Reliable Variational Learning for Hierarchical Dirichlet Processes

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Learning Structured BNP Models

Genetics, Climate Change, Politics, ...

There are reasons to believe that the genetics of an organism are likely to shift due to the extreme changes in our climate. To protect them, our politicians must pass environmental legislation that can protect our future species from becoming extinct...



- \mathcal{M} X z_{dn} x_{dn}
- Nonparametric: Data-driven discovery of model structure: topics, behaviors, objects, communities...
- Reliable: Structure driven by data and modeling assumptions, not heuristic algorithm initializations
- Parsimonious: Want a single model structure with good predictive power, not full posterior uncertainty

Hierarchical Dirichlet Process (Teh et al., JASA 2006)

Memoized Variational Inference for Dirichlet Process Mixture Models

Michael Hughes & E. Sudderth

2013 Conference on Neural Information Processing Systems





Dirichlet Process Stick-Breaking

GOAL: Partition data into an a priori unknown number of discrete clusters.



Dirichlet Process Mixtures

GOAL: Partition data into an a priori unknown number of discrete clusters.



Each cluster k = 1, 2, ...

- > Cluster shape: $\phi_k \sim H(\lambda_0)$
- > Stick proportion: $v_k \sim \text{Beta}(1, \alpha)$
- \succ Cluster frequency: π_k

Each observation n = 1, 2, ..., *N*:

 \succ Cluster assignment: $z_n \sim \operatorname{Cat}(\pi)$ > Observed value: $x_n \sim F(\phi_{z_m})$

 $f(x_n \mid \phi_k) = \exp(\phi_k^T t(x_n) - a(\phi_k))$ $h(\phi_k \mid \lambda_0) = \exp(\lambda_0^T \bar{t}(\phi_k) - \bar{a}(\lambda_0)),$

Assume exponential family likelihoods with conjugate priors

$$\bar{t}(\phi_k) = [\phi_k, -a(\phi_k)]$$

Dirichlet Process Mixtures

GOAL: Partition data into an a priori unknown number of discrete clusters.



Visually summarize model structure via directed graphical model

MCMC for DP Mixtures

Can we sample from the posterior distribution over data clusterings?

 $v_1, v_2, v_3 \dots$

0.3

 $\overline{\pi_1} \ \overline{\pi_2} \ \overline{\pi_3}$

 $\pi \sim \text{Stick}(\alpha)$

0.2

 z_n

 x_n

0.5



 \mathcal{X}_{n}

- Marginalize stick-breaking weights via Chinese Restaurant Process, assigning positive probability to all partitions of data (large support)
- Via conjugacy of base measure to exponential family likelihood, marginalize cluster shape parameters

Gibbs Sampler: (Neal 1992, MacEachern 1994)

Iteratively resample cluster assignment for one observation, fixing all others.



Five random initializations from K=1, K=50, K=300 clusters
 Reversible jump MCMC? Proposals slow, acceptance low.

Variational Bounds

What is the marginal likelihood of our observed data?

$$\log p(x \mid \alpha, \lambda_{0}) = \log \sum_{z} \iint p(x, z, v, \phi \mid \alpha, \lambda_{0}) \, dv d\phi$$

$$= \log \sum_{z} \iint \frac{q(z, v, \phi)p(x, z, v, \phi \mid \alpha, \lambda_{0})}{q(z, v, \phi)} \, dv d\phi$$

$$= \log \mathbb{E}_{q} \left[\frac{p(x, z, v, \phi \mid \alpha, \lambda_{0})}{q(z, v, \phi)} \right] \quad \text{Expectation with respect to some variational distribution } q(z, v, \phi)$$

$$\overset{\text{Jensen's}}{\underset{\text{Inequality}}{\text{Jensen's}}} \geq \mathbb{E}_{q} [\log p(x, z, v, \phi \mid \alpha, \lambda_{0})] - \mathbb{E}_{q} [\log q(z, v, \phi)] = \mathcal{L}(q)$$

$$\overset{\text{Expected log-likelihood (negative of "average energy")} \quad \text{Variational entropy}} \quad (\pi \cap \alpha)$$

$$\overset{\text{Maximizing this bound recovers true posterior:}}{\mathcal{L}(q) = \log p(x \mid \alpha, \lambda_{0}) - \mathrm{KL}(q(z, v, \phi) \mid |p(z, v, \phi \mid x, \alpha, \lambda_{0}))} \quad (z, v, \phi)$$

 z_n

 x_n

The simplest mean field variational methods create tractable algorithms via assumed independence:

 $q(z, v, \phi) = q(z)q(v, \phi)$

Approximating Infinite Models

$$q(z_n = k) = r_{nk} \xrightarrow{\text{Beta}}_{\text{Distribution}} \xrightarrow{\text{Exponential Family}}_{\text{from Conjugate Prior}} q(z, v, \phi) = q(z)q(v, \phi) = \left[\prod_{n=1}^{N} q(z_n)\right] \cdot \left[\prod_{k=1}^{\infty} q(v_k)q(\phi_k)\right]$$

Categorical distribution with unbounded support, and infinitely many potential clusters!

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Bottom-Up Assignment Truncation Bryant & Sudderth, 2012; Teh, Kurihara, & Welling, 2008 $q(z_n) = \operatorname{Cat}(z_n \mid r_{n1}, r_{n2}, \dots, r_{nK}, 0, 0, 0, \dots)$ $q(v, \phi) = \prod_{k=1}^{\infty} q(v_k)q(\phi_k)$ For any k>K, optimal variational distributions equal prior & need not be explicitly represented

Batch Variational Updates

A Bayesian nonparametric analog of Expectation-Maximization (EM)

$$q(z, v, \phi) = \left[\prod_{n=1}^{N} q(z_n \mid r_n)\right] \cdot \left[\prod_{k=1}^{\infty} \operatorname{Beta}(v_k \mid \alpha_{k1}, \alpha_{k0}) h(\phi_k \mid \lambda_k)\right]$$

 $q(z_n) = \operatorname{Cat}(z_n \mid r_{n1}, r_{n2}, \dots, r_{nK}, 0, 0, 0, \dots)$ for some K>0

Update Assignments (The Expectation Step): For all N data,

$$r_{nk} \propto \exp(\mathbb{E}_q[\log \pi_k(v)] + \mathbb{E}_q[\log p(x_n \mid \phi_k)]) \quad \text{for } k \leq K$$
$$\mathbb{E}_q[\log \pi_k(v)] = \mathbb{E}_q[\log(v_k)] + \sum_{\ell=1}^{k-1} \mathbb{E}_q[\log(1 - v_\ell)]$$
$$\psi(\alpha_{k1}) - \psi(\alpha_{k1} + \alpha_{k0}) \quad \psi(\alpha_{k0}) - \psi(\alpha_{k1} + \alpha_{k0})$$

Update Cluster Parameters (The Other Expectation Step):

$$N_k^0 = \sum_{n=1}^N r_{nk} \qquad s_k^0 \leftarrow \sum_{n=1}^N r_{nk} t(x_n) \qquad \lambda_k \leftarrow \lambda_0 + s_k^0$$

Expected counts and sufficient statistics are only non-zero for first K clusters

$$\alpha_{k1} \leftarrow 1 + N_k^0 \qquad \qquad \mathbb{E}_q[v_k] = \frac{\alpha_{k1}}{\alpha_{k1} + \alpha_{k0}}$$
$$\alpha_{k0} \leftarrow \alpha + \sum_{\ell=k+1}^{\infty} N_\ell^0 = \alpha + \sum_{\ell=k+1}^K N_\ell^0$$

Likelihood Bounds & Convergence

$$\mathcal{L}(q) = \mathbb{E}_q[\log p(x, z, v, \phi \mid \alpha, \lambda_0)] - \mathbb{E}_q[\log q(z, v, \phi)]$$

Immediately after global parameter update, bound simplifies:

$$\mathcal{L}(q) = \mathbb{H}[r] + \sum_{k=1}^{K} \left[\bar{a}(\lambda_k) - \bar{a}(\lambda_0) + \log B(\alpha_{k1}, \alpha_{k0}) - \log B(1, \alpha) \right]$$
$$\mathbb{H}[r] = -\sum_{n=1}^{N} \sum_{k=1}^{\infty} r_{nk} \log r_{nk} = -\sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \log r_{nk}$$



Likelihood Bounds & Convergence

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Properties of variational optimization algorithm:

- + Likelihood bound monotonically increasing, guaranteed convergence to posterior mode
- + Unlike classical EM for MAP estimation, allows Bayesian comparison of hypotheses with varying complexity *K*, crucial for BNP models
- Truncation level K is assumed fixed
- Sensitive to initialization (many modes)
- Each iteration must examine all data (SLOW)



Stochastic Variational Inference

Hoffman, Blei, Paisley, & Wang, JMLR 2013

Stochastically partition large dataset into *B* smaller *batches*:



Properties of stochastic inference:

- + Per-iteration cost is low
- + Initial iterations often very effective
- Objective is highly non-convex, so convergence guarantee is weak
- $\begin{array}{c} 0.4 \\ 0.2 \\ 0.2 \\ 0 \\ 0 \\ 10^{0} \\ 10^{1} \\ 10^{2} \\ 10^{3} \\ 10^{4}$
- Batch size and learning rate significantly impact efficiency & accuracy

Memoized Variational Inference

Hughes & Sudderth, NIPS 2013; Neal & Hinton 1999

Memoization: Storage (caching) of results of previous computations



Properties of memoized inference:

- + Per-iteration cost is low
- + Initial iterations often very effective
- + Insensitive to chosen B, no learning rate
- + Foundation for inferring number of clusters K
- Requires storage proportional to number of batches (NOT number of observations)

Entropy for $\mathcal{L}(q)$ $H_k^0 = H_k^1 + H_k^2 + \dots H_k^B$ $H_k^b = -\sum_{n \in \mathcal{B}_b} r_{nk} \log r_{nk}$

 $\begin{vmatrix} s_1^0 & s_2^0 & \cdots & s_K^0 \end{vmatrix}$

 $s_k^0 = s_k^1 + s_k^2 + \dots s_k^B$

Memoized Cluster Births



Principles guiding memoized births:

- > BNP models support rare clusters, so random sampling ineffective
- > Target data grouped by some current cluster (likelihood-independent)
- Memoized updates allow efficient marginal likelihood verification

Memoized Cluster Merges

Merge two clusters into one for parsimony, accuracy, efficiency.



> New cluster takes over all responsibility for data assigned to old clusters:

 $r_{nk_m} \leftarrow r_{nk_a} + r_{nk_b} \quad \Longrightarrow \quad N_{k_m}^0 \leftarrow N_{k_a}^0 + N_{k_b}^0, \, s_{k_m}^0 \leftarrow s_{k_a}^0 + s_{k_b}^0$

> No batch processing required, efficiently evaluate via memoized statistics: $\mathcal{L}(q) = \mathbb{H}[r] + \sum_{k=1}^{K} \left[\bar{a}(s_k^0 + \lambda_0) - \bar{a}(\lambda_0) + \log B(1 + N_k^0, \alpha + N_{>k}^0) - \log B(1, \alpha) \right]$

 Accept or reject via exact full-dataset likelihood bound: L(q_{merge}) > L(q)?
 Requires memoized entropy sums for candidate pairs of clusters; more efficient alternatives under development.

Example: Finite Gaussian Mixture

- > N=100,000 samples from mixture of 8 Gaussians
- > 25-dim. covariance motivated by 5x5 image patches
- > DP mixture variational approximations allow K=25 clusters



Clustering Handwritten Digits

MNIST: 60,000 digits projected to 50 dimensions via PCA.



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MNIST: 60,000 digits projected to 50 dimensions via PCA.



MNIST: Variational versus Gibbs



Five random initializations from K=1, K=50, K=300 clusters

Diagonal-covariance Gaussians (change from previous slides)

Clustering Image Patches

SUN Database of Natural Scene Categories: N=108,754



> Memoized birth-merge learns a more accurate model with only K=28 clusters

8x8 Image Patches (Berkeley Segmentation): N=1.88 million

Memoized birth-merge allows growth in model complexity

Effective performance as density model for image denoising





Memoized Variational Inference for Hierarchial DP Topic Models

Michael Hughes, Dae II Kim, & E. Sudderth

estimation data density approach em probability model number set mixture gaussian figure posterior bayesian distribution parameters models log likelihood prior



What are Topic Models?

GOAL: Summarize semantic content of a large document corpus.



Hierarchical DP Topic Model

Generalization of Latent Dirichlet Allocation (LDA, Blei 2003) by Teh et al. JMLR 2006. Dependent Dirichlet process (DDP, MacEachern 1999) with group-specific weights.

Global topic frequencies and parameters:

- $\beta_k = u_k \prod_{\ell=1}^{k-1} (1 u_\ell) \quad u_k \sim \text{Beta}(1, \gamma)$ $\phi_k \sim \text{Dirichlet}(\lambda_0)$ (sparse) \succ For each of *D* documents (groups): π_d > Topic frequencies: $\pi_d \sim DP(\alpha\beta)$ Generalized $\pi_{dk} = v_{dk} \prod_{\ell=1}^{k-1} (1 - v_{d\ell})$ z_{dn} Dirichlet. $v_{dk} \sim \text{Beta}(\alpha_k u_k, \alpha_k (1 - u_k))$ Connor & Mosimann $\alpha_k = \alpha \prod_{\ell=1}^{k-1} (1 - v_{d\ell})$ 1969 x_{dn} \succ For each of N_d words in document d:
 - > Topic assignment: $z_{dn} \sim \operatorname{Cat}(\pi_d)$ > Observed value: $x_{dn} \sim \operatorname{Cat}(\phi_{z_{dn}})$



Variational Learning of HDP Topics

 $q(z_{dn}) = \text{Cat}(z_{dn} \mid r_{dn1}, r_{dn2}, \dots, r_{dnK}, 0, 0, 0, \dots)$ for some K>0

Update Document Distributions: For $k \leq K$,

 $r_{dnk} \propto \exp(\mathbb{E}_q[\log \pi_{dk}(v_d)] + \mathbb{E}_q[\log p(x_{dn} \mid \phi_k)])$

 $\mathbb{E}_q[\log \pi_{dk}(v_d)] = \mathbb{E}_q[\log(v_{dk})] + \sum_{\ell=1}^{k-1} \mathbb{E}_q[\log(1-v_{d\ell})]$

Closed form update for beta stick-breaking weights

Local iteration between assignments and weights

Update Global Parameters:

$$q(\phi_k) = \operatorname{Dir}(\phi_k \mid \lambda_0 + s_k^0)$$
$$s_k^0 \leftarrow \sum_{d=1}^D \sum_{n=1}^{N_d} r_{dnk} t(x_{dn})$$

Closed form for topic-specific word distributions

Beta normalization constants have non-conjugate dependence on topic frequencies, requires additional bound and numerical optimization

Iterate: Batch, Stochastic, or Memoized



Analysis of Document Corpora



- Variational: Memoized versus stochastic rate A, stochastic rate C
- Baseline: Stochastic variational on "expanded" HDP (Wang et al. 2011)

Stochastic Variational Inference for Hierarchial DP Relational Models

D. Kim, P. Gopalan, D. Blei, & E. Sudderth 2013 Conference on Neural Information Processing Systems



What are Relational Models?

GOAL: Unsupervised community discovery from observed relationships.



Stochastic Block Model: (Wang et al., JASA 1987)
 Assign each node to one latent block/community
 Predict edge presence or absence from block assignments of source and receiver nodes

Mixed Membership Blockmodels

Parametric mixed membership stochastic blockmodel, Airoldi et al. JMLR 2008



- Source Community Assignment
- Receiver Community Assignment
- Community Link Probability
- Binary Edge Indicator

 $s_{ij} \sim \operatorname{Cat}(\pi_i)$ $r_{ij} \sim \operatorname{Cat}(\pi_j)$ $\phi_{k\ell} \sim \operatorname{Beta}(\tau_a, \tau_b)$ $y_{ij} \sim \operatorname{Bern}(s_{ij}\phi r_{ij}^T)$

HDP Relational Models



Variational Learning of Relations

Assortative Likelihoods:



Stochastic Variational:



Analysis of Collaboration Networks



LittleSis Network: Raw Data



LittleSis Network Communities





Reliable Variational Learning for Hierarchical Dirichlet Processes

- Scalable: Large-scale learning via stochastic or memoized updates
- Reliable: Birth-merge recovers structure informed by model & data, not inference algorithm limitations
- Flexible: Designed to be broadly applicable: space, time, scale, ...



BNPy: Bayesian Nonparametric Learning in Python Erik Sudderth @ Brown CS: http://cs.brown.edu/~sudderth/