Probabilistic Models for Graphs, and Intro to Nonparametric Bayesian Modeling

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Topics in Probabilistic Modeling and Inference (CS698X)

March 25, 2019

Modeling Graphs

- Often we wish to understand the underlying structure (e.g., communities/groups/topics) in a graph, predict links, classify nodes, visualize, etc.
- An example graph† (a 575,000 node citation network of papers; each node is a paper):

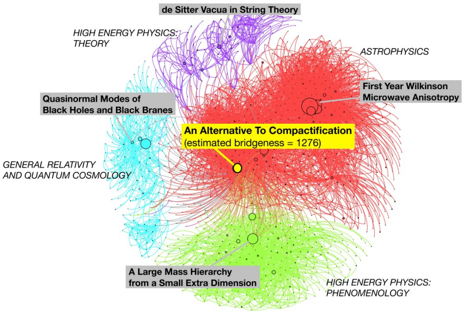

Fig. 1. The discovered community structure in a subgraph of the arXiv citation network (21). The figure shows the top four link communities that include citations to "An alternative to compactification" (22), an article that bridges several communities. We visualize the links between the articles and show some highly cited titles. Each community is labeled with its dominant subject area; nodes are sized by their bridgeness (39), an inferred measure of their impact on multiple communities. This is taken from an analysis of the full 575,000 node network.

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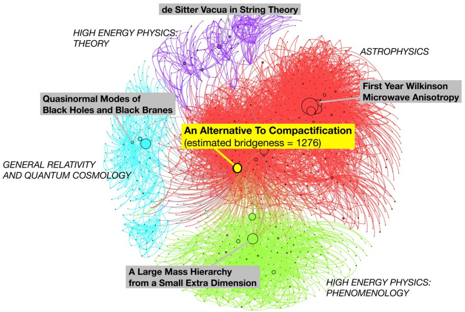

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- Statistical models of graphs can help us solve these problems

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- Some representative models
  - Latent Space Model
  - Stochastic Blockmodel
  - Mixed-Membership Blockmodel (MMSB)

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[†] Latent space approaches to social network analysis (Hoff et al, 2002)

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- Blockmodels and its variants has such properties as we will see next

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Stochastic Blockmodel

- SBM† assumes each node belongs to a cluster/community or "block" (total K clusters)

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- Note: In the fully Bayesian version, π and η can also be given priors

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- Unlike SBM in which node n has a unique one-hot $\boldsymbol{z}_n$ vector, in MMSB, each node n has an interaction-specific cluster assignment

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- A lot of work on scalable Bayesian inference# in these models (e.g., online MCMC/VI)

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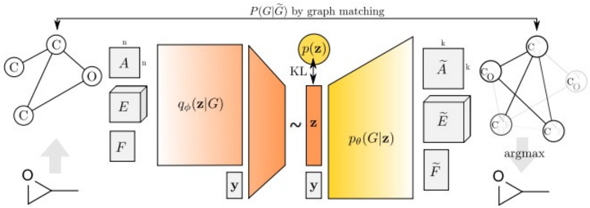
  - Combining classical prob. models of graphs with graph neural nets (e.g., Graph Convolutional Net†)
  - Learning to generate graphs‡ (just like image or text generation in deep learning)



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Nonparametric Bayesian Modeling

(A way of learning the “right” model size/complexity)

Motivating Problem: Mixture Models

- A mixture model can be used to cluster/partition the data into multiple groups
- Defined by K component distributions (e.g., K Gaussians for a Gaussian Mixture Model)
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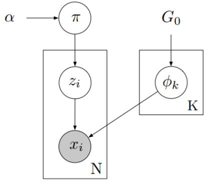
Motivating Problem: Mixture Models

- A mixture model can be used to cluster/partition the data into multiple groups
- Defined by K component distributions (e.g., K Gaussians for a Gaussian Mixture Model)
- Every component distribution $p(\boldsymbol{x}|\phi_k)$ has a mixing weight $\pi_k \in (0,1)$, and $\sum_{k=1}^{K} \pi_k = 1$
- The distribution of any observation $\boldsymbol{x}$

$$p(\boldsymbol{x}|\pi,\phi) = \sum_{k=1}^{K} \pi_k p(\boldsymbol{x}|\phi_k)$$

  where $\pi = \{\pi_k\}_{k=1}^{K}$ and $\phi = \{\phi_k\}_{k=1}^{K}$
- Question: What's the "right" number of clusters? Can do Bayesian model comparison (try different K's and compute marginal likelihood for each choice of K). But that can be expensive.
- How about having a single model but allowing the number of clusters to "grow" with data?

Prelude: A Bayesian Mixture Model (with fixed K)



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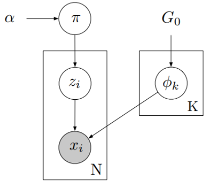

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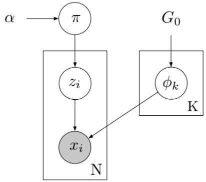

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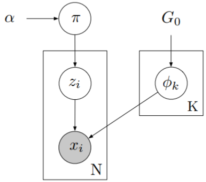

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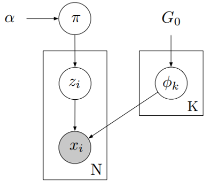

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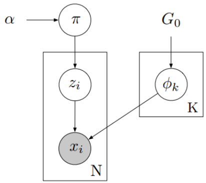

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    - Suppose $\boldsymbol{z}_i = k$. Draw $\boldsymbol{x}_i$ from $p(\boldsymbol{x}|\phi_k)$

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    - Sample each $\boldsymbol{z}_i$ using

$$p(\boldsymbol{z}_i = k|\mathbf{Z}_{-i}, \pi, \phi, \mathbf{X}) \propto p(\boldsymbol{z}_i|\pi) \times p(\boldsymbol{x}_i|\phi_k) = \pi_k \times p(\boldsymbol{x}_i|\phi_k)$$

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    - Sample $\phi_k = (\mu_k, \Sigma_k)$ from NIW posterior given $\mathbf{Z}$ and $\mathbf{X}$ (NIW posterior also has a closed form).

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Nonparametric Bayesian Mixture Model

(.. which you get when you allow unbounded K)

(.. i.e., you allow $K \to \infty$)

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- The probability of $\boldsymbol{x}_i$ being assigned to this new (so far empty) cluster

$$p(\boldsymbol{z}_i = k_{new}|\mathbf{Z}_{-i}, \phi, \mathbf{X}) \propto \alpha \times p(\boldsymbol{x}_i|G_0) \qquad \text{(WHY? Reason on the next slide!)}$$

where $p(\boldsymbol{x}_i|G_0) = \int p(\boldsymbol{x}_i|\phi_{new})p(\phi_{new}|G_0)d\phi_{new}$

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A brief sketch of a basic Gibbs sampler (samples $\mathbf{Z}$ and $\{\phi_k\}_{k=1}^K$) for this model with unbounded K (note: The mixing proportions π_k's were collapsed from the prior $p(\boldsymbol{z}_i|\pi)$)

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A brief sketch of a basic Gibbs sampler (samples $\mathbf{Z}$ and $\{\phi_k\}_{k=1}^K$) for this model with unbounded K (note: The mixing proportions π_k's were collapsed from the prior $p(\boldsymbol{z}_i|\pi)$)

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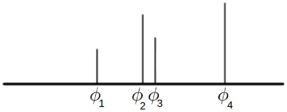
Note: "Markov Chain Sampling Methods for Dirichlet Process Mixture Models" (Neal, 2000) is an excellent reference for various MCMC sampling algorithms for nonparametric Bayesian mixture models (including collapsed versions that don't require sampling for $\{\phi_k\}_{k=1}^K$

Nonparametric Bayesian Mixture Models (A More Formal Perspective..)

A Gentle Start: A Discrete Distribution

- Assume some space Ω (e.g., the real line) and K "locations" $\phi_1, \ldots, \phi_K$ in that space



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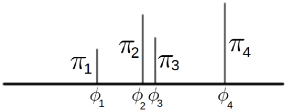

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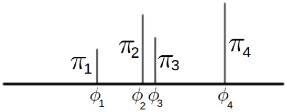

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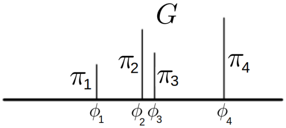

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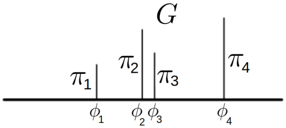

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- Important: The support of this discrete distribution G is $\{\phi_k\}_{k=1}^{K}$

A Bayesian Construction of G

- Let's define appropriate priors on $\{\phi_k\}_{k=1}^K$ and $\{\pi_k\}_{k=1}^K$

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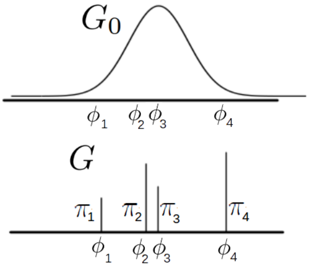

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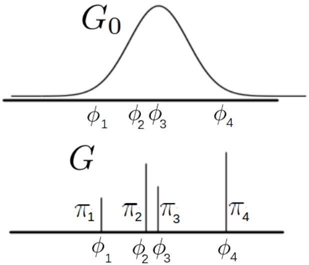
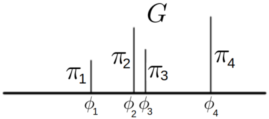


- Note that G is now a random distribution (or a random measure)

Discrete Distributions Induce Clustering!

- Drawing values repeatedly from a discrete distribution leads to repetitions



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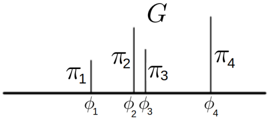

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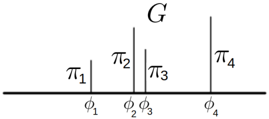

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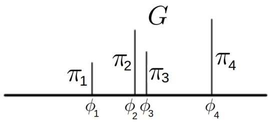

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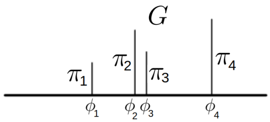

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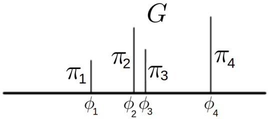

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- Therefore G can be used in a mixture model where θ_i's define the params of mixture distributions

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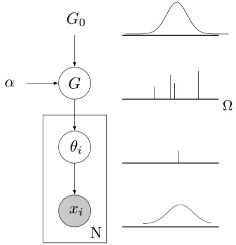

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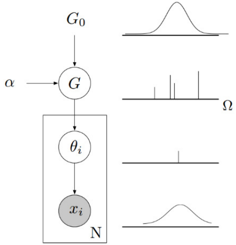

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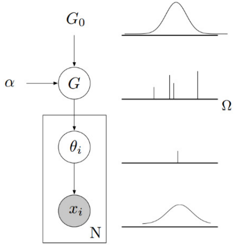

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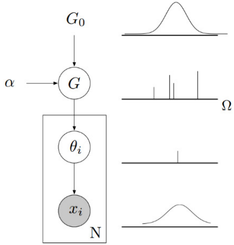

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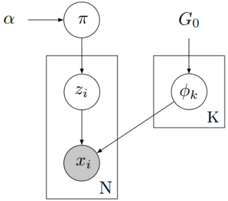
  - Thus effectively the data is generated from not N separate distributions but only $K < N$ unique distributions $\{p(\boldsymbol{x}|\phi_k)\}_{k=1}^K$, which naturally results in a clustering of data

Two Equivalent Views

View-1 (the familiar one!): Clustering is explicitly described by the indicator $\boldsymbol{z}_i$

$$
\begin{aligned}
\pi &\sim \text{Dirichlet}(\alpha/K, \ldots, \alpha/K) \\
\phi_k &\sim G_0 \\
z_i &\sim \text{multinoulli}(\pi) \\
\boldsymbol{x}_i &\sim p(x|\phi_k) \text{ if } z_i = k
\end{aligned}
$$



(Equivalent) View-2: Clustering is implicit (non-uniqueness of θ_i's denotes clustering of $\boldsymbol{x}_i$'s)

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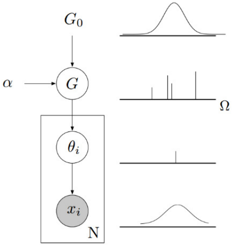

An Infinite Mixture Model

- Recall that our Bayesian mixture model construction for the finite K was

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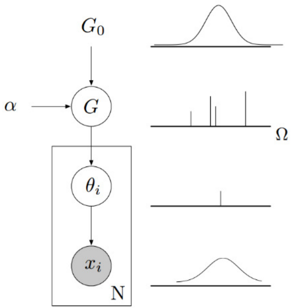

- To get a mixture model with unbounded number of cluster, we need G of the form

$$G = \sum_{k=1}^{\infty} \pi_k \delta_{\phi_k}$$

- How can we formally construct such a G that has potentially infinite mixture components?

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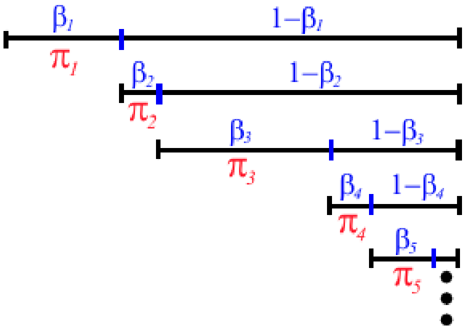
$$\begin{aligned}
\beta_k &\sim \text{Beta}(1,\alpha) \qquad k = 1,\ldots,\infty \\
\pi_1 &= \beta_1 \\
\pi_k &= \beta_k \prod_{\ell=1}^{k-1} (1-\beta_{k-1}) \qquad k = 2,\ldots,\infty
\end{aligned}$$

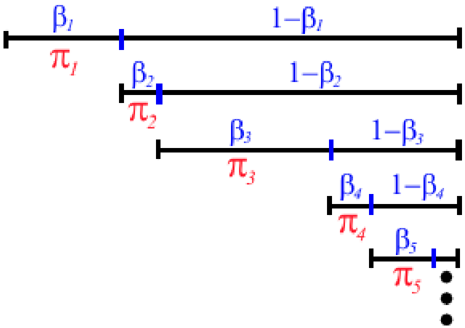
The Stick-Breaking Construction

- Assume a stick of length 1 to begin with. Now recursively break it as follows:
  - Choose a random location $\beta_k \in (0,1)$ drawn from $\text{Beta}(1,\alpha)$ at which to break the stick
  - Record π_k as "β_k times the length of the remaining stick"



The Stick-Breaking Construction

- Assume a stick of length 1 to begin with. Now recursively break it as follows:
  - Choose a random location $\beta_k \in (0, 1)$ drawn from $\text{Beta}(1, \alpha)$ at which to break the stick
  - Record π_k as "β_k times the length of the remaining stick"



- Can show that $\sum_{k=1}^{K} \pi_k = 1$ as $K \to \infty$. One easy way to verify this is by showing that $1 - \sum_{k=1}^{K} \pi_k \to 0$ as $K \to \infty$

Next Class

- Some other (equivalent) ways of looking at nonparametric Bayesian mixture models
  - Dirichlet Process
  - Chinese Restaurant Process
  - Pólya-Urn Scheme
  - Hierarchical Dirichlet Process
- Some other examples of nonparametric Bayesian models