DETAILED DERIVATIONS OF SMALL-VARIANCE ASYMPTOTICS FOR SOME HIERARCHICAL BAYESIAN NONPARAMETRIC MODELS

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Abstract. In this note we provide detailed derivations of two versions of small-variance asymptotics for hierarchical Dirichlet process (HDP) mixture models and the HDP hidden Markov model (HDP-HMM, a.k.a. the infinite HMM). We include derivations for the probabilities of certain CRP and CRF partitions, which are of more general interest.

1. Introduction

Numerous flexible Bayesian nonparametric models and associated inference algorithms have been developed in recent years for solving problems such as clustering and time series analysis. However, simpler approaches such as $k$-means remain extremely popular due to their simplicity and scalability to the large-data setting.

The $k$-means optimization problem can be viewed as the small-variance limit of MAP inference in a $k$-component Gaussian mixture model. That is, with observed data $X = (x_n)_{n=1}^N, x_n \in \mathbb{R}^D$, the Gaussian mixture model log joint density with means $\mu_1, \ldots, \mu_n \in \mathbb{R}^D$, cluster assignments $Z = (z_n)_{n=1}^N$ with $z_n \in \{1, 2, \ldots, K\}$, and spherical variance $\sigma^2$ is

$$
\log p(\mu, Z, X) = \log p(\mu)p(Z) - \frac{1}{2}ND \log 2\pi \sigma^2 - \frac{1}{2}\sum_{n=1}^N \|x_n - \mu_{z_n}\|^2 - \omega(\beta),
$$

where $\beta \triangleq \frac{1}{2\sigma^2}$. As $\sigma^2 \rightarrow 0$, or equivalently $\beta \rightarrow \infty$, the term that is linear in $\beta$ dominates and the MAP problem becomes the $k$-means problem in the sense that

$$
\lim_{\sigma^2 \rightarrow 0} \arg \max_{\beta \rightarrow \infty} \log p(\mu, Z, X)' = \lim_{\beta \rightarrow \infty} \arg \min_{Z, \mu} \beta \sum_{n=1}^N \|x_n - \mu_{z_n}\|^2 + \omega(\beta)
$$

$$
= \arg \min_{Z, \mu} \sum_{n=1}^N \|x_n - \mu_{z_n}\|^2.
$$

Note that we have assumed the priors $p(Z)$ and $p(\mu)$ are positive and independent of $\sigma^2$.

Recently developed small-variance asymptotics (SVA) methods generalize the above derivation of $k$-means to other Bayesian models, with nonparametric Bayesian models such as those based on the Dirichlet process (DP) and the Indian buffet process being of particular interest. While obtaining $k$-means from the Gaussian mixture model is straightforward, the SVA derivations for nonparametric models can be quite subtle, especially for hierarchical models. Indeed, we are not
aware of a reference with the derivations for many important DP and hierarchical DP (HDP) probability expressions. This note is meant to serve as a self-contained reference to some DP and HDP material of general interest as well as SVA derivations for HDP-based models. In particular, we provide derivations for the HDP mixture model and the HDP-HMM (a.k.a. the iHMM).

A Caution. This note is not meant to serve as an introduction to SVA methods or Bayesian nonparametric modeling tools. Thus, we assume the reader is familiar with the MAD-Bayes approach to SVA [4] and scaled exponential family distributions [3]. We also assume basic familiarity with the Chinese restaurant process (CRP) and Chinese restaurant franchise (CRF) representations of, respectively, the DP and the HDP [1, 8].

2. Preliminaries

2.1. Notation. For an arbitrary real-valued vector \( v \in \mathbb{R}^D \) and indices \( 1 \leq i \leq j \leq D \), let \( v_{i:j} \triangleq (v_i, v_{i+1}, \ldots, v_j) \), \( \bar{v}_j \triangleq \sum_{i=1}^j v_i \), and \( v_\cdot \triangleq \bar{v}_D \); we extend the range and dot notations in the obvious way to matrices and tensors. By convention \( \prod_\emptyset = 1 \) and \( \sum_\emptyset = 0 \).

2.2. Dirichlet process, Chinese restaurants, and all that. Recall that for a CRP with concentration parameter \( \kappa \), given that there are \( c \) observations, the probability of observing \( L \) tables with counts \( c_1, \ldots, c_L \) is:

\[
\mathbb{P}_{\text{CRP}}(c) = \prod_{\ell=1}^L \frac{\kappa \cdot c_\ell!}{\Gamma(\kappa + \ell)} = \frac{\kappa^L \Gamma(\kappa)}{\Gamma(\kappa + c)} \prod_{\ell=1}^L c_\ell! \tag{3}
\]

\[
= \frac{\kappa^{L-1} \Gamma(\kappa + 1)}{\Gamma(\kappa + c)} \prod_{\ell=1}^L c_\ell!, \tag{4}
\]

where we have used the exchangeability of the CRP.

For a CRF with concentration parameters \( \kappa \) and \( \alpha \) and \( c \) observations, let \( K \) be the number of tables in the top-level restaurant, let \( N \) be the number of franchises, let \( t_{ij} \) be the number of tables in restaurant franchise \( i \) serving dish \( j \), and let \( c_{ijt} \) be the number of customers at the \( t \)-th table serving dish \( j \) in restaurant \( i \). For the top-level restaurant, the “customer” counts are \((t_i)\), and for \( i \)-th franchise, the customer counts are \((c_{i,j})\). Hence, repeatedly using Eq. (5), we have

\[
\mathbb{P}_{\text{CRF}}(t, c | \alpha, \kappa)
= \frac{\kappa^{K-1} \Gamma(\kappa + 1)}{\Gamma(\kappa + t)} \prod_{j=1}^K \alpha^{t_j} \prod_{i=1}^N \frac{\alpha^{t_j - 1} \Gamma(\alpha + 1)}{\Gamma(\alpha + c_{ij})} \prod_{j=1}^K \prod_{t=1}^{t_{ij}} c_{ijt}! \tag{6}
\]

We can integrate over all possible seating arrangements for the customers in the franchises. That is, if \( C_{ij} = c_{ij} \) is the number of customers eating dish \( j \) at
restaurant $i$, then
\[
P_{C_{RF}}(t, C | \alpha, \kappa) = \frac{\kappa^{K-1} \Gamma(k+1)}{\Gamma(k+t_i)} \prod_{j=1}^{K} t_j^{-1} \prod_{i=1}^{N} \left( \frac{\alpha_i^{t_i} - 1 \Gamma(\alpha + 1)}{\Gamma(\alpha + C_i)} \prod_{j=1}^{K} \left[ C_{ij} \right] \right),
\]
where $\left[ C_{ij} \right]$ is an unsigned Stirling number of the first kind \( \mathbb{G} \), which can be interpreted as the number of ways to seat $C_{ij}$ customers at $t_{ij}$ tables such that each table has at least one customer (more formally, the number of permutations of $C_{ij}$ objects with $t_{ij}$ disjoint cycles).

3. SVA FOR HDP MIXTURE MODELS

The generative model for the HDP \[ \text{[8]} \] with $N$ groups and $J_i$ Gaussian observations in group $i$ is:
\[
\begin{align*}
\beta & \sim \text{GEM}(\gamma) \\
\pi_i & \sim \mathcal{DP}() \alpha \beta, \quad i \geq 1 \\
\mu_k & \sim \mathcal{N}(0, \sigma_k^2), \quad k \geq 1 \\
z_{ij} & \sim \text{Multi}(\pi_i), \quad j, i \geq 1 \\
y_{ij} | z_{ij} & \sim \mathcal{N}(\mu_{z_{ij}}, \sigma^2), \quad j, i \geq 1,
\end{align*}
\]
Here $\text{GEM}(\gamma)$ is the stick-breaking prior with concentration parameter $\gamma$ \[ \mathbb{G} \] and $y_{ij}$ is the $j^{th}$ observation in the $i^{th}$ group. Let $Z_i \triangleq (z_{ij})_{j=1}^{J_i}$, $Y_i \triangleq (y_{ij})_{j=1}^{J_i}$, and $K \triangleq \max z_{ij}$. For the joint density of the HDP we have:
\[
\mathbb{P}(Z_{1:N}, Y_{1:N}, \mu_{1:N}, \pi_{1:N, 1:K}, \beta_{1:K} | \sigma_0, \sigma, \alpha, \gamma)
= \mathbb{P}(Z_{1:N}, \beta_{1:K}, \pi_{1:N, 1:K} | \alpha, \gamma) \prod_{k=1}^{K} \prod_{i:j,z_{ij}=k} \mathbb{N}(y_{ij} | \mu_k, \sigma^2) \prod_{k=1}^{K} \mathbb{N}(\mu_k | 0, \sigma_0^2),
\]
where
\[
\mathbb{P}(Z_{1:N}, \beta_{1:K}, \pi_{1:N, 1:K} | \alpha, \gamma)
\triangleq \text{GEM}(\beta_{1:K}; \gamma) \prod_{i=1}^{N} \mathcal{DP}(\pi_{i,1:K}; \alpha \beta_{1:K}) \prod_{i=1}^{N} \prod_{j=1}^{J_i} \text{Multi}(z_{ij}; \pi_{i,1:K}).
\]
Integrating out $\beta_{1:K}$ and $\pi_{1:N}$, we obtain the CRF representation in Eq. \[ \text{[7]} \] :
\[
P(t, Z_{1:N} | \alpha, \gamma) = \frac{\gamma^{K-1} \Gamma(\gamma + 1)}{\Gamma(\gamma + t_i)} \prod_{j=1}^{K} t_j^{-1} \prod_{i=1}^{N} \left( \frac{\alpha_i^{t_i} \Gamma(\alpha + 1)}{\Gamma(\alpha + z_{ij})} \prod_{j=1}^{K} \left[ z_{ij} \right] \right),
\]
As in the introduction, define $\beta = \frac{1}{2\sigma^2}$, so we are interested in the limit $\beta \rightarrow \infty$ (i.e., $\sigma^2 \rightarrow 0$). To maintain the effects of the hyperparameters in the small-variance limit, we set $\gamma = \exp(-\lambda_1 \beta)$ and $\alpha = \exp(-\lambda_2 \beta)$, where $\lambda_1 > 0$ and $\lambda_2 > 0$ are free
parameters. Taking the logarithm of Eq. (7), we obtain
\[
\log p(t, Z_{1:N} | \alpha, \gamma) = (K - 1) \log \gamma + \log \Gamma(\gamma + 1) + \sum_{j=1}^{K} \log t_{-j}!
\]
\[
+ \sum_{i=1}^{N} \left\{ (t_i - 1) \log \alpha + \log \Gamma(\alpha + 1) + \sum_{j=1}^{K} \log \left[ z_{ij} \right] \right\}
\]
\[
= -\beta \lambda_1 (K - 1) + \text{O}(1) - N \sum_{i=1}^{N} \left\{ \beta \lambda_2 (t_i - 1) + \text{O}(1) \right\}.
\]
(17)

If \( m_i \triangleq \# \{ z_{ij} \}_{j=1}^{L_i} \) is the number of distinct indices in \( Z_i \), then
\[
\max_{t \sim Z_{1:T}} -\lambda_1 (K - 1) - \lambda_2 \sum_{i=1}^{K} (t_i - 1) = -\lambda_1 (K - 1) - \lambda_2 \sum_{i=1}^{K} (m_i - 1),
\]
(18)
where \( t \sim Z_{1:T} \) denotes that \( t \) is consistent with \( Z_{1:T} \). Hence, after setting the variance of \( \mu_k \) to be \( \sigma_0^2 = \sigma^2 / \lambda_3 \), where \( \lambda_3 \geq 0 \) is a free parameter, the SVA objective function for the HDP mixture model is
\[
\min_{K, Z, \mu} \left\{ \sum_{k=1}^{K} \sum_{i:j \mid z_{ij} = k} \| y_{ij} - \mu_k \|^2 + \lambda_1 (K - 1) + \lambda_2 \sum_{i=1}^{N} (m_i - 1) + \lambda_3 \sum_{k=1}^{K} \| \mu_k \|^2 \right\}.
\]
(19)

This cost function is in fact the \( k \)-means objective function with some additional penalty terms. The second and third terms in Eq. (19) penalize the number of global and local clusters, respectively. The final term introduces the additional cost for the prior over the cluster means.

4. SVA FOR THE HDP-HMM

The HDP-HMM generative model with Gaussian observations is [9]:
\[
\beta \sim \text{GEM}(\gamma)
\]
(20)
\[
\pi_k \sim \text{DP}(\alpha \beta), \quad k \geq 1
\]
(21)
\[
\mu_k \sim N(0, \sigma_0^2), \quad k \geq 1
\]
(22)
\[
\begin{align*}
\gamma_{t-1} | \gamma_{t-1} & \sim \text{Multi}(\pi_{\gamma_{t-1}}), \quad t \geq 2 \\
y_t | \gamma_t & \sim N(\mu_{\gamma_t}, \sigma^2), \quad t \geq 1,
\end{align*}
\]
(23)
(24)
with \( z_1 \triangleq 1 \). Let \( Z \triangleq (z_{i,t})_{t=1}^{T} \), \( Y \triangleq (y_{i,t})_{t=1}^{T} \), and \( K \triangleq \max_{t=1,...,T} z_t \). The joint density of the model is
\[
\begin{align*}
P(Z, Y, \mu_{1:K}, \pi_{1:K,1:K}, \beta_{1:K} | \sigma_0, \sigma, \alpha, \gamma) \\
= P(Z, \beta_{1:K}, \pi_{1:K,1:K} | \alpha, \gamma) \prod_{t=1}^{T} N(y_t | \mu_{z_t}, \sigma^2) \prod_{k=1}^{K} N(\mu_k | 0, \sigma_0^2),
\end{align*}
\]
(25)
where
\[
P(Z, \beta_{1:K}, \pi_{1:K,1:K} \mid \alpha, \gamma) = GEM(\beta_{1:K}; \gamma) \prod_k \mathcal{D} \mathcal{P}(\pi_{k,1:K} \mid \alpha \beta_{1:K}) \prod_{t=1}^T \text{Mult}(z_t; \pi_{z_{t-1},1:K}).
\] (26)

We consider two approaches to obtaining the SVA for the HDP-HMM. The first is a “combinatorial” approach, in which we integrate out $\beta_{1:K}$ and $\pi_{1:K,1:K}$. The second is a “direct” approach, in which we do not integrate out $\beta_{1:K}$ and $\pi_{1:K,1:K}$.

4.1. Combinatorial Approach. By integrating out $\beta_{1:K}$ and $\pi_{1:K,1:K}$, we obtain the CRF representation, which is the same urn scheme representation used in the original iHMM paper \cite{3,8}. The development is exactly the same as the HDP mixture model case, see Eqs. (15) to (17). As before $\beta = \frac{\lambda t}{2\beta^2}$, $\gamma = \exp(-\lambda_1 \beta)$, and $\alpha = \exp(-\lambda_2 \beta)$, where $\lambda_1$ and $\lambda_2$ are free parameters:

\[
\log P(t, Z \mid \alpha, \gamma) = -\beta \lambda_1 (K - 1) - \beta \lambda_2 \sum_{i=1}^K (t_i - 1) + O(1).
\] (27)

If $s_i$ is the number of distinct transitions out of state $i$, then

\[
\max_{t \mid t \sim Z} -\lambda_1 (K - 1) - \lambda_2 \sum_{i=1}^K (t_i - 1) = -\lambda_1 (K - 1) - \lambda_2 \sum_{i=1}^K (s_i - 1).
\] (28)

If we use the free parameter $\lambda_3$ introduced in Section \cite{3} then the SVA optimization problem for the HDP-HMM is

\[
\min_{K, Z, \mu} \left\{ \sum_{t=1}^T \| y_t - \mu_{z_t} \|^2 + \lambda_1 (K - 1) + \lambda_2 \sum_{i=1}^K (s_i - 1) + \lambda_3 \sum_{i=1}^K \| \mu_i \|^2 \right\}.
\] (29)

In this cost function, the $\lambda_1$ term adds the cost for the total number of states and $\lambda_2$ term penalizes the total number of distinct transitions out of the states. As in Eq. \cite{19}, the last term represents the cost corresponding to the prior over the means of the states.

4.2. Direct Approach. Alternatively, we can choose not to integrate out $\beta_{1:K}$ and $\pi_{1:K,1:K}$. If we let $\beta_{K+1} = \frac{1}{1 - \beta_K}$ and $\pi_{i,K+1} = \frac{1 - \pi_i}{1 - \pi_{K+1}}$, then

\[
P(Z, \beta_{1:K}, \pi_{1:K,1:K} \mid \alpha, \gamma) = \prod_{i=1}^K \text{Beta} \left( \frac{\beta_i}{1 - \beta_{i-1}}, 1, \gamma \right) \text{Dir}(\pi_{i,1:K+1} \mid \alpha \beta_{1:K+1}) \prod_{t=2}^T \pi_{z_{t-1},z_t}
\]

\[
= \prod_{i=1}^K \left\{ \frac{\Gamma(1 + \gamma)}{\Gamma(\gamma)} \left( \frac{1 - \beta_i}{1 - \beta_{i-1}} \right) \gamma^{-1} \Gamma(\alpha) \prod_{j=1}^{K+1} \frac{\alpha^2}{\Gamma(\alpha \beta_j)} \right\} \prod_{t=2}^T \pi_{z_{t-1},z_t}.
\] (30)
Let $\gamma = \exp(-\lambda_1 \beta)$ and $\alpha = \lambda_2 \beta$. Taking the logarithm of the product from $i = 1$ to $K$ yields
\[
\sum_{i=1}^{K} \left\{ -\log \Gamma(\gamma) + \alpha \log \alpha - \alpha + o(\beta) \right. \\
+ \sum_{j=1}^{K+1} \left\{ -\alpha \beta_j \log(\alpha \beta_j) + \alpha \beta_j + \alpha \beta_j \log \pi_{ij} + o(\beta) \right\} \\
= \beta \sum_{i=1}^{K} \left\{ -\lambda_1 + \sum_{j=1}^{K+1} \{-\lambda_2 \beta_j \log(\beta_j) + \lambda_2 \beta_j \log \pi_{ij} \} + o(\beta) \right. \\
\left. \right\} + o(\beta). 
\]
(31)
\[
= -\beta \left\{ \lambda_1 K + \lambda_2 \sum_{i=1}^{K} \text{KL}(\beta_{1:K+1} || \pi_{i,1:K+1}) \right\} + o(\beta). 
\]
(32)

Here we have used the asymptotic expansions of $\log \Gamma(z)$:
\[
\log \Gamma(z) = z \log z - z + o(z), \quad z \to \infty
\]
(34)
\[
\log \Gamma(z) = -\log z + O(z), \quad z \downarrow 0.
\]
(35)

Hence, the SVA minimization problem for the HDP-HMM is:
\[
\min_{K,z,\beta,\pi} \left\{ \sum_{t=1}^{T} \| y_t - \mu_{z_t} \|^2 - \zeta \sum_{i=2}^{T} \log \pi_{z_{t-1},z_{t}} \\
+ \lambda_1 K + \lambda_2 \sum_{i=1}^{K} \text{KL}(\beta_{1:K+1} || \pi_{i,1:K+1}) + \lambda_3 \sum_{i=1}^{K} \| \mu_i \|^2 \right\}.
\]
(36)

Compared to Eq. (29), the main difference is in the terms involving hyperparameters $\zeta$ and $\lambda_2$. In this cost function, the $\zeta$ term penalizes transition probabilities very close to zero. The KL divergence term between $\beta_{1:K+1}$ and $\pi_{i,1:K+1}$ is due to the hierarchical structure of the prior and it biases the transition probabilities $\pi_{i,1:K+1}$ to be similar to the prior $\beta_{1:K+1}$.

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