# GURLS\_mkl: A PFBS-based Implementation for Multiple Kernel Learning

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#### 1 Introduction

#### 2 Hierarchical Dirichlet Process

## **A Hierarchical Dirichlet Process**

#### A.1 Model

Classic view:

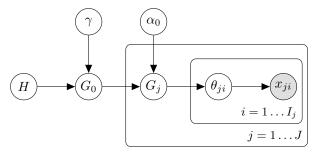
$$\begin{aligned} G_0|\gamma, H &\sim DP(\gamma, H) \\ G_j|\alpha_0, G_0 &\sim DP(\alpha_0, G_0) \\ \theta_{ji}|G_j &\sim G_j \\ x_{ji}|\theta_{ji} &\sim F(\theta_{ji}) \end{aligned}$$

where  $P \sim DP(\alpha,G)$  adopts the stick breaking representation w.p. 1:

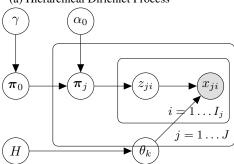
$$P = \sum_{k=1}^{\infty} \pi_k \delta_{\phi_k} \qquad \text{where:} \qquad \pi_k \sim GEM(\alpha), \quad \phi_k \sim G$$

Alternatively, one may describe the generative processes of  $\pi_k$  and  $\theta_k$  separately as:

$$\begin{aligned} & \boldsymbol{\pi}_0 | \boldsymbol{\gamma} & \sim GEM(\boldsymbol{\gamma}) & \boldsymbol{\theta}_k | \boldsymbol{H} \sim \boldsymbol{H} \\ & \boldsymbol{\pi}_j | \boldsymbol{\alpha}_0, \boldsymbol{\pi}_0 & \sim DP(\boldsymbol{\alpha}_0, \boldsymbol{\pi}_0) & & \\ & z_{ji} | \boldsymbol{\pi}_j & \sim \boldsymbol{\pi}_j \\ & x_{ji} | z_{ji}, (\boldsymbol{\theta}_k)_{k=1}^{\infty} \sim F(\boldsymbol{\theta}_{z_{ji}}) & & \end{aligned}$$



(a) Hierarchical Dirichlet Process



(b) Hierarchical Dirichlet Process

Figure 1: Hierarchical Dirichlet Process

## A.2 Inference

Assuming conjugacy between H and  $F^{-1}$  and holding  $(\gamma, \alpha_0)$  fixed,

<sup>&</sup>lt;sup>1</sup>so we can integrate out the mixture component parameters

we now describe a simplied Gibbs approach to sample parameters  $(z_{ji}, m_{jk}, \pi_0)$  from the Chinese Restaurant Franchise (see Appendix C) representation of the posterior, where the parameter  $z_{ji}$  are referred to respectively as customer-specific dish assignment,  $m_{jk}$  as dish-specific table count, and  $\pi_0$  as global dish distribution. This particular method is referred to as "direct assignment" in Teh et al. [2006] since it circumvented the issue of bookkeeping for every  $t_{ij}$  (customer-specific table assignment) and  $k_{jt}$  (table-specific dish assignment) variables

In each Gibbs iteration, denote  $f_k^{-x_{ji}}(x_{ji}) = \frac{\int f(\mathbf{x}|\theta_k)h(\theta_k)d_{\theta_k}}{\int f(\mathbf{x}_{-(ji)}|\theta_k)h(\theta_k)d_{\theta_k}}$  the conditional distribution  $x_{ji}|\mathbf{x}_{-(ji)}$  under  $\theta = \theta_k$ , and assume there are currently K dishes and T tables, we sample  $(z_{ji}, m_{jk}, \pi_0)$  iteratively as:

1. Sample  $z_{ji} = k | \mathbf{z}_{-(ji)}, \mathbf{m}, \boldsymbol{\pi}_0$  from the distribution:

$$z_{ji} = k | \mathbf{z}_{-(ji)}, \mathbf{m}, \boldsymbol{\pi}_0 \propto \begin{cases} f_k^{-x_{ji}}(x_{ji}) * (n_{jk}^{-(ji)} + \alpha_0 \pi_{0,k}) & k \leq K \\ f_{K+1}^{-x_{ji}}(x_{ji}) * \alpha_0 \pi_{0,u} & k = K+1 \end{cases}$$

2. Sample  $m_{jk} = m|\mathbf{z}, \mathbf{m}_{-(jk)}, \boldsymbol{\pi}_0$ , by setting  $m_{jk} = \sum_i I(t_{ji} = t_{new}|k_{jt_{new}} = k)$ , we can sample  $t_{ji}$  from:

$$t_{ji} = t | k_{jt} = k, \mathbf{t}_{-(ji)}, \boldsymbol{\pi}_0 \propto \begin{cases} n_{jt}^{-(ji)} & t \le T \\ \alpha_0 \boldsymbol{\pi}_{0,k} & t = T+1 \end{cases}$$

and as in Fox [2009], sample  $I(t_{ji}=t_{new}|k_{jt_{new}}=k)$  directly from:

$$Bern\Big(\frac{\alpha_0\pi_{0,k}}{n_{ik}+\alpha_0\pi_{0,k}}\Big)$$

3. Sample  $\pi_0$  from distribution:

$$\boldsymbol{\pi}_0 \sim Dir(m_1, \dots, m_K, \gamma)$$

#### Algorithm 1 HDP, Gibbs Sampler through Direct Assignment

```
1: procedure hdp_gibbs_ds(\mathbf{K}, \mathbf{y}, (\tau, \mu, \sigma))
2: \boldsymbol{\alpha}^0 = \mathbf{0}
3: for p = 1 to MAX_ITER do
4: \boldsymbol{\alpha}_0^p = (1 - \frac{\mu}{\sigma})\boldsymbol{\alpha}^{p-1} - \frac{1}{\sigma n}(\mathbf{K}\boldsymbol{\alpha}^{p-1} - \mathbf{y})
5: \boldsymbol{\alpha}^p = \mathbf{S}_{\frac{\tau}{\sigma}}(K, \boldsymbol{\alpha}_0^p)
6: end for
7: return f^{\text{MAX_ITER}} = (\boldsymbol{\alpha}^{\text{MAX_ITER}})^T \mathbf{k}
8: end procedure
```

## A.3 Application: Clustering Hierarchical Gaussian Data

Consider mixture of Gaussian data  $\mathbf{x} = \{\mathbf{x}_1, \dots, \mathbf{x}_K\}$  with  $\mathbf{x}_k \stackrel{iid}{\sim} MVN(\boldsymbol{\theta}_{k,2\times 1}, \mathbf{I}_{2\times 2})$  with unknown mean  $\boldsymbol{\theta}$ . Assuming diffused Gaussian prior  $\boldsymbol{\theta} \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$ , the form of likelihood F and base measure H are:

$$f(x_{ji}|\boldsymbol{\theta}_k) \propto exp(-\frac{1}{2\sigma^2}(x_{ji} - \boldsymbol{\theta}_k)^T(x_{ji} - \boldsymbol{\theta}_k))$$
$$h(\boldsymbol{\theta}_k) \propto exp(-\frac{1}{2\sigma_0^2}\boldsymbol{\theta}_k^T\boldsymbol{\theta}_k)$$

Then  $f_k^{-x_{ji}}(x_{ji})$  should be:

$$f_k^{-x_{ji}}(x_{ji}) \sim N(\frac{n_k^{-(ji)}\sigma_0^2}{n_k^{-(ji)}\sigma_0^2 + \sigma^2}\bar{\mathbf{x}}_k^{-(ji)}, (1 + \frac{\sigma_0^2}{n_k^{-(ji)}\sigma_0^2 + \sigma^2})\mathbf{I})$$

#### **B** HDP for Hidden Markov Model

#### **B.1** Hidden Markov Model

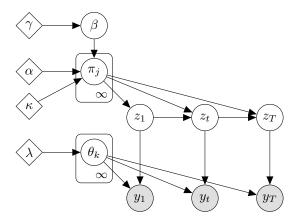


Figure 2: Hidden Markov Model

$$\beta|\gamma \sim GEM(\gamma)$$

$$\pi_{j}|\beta,\alpha \sim DP(\alpha,\beta)$$

$$\theta_{k}|H,\lambda \sim H(\lambda)$$

$$z_{t}|z_{t-1},\boldsymbol{\pi} \sim \pi_{z_{t-1}}$$

$$y_{t}|z_{t},\boldsymbol{\theta} \sim F(\theta_{z_{t}})$$

$$f_k(y_t) = p(y_t|\boldsymbol{\theta}_{z_t})p(z_t|z_{t-1})$$

### **B.2** Sticky HDP

Though flexible, the fact that HDP-HMM is deploying  $\pi_k \sim DP(\alpha, \beta)$  leads to:

- 1. large posterior probability for unrealistically transition dynamics
- 2. once instantiated, the unrealistically transition dynamics will be reinforced by CRF

Sticky HDP address above issues by encouraging self-transition. More specifically, the base measure for  $\pi_k$  is augmented *a priori* from  $\beta$  to:

$$\pi_j \sim DP(\alpha + \kappa, \frac{\alpha\beta + \kappa\delta_j}{\alpha + \kappa})$$

#### **B.3** Inference

Inference for HMM with Sticky HDP prior follows the sticky extension of CRF. For a observation  $y_t$  at time t, "restaurant" corresponds to the state  $z_t$  that  $y_t$  is at, and dishes at restaurant  $z_t$  indicates the potential states that  $y_{t+1}$  can transit to. To improve mixing rate of state sequence  $\mathbf{z}$ , we deploy the blocked sampler which uses a weak limit approximation of the infinite-dimension DP prior. More specifically, we assume there are L states, and  $\beta$  and  $\pi$  follows:

$$\beta | \gamma \sim Dir(\frac{\gamma}{L}, \dots, \frac{\gamma}{L})$$
  
$$\pi_j | \alpha, \beta, \kappa \sim Dir(\alpha \beta_1, \dots, \alpha \beta_j + \kappa, \dots, \alpha \beta_L)$$

Define  $\theta_k$  as emission parameter for state k, we sample  $(\mathbf{z}, \mathbf{m}, \pi_0, \boldsymbol{\theta})$  as follows:

1. Sample  $z_t$  from the distribution:

$$z_t|\mathbf{z}_{-(ii)}, \mathbf{m}, \boldsymbol{\pi}_0, \boldsymbol{\theta} \sim f(z_t = k|\mathbf{y}, \mathbf{m}, \boldsymbol{\pi}_0, \boldsymbol{\theta})$$

where  $f(z_t = k|\mathbf{y})$  is calculated using the forward-backward message passing algorithm in B.3.1).

- 2. Sample  $m_{jk}$  through override correction:
  - (a) Sample  $m'_{jk} = \sum_{i} I(t_{ji} = t_{new} | k_{jt_{new}} = k)$ , where:

$$I(t_{ji} = t_{new} | k_{jt_{new}} = k) \sim Bern\left(\frac{\alpha \pi_{0,k} + \kappa \delta_j(k)}{n_{jk} + \alpha \pi_{0,k} + \kappa \delta_j(k)}\right)$$

(b) Sample override variable:

$$w_j \sim Binom\left(m'_{jj}, \frac{\kappa}{\kappa + \alpha \pi_{0,j}}\right)$$

(c) Finally calculate  $m_{jk}$  as:

$$m_{jk} = \begin{cases} m'_{ij} & j \neq k \\ m'_{ij} - w_j & j = k \end{cases}$$

3. Sample  $\pi_0$  from distribution:

$$\boldsymbol{\pi}_0 \sim Dir(\frac{\gamma}{L} + m_1, \dots, \frac{\gamma}{L} + m_K)$$

4. Sample  $\theta$  from distribution:

$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta}|\lambda, \mathbf{y})$$

#### **B.3.1** Forward-backward Message Passing

The forward-backward algorithm provide an efficient method for computing node marginals  $p(y_t)$ . Define:

Backward Message :  $\beta_t(z_t) = p(\mathbf{y}_{T>t}|z_t)$ Forward Message :  $\alpha_t(z_t) = p(\mathbf{y}_{T\leq t}, z_t)$ Joint Message :  $\alpha_t(z_t)\beta_t(z_t) = p(\mathbf{y}, z_t)$ 

which can be alternatively defined using message  $m_{t_1,t_2}$ 

Backward Message :  $\beta_t(z_t) = p(\mathbf{y}_{T>t}|z_t) = m_{t+1,t}(z_t)$ Forward Message :  $\alpha_t(z_t) = p(y_t|z_t)p(\mathbf{y}_{T< t}, z_t) = p(y_t|z_t)m_{t-1,t}(z_t)$ 

These two types of messages can be computed  $\beta_t$  backward and  $\alpha_t$  forward in time as:

$$\begin{split} \beta_{t-1} &= \sum_{z_t} p(y_t|z_t) \qquad p(z_t|z_{t-1})\beta_t(z_t) \qquad \text{with} \quad \beta_T(z_T) = 1 \\ \alpha_{t+1} &= \sum_{z_t} p(y_{t+1}|z_{t+1})p(z_{t+1}|z_t)\alpha_t(z_t) \qquad \text{with} \quad \alpha_1(z_1) = p(y_1,z_1) = p(y_1|z_1)\pi^0(z_1) \end{split}$$

Using the forward and backward messages, we can compute state assignment posterior as:

$$p(z_t|\mathbf{y}) = \frac{p(z_t, \mathbf{y})}{\sum_{z_t} p(z_t, \mathbf{y})} = \frac{\alpha_t(z_t)\beta_t(z_t) = p(\mathbf{y}, z_t)}{\sum_{z_t} \alpha_t(z_t)\beta_t(z_t) = p(\mathbf{y}, z_t)}$$

#### C Chinese Restaurant Franchise

A hierarchical analogy of Chinese Restaurant Process, the Chinese Restaurant Franchise offers a convenient scheme to sample from the posterior of cluster-specific  $\theta$ 's in HDP. This process draw below analogy:

- H as the dish distribution for all possible dishes in the world, with the types of possible dishes being  $(\theta_k)_{k=1}^{\infty}$ .
- $G_0 \sim DP(\gamma, H)$  as the dish distribution for the franchise
- $G_j \sim DP(\alpha_0, G_0)$  as the dish distribution for restaurant j in the franchise
- $\psi_{jt} \sim G_0$  as the dish served at table t in restaurant j.  $k_{jt} \sim \pi_0$  as the index of dish choice for this table.
- $\theta_{ji} \sim G_j$  as the dish will be enjoyed by customer i in restaurant j.  $t_{ji} \sim \pi_j$  as the index of table choice for this customer.

Integrating over  $G_j$ , the sampling scheme for subject-specific dish  $\theta_{ji} \sim G_j$  is:

$$\theta_{ji} | \boldsymbol{\theta}_{j(-i)}, \alpha_0, G_0 \sim \sum_{k=1}^{K} \frac{n_{jt.}}{\alpha_0 + n_{j..}} \delta_{\psi_{jt}} + \frac{\gamma}{n_{j..} + \gamma} G_0$$

Integrating over  $G_0$ , the sampling scheme for table-specific dish  $\psi_{jt}\sim G_0$  is:

$$\psi_{jk}|\Psi_{j(-k)}, \gamma, H \sim \sum_{k=1}^{K} \frac{m_{.k}}{\gamma + m_{..}} \delta_{\theta_k} + \frac{\gamma}{m_{..} + \gamma} H$$

# **D** References

## References

Yee Whye Teh, Michael I. Jordan, Matthew J. Beal, and David M. Blei. Hierarchical Dirichlet Processes. *Journal of the American Statistical Association*, 101(476):1566–1581, 2006. ISSN 0162-1459. URL http://www.jstor.org/stable/27639773.

Emily Beth Fox. *Bayesian nonparametric learning of complex dynamical phenomena*. Thesis, Massachusetts Institute of Technology, 2009. URL http://dspace.mit.edu/handle/1721.1/55111.