

Advanced Machine Learning Lecture 13

Hierarchical Dirichlet Processes

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This Lecture: Advanced Machine Learning

- Regression Approaches
 - Linear Regression
 - Regularization (Ridge, Lasso)
 - Kernels (Kernel Ridge Regression)
 - Gaussian Processes



Bayesian Estimation & Bayesian Non-Parametrics

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- Prob. Distributions, Approx. Inference
- » Mixture Models & EM
- Dirichlet Processes
- Latent Factor Models
- » Beta Processes

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Advanced Machine

- SVMs and Structured Output Learning
 - SV Regression, SVDD
 - Large-margin Learning



 $f: \mathcal{X} \to \mathcal{Y}$



Topics of This Lecture

• Applying DPs

- Recap: DPs
- Efficient Gibbs sampling

Hierarchical Dirichlet Processes

- Definition
- > Properties
- > Chinese Restaurant Franchise
- Gibbs sampling for HDPs

Applications

Topic modeling

RWTHAACHEN UNIVERSITY Recap: Dirichlet Process Mixture Models



Base distribution G_0

Infinite discrete distribution on Θ , defines the clusters

Parameters of the cluster that generates \mathbf{x}_n

Likelihood of \mathbf{x}_n given the cluster

Distributional form

 α

- \succ Explicit representation of the DP through the node G.
- > Useful when we want to use the DPMM's predictive distribution.

Recap: Pólya Urn Scheme

- Pólya Urn scheme
 - Simple generative process for the predictive distribution of a DP

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Consider a set of N observations \$\bar{\theta}_n \$\$ ~ G\$ taking K distinct values \$\$ {\theta_k\$}_{k=1}^K\$. The predictive distribution of the next observation is then

$$p(\bar{\theta}_N = \theta | \bar{\theta}_{1:N-1}, \alpha, H) = \frac{\alpha H(\theta) + \sum_{k=1}^{K} N_k \delta(\theta, \theta_k)}{N - 1 + \alpha}$$

Remarks

- > This procedure can be used to sample observations from a DP without explicitly constructing the underlying mixture.
- ⇒ DPs lead to simple predictive distributions that can be evaluated by caching the number of previous observations taking each distinct value.



α

Recap: Chinese Restaurant Process (CRP)

- Procedure
 - Imagine a Chinese restaurant with an infinite number of tables, each of which can seat an infinite number of customers.
 - The 1st customer enters and sits at the first table.
 - > The N^{th} customer enters and sits at table

$$\left\{egin{array}{cc} k & {
m with \ prob} \ rac{N_k}{N-1+lpha} \ {
m for} \ k=1,\ldots,K \ K+1 \ {
m with \ prob} \ rac{lpha}{N-1+lpha} & {
m (new \ table)} \end{array}
ight.$$

where N_k is the number of customers already sitting at table k.



Recap: CRPs & De Finetti's Theorem

- Putting all of this together...
 - De Finetti's theorem tells us that the CRP has an underlying mixture distribution with a prior distribution over measures.
 - The Dirichlet Process is the De Finetti mixing distribution for the CRP.

• Graphical model visualization

This means, when we integrate out G, we get the CRP:

$$p(\theta_1, \dots, \theta_N) = \int \prod_{n=1}^N p(\theta_n | G) dP(G)$$

 \Rightarrow If the DP is the prior on G, then the CRP defines how points are assigned to clusters when we integrate out G.



/ Image source: Kurt Miller

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Recap: CRPs and Efficient Inference

- Taking advantage of exchangeability...
 - > In clustering applications, we are ultimately interested in the cluster assignments z_1, \dots, z_N .
 - Equivalent question in the CRP: Where should customer n sit, conditioned on the seating choices of all the other customers?
 - This is easy when customer \boldsymbol{n} is the last customer to arrive:

$$p(\mathbf{z}_N = \mathbf{z} | \mathbf{z}_1, ..., \mathbf{z}_{N-1}, \alpha) = \frac{1}{N-1+\alpha} \left(\sum_{k=1}^K N_k \delta(\mathbf{z}, k) + \alpha \delta(\mathbf{z}, \bar{k}) \right)$$

- (Seemingly) hard otherwise...
- ⇒ Because of exchangeability, we can always swap customer n with the final customer and use the above formula!
 ⇒ We'll use this for efficient Gibbs sampling later on...

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Recap: Stick-Breaking Construction

- Explicit construction for the weights in DP realizations
 - > Define an infinite sequence of random variables

$$\beta_k \sim \text{Beta}(1, \alpha)$$
 $k = 1, 2, \dots$

> Then define an infinite sequence of mixing proportions as

$$\pi_1 = \beta_1$$

$$\pi_k = \beta_k \prod_{l=1}^{k-1} (1 - \beta_l) \qquad k = 2, 3, \dots$$

> This can be viewed as breaking off portions of a stick

> When the π_k are drawn this way, we can write $\pi \sim \text{GEM}(\alpha)$. (where GEM stands for Griffiths, Engen, McCloskey)

Slide adapted from Kurt Miller, Mike Jordan

RWTHAACHEN UNIVERSITY Summary: Pólya Urns, CRPs, and Stick-Breaking



Slide adapted from Kurt Miller, Mike Jordan

Summary: Pólya Urns, CRPs, and Stick-Breaking

- Better understanding of the properties of DPs
 - > All three schemes lead to proofs that DPs exist.
 - Using the Polya urn scheme, we showed that we can sample from DPs without constructing the underlying mixture explicitly.
 - > Using the Chinese Restaurant Process, we showed that the expected number of clusters grows with $\mathcal{O}(\alpha \log N)$.
 - Using the Stick-Breaking Construction, we showed that Dirichlet measures are discrete with probability one.

Uses for inference

- All three schemes can be used to construct efficient inference methods.
- We will mostly look at Gibbs samplers that are derived from the CRP.



Topics of This Lecture

- Applying DPs
 - Recap: DPs
 - Efficient Gibbs sampling
- Hierarchical Dirichlet Processes
 - Definition
 - > Properties
 - > Chinese Restaurant Franchise
 - > Gibbs sampling for HDPs
- Applications
 - Topic modeling

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Dirichlet Process Mixture Models

• Back to the clustering problem...



Indicator variable representation



Distributional form



Collapsed DP Mixture Sampler

- Efficient algorithm
 - Generalize the collapsed (Rao-Blackwellized) Gibbs sampler we derived for finite mixtures
 - > As before, sample the indicator variables z_n assigning observations to latent clusters, marginalizing mixture weights π_k and parameters θ_k .
 - > Assume the cluster priors $H(\lambda)$ are conjugate.
- Derivation
 - The model implies the factorization

 $p(\mathbf{z}_n | \mathbf{z}_{-n}, \mathbf{x}, \alpha, \lambda) \propto p(\mathbf{z}_n | \mathbf{z}_{-n}, \alpha) p(\mathbf{x}_n | \mathbf{z}, \mathbf{x}_{-n}, \lambda)$

Prior on partitions expressed by the CRP!



17 Image source: Yee Whye Teh



Collapsed DP Mixture Sampler

- Derivation (cont'd)
 - \succ Exchangeability: Think of \mathbf{z}_n as the last observation in sequence

$$p(\mathbf{z}_n | \mathbf{z}_{-n}, \alpha) = \frac{1}{N - 1 + \alpha} \left(\sum_{k=1}^K N_{-n,k} \delta(\mathbf{z}_n, k) + \alpha \delta(\mathbf{z}_n, \bar{k}) \right)$$

The predictive likelihood of x_n is computed as for finite mixtures:

$$p(\mathbf{x}_n | \mathbf{z}_n = k, \mathbf{z}_{-n}, \mathbf{x}_{-n}, \lambda) = p(\mathbf{x}_n | \{\mathbf{x}_m | \mathbf{z}_{mk} = 1, m \neq n\}, \lambda)$$

 \succ New clusters k are based on the predictive likelihood implied by the hyperparameters λ

$$p(\mathbf{x}_n | \mathbf{z}_n = \bar{k}, \mathbf{z}_{-n}, \mathbf{x}_{-n}, \lambda) = p(\mathbf{x}_n | \lambda) = \int_{\Theta} p(\mathbf{x}_n | \theta) h(\theta | \lambda) d\theta$$



Collapsed DP Mixture Sampler

- Algorithm
 - 1. Sample a random permutation $au\left(\cdot\right)$ of the integers $\{1,\ldots,N\}$.
 - 2. Set $\alpha = \alpha^{(t-1)}$ and $z = z^{(t-1)}$. For each $n \in \{\tau(1), ..., \tau(N)\}$, sequentially resample z_n as follows
 - a) For each of the K existing clusters, determine the predictive likelihood

$$p_k(\mathbf{x}_n | \mathbf{z}_{-n}, \lambda) = p(\mathbf{x}_n | \{\mathbf{x}_m | z_{mk} = 1, m \neq n\}, \lambda)$$

Also determine the likelihood $p_{ar{k}}(\mathbf{x}_n)$ of a potential new cluster $ar{k}$

$$p_{\bar{k}}(\mathbf{x}_n | \mathbf{z}_{-n}, \lambda) = p(\mathbf{x}_n | \lambda) = \int_{\Omega} p(\mathbf{x}_n | \theta) h(\theta | \lambda) \mathrm{d}\theta$$

b) Sample a new assignment \mathbf{z}_n from the multinomial distribution

$$\mathbf{z}_{n} \sim \frac{z_{n\bar{k}} \alpha p_{\bar{k}}(\mathbf{x}_{n} | \mathbf{z}_{-n}, \lambda) + \sum_{k=1}^{K} z_{nk} N_{-n,k} p_{k}(\mathbf{x}_{n} | \mathbf{z}_{-n}, \lambda)}{\alpha p_{\bar{k}}(\mathbf{x}_{n} | \mathbf{z}_{-n}, \lambda) + \sum_{j=1}^{K} (N_{-n,j} p_{j}(\mathbf{x}_{n} | \mathbf{z}_{-n}, \lambda))}$$

c) Update cached sufficient statistics to reflect assignment z_{nk} . If $\mathbf{z}_n = \bar{k}$, create a new cluster and increment K.

Slide adapted from Erik Sudderth

Collapsed DP Mixture Sampler (cont'd)

- Algorithm (cont'd)
 - 3. Set $z^{(t)} = z$. Optionally, mixture parameters for the K currently instantiated clusters may be sampled as in step 3 of the standard finite mixture sampler.
 - 4. If any current clusters are empty ($N_k = 0$), remove them and decrement K accordingly.
- Remarks
 - > Algorithm is valid if the cluster priors $H(\lambda)$ are conjugate.
 - > Cluster assignments $z^{(t)}$ produced by Gibbs sampler provide estimates $K^{(t)}$ of the number of clusters underlying the observations X, as well as their associated parameters.
 - Predictions based on samples average over mixtures of varying size, avoiding difficulties in selecting a single model.

Collapsed DP Sampler: 2 Iterations



Slide credit: Erik Sudderth

Collapsed DP Sampler: 10 Iterations



Slide credit: Erik Sudderth

Collapsed DP Sampler: 50 Iterations





 $\log p(x \mid \pi, \theta) = -396.71$

DPMMs vs. Finite Mixture Samplers



Observations

- Despite having to search over mixtures of varying order, the DP sampler typically converges faster.
- > Avoids local optima by creating redundant clusters at beginning.



DP Posterior Number of Clusters



Slide credit: Erik Sudderth

Summary: Nonparametric Bayesian Clustering

- DPMMs for Clustering
 - > First specify the likelihood. This is application dependent.
 - > Next, specify a prior on all parameters the Dirichlet Process!
 - Exact posterior inference is intractable. But we can use a Gibbs sampler for approximate inference. This is based on the CRP representation.



DPMM Software Packages

• Matlab packages for CRP mixture models

Algorithm	Author	Link
MCMC	J. Eisenstein	http://people.csail.mit.edu/jacobe/software.html
Variational	K. Kurihara	<u>http://sites.google.com/site/kenichikurihara/</u> <u>academic-software</u>



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Topic modeling



Hierarchical Bayesian Models

- Original Bayesian idea
 - > View parameters as random variables place a prior on them.
- Problem
 - > Often the priors themselves need parameters (hyperparameters)
- Solution
 - Place a prior on these parameters!



Multiple Learning Problems

- We often face multiple, related learning problems
 - > E.g., multiple related Gaussian means: $x_{ij} \sim \mathcal{N}(\theta_i, \sigma_i^{-2})$



- > Maximum likelihood: $\hat{ heta}_i = rac{1}{N_i} \sum_{j=1}^{N_i} x_{ij}$
- ML often does not work very well...
- Want to "share statistical strength" (i.e., smooth)



Hierarchical Bayesian Approach

- Bayesian solution
 - > Treat the parameters θ_i as random variables sampled from an underlying prior θ_0 .



- Bayesian inference yields shrinkage
 - > Posterior mean for each θ_k combines data from all of the groups, without simply lumping the data into one group.

Slide credit: Mike Jordan



Multiple Clustering Problems

• What to do if we have DPs for multiple related datasets?



Slide credit: Kurt Miller, Mike Jordan



Attempt 1



- > What kind of distribution do we use for G_0 ? What for H?
- > Suppose $\theta_{\rm ij}$ are mean parameters for a Gaussian where

 $G_i \sim \mathrm{DP}(\alpha, G_0)$

and G_0 is a Gaussian with unknown mean?

$$G_0 = \mathcal{N}(\theta_0, \sigma_0^2)$$

> This does NOT work! Why?



Attempt 1



- > Problem: if G_0 is continuous, then with probability ONE, G_i and G_j will share ZERO atoms.
- \Rightarrow This means NO clustering!





Hierarchical Dirichlet Processes

- We need to have the base measure G_0 be discrete
 - > But also need it to be flexible and random.
- Solution:
 - > Let G_0 itself be distributed according to a DP:

$$G_0|\gamma, H \sim \mathrm{DP}(\gamma, H)$$

> Then

$$G_j | \alpha, G_0 \sim \mathrm{DP}(\alpha_0, G_0)$$

has at its base measure a (random) atomic distribution. \Rightarrow Samples of G_i will resample from those atoms.

Hierarchical Dirichlet Processes [Teh et al., 2006]



Slide credit: Kurt Miller, Mike Jordan

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Comparison

Dirichlet Process

Useful in models for which a component of the model is a discrete random variable of unknown cardinality.

• Hierarchical Dirichlet Processes [Teh et al., 2006]

- Useful in problems in which there are multiple groups of data, where the model for each group of data incorporates a discrete variable of unknown cardinality, and where we wish to tie these variables across groups.
- Similar representations for HDP to derive its properties
 - Stick-Breaking construction
 - > Chinese Restaurant Franchise

- Chain of Chinese restaurants
 - Each restaurant has an unbounded number of tables.
 - There is a global menu with an unbounded number of dishes.
 - The first customer at a table selects the dish for that table from the global menu.



Reinforcement effects

- Customers prefer to sit at tables with many other customers, and prefer dishes that are chosen by many other customers.
- Dishes are chosen with probability proportional to the number of tables (franchise-wide) that have previously served that dish.

- Examine marginal properties of HDP
 - > First integrate out G_i , then G_0 .



Slide adapted from Kurt Miller

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- Step 1: Integrate out G_i:
 - Variable definitions
 - θ_{ij} : RV for customer i in restaurant j.
 - θ_{jt}^* : RV for table t in restaurant j.
 - ${\theta_k}^{**}$: RV for dish k.
 - m_{jk} : number of tables in rest. j serving dish k.
 - n_{jtk} : number of customers in rest. j sitting at table t and being served dish k.
 - We denote marginal counts by dots, e.g. $m_{j\cdot} = \sum_{k=1}^{K} m_{jk}$
 - > Integration yields a set of conditional distributions described by a Polya urn scheme m_{i} .

$$heta_{ij}| heta_{1j},..., heta_{i-1,j},lpha,G_0 \sim \sum_{t=1}^{J}rac{n_{jt.}}{lpha+n_{j..}}\delta_{ heta_{jt}^*}+rac{lpha}{lpha+n_{j..}}G_0$$

40 Image source: Kurt Miller

m



H

- Step 2: Integrate out G₀:
 - Variable definitions
 - θ_{ij} : RV for customer i in restaurant j.
 - θ_{jt}^* : RV for table t in restaurant j.
 - θ_k^{**} : RV for dish k.
 - m_{jk} : number of tables in rest. j serving dish k.
 - n_{jtk} : number of customers in rest. j sitting at table t and being served dish k.
 - We denote marginal counts by dots, e.g. $m_{j\cdot} = \sum_{k=1}^{K} m_{jk}$
 - > Again, we get a Polya urn scheme

$$\theta_{jt}^{*}|\theta_{11}^{*},...,\theta_{1,m_{1,\cdot}}^{*},...,\theta_{j,t-1}^{*},\gamma,H$$







Inference for HDP: CRF Sampler

- Using the CRF representation of the HDP
 - > Customer i in restaurant j is associated with i.i.d draw from G_i and sits at table t_{ij} .
 - \succ Table t in restaurant j is associated with i.i.d draw from G_0 and serves dish $k_{jt}.$
 - > Dish k is associated with i.i.d draw from H.

Gibbs sampling approach

- Iteratively sample the table and dish assignment variables, conditioned on the state of all other variables.
- > The parameters θ_{ij} are integrated out analytically (assuming conjugacy).
- To resample, make use of exchangeability.
- \Rightarrow Imagine each customer i being the last to enter restaurant j.



Inference for HDP: CRF Sampler

- Procedure
 - **1.** Resample t_{ij} according to the following distribution

 $\begin{cases} t_{ij} = t & \text{with prob.} \quad \propto \frac{n_{jt}^{\neg ij}}{n_{j\cdot\cdot}^{\neg ij} + \alpha} f_{k_{jt}}(\{x_{ij}\}) \\ t_{ij} = t^{\text{new}}, k_{jt^{\text{new}}} = k & \text{with prob.} \quad \propto \frac{\alpha}{n_{j\cdot\cdot}^{\neg ij} + \alpha} \propto \frac{m_{\cdot k}^{\neg ij}}{m_{\cdot\cdot}^{\neg ij} + \gamma} f_k(\{x_{ij}\}) \\ t_{ij} = t^{\text{new}}, k_{jt^{\text{new}}} = k^{\text{new}} & \text{with prob.} \quad \propto \frac{\alpha}{n_{j\cdot\cdot}^{\neg ij} + \alpha} \propto \frac{\gamma}{m_{\cdot\cdot}^{\neg ij} + \gamma} f_{k^{\text{new}}}(\{x_{ij}\}) \end{cases}$

where $\neg ij$ denotes counts in which customer i in restaurant j is removed from the CRF. (If this empties a table, we also remove the table from the CRF, along with the dish on it.)

> The terms $f_k(\{x_{ij}\})$ are defined as follows $f_k(\{x_{ij}\}_{ij\in D}) = \frac{\int h(\theta) \prod_{i'j'\in D_k\cup D} f_{\theta}(x_{i'j'}) \mathrm{d}\theta}{\int h(\theta) \prod_{i'j'\in D_k\setminus D} f_{\theta}(x_{i'j'}) \mathrm{d}\theta}$

where D_K denotes the set of indices associated with dish k.



Inference for HDP: CRF Sampler

- Procedure (cont'd)
 - 2. Resample k_{jt} (Gibbs update for the dish)

$$k_{jt} = \begin{cases} k & \text{with prob.} \quad \propto \frac{m_{\cdot k}^{\gamma t}}{m_{\cdot \gamma}^{\gamma t} + \gamma} f_k(\{x_{ij} : t_{ij} = t\}) \\ k^{\text{new}} & \text{with prob.} \quad \propto \frac{\gamma}{m_{\cdot \gamma}^{\gamma t} + \gamma} f_{k^{\text{new}}}(\{x_{ij} : t_{ij} = t\}) \end{cases}$$

- Remarks
 - > Computational cost of Gibbs updates is dominated by computation of the marginal conditional probabilities $f_k(\cdot)$.
 - Still, the number of possible events that can occur at one Gibbs step is one plus the total number of tables and dishes in all restaurants that are ancestors of j.
 - This number can get quite large in deep or wide hierarchies...



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Applications

Topic modeling



- Example: Document topic modelling
 - > Topic: probability distribution over a set of words
 - > Model each document as a probability distribution over topics.





Latent Dirichlet Allocation

[Blei et al., 2003]

> Popular topic modelling approach with fixed number of topics k



- Random variables
 - A word is represented as a multinomial random variable \boldsymbol{w}
 - A topic is represented as a multinomial random variable z
 - A document is represented as a Dirichlet random variable heta



HDPs can be used to define a BNP version of LDA

- Number of topics is open-ended
- Multiple infinite mixture models, linked via shared topic distribution.





\Rightarrow HDP-LDA avoids the need for model selection.

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- There are many other generalizations I didn't talk about
 - Dependent DPs
 - Nested DPs
 - > Pitman-Yor processes
 - Infinite HMMs
 - **>** • •

• And some that I will talk about in Lectures 15/16...

- Infinite Latent Factor Models
- Beta Processes
- Indian Buffet Process
- Hierarchical Beta Process



References and Further Reading

- Unfortunately, there are currently no good introductory textbooks on the Dirichlet Process. We will therefore post a number of tutorial papers on their different aspects.
 - > One of the best available general introductions
 - E.B. Sudderth, "<u>Graphical Models for Visual Object Recognition and</u> <u>Tracking</u>", PhD thesis, Chapter 2, Section 2.5, 2006.
 - A tutorial on Hierarchical DPs
 - Y.W. Teh, M.I. Jordan, <u>Hierarchical Bayesian Nonparametric Models</u> <u>with Applications</u>. Bayesian Nonparametrics, Cambridge Univ. Press, 2010.
 - Good overview of MCMC methods for DPMMs
 - R. Neal, <u>Markov Chain Sampling Methods for Dirichlet Process</u> <u>Mixture Models</u>. Journal of Computational and Graphical Statistics, Vol. 9(2), p. 249-265, 2000 <u>B. Leibe</u>