as $\beta \to \infty$ the conditional distribution of $\mu_k$ will be concentrated on the empirical mean. See Appendix A for details.

For $z_i$: since we are performing both classification and clustering, we need both the likelihood (e.g. $D_\phi(x_i, \mu_k)$) and hinge loss (e.g. $\phi(y_i | z_i, \eta)$) to play a role in determining $z_i$. A straightforward application of existing SVA techniques will drop the hinge loss. To avoid such artifacts, we develop a new analysis by scaling the regularization parameter $c$. Specifically, let $\tilde{c} = \beta^c c$ and $\phi(y_i | z_i = k, \eta, \beta') = \exp(-2\tilde{c}(\zeta_i^k_1))$. We also set a connection between the two scaling constants $\beta = (\beta, \beta')$ as $\beta = \beta$, where $s$ is a constant. Then, by Eq. (19), the conditional in Eq. (15) becomes

$$q(z_i = k | z_i, \mu, \eta, \beta) = \frac{n_i - k}{Z} f_\beta(x_i) \cdot \exp \left( -\beta' \left( s \cdot D_\phi(x_i, \mu_k) + 2c(\zeta_i^k_1) \right) \right).$$

(22)

When generating new clusters, we need to retain the regularization term (i.e. prior) of $\eta$. Therefore, the variance of the prior distribution, $\nu^2$, should be properly scaled. To this end, we use the scaling $\nu^2 = \nu^2 / \beta'$. Then, the conditional probability in Eq. (16) can be expressed as

$$q(z_i = z_{\text{new}} | \alpha, \beta) = \frac{\alpha}{Z} I_1 \cdot I_2,$$

(23)

where the two integrals are $I_1 := \int p(x_i | \tilde{\theta}) p(\tilde{\theta}) d\tilde{\theta}$ and $I_2 := \int \phi(y_i | z_i, \eta, \beta') p(\eta | \nu^2) d\eta$. Though the integrals are hard to compute, we can apply the Laplace’s method to derive meaningful SVA results, as detailed below.

For integral $I_1$, using Eqs. (19,20), we can expand it as

$$I_1 = f_\beta(x_i) g_\beta \left( \frac{\tau}{\beta}, \frac{\kappa}{\beta} \right) A(\tilde{\phi}, \tau, \kappa, \beta) (x_i) \cdot \beta^2 J,$$

(24)

where $A(\tilde{\phi}, \tau, \kappa, \beta) (x_i)$ := $\exp(-\beta \varphi(x_i) + \kappa \varphi(x_i) - (\beta + \kappa) \varphi(\tilde{\phi}(x_i) + \beta \varphi(x_i))$ arises when combining the exponential family distribution with its conjugate prior; and $J := \int \exp \left( -\beta \varphi(x_i) + \frac{\tau}{\beta} \varphi(x_i) + \frac{\kappa}{\beta} \varphi(x_i) \right) d\varphi$ is another integral, which can be further expanded via the Laplace’s method. Let $\tilde{\theta} = \tilde{\theta}(\mu)$ be a local minimum of $D(\tilde{\theta}) = D(\frac{\partial \varphi}{\partial \mu} + \mu(\tilde{\theta}))$. We then have

$$J = \exp \left( -\beta \varphi(x_i) + \frac{\tau}{\beta} \varphi(x_i) + \frac{\kappa}{\beta} \varphi(x_i) \right) \left( \frac{\partial^2 D(\tilde{\theta})}{\partial \beta^2} \right)^{-1/2} + o(1).$$

(25)

As $\lim_{\beta \to \infty} \frac{\tau}{\beta} = \varphi(x_i)$, we have $D(\tilde{\theta}) = D(\theta(x_i)) = 0$. Thus, $\lim_{\beta \to \infty} J = (2\tau / (\beta + \kappa))^{1/2} \cdot \varphi(x_i)^{-1/2}$. Note also that $\lim_{\beta \to \infty} A(\tilde{\phi}, \tau, \kappa, \beta) (x_i) = \exp(-\kappa(\varphi(\tau / \kappa) - \varphi(x_i)))$ (Jiang, Kulis, and Jordan 2012). Since $\varphi(x_i)$ and $A(\tilde{\phi}, \tau, \kappa, \beta) (x_i)$ do not scale with $\beta$, we have

$$I_1 = f_\beta(x_i) g_\beta \left( \frac{\tau}{\beta}, \frac{\kappa}{\beta} \right) (2\pi\beta)^{1/2} \cdot C_1(x_i),$$

(26)

as $\beta \to \infty$, where $C_1(\cdot)$ is a function independent of $\beta$.

The integral $I_2$ can be analyzed similarly via the Laplace’s method. Let $L(\eta) = 2c(l - y_i \eta^T x_i)_+ + \frac{\nu^2}{2\beta'}$ be the hinge loss and regularization term induced by the classifier $\eta$. Then we have $I_2 = \int \left( 2\pi \nu^2 / \beta' \right)^{-d/2} \exp(-\beta^2 L(\eta) / \beta^2) \cdot \exp(-\beta^2 L(\eta^*) / \beta^2) \cdot \exp(-\beta^2 L(\eta^*) / \beta^2) \cdot C_2(x_i) d\eta$. Thus, we can compute $\eta^*$ for each instance $x_i$ in a constant time. Finally, the above analysis can be generalized to multi-classification. See Appendix C for details.
Algorithm 1 The M$^2$DPM algorithm

Initialize: $z^{(0)}, \mu^{(0)}, \eta^{(0)}, \omega^{(0)}; g \leftarrow 0.$
repeat
\begin{itemize}
  \item For each instance $i$: $z_i^{(g+1)} \leftarrow \arg\min_k Q_i(k).
  \item For each cluster $k$: $\mu_k^{(g+1)} \leftarrow (\sum_i \delta_{z_i,k} x_i) / (\sum_i \delta_{z_i,k}).$
  \item For each instance $i$: $\omega_i^{(g+1)} \leftarrow c \cdot |\zeta_i|.$
  \item For each cluster $k$: $\eta_k^{(g+1)} \leftarrow \lambda_k.$
\end{itemize}
Update: $g \leftarrow g + 1.$
until converge

Asymptotics of the posterior distribution

We now perform SVA analysis to posterior in Eq. (11) directly and derive an optimization objective. The analysis is based on the fact that the CRP prior can be written as an exchangeable partition probability function (Pitman 1995; Aldous 1985):
\begin{equation}
p_0(z|\alpha) = \alpha^{K-1} \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha+n)} \prod_{k=1}^K (n_k - 1)!, \tag{33}
\end{equation}
where $K$ is the number of nonempty clusters. Since $\Gamma(\alpha+1)/\Gamma(\alpha+n)$ only depends on $D$, the posterior (11) can be written as
\begin{equation}
q(\Theta) \propto \alpha^{K-1} \psi(n) \prod_{k=1}^K p(\mu_k, \eta_k) \prod_{i=1}^n p(x_i | \mu_k) \phi(y_i | z_i, \eta),
\end{equation}
where $\psi(n) := \prod_{k=1}^K (n_k - 1)!$. Scaling $\theta$, $c$ and $\nu^2$ by putting $\hat{\theta} = \beta \theta$, $\hat{\nu^2} = \nu^2 / \beta^2$ and $\beta = \beta'$, the posterior $q(\Theta)$ becomes
\begin{equation}
q(\Theta | \beta) \propto \alpha^K \psi(n) \left( \frac{\tau}{\beta} \right)^{K} \prod_{i=1}^n f_{\beta}(x_i) \cdot \exp \left( -\beta' \mathcal{L}(z, \mu, \eta) - \sum_{k=1}^K \kappa D_{\beta'} \left( \frac{\tau}{\beta}, \mu_k \right) \right),
\end{equation}
where $\mathcal{L}(z, \mu, \eta) = \sum_{k=1}^K \|y_i - \mu_k\|^2_{2p} + 2c \sum_{i=1}^n (\zeta_i^2) + s \sum_{i=1}^n D_{\beta'}(x_i, \mu_k)$. Assuming the scaling of the concentration parameter $\alpha$ in Eq. (30) and noting the fact that $f_{\beta}(x_i)$ only depends on data $x_i$, the posterior distribution (34) then concentrate on the values of $z, \mu, \eta$ that minimize the loss function in Eq. (35) when $\beta$ and $\beta'$ approach infinity$^2$:
\begin{equation}
\mathcal{L}^\nu(z, \mu, \eta) = \mathcal{L}(z, \mu, \eta) + \lambda \cdot K. \tag{35}
\end{equation}

Theorem 1 (with a proof in Appendix B) characterizes the consistency between Alg. 1 and the objective in Eq. (35). Specifically, it states that each iteration of Alg. 1 decreases the loss function in Eq. (35) monotonically. This consistency is desirable, as we are adopting the same set of scaling assumptions in small-variance asymptotic analysis on both the Gibbs sampler and the posterior distribution.

**Theorem 1.** Let $\mathcal{L}^\nu(z, \mu, \eta)$ be the loss function defined in Eq. (35). After each iteration of Algorithm 1, we have
\begin{equation}
\mathcal{L}^\nu(z^{(g+1)}, \mu^{(g+1)}, \eta^{(g+1)}) \leq \mathcal{L}^\nu(z^{(g)}, \mu^{(g)}, \eta^{(g)}). \tag{36}
\end{equation}

Experiments

Results on synthetic datasets

We first compare M$^2$DPM with various competitors on synthetic data generated under 2 settings. For each setting, we generate 20 datasets at random and report the average accuracy and running time. In each dataset, we randomly pick 80% instances for training and use the rest 20% for testing. Hyper-parameters are determined by 5-fold cross-validation on training data. The algorithm terminates when the relative change of the loss function is less than $\epsilon = 10^{-3}$.

**Setting I:** we first assign each of the 1,000 instances to a cluster according to a CRP with the concentration parameter $\alpha = 1$. For each instance in cluster $k$, we then sample its 10-dimensional feature vector from a Gaussian distribution $N(\mu_k, \sigma^2 I_d)$, where we set $\sigma = 0.5$ and $\mu_k = (k, \cdots, k)^T$. Note that the instances from different clusters may overlap due to the random samples from Gaussian distributions. The maximum number of clusters is 10. For each cluster $k$, we sample a linear classifier $\eta_k$ from a Gaussian distribution $N(0, I_d)$. We sample binary labels from a Bernoulli model $p(y_i = 1 | x_i, \eta) = \text{Sigmoid}(\eta_k^T (x_i - \mu_k))$.

**Setting II:** we uniformly divide 10,000 10-dimensional instances into 10 clusters. For each cluster $k$, values of each feature are sampled from a uniform distribution $U[k - 0.5, k + 0.5]$, and a linear classifier is generated as in Setting I. The true labels are sampled from the same Bernoulli model as in Eq. (37). Note that the clusters are disjoint.

Table 1 shows the average accuracy and running time of M$^2$DPM (std in parentheses), compared to Gibbs iSVM$^3$, dpMNL (Shahbaba and Neal 2009) and other baseline algorithms. We also compare with a pipeline algorithm that first uses DP-means to cluster the data and then trains an SVM classifier for each cluster. The results show that M$^2$DPM achieves comparable performance with the best methods in both settings, while requires much less running time than other sampling methods (e.g. dpMNL, Gibbs-iSVM) and kernel SVMs (e.g. RBF-SVM) when the data size is large.

Though RBF-SVM has slightly higher accuracy in Setting II, M$^2$DPM has the advantage of identifying latent cluster structures. As a nonparametric method, M$^2$DPM can infer the number of clusters adaptively. Table 2 illustrates how the number of clusters is automatically resolved from...
datasets with different sizes. Here, we generated 10,000 10-dimensional instances from a DP mixture and used the first \( n_0 \) ones as training data for each run of \( M^2DPM \), under the same set of hyper-parameters. Note that the first \( n_0 \) instances may belong to fewer latent clusters due to the nature of DP. We can see that \( M^2DPM \) gave quite accurate predictions of the number of latent clusters and it can adapt to datasets with different sizes very well. Table 2 also shows that the running time of \( M^2DPM \) scales near linearly with respect to the data size, a desirable property for learning on large datasets.

### Results on Real Datasets

#### Protein Fold Classification

The first real dataset was created in (Ding and Dubchak 2001) for protein fold classification. It consists of 698 samples, each classified into one of the 27 different 3-d folding patterns. Each sample is represented by its percentage composition of 20 amino acids as well as its length of the protein sequence. Our objective is to classify data samples into one of the 27 classes given these types of features. We follow the previous setup that uses 313 samples as training data and the remaining 385 as testing data. The classification accuracy, \( F_1 \) scores and running time are reported in Table 3. We select the hyper-parameters of \( M^2DPM \) by a 5-fold cross-validation on the training set.

We can see that our method outperforms all the other algorithms except dpMNL and Gibbs-iSVM, in terms of both accuracy and \( F_1 \) scores. Though dpMNL and Gibbs-iSVM give better accuracy, they require significantly longer time to train and predict. This demonstrates that our algorithm can perform training and predicting with extraordinarily fast speed while still maintaining adequate performance.

#### Detecting Parkinson’s Disease

The second real dataset is described in (Little et al. 2009) for detecting Parkinson’s disease. It consists of 195 instances (i.e., patients), each associated with 22 real-valued features and a binary label indicating whether the patient has Parkinson’s disease. We follow the previous setup (i.e., performing 5-fold cross-validation) and compare with the results reported in (Shahbaba and Neal 2009) in Table 4. The results are reported using hyper-parameters \( \lambda = 150, s = 0.01, \nu = 1 \) and \( c = 2.5 \), which were selected by a 5-fold cross-validation performed on the data set. The results show that our method achieves comparable performance compared to the best competitors while requires much less running time.

Apart from having good accuracy, \( M^2DPM \) is also able to cluster patients into several groups that have different characteristics. Our algorithm divides patients into five groups, and Table 5 shows average ages and disease stages of the five groups. Note that the age and disease stage information are not contained in the original dataset and are cited from Table 1 in (Little et al. 2009). It is clear that patients in the 4-th group are senior than patients in the other groups, and are in more serious conditions in terms of disease stages.

### Conclusions

We present max-margin DP-means (\( M^2DPM \)), an efficient algorithm for both clustering and classification, with the number of clusters automatically resolved from data. \( M^2DPM \) was developed by performing small-variance asymptotic analysis to a Gibbs sampler of DP mixtures of SVMs. By exploring the similar analysis, we show that \( M^2DPM \) monotonically minimizes an objective function. Experiments on synthetic and real-world datasets demonstrate that \( M^2DPM \) runs much faster than various competitors while still maintaining accurate predictions.
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