Multi-level clustering with contexts via hierarchical nonparametric Bayesian inference

Long Nguyen

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Biostatistics Seminar, October 2016

# Multi-level clustering analysis

I'd like to ...

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- cluster images into meaningful categories
- cluster the users into typical profiles based on recorded activities

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I'd like to ...

- cluster the collection of documents into meaningful topics
- cluster images into meaningful categories
- cluster the users into typical profiles based on recorded activities

I also want to exploit contextual information that may be available

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# Topic modeling

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Topic modeling a popular tool for mining and analyzing patterns from texts in news articles, scientific papers, blogs, but also tweets, query logs, digital books, metadata records...



News articles





Scientific papers





Tweets







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also applicable to ther data formats (images, networks)

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also applicable to ther data formats (images, networks)

in diverse domains in computer sciences, biomedical sciences, scientometrics, social and political science, and digital humanities.

(4) (日本)

#### Take a document from the AP corpus (Blei, Ng, Jordan, 2003)

The William Randolph Heart Foundation will give \$1.25 million to Lincoln Center, Metropolitan Opera Co., New York Philhamonic and pulling School. "Our Yourd felt that we had a real opportunity to make a mark on the future of the performing arts with these grants an act every bit a simportant as our tradinonal areas of support in health, medical research, education and the social services," Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center Share will be \$200,000 for its new balding, which will house young artists and provider as whare will be \$200,000 for its new balding. Which the performing artists and provide new public radinities. The Metropolitan Opera Co. and New York Philharmonic will receive \$400,000 each. The Juilland School, where music and the performing at sea taught, will get \$250,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual \$100,000 donation, too.

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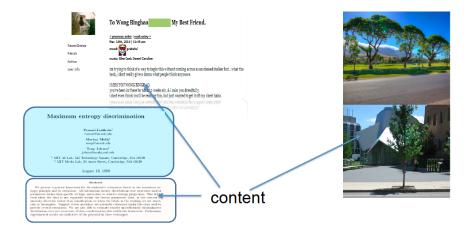
The William Randolph Hearst Foundation will give \$125 million to Lincoln Center, Metropolitan Opera Co., New York Philhamonic and Juilliad School. "Our Yourd felt that we had a real orgoportunity to make a mark on the future of the performing arts with these grants and every bit as important as our traditional areas of support in health, medical research, education and the social services," Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center's share will be \$200000 for its new bailding, which will house young artists and provide new public facilities. The Metropoltan Opera Co. and New York Philharmonic will receive \$400,000 each. The Juilland School, where music and the performing at sea taught, will get \$2500,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual \$100,000 donation, too.

#### after feeding to Latent Dirichlet Allocation (LDA) model:

"Arts"	"Budgets"	"Children"	"Education"
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
MUSIC	BUDGET	CHILD	EDUCATION
MOVIE	BILLION	YEARS	TEACHERS
PLAY	FEDERAL	FAMILIES	HIGH
MUSICAL	YEAR	WORK	PUBLIC
BEST	SPENDING	PARENTS	TEACHER
ACTOR	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANIGAT
YORK	PLAN	WELFARE	NAMPHY
OPERA	MONEY	MEN	STATE
THEATER	PROGRAMS	PERCENT	PRESIDENT
ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	LIFE	HAITI

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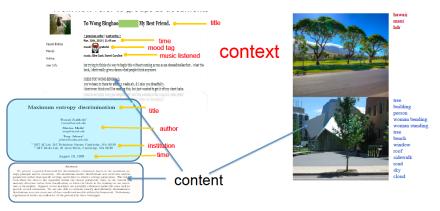
# This talk: modeling both content and context



"content data": words/documents/images

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# Modeling both content and context



"content data": words/documents/images "context data": time, location, hashtags, etc

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• Goal: jointly discover clusters of contents and contexts, e.g., words and time/locations

• Probabilistic modeling for jointly model both contents and document contexts Bayesian nonparametric approach

- Multiple advantages:
  - context-aware topic modeling of contents
  - context clusters share content topics
  - infer context given content and vice-versa

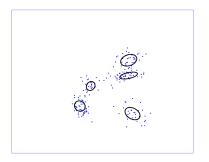
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# Mixture models

Long Nguyen (UM)

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# Mixture modeling



Mixture density:

$$p_G(x) = \sum_{i=1}^k p_i f(x|\theta_i)$$

 $G = \sum_{i=1}^{k} p_i \delta_{\theta_i}$  is mixing measure

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Nonparametric Bayesian inference

$$G \sim \Pi,$$
  
$$x_1,\ldots,x_n | G \sim p_G$$

Clusters are drawn from posterior distribution  $\Pi(G|x_1,\ldots,x_n)$ 

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#### Dirichlet process prior $G \sim \mathcal{D}_{\alpha G_0}$

(Ferguson, 1973)

- D<sub>αG0</sub> (also, DP(α, G<sub>0</sub>)): Dirichlet distribution on the space of probability measure on Θ
- G is called a Dirichlet process (a random PM on  $\Theta$ )
- *G* is discrete with probability one, and admit Sethuraman's stick-breaking representation

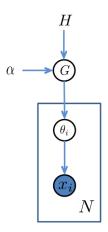
$$G=\sum_{i=1}^{\infty}\pi_i\delta_{\eta_i},$$

where both  $\pi_i$ s and  $\eta_i$ s are random variables obeying suitable laws

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# Dirichlet process mixture

[Antoniak (1974), Lo (1984), Escobar & West (1992), Mueller & McEachern (1998),...]



$$egin{array}{rcl} G &\sim & \mathcal{D}_{lpha H} \ ec{ heta}_i | G & \stackrel{iid}{\sim} & G \ ec{ heta}_i | heta_i & \stackrel{indep}{\sim} & f(\cdot | heta_i) \end{array}$$

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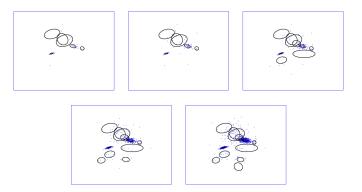
Data are naturally organized as a multi-level collection of data sets

- text corpus as collection of documents, document as collection of words
- image db as collection of images, image as collection of patches
- collection of users, user as collection of activities

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### Exchangeable collection of data sets

Each data set is a collection of exchangeable elements  $\implies$  mixture of mixture of distributions



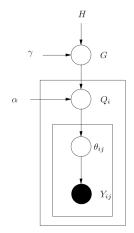
[courtesy M. Jordan's slides]

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This gives rise naturally to a hierarchical model

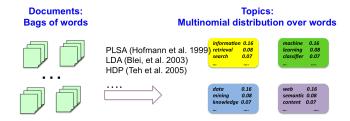
#### Hierarchical Dirichlet Processes (HDP)

(Teh, Jordan, Blei and Beal, JASA 2006)



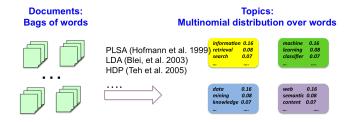
$$\begin{array}{rcl} G & \sim & \mathcal{D}_{\gamma H} \\ Q_1, \dots, Q_m | G & \stackrel{iid}{\sim} & \mathcal{D}_{\alpha G} \\ Y_{i1}, \dots, Y_{in} | Q_i & \stackrel{iid}{\sim} & \rho_{Q_i} \ \mathrm{for} \ i = 1, \dots, m \end{array}$$

### Back to earth: topic modeling for documents

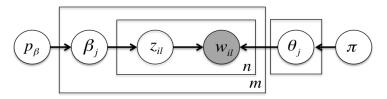


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# Back to earth: topic modeling for documents



The hierarchical model from the previous slide is this:

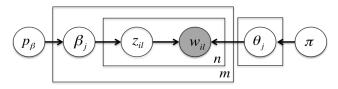


 $w_{il}$ : (observed) word l in document i

 $z_{il}$ : (latent) topic index that word  $w_{il}$  is associated with

Long Nguyen (UM)

### Latent Dirichlet allocation model

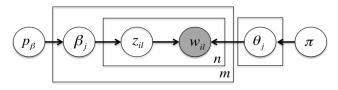


Generative process:

- For each  $j = 1, \ldots, k$ , sample a vector of frequencies  $\theta_j \in \Delta^{d-1}$ 
  - these are called "topics", distributed by a Dirichlet
  - d = vocabulary size

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### Latent Dirichlet allocation model



Generative process:

- For each  $j = 1, \ldots, k$ , sample a vector of frequencies  $\theta_j \in \Delta^{d-1}$ 
  - these are called "topics", distributed by a Dirichlet
  - d = vocabulary size
- For each document  $i = 1, \ldots, m$ ,
  - ▶ sample a topic proportion  $\beta \in \Delta^{k-1}$  (e.g., another Dirichlet)
  - for each word position in document i
    - **\*** sample a topic label  $z \sim \text{Multinomial}(\beta)$ ;
    - **\*** given z, sample a word  $w \sim \text{Multinomial}(\theta_z)$ .

Inferential goal: given data of size  $m \times n$ , estimate the topic vectors  $\theta_j$ 's

Long Nguyen (UM)

#### Feeding AP corpus of documents, e.g.:

The William Randolph Hearst Foundation will give \$1.25 million to Lincoln Center. Metropolitan Opera Co., New York Philhamonic and philling School. "Our Yound fift that we had a real opportunity to make a mark on the future of the performing arts with these grants an act every bit as important as our traditional areas of support in health, medical research, education and the social services," Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center Santae will be \$200000 for its new balding, which will house young artists and provider so share will be \$200000 for its new balding. Where music and he performing artists and provide new public facilities. The Metropolitan Opera Co. and New York Philhamonic will receive \$400.000 each. The Juilland School, where music and he performing at sea taught, will get \$2500.000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual \$100,000 donation, too.

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#### Feeding AP corpus of documents, e.g.:

The William Randolph Hearst Foundation will give \$125 million to Lincoln Center. Metropolitan Opera Co., New York Philhamonic and pulling School - 'Oor Yoood fift that we had a real opportunity to make a mark on the future of the performing arts with these grants na cievery bit as important as our traditional areas of support in health, medical research, education and the social asvices, 'Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center's share will be \$20000 for its new bailding, which will house young artists and provide new public facilities. The Metropoltan Opera Co. and New York Philharmonic will receive \$400,000 each. The Juillard School, where music and the performing as the taght, will get \$250,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual \$100,000 donation, too.

#### to LDA/HDP model, we obtain

"Arts"	"Budgets"	"Children"	"Education"
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
MUSIC	BUDGET	CHILD	EDUCATION
MOVIE	BILLION	YEARS	TEACHERS
PLAY	FEDERAL	FAMILIES	HIGH
MUSICAL	YEAR	WORK	PUBLIC
BEST	SPENDING	PARENTS	TEACHER
ACTOR	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANIGAT
YORK	PLAN	WELFARE	NAMPHY
OPERA	MONEY	MEN	STATE
THEATER	PROGRAMS	PERCENT	PRESIDENT
ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	LIFE	HAITI

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#### Back to our work

• HDP does not help us cluster documents (yet)

• nor does it help us handle contextual information (time/location/hashtags)

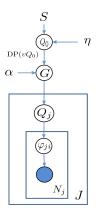
• since documents is associated with distribution over words, we need to be able to cluster over the space of distributions!

# Clustering in space of distributions

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### Nested Dirichlet processes

[Rodriguez, Dunson and Gelfand, JASA 2008]

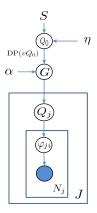


 $Q_1,\ldots,Q_m|G \stackrel{iid}{\sim} G,$ 

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# Nested Dirichlet processes

[Rodriguez, Dunson and Gelfand, JASA 2008]



 $Q_1,\ldots,Q_m|G \stackrel{iid}{\sim} G,$ 

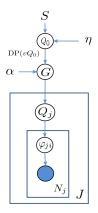
where

$$G \sim \mathcal{D}_{\alpha \mathcal{D}_{vQ_0}}$$

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### Nested Dirichlet processes

[Rodriguez, Dunson and Gelfand, JASA 2008]



$$Q_1,\ldots,Q_m|G\overset{iid}{\sim}G,$$

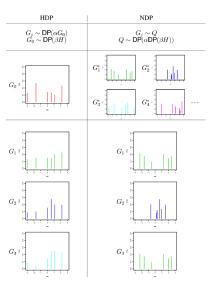
where

$$G \sim \mathcal{D}_{\alpha \mathcal{D}_{vQ_0}}$$

E.g.,  $Q_0$  is a distribution over a space of atoms (words/image patches/ human activities)

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### HDP vs NDP



Long Nguyen (UM)

(Rodriguez et al, 2008) Oct 2016 22 / 54

#### Multi-level clustering with contexts: MC2

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Multi-level clustering with contexts: MC2

(Nguyen et al, ICML, 2014; Huynh et al, UAI, 2016)

- pairing up context (document-level) with content (word-level) is unnatural since they lie on different levels of abstraction
- first idea: treat context as index for distributions over contents
  - but, raw contextual data are noisy (e.g., noisy tags, continuous location coordinates)

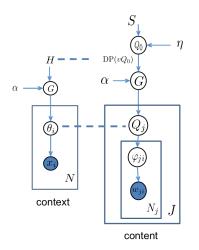
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## Multi-level clustering with contexts: MC2

(Nguyen et al, ICML, 2014; Huynh et al, UAI, 2016)

- pairing up context (document-level) with content (word-level) is unnatural since they lie on different levels of abstraction
- first idea: treat context as index for distributions over contents
  - but, raw contextual data are noisy (e.g., noisy tags, continuous location coordinates)
- second idea: make context indices random
  - context cluster acts as an index into a distribution of contents
  - this allows context (time/space) to influence both topics and document clusters.
- how to make this concrete?

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Pairing up context atoms  $\theta_i$  with content distributions  $Q_i$ :

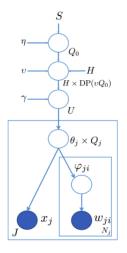
$$(\theta_j, Q_j)|U \sim U,$$

where

$$U \sim \mathcal{D}_{\gamma(H \times \mathcal{D}_{vQ_0})}$$

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MC2



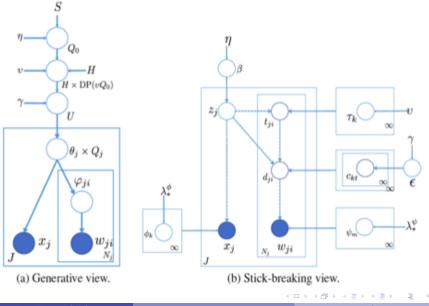
- form a product of base measure  $H \times \mathcal{D}_{\nu Q_0}$
- use this as base measure in a nested DP fashion

$$U \sim \mathcal{D}_{\gamma(H \times \mathcal{D}_{vQ_0})}$$

- marginalizing out content yields a DP mixture over context data
- marginalizing out context yields a nested DP mixture over content

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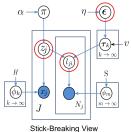
# MC2 grounded in stick-breaking representation



Long Nguyen (UM)

Oct 2016 27 / 54

# Gibbs sampling for MC2



Variables sampled during collapsed Gibbs

• sampling z<sub>j</sub>

$$p(z_j = k | \cdot) \propto p(z_j = k | z_{-j}, \alpha)$$
  
 
$$\times p(x_j | z_j = k, z_{-j}, x_{-j}, H)$$
  
 
$$\times p(l_{j^*} | z_j = k, l_{-j^*}, z_j, \epsilon, \nu)$$

• sampling *l<sub>ji</sub>* 

$$p(l_{ji} = m | \cdot) \propto p(w_{ji} | l, w_{-ji}, S)$$
$$\times p(l_{ji} = m | l_{-ji}, z_j = k, z_{-j}, \epsilon, v)$$

- sampling  $\epsilon$ 
  - > p(o<sub>km</sub> = h|·) ∝ Stirl(h, n<sub>km</sub>)(vε<sub>m</sub>)<sup>h</sup>, h = 0, 1, ..., n<sub>km</sub>> p(ε|·) ∝ ε<sup>η-1</sup><sub>new</sub> ∏<sup>M</sup><sub>m=1</sub> ε<sup>∑<sub>k</sub> o<sub>km</sub>-1</sup>

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# Application 1: document modeling

#### PNAS dataset

- 79,800 documents (only titles and timestamps)
- Vocabulary size is 36,782 (remove stop words)
- Context observations are document timestamps (1915–2005)
- NIPS abstract dataset
  - 1740 documents; vocabulary size: 13,649 words
  - Three types of context information: timestamps, authors (2037 unique authors), article titles

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# Perplexity (goodness of fit)

Method	Perplexity (on words only)				Feature used
Method	PNAS	(K,M)	NIPS	(K,M)	reature used
HDP (Teh et al., 2006b)	3027.5	(-, 86)	1922.1	(-, 108)	words
npTOT (Dubey et al., 2012; Phung et al., 2012)	2491.5	(-, 145)	1855.33	(-, 94)	words+timestamp
MC <sup>2</sup> without context	1742.6	(40, 126)	1583.2	(19, 61)	words
MC <sup>2</sup> with titles	-	-	1393.4	(32, 80)	words+title
MC <sup>2</sup> with authors	-	-	1246.3	(8, 55)	words+authors
MC <sup>2</sup> with timestamp	895.3	(12, 117)	984.7	(15, 95)	words+timestamp

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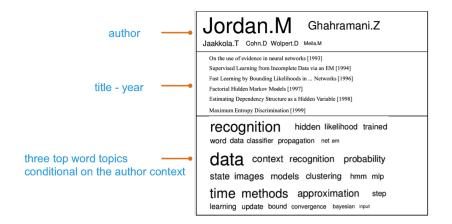
### Context-aware topics



Manual count statistic of keyword "albinism" in Google Scholar

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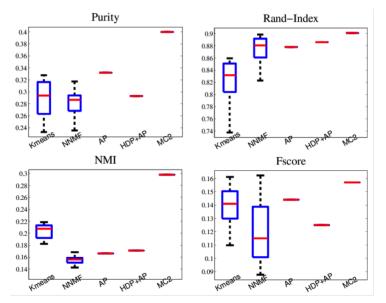
### Context-aware topics



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# Application 2: image clustering

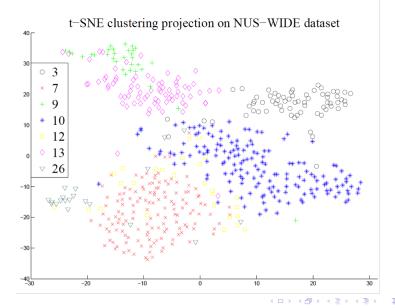


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Long Nguyen (UM)

### Application 2: image clustering



Long Nguyen (UM)

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# Application 2: image clustering

Missing(%)	Purity	NMI	RI	F-score
0%	0.407	0.298	0.901	0.157
25%	0.338	0.245	0.892	0.149
50%	0.32	0.236	0.883	0.137
75%	0.313	0.187	0.860	0.112
100%	0.306	0.188	0.867	0.119

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# Scaling up

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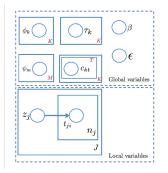
# Scaling up

• Wikipedia: 1.1 million documents from wikipedia.com context: first author and top-level categories

 PubMed: 1.4 million documents from pubmed.gov context: medical subject headings (MeSH)

• AUA (application user activities): > 1M users context: background softwares

### Stochastic mean-field approximation



- factorized posterior distribution into that of local and global variables
- gradient-based update for local variables via structured mean-field approximation (can be parallelized)
- update for global variables using natural gradient and via stochastic optimization

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• Not possible to fit via a Gibbs sampler

Run times on 8-node SPARK cluster

• stochastic mean-field approximation take, resp., 17 hours, 18.5 hours, and 18 hours

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# Scaling up

	Context availability		LDA
	100%	0%	
Wikipedia - writer	2,167	2,280	2,635
Pubmed - MeSH	2,294	2.448	3,178
AUA - other products	142.3	149.7	209.3

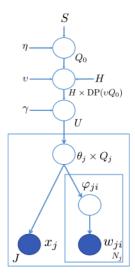
Table 2: Log perplexity of Wikipedia and PubMed data

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# Identifiability and posterior contraction

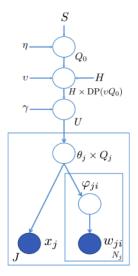
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What is going on in the layers of latent variables?



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What is going on in the layers of latent variables?





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#### Battleship USS Texas

## Posterior concentration of mixing measure G

Suppose

$$X_1,\ldots,X_n \stackrel{iid}{\sim} p_G(x) := \int f(x|\theta)G(d\theta)$$

f is known, while  $G = G_0$  unknown discrete mixing measure

 Consistency: does the posterior distribution Π(G|X<sub>1</sub>,...,X<sub>n</sub>) concentrate most of its mass around the "truth" G<sub>0</sub>?

• Rate: what is the rate of concentration (convergence) as  $n \to \infty$ ?

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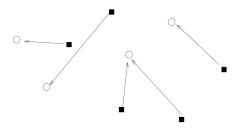
### Optimal transport distance

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### Optimal transportation problem (Monge-Kantorovich)

how to move the mass from one distribution to another?

Originally: how to transport goods from a collection of producers to a collection of consumers located in a common space



squares: locations of producers; circles: locations of consumers

The optimal cost of transportation defines a distance from "production density" — to — "consumption density".

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### Wasserstein distance

Let G, G' be two prob. measures on  $\Theta$ 

A coupling  $\kappa$  of G, G' is a joint dist on  $\Theta \times \Theta$  which induces marginals G, G'

#### Definition

Let  $\rho$  be a distance function on  $\Theta$ , the Wasserstein distance is defined by:

$$d_{\rho}(G,G') = \inf_{\kappa} \int \rho(\theta,\theta') d\kappa.$$

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$$d_{\rho}(G,G') = \inf_{\kappa} \int \rho(\theta,\theta') d\kappa.$$

When  $\Theta = \mathbb{R}^d$ , for  $r \ge 1$ , we obtain  $L_r$  Wasserstein metric:

$$W_r(G, G') := \left[\inf_{\kappa} \int \|\theta - \theta'\|^r d\kappa\right]^{1/r}$$

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Wasserstein distance  $W_r$  metrizes weak convergence in the space of probability measures on  $\Theta$ .

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If  $G = \sum_{i=1}^{k} \frac{1}{k} \delta_{\theta_i}$ ,  $G' = \sum_{j=1}^{k} \frac{1}{k} \delta_{\theta'_j}$ , then  $W_1(G, G') = \inf_{\pi} \sum_{i=1}^{k} \frac{1}{k} \|\theta_i - \theta'_{\pi(i)}\|,$ 

where  $\pi$  ranges over the set of permutations on  $(1, \ldots, k)$ .

Long Nguyen (UM)

### Finite mixtures

(Nguyen, AOS 2013; Ho & Nguyen, EJS 2016)

For strongly identifiable mixture models the posterior  $\Pi(G|X_1, \ldots, X_n)$  contracts to true  $G_0$  at the rate  $\epsilon_n$ ,

$$\Pi(W_r(G,G_0) \leq \epsilon_n | X_1,\ldots,X_n) \stackrel{P}{\longrightarrow} 1$$

- if the number of mixing components known,  $\epsilon_n \simeq n^{-1/2}$  under  $W_1$
- if only an upper bound of the number of mixing component is known,  $\epsilon_n \asymp n^{-1/4}$  under  $W_2$

Strongly identifiable finite mixtures:

• location Gaussian mixtures, scale Gaussian mixtures, etc

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### Infinite mixtures

(Nguyen, AOS 2013)

For infinite mixtures using Dirichlet process prior on a compact Euclidean space, the posterior  $\Pi(G|X_1, \ldots, X_n)$  contracts to true  $G_0$  at the rate  $\epsilon_n$ ,

$$\Pi(W_2(G,G_0) \leq \epsilon_n | X_1,\ldots,X_n) \stackrel{P}{\longrightarrow} 1$$

- if the mixture's kernel is "ordinary smooth" (e.g., Laplace), then  $\epsilon_n \simeq n^{-1/(4+\beta)}$ , where  $\delta$  is determined by the smoothness parameter
- if the mixture's kernel is "supersmooth" (e.g., Gaussian), then  $\epsilon_n \simeq (\log n)^{-1/\beta}$

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# Weakly identifiably models

(Ho & Nguyen, AOS 2016)

#### location-scale and finite Gaussian mixtures

The posterior of G contracts very slowly, as the number of extra number of mixing components

- $n^{-1/8}$  if overfitting by one
- $n^{-1/12}$  if overfitting by two
- and so on

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- and so on

There is a more general theory behind this phenomenon based on the singularity structures of the mixture model's parameter space

### Posterior contraction in hierarchical models

(4) (3) (4) (4) (4)

### Distance between nonparametric Bayesian hierarchies

Need a notion of distance between, say  $\mathcal{D}_{\alpha \textit{G}}$  and  $\mathcal{D}_{\alpha'\textit{G}'}$ 

**Recall**: for  $G, G' \in \mathcal{P}(\Theta)$ , space of Borel probability measures on  $\Theta$ ,

$$W_r(G,G') := \inf_{\kappa \in \mathcal{T}(G,G')} \left[ \int \|\theta - \theta'\|^r d\kappa(\theta,\theta') 
ight]^{1/r}.$$

 $\mathcal{T}(G, G')$  is the space of all couplings of G, G'.

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#### Distance between measures of measures in Bayesian hierarchy:

Let  $\mathcal{D}, \mathcal{D}' \in \mathcal{P}(\mathcal{P}(\Theta))$  (the space of Borel probability measures on  $\mathcal{P}(\Theta)$ ). Define Wasserstein distance between  $\mathcal{D}, \mathcal{D}'$ 

$$W_r(\mathcal{D},\mathcal{D}') := \inf_{\mathcal{K}\in\mathcal{T}(\mathcal{D},\mathcal{D}')} \left[ \int W_r^r(\mathcal{G},\mathcal{G}') \, d\mathcal{K}(\mathcal{G},\mathcal{G}') \right]^{1/r}$$

 $\mathcal{T}(\mathcal{D},\mathcal{D}')$  is the space of all couplings of  $\mathcal{D},\mathcal{D}'\in\mathcal{P}(\mathcal{P}(\Theta))$ 

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### Hierarchical Dirichlet processes

(Nguyen, Bernoulli 2016)

- rates of posterior contraction of the Dirichlet base measure residing at the top of the latent hierarchy
- there is a striking effect of "borrowing of strength" phenomenon, which can be quantified
  - parameteric rate of contraction can be achieved at individual group-level distributions if there are sufficiently many groups supported by data residing in the same level of the model's hierarchy

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# Summary

- MC2: nonparametric Bayesian modeling for joint context/content inference
- scaling up via stochastic variational inference and parallel computing
- posterior contraction behavior of latent variables

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