# Applied Nonparametric Bayes

Michael I. Jordan

*Department of Electrical Engineering and Computer Science*
*Department of Statistics*
*University of California, Berkeley*

**http://www.cs.berkeley.edu/∼jordan**

*Acknowledgments*: Yee Whye Teh, Romain Thibaux, Erik Sudderth

# Computer Science and Statistics

- Separated in the 40's and 50's, but merging in the 90's and 00's
- What computer science has done well: data structures and algorithms for manipulating data structures
- What statistics has done well: managing uncertainty and justification of algorithms for making decisions under uncertainty
- What machine learning attempts to do: hasten the merger along
  - machine learning isn't a new field per se

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- What computer science has done well: data structures and algorithms for manipulating data structures
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- What machine learning attempts to do: hasten the merger along
  - machine learning isn't a new field per se
- An issue to be grappled with: the two flavors of statistical inference (frequentist and Bayesian)

# Nonparametric Bayesian Inference (Theme I)

- At the core of Bayesian inference lies Bayes' theorem:

$$posterior \propto likelihood \times prior$$

- For parametric models, we let $\theta$ be a Euclidean parameter and write:

$$p(\theta|x) \propto p(x|\theta)p(\theta)$$

- For nonparametric models, we let $G$ be a general stochastic process (an "infinite-dimensional random variable") and write:

$$p(G|x) \propto p(x|G)p(G)$$

which frees us to work with flexible data structures

# Nonparametric Bayesian Inference (cont)

- Examples of stochastic processes we'll mention today include distributions on:
  - directed trees of unbounded depth and unbounded fan-out
  - partitions
  - sparse binary infinite-dimensional matrices
  - copulae
  - distributions
- General mathematical tool: completely random processes

# Hierarchical Bayesian Modeling (Theme II)

- Hierarchical modeling is a key idea in Bayesian inference
- It's essentially a form of recursion
  - in the parametric setting, it just means that priors on parameters can themselves be parameterized
  - in our nonparametric setting, it means that a stochastic process can have as a parameter another stochastic process
- We'll use hierarchical modeling to build structured objects that are reminiscent of graphical models—but are nonparametric
  - statistical justification—the freedom inherent in using nonparametrics needs the extra control of the hierarchy

# What are "Parameters"?

- *Exchangeability*: invariance to permutation of the joint probability distribution of infinite sequences of random variables

  **Theorem (De Finetti, 1935).** *If* $(x_1, x_2, \ldots)$ *are infinitely exchangeable, then the joint probability* $p(x_1, x_2, \ldots, x_N)$ *has a representation as a mixture*:

  $$p(x_1, x_2, \ldots, x_N) = \int \left( \prod_{i=1}^{N} p(x_i \,|\, G) \right) dP(G)$$

  *for some random element* $G$.

- The theorem would be false if we restricted ourselves to finite-dimensional $G$

# Computational Consequences

- Having infinite numbers of parameters is a good thing; it avoids placing artificial limits on what one can learn
- But how do we compute with infinite numbers of parameters?
- Important relationships to combinatorics

# Stick-Breaking

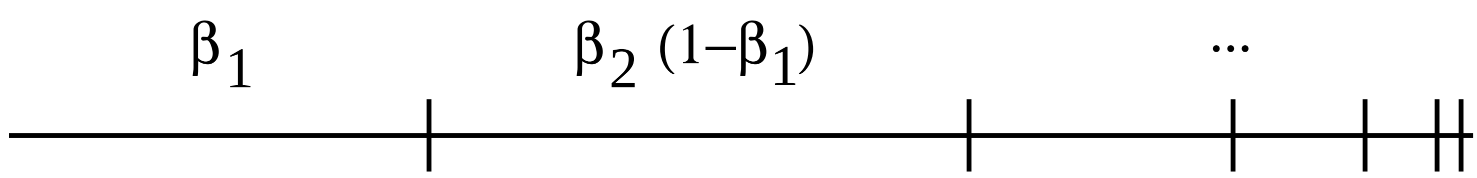
- A general way to obtain distributions on countably infinite spaces
- *A canonical example*: Define an infinite sequence of beta random variables:

$$\beta_k \sim \mathrm{Beta}(1, \alpha_0) \qquad\qquad k = 1, 2, \ldots$$

- And then define an infinite random sequence as follows:

$$\pi_1 = \beta_1, \qquad \pi_k = \beta_k \prod_{l=1}^{k-1} (1 - \beta_l) \qquad\qquad k = 2, 3, \ldots$$

- This can be viewed as breaking off portions of a stick:



# Constructing Random Measures

- It's not hard to see that $\sum_{k=1}^{\infty} \pi_k = 1$ (with probability one)

- Now define the following object:

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

  where $\phi_k$ are independent draws from a distribution $G_0$ on some space

- Because $\sum_{k=1}^{\infty} \pi_k = 1$, $G$ is a probability measure—it is a random measure

- The distribution of $G$ is known as a Dirichlet process: $G \sim \mathrm{DP}(\alpha_0, G_0)$

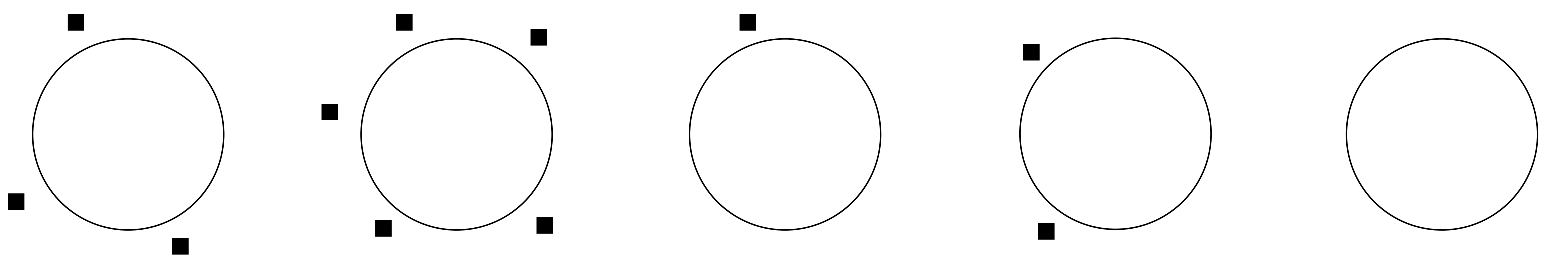
- What exchangeable marginal distribution does this yield when integrated against in the De Finetti setup?

# Chinese Restaurant Process (CRP)

- A random process in which $n$ customers sit down in a Chinese restaurant with an infinite number of tables
  - first customer sits at the first table
  - $m$th subsequent customer sits at a table drawn from the following distribution:

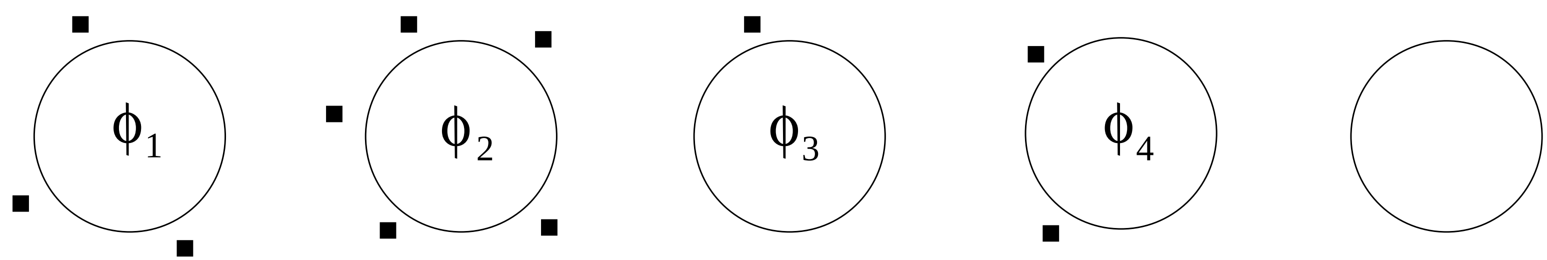
$$\begin{aligned} P(\text{previously occupied table } i \,|\, \mathcal{F}_{m-1}) &\propto n_i \\ P(\text{the next unoccupied table} \,|\, \mathcal{F}_{m-1}) &\propto \alpha_0 \end{aligned} \tag{1}$$

where $n_i$ is the number of customers currently at table $i$ and where $\mathcal{F}_{m-1}$ denotes the state of the restaurant after $m-1$ customers have been seated



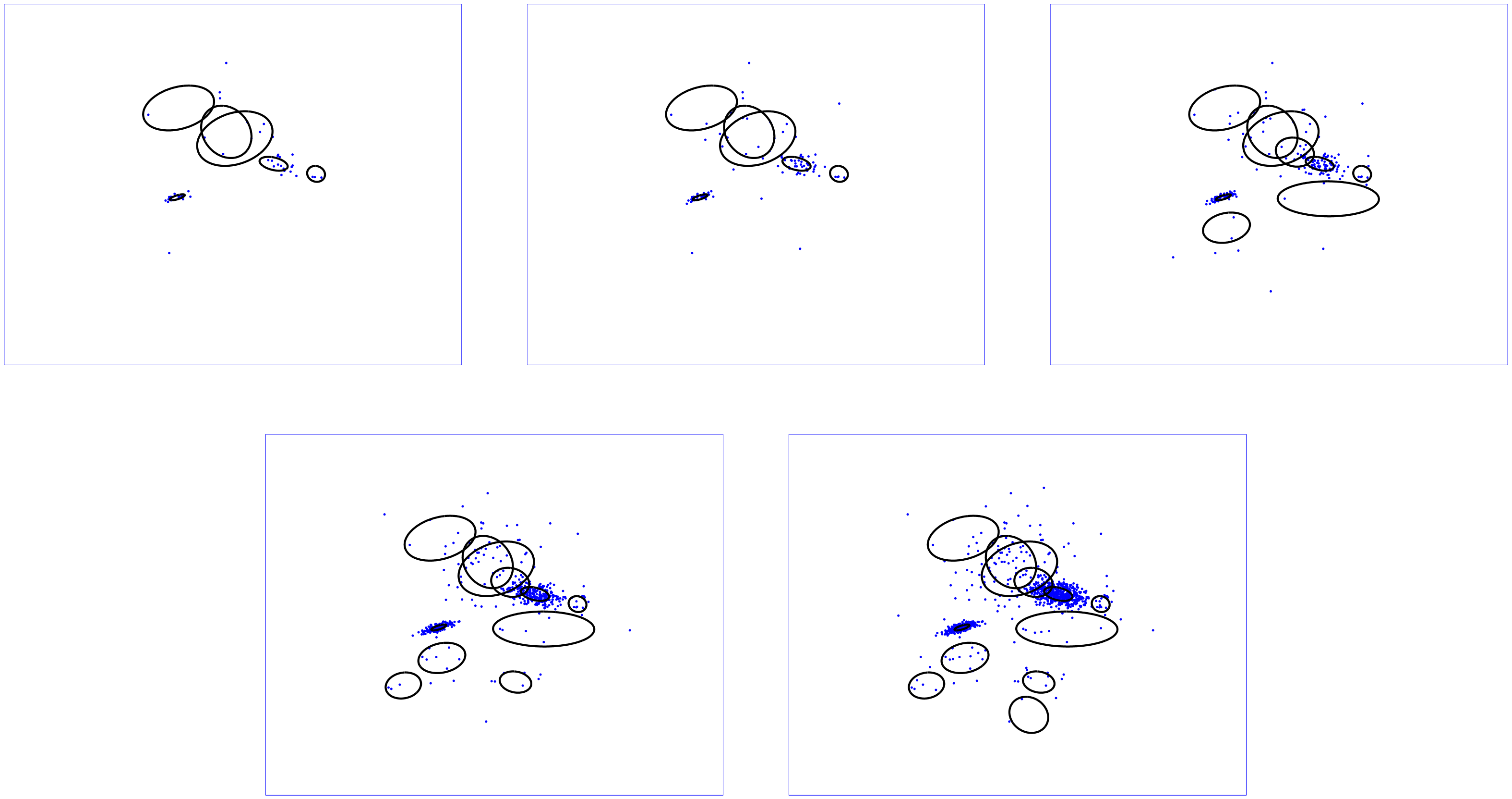
# The CRP and Clustering

- Data points are customers; tables are clusters
  - the CRP defines a prior distribution on the partitioning of the data and on the number of tables
- This prior can be completed with:
  - a likelihood—e.g., associate a parameterized probability distribution with each table
  - a prior for the parameters—the first customer to sit at table $k$ chooses the parameter vector for that table ($\phi_k$) from a prior $G_0$




- So we now have a distribution—or can obtain one—for any quantity that we might care about in the clustering setting

# CRP Prior, Gaussian Likelihood, Conjugate Prior



$$\phi_k = (\mu_k, \Sigma_k) \sim N(a,b) \otimes IW(\alpha, \beta)$$

$$x_i \sim N(\phi_k)$$ for a data point $i$ sitting at table $k$

# Posterior Inference for the CRP

- We've described how to generate data from the model; how do we go backwards and generate a model from data?
- A wide variety of variational, combinatorial and MCMC algorithms have been developed
- E.g., a Gibbs sampler is readily developed by using the fact that the Chinese restaurant process is exchangeable
  - to sample the table assignment for a given customer given the seating of all other customers, simply treat that customer as the last customer to arrive
  - in which case, the assignment is made proportional to the number of customers already at each table (cf. preferential attachment)
  - parameters are sampled at each table based on the customers at that table (cf. K means)
- (This isn't the state of the art, but it's easy to explain on one slide)

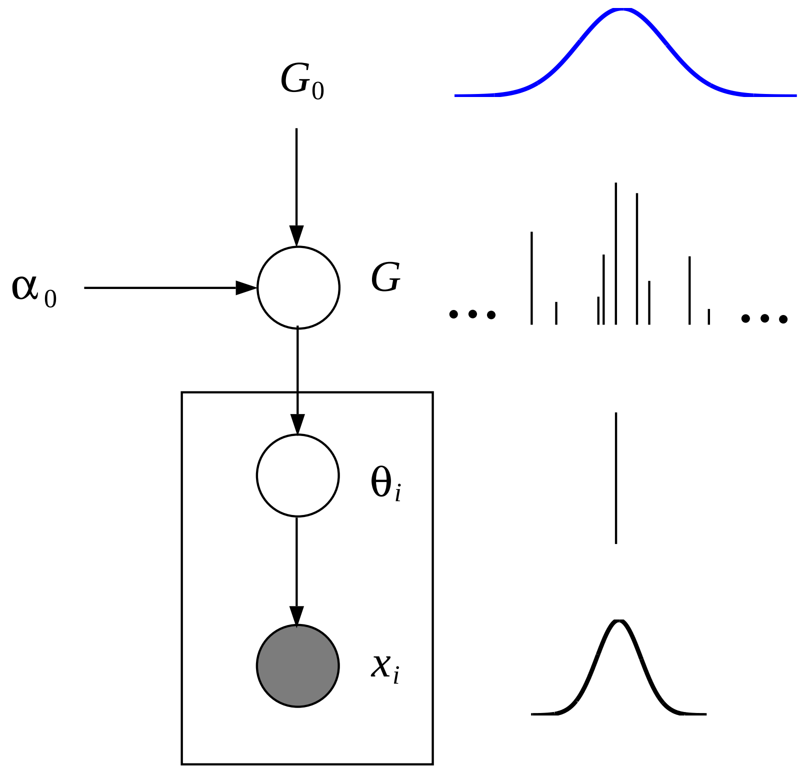
# Exchangeability

- As a prior on the partition of the data, the CRP is exchangeable
- The prior on the parameter vectors associated with the tables is also exchangeable
- The latter probability model is generally called the Pólya urn model. Letting $\theta_i$ denote the parameter vector associated with the $i$th data point, we have:

$$\theta_i \,|\, \theta_1, \ldots, \theta_{i-1} \;\sim\; \alpha_0 G_0 + \sum_{j=1}^{i-1} \delta_{\theta_j}$$

- From these conditionals, a short calculation shows that the joint distribution for $(\theta_1, \ldots, \theta_n)$ is invariant to order (this is the exchangeability proof)
- As a prior on the number of tables, the CRP is nonparametric—the number of occupied tables grows (roughly) as $O(\log n)$—we're in the world of nonparametric Bayes

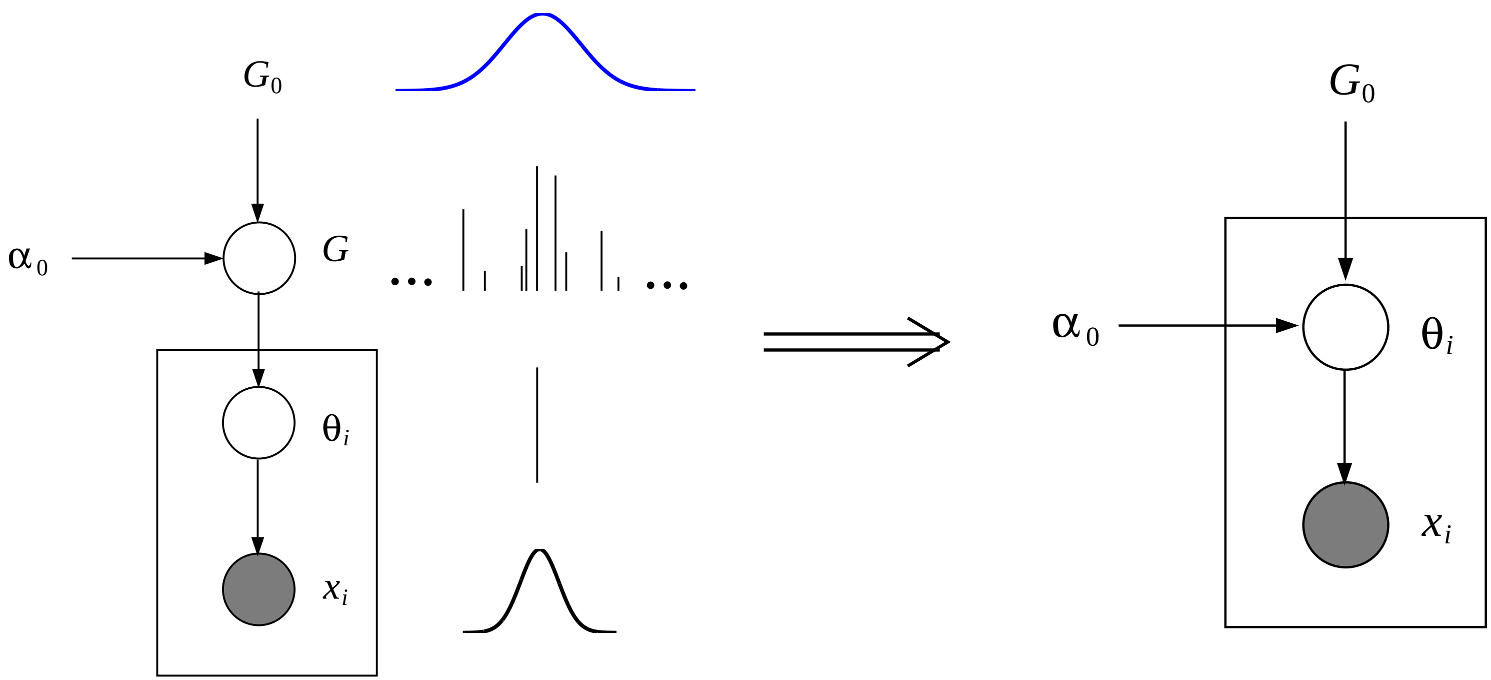
# Dirichlet Process Mixture Models




$$
\begin{aligned}
G &\sim \mathrm{DP}(\alpha_0 G_0) \\
\theta_i \,|\, G &\sim G \qquad\qquad\quad i \in 1, \ldots, n \\
x_i \,|\, \theta_i &\sim F(x_i \,|\, \theta_i) \qquad i \in 1, \ldots, n
\end{aligned}
$$

# Marginal Probabilities

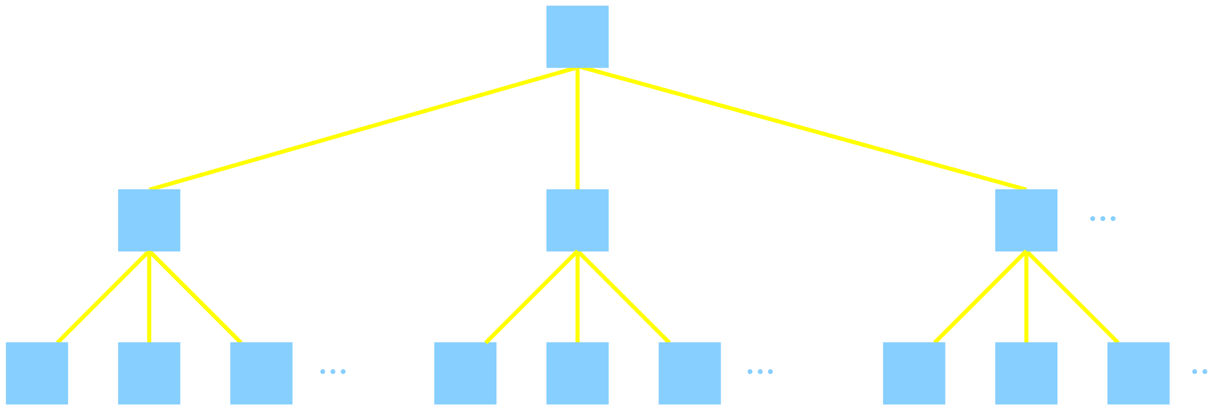
- To obtain the marginal probability of the parameters $\theta_1, \theta_2, \ldots$, we need to integrate out $G$




- This marginal distribution turns out to be the Chinese restaurant process (more precisely, it's the Pólya urn model)

# The Nested CRP

(Blei, Griffiths, & Jordan, 2009)



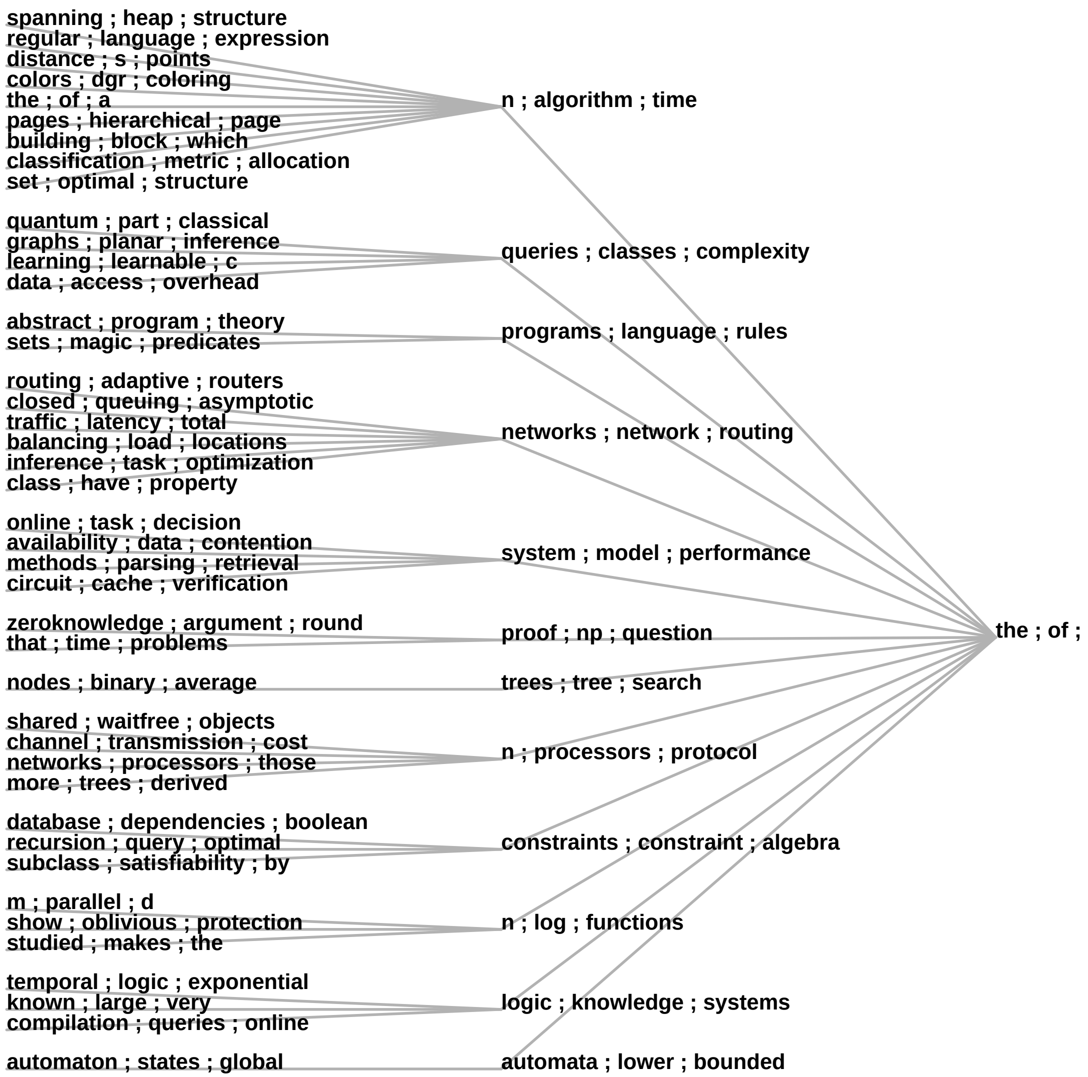
- Each node in the tree is an entire Chinese restaurant
- Each table in a given restaurant points to another restaurant
- A customer starts at the root and selects a table, which leads to another restaurant, and the process repeats infinitely often
- We obtain a measure on trees of unbounded depth and unbounded branching factors—the nested CRP

# Hierarchical Topic Models

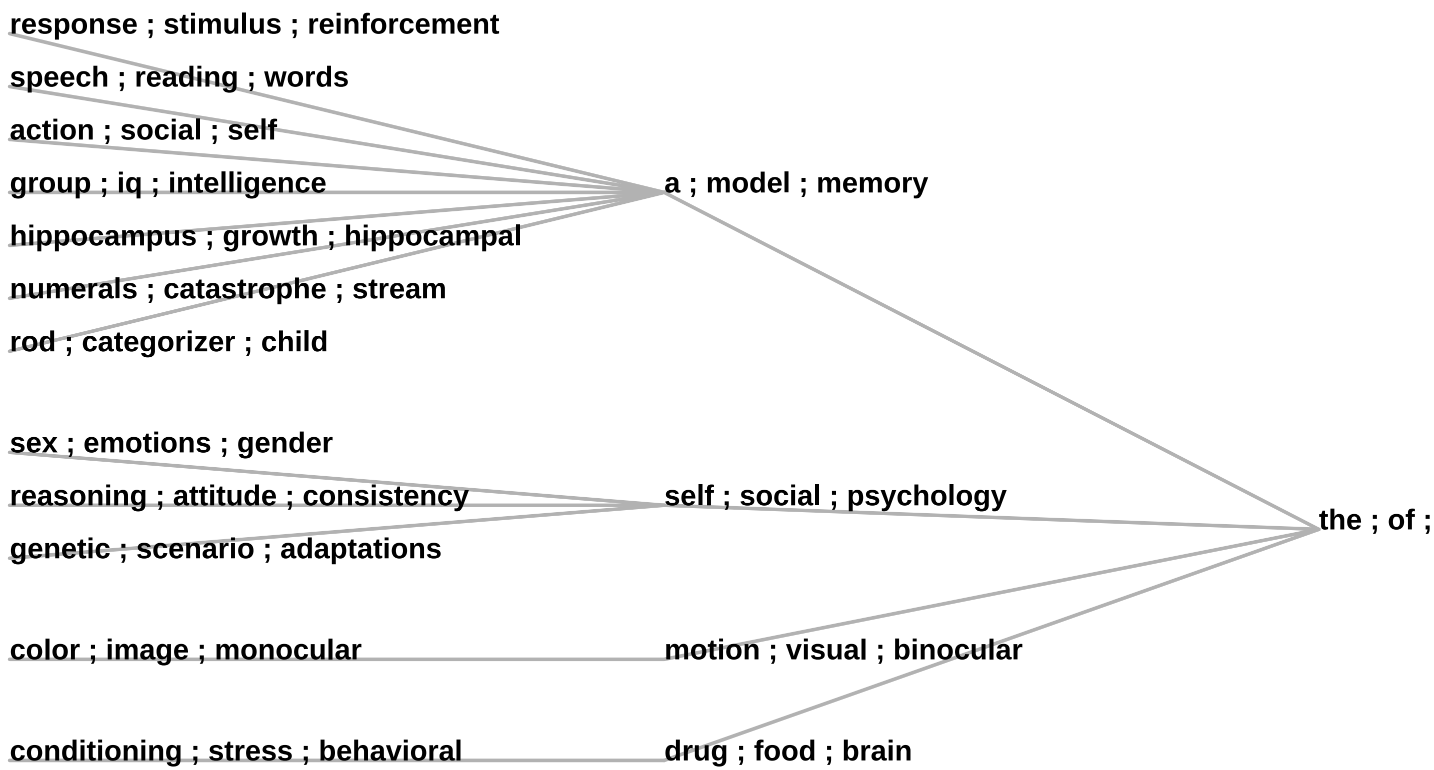
(Blei, Griffiths, & Jordan, 2008)

- The nested CRP defines a distribution over paths in a tree
- At every node in the tree place a distribution on words (a "topic") drawn from a prior over the vocabulary
- To generate a document:
  - pick a path down the infinite tree using the nested CRP
  - repeatedly
    - pick a level using the stick-breaking distribution
    - select a word from the topic at the node at that level in the tree

# Topic Hierarchy from *JACM*

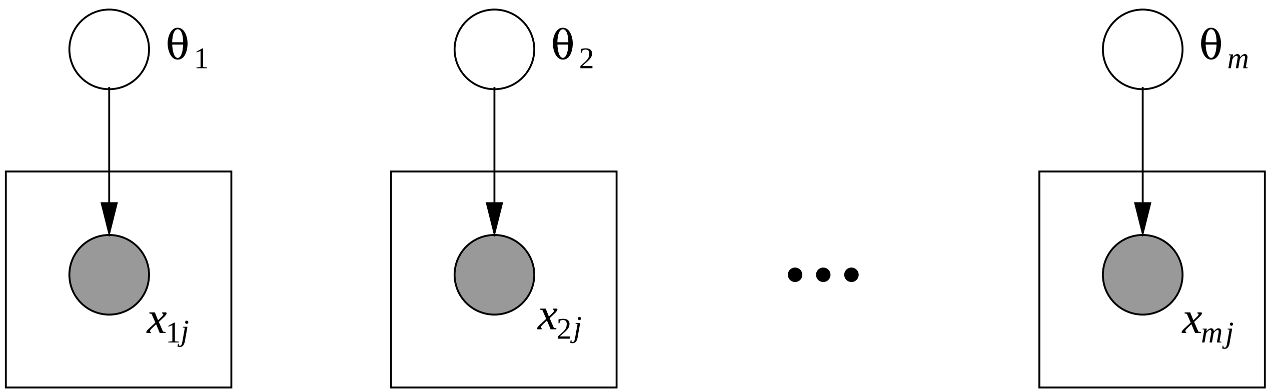


# Topic Hierarchy from *Psychology Today*



# Multiple Estimation Problems

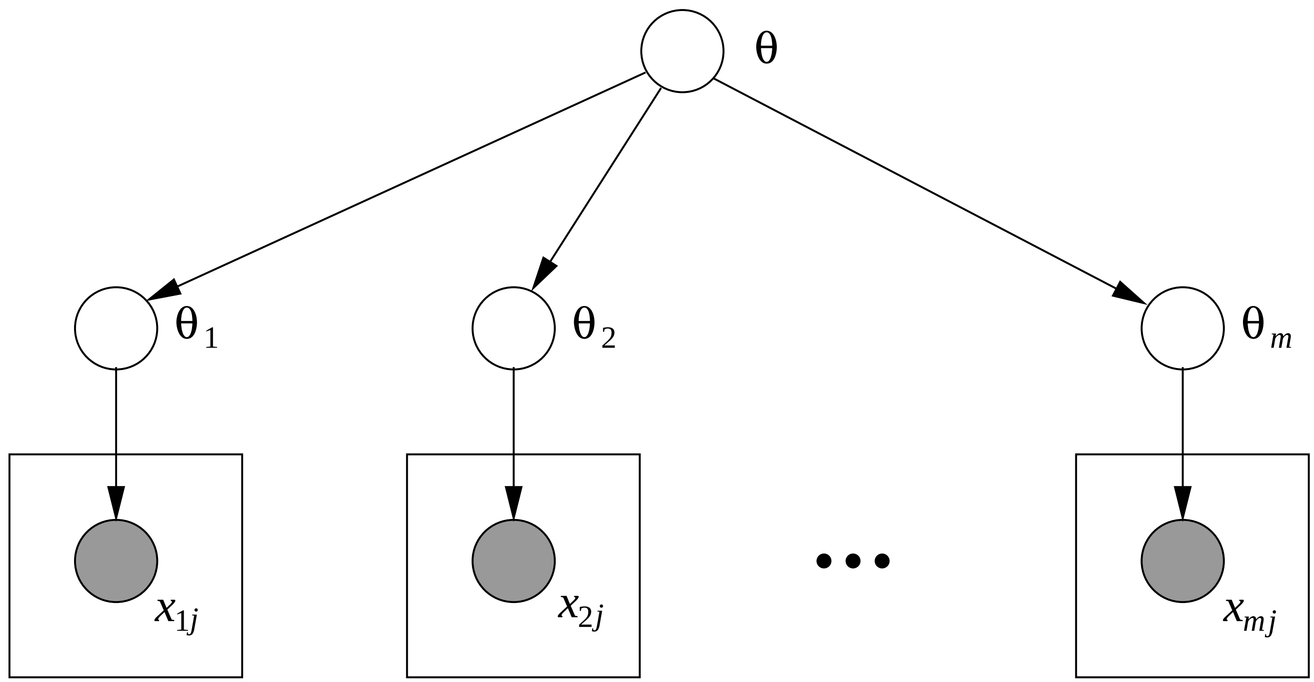
- We often face multiple, related estimation problems
- E.g., multiple Gaussian means: $x_{ij} \sim N(\theta_i, \sigma_i^2)$




- Maximum likelihood: $\hat{\theta}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij}$
- Maximum likelihood often doesn't work very well
  - want to "share statistical strength" (i.e., "smooth")

# Hierarchical Bayesian Approach

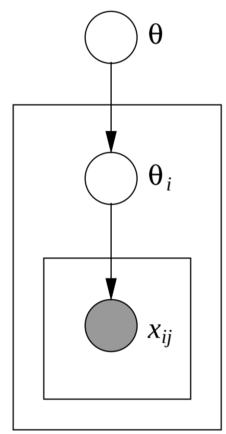
- The Bayesian or empirical Bayesian solution is to view the parameters $\theta_i$ as random variables, sampled from an underlying variable $\theta$



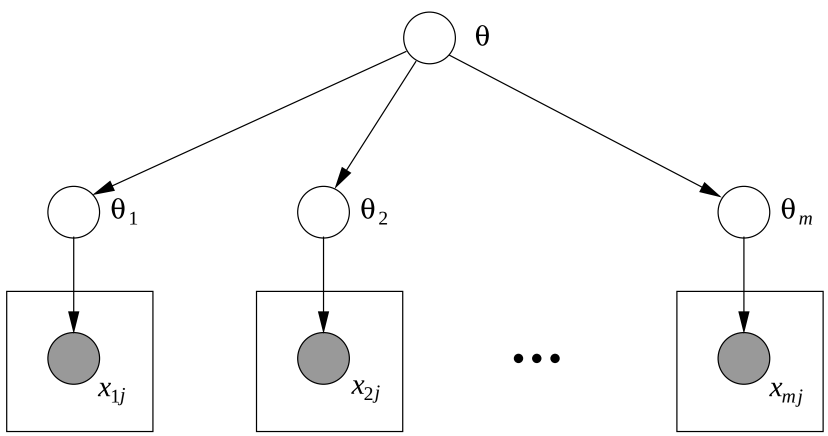

- Given this overall model, posterior inference yields *shrinkage*—the posterior mean for each $\theta_k$ combines data from all of the groups

# Hierarchical Modeling

- Recall the plate notation:




- Equivalent to:

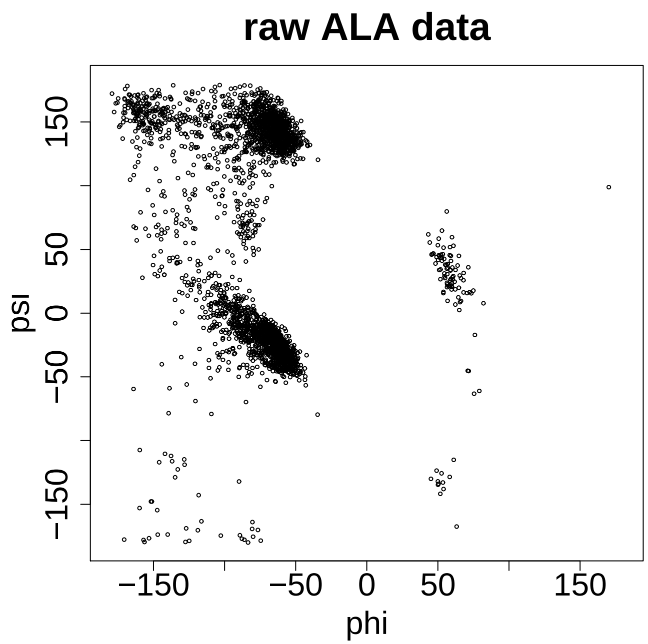


# Multiple Clustering Problems

- Suppose that we have $M$ groups of data, each of which is to be clustered
- Suppose that the groups are related, so that evidence for a cluster in one group should be transferred to other groups
- But the groups also differ in some ways, so we shouldn't lump the data together
- How do we solve the multiple group clustering problem?
- How do we solve problem when the number of clusters is unknown (within groups and overall)?

# Protein Folding

- A protein is a folded chain of amino acids
- The backbone of the chain has two degrees of freedom per amino acid (phi and psi angles)
- Empirical plots of phi and psi angles are called *Ramachandran diagrams*



# Protein Folding (cont.)

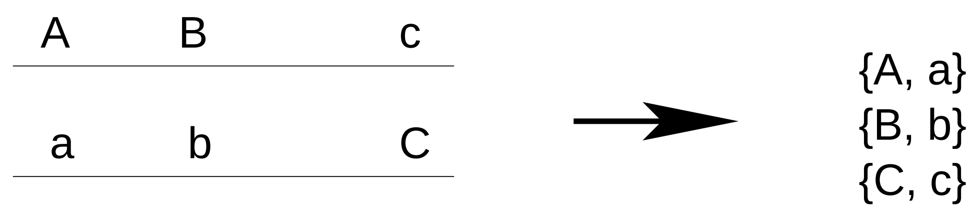
- We want to model the density in the Ramachandran diagram to provide an energy term for protein folding algorithms

- We actually have a linked set of Ramachandran diagrams, one for each amino acid neighborhood

- We thus have a linked set of clustering problems
  - note that the data are *partially exchangeable*

# Haplotype Modeling

- Consider $M$ binary markers in a genomic region
- There are $2^M$ possible haplotypes—i.e., states of a single chromosome
  - but in fact, far fewer are seen in human populations
- A genotype is a set of unordered pairs of markers (from one individual)



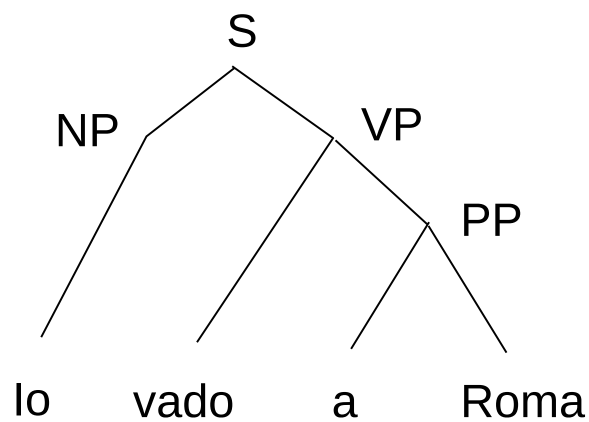

- Given a set of genotypes (multiple individuals), estimate the underlying haplotypes
- This is a clustering problem

# Haplotype Modeling (cont.)

- A key problem is inference for the number of clusters
- Consider now the case of multiple groups of genotype data (e.g., ethnic groups)
- Geneticists would like to find clusters within each group but they would also like to share clusters between the groups

# Natural Language Parsing

- Given a corpus of sentences, some of which have been parsed by humans, find a grammar that can be used to parse future sentences

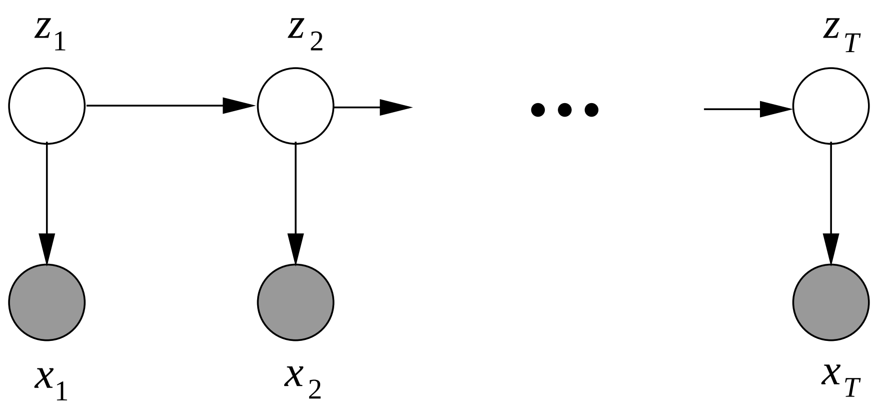



- Much progress over the past decade; state-of-the-art methods are statistical

# Natural Language Parsing (cont.)

- Key idea: *lexicalization* of context-free grammars
  - the grammatical rules (S $\rightarrow$ NP VP) are conditioned on the specific lexical items (words) that they derive
- This leads to huge numbers of potential rules, and (adhoc) shrinkage methods are used to control the counts
- Need to control the numbers of clusters (model selection) in a setting in which many tens of thousands of clusters are needed
- Need to consider related groups of clustering problems (one group for each grammatical context)

# Nonparametric Hidden Markov Models




- An open problem—how to work with HMMs and state space models that have an unknown and unbounded number of states?

- Each row of a transition matrix is a probability distribution across "next states"

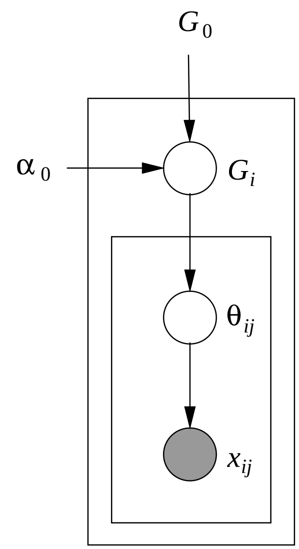
- We need to estimation these transitions in a way that links them across rows

# Image Segmentation

- Image segmentation can be viewed as inference over partitions
  - clearly we want to be nonparametric in modeling such partitions
- Standard approach—use relatively simple (parametric) local models and relatively complex spatial coupling
- Our approach—use a relatively rich (nonparametric) local model and relatively simple spatial coupling
  - for this to work we need to combine information across images; this brings in the hierarchy

# Hierarchical Nonparametrics—A First Try

- Idea: Dirichlet processes for each group, linked by an underlying $G_0$:




- Problem: the atoms generated by the random measures $G_i$ will be distinct
  - i.e., the atoms in one group will be distinct from the atoms in the other groups—no sharing of clusters!

- Sometimes ideas that are fine in the parametric context fail (completely) in the nonparametric context... :-(

# Hierarchical Dirichlet Processes

(Teh, Jordan, Beal & Blei, 2006)

- We need to have the base measure $G_0$ be discrete
  - but also need it to be flexible and random

# Hierarchical Dirichlet Processes

(Teh, Jordan, Beal & Blei, 2006)

- We need to have the base measure $G_0$ be discrete
  - but also need it to be flexible and random
- The fix: Let $G_0$ itself be distributed according to a DP:

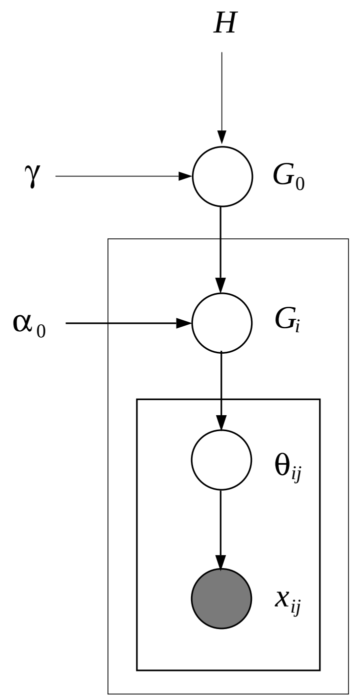
$$G_0 \,|\, \gamma, H \;\sim\; \mathrm{DP}(\gamma H)$$

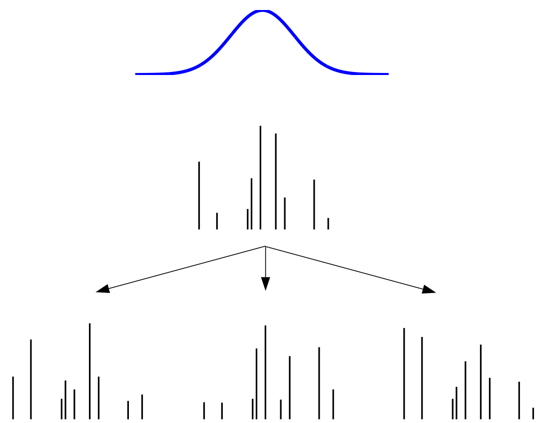
- Then

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

  has as its base measure a (random) atomic distribution—samples of $G_j$ will resample from these atoms

# Hierarchical Dirichlet Process Mixtures

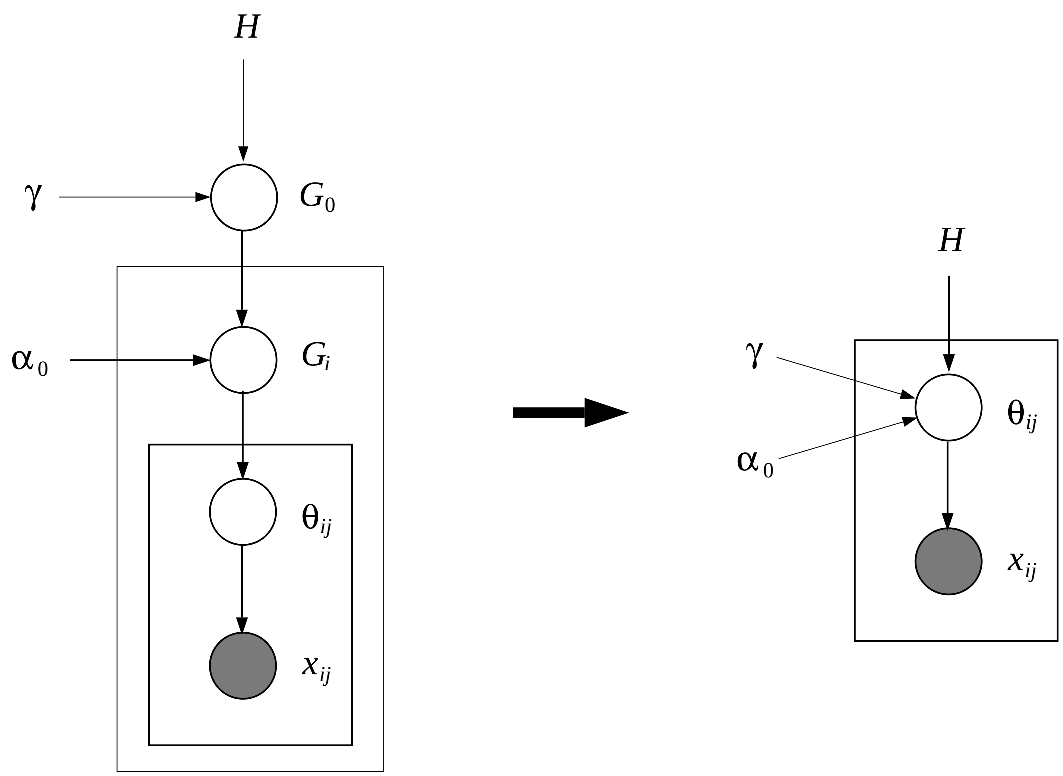


$$
\begin{aligned}
G_0 \mid \gamma, H &\sim \mathrm{DP}(\gamma H) \\
G_i \mid \alpha, G_0 &\sim \mathrm{DP}(\alpha_0 G_0) \\
\theta_{ij} \mid G_i &\sim G_i \\
x_{ij} \mid \theta_{ij} &\sim F(x_{ij}, \theta_{ij})
\end{aligned}
$$

# Chinese Restaurant Franchise (CRF)

- First integrate out the $G_i$, then integrate out $G_0$



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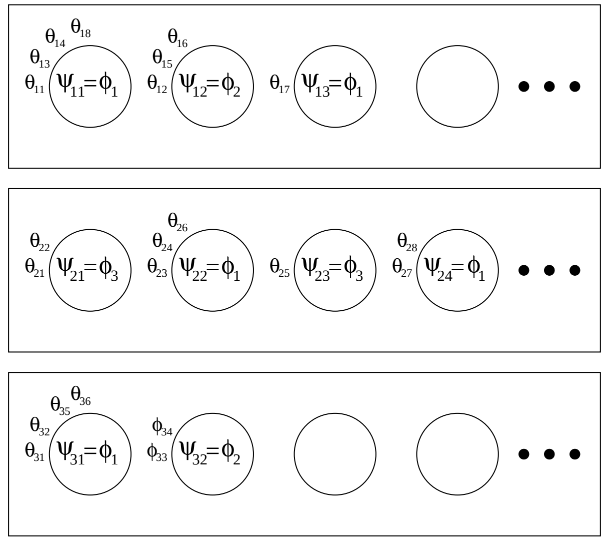
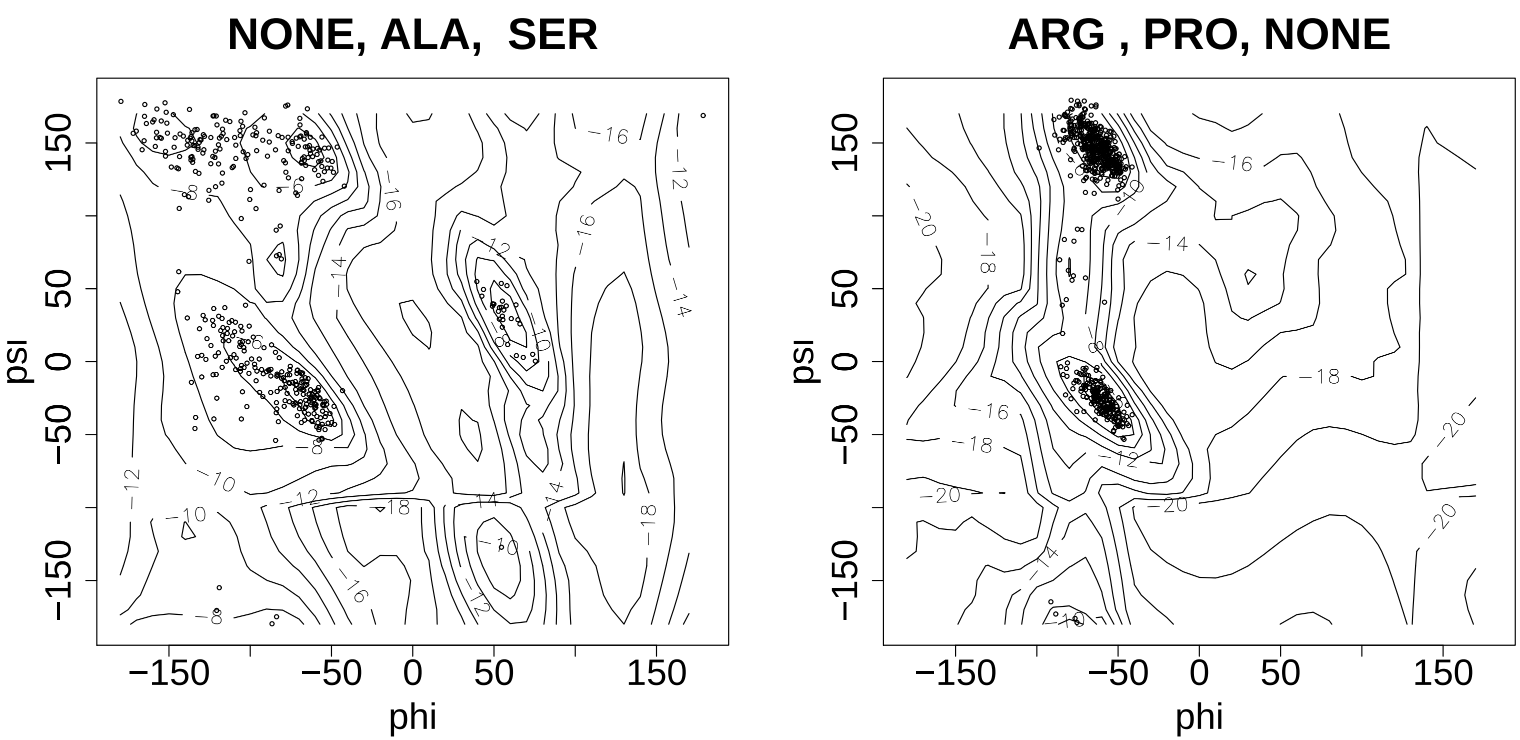


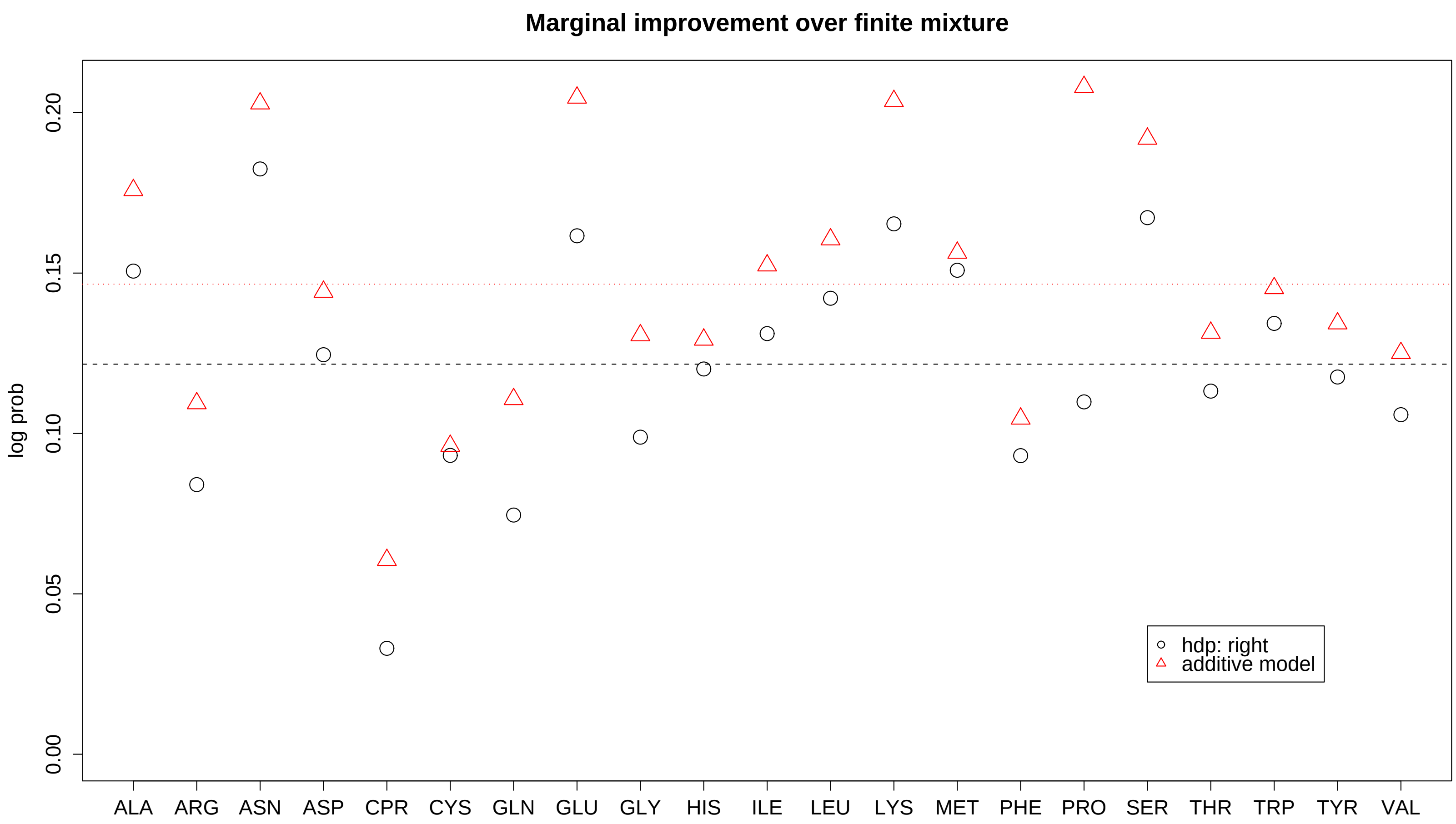

- To each group there corresponds a *restaurant*, with an unbounded number of *tables* in each restaurant
- There is a global *menu* with an unbounded number of *dishes* on the menu
- The first customer at a table selects a dish for that table from the global menu
- Reinforcement effects—customers prefer to sit at tables with many other customers, and prefer to choose dishes that are chosen by many other customers

# Protein Folding (cont.)

- We have a linked set of Ramachandran diagrams, one for each amino acid neighborhood



# Protein Folding (cont.)



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- Key idea: *lexicalization* of context-free grammars
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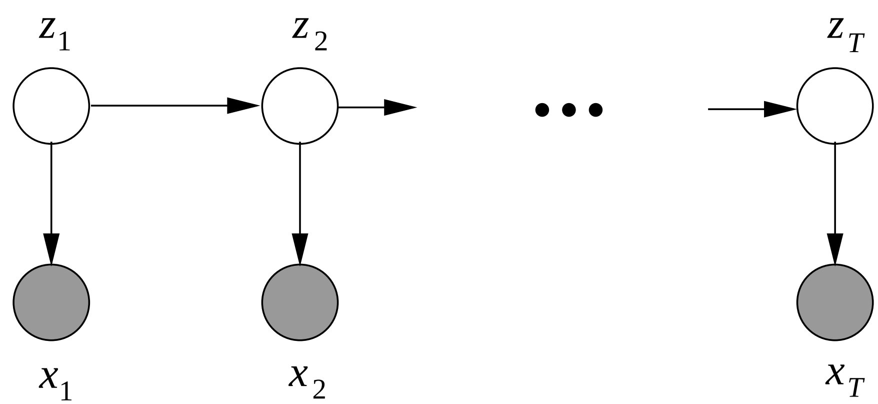
# HDP-PCFG

(Liang, Petrov, Jordan & Klein, 2007)

- Based on a training corpus, we build a lexicalized grammar in which the rules are based on word clusters
- Each grammatical context defines a clustering problem, and we link the clustering problems via the HDP

| T | PCFG | | HDP-PCFG | |
|---|---|---|---|---|
| | $F_1$ | Size | $F_1$ | Size |
| 1 | 60.4 | 2558 | 60.5 | 2557 |
| 4 | 76.0 | 3141 | 77.2 | 9710 |
| 8 | 74.3 | 4262 | 79.1 | 50629 |
| 16 | 66.9 | 19616 | 78.2 | 151377 |
| 20 | 64.4 | 27593 | 77.8 | 202767 |

# Nonparametric Hidden Markov models



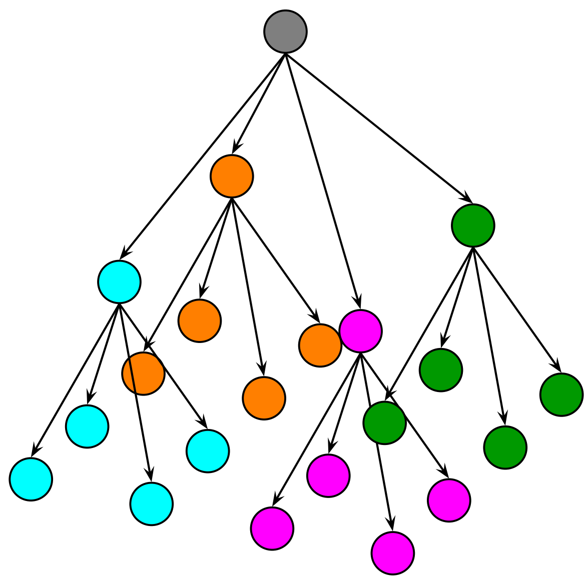

- A perennial problem—how to work with HMMs that have an unknown and unbounded number of states?

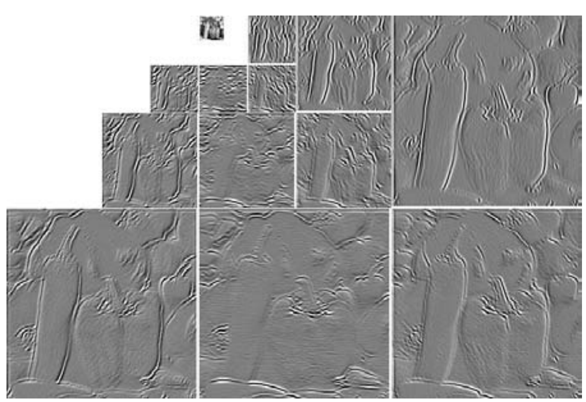
- A straightforward application of the HDP framework
  - multiple mixture models—one for each value of the "current state"
  - the DP creates new states, and the HDP approach links the transition distributions

# Nonparametric Hidden Markov Trees

(Kivinen, Sudderth & Jordan, 2007)

- Hidden Markov trees in which the cardinality of the states is unknown a priori
- We need to tie the parent-child transitions across the parent states; this is done with the HDP





# Nonparametric Hidden Markov Trees (cont.)

- Local Gaussian Scale Mixture (31.84 dB)

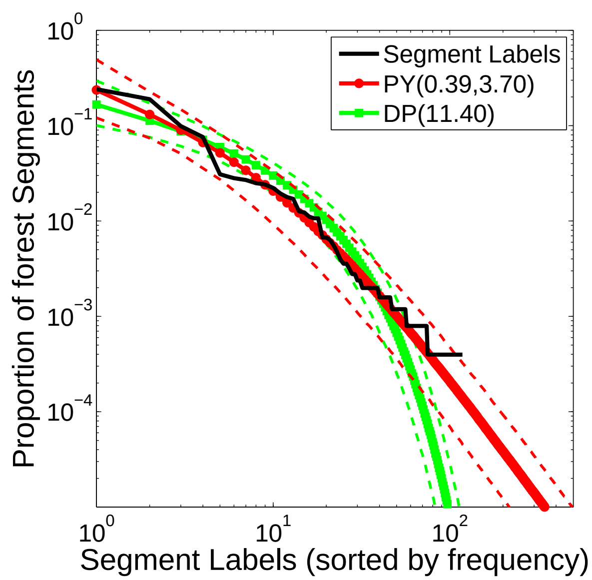
# Nonparametric Hidden Markov Trees (cont.)

- Hierarchical Dirichlet Process Hidden Markov Tree (32.10 dB)

# Image Segmentation

(Sudderth & Jordan, 2009)

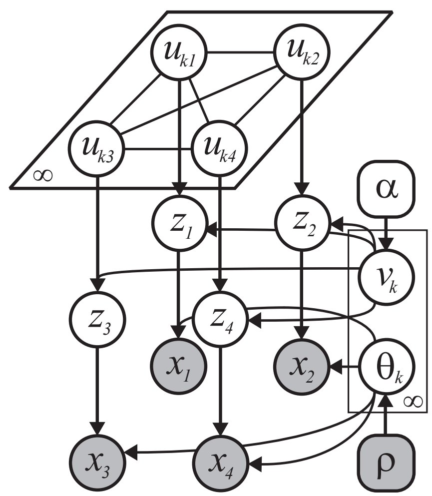
- Image segmentation can be viewed as inference over partitions
- Image statistics are better captured by the Pitman-Yor stick-breaking processes than by the Dirichlet process
  - Pitman-Yor is based on $\mathrm{Beta}(1-\gamma_1, \gamma_2 + k\gamma_1)$ instead of $\mathrm{Beta}(1, \alpha)$; this yields power laws



# Image Segmentation (cont)

(Sudderth & Jordan, 2009)

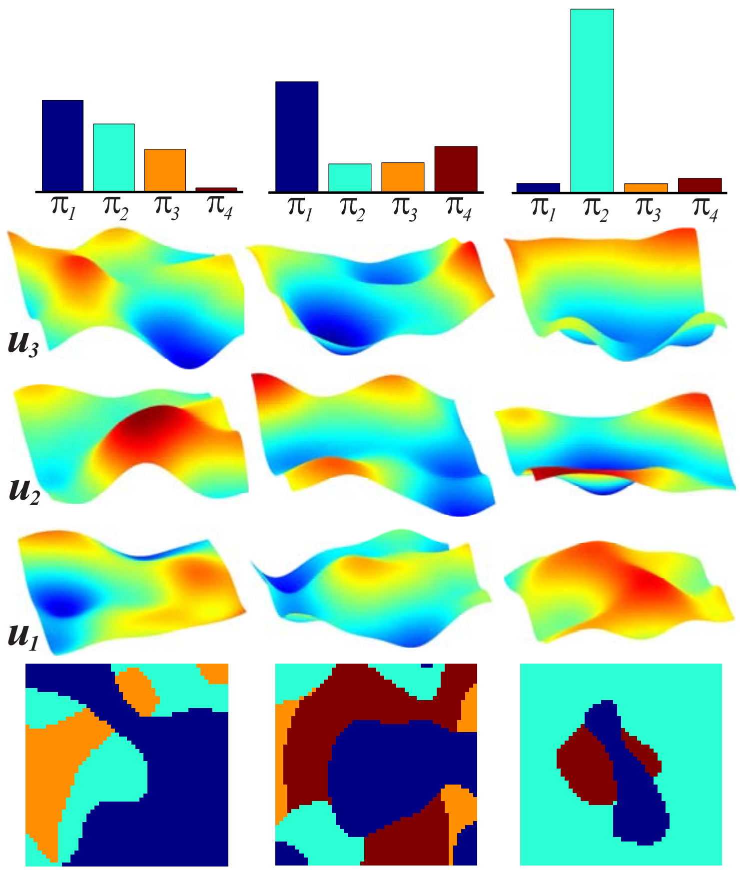
- So we want Pitman-Yor marginals at each site in an image
- The (perennial) problem is how to couple these marginals spatially
  - to solve this problem, we again go nonparametric—we couple the PY marginals using Gaussian process copulae



# Image Segmentation (cont)

(Sudderth & Jordan, 2009)

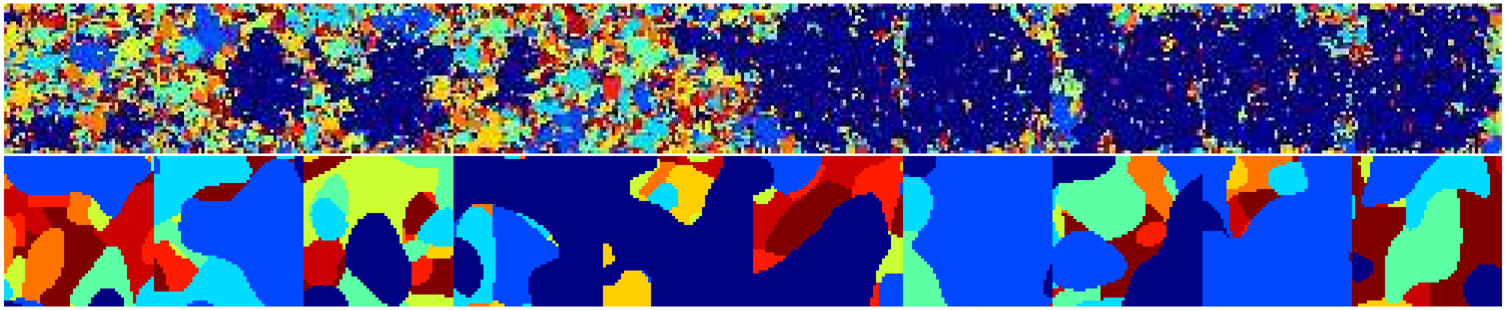
- A sample from the coupled HPY prior:



# Image Segmentation (cont)

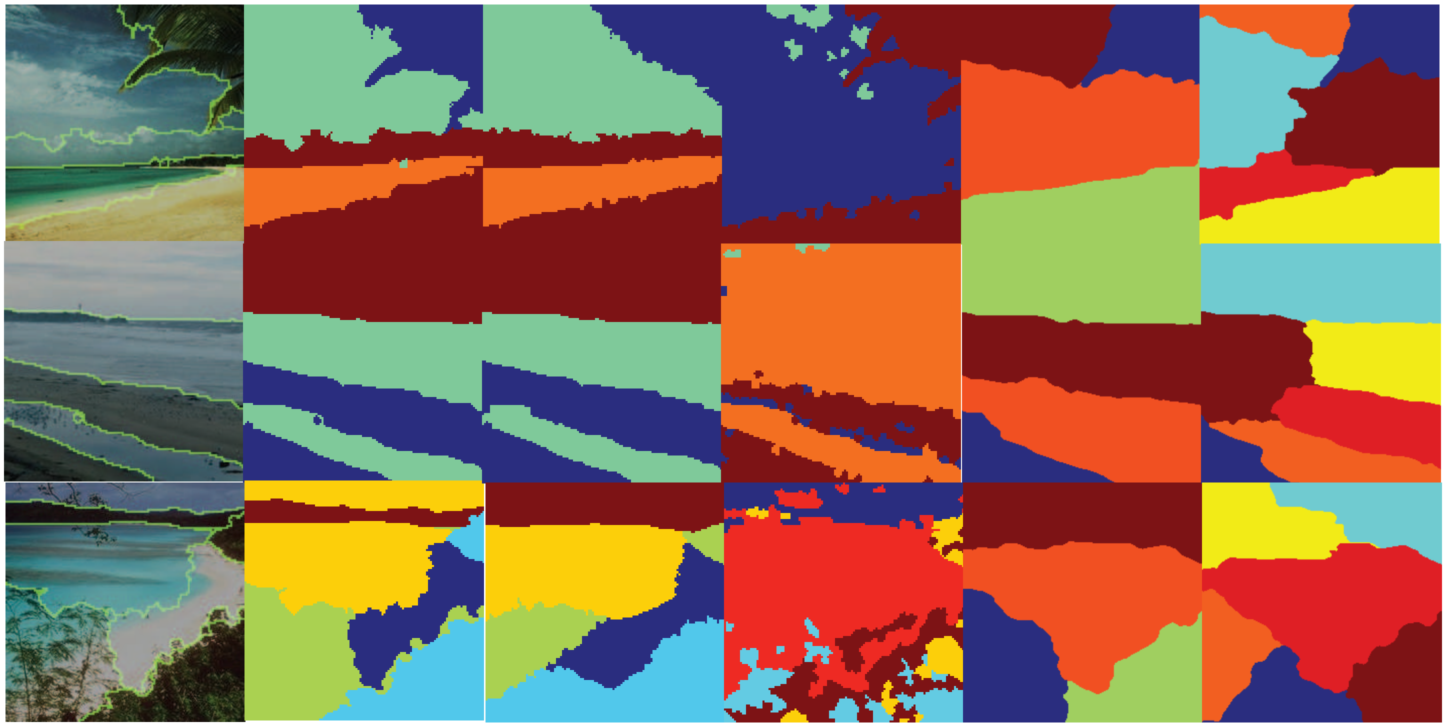
(Sudderth & Jordan, 2009)

- Comparing the HPY prior to a Markov random field prior



# Image Segmentation (cont)

(Sudderth & Jordan, 2009)



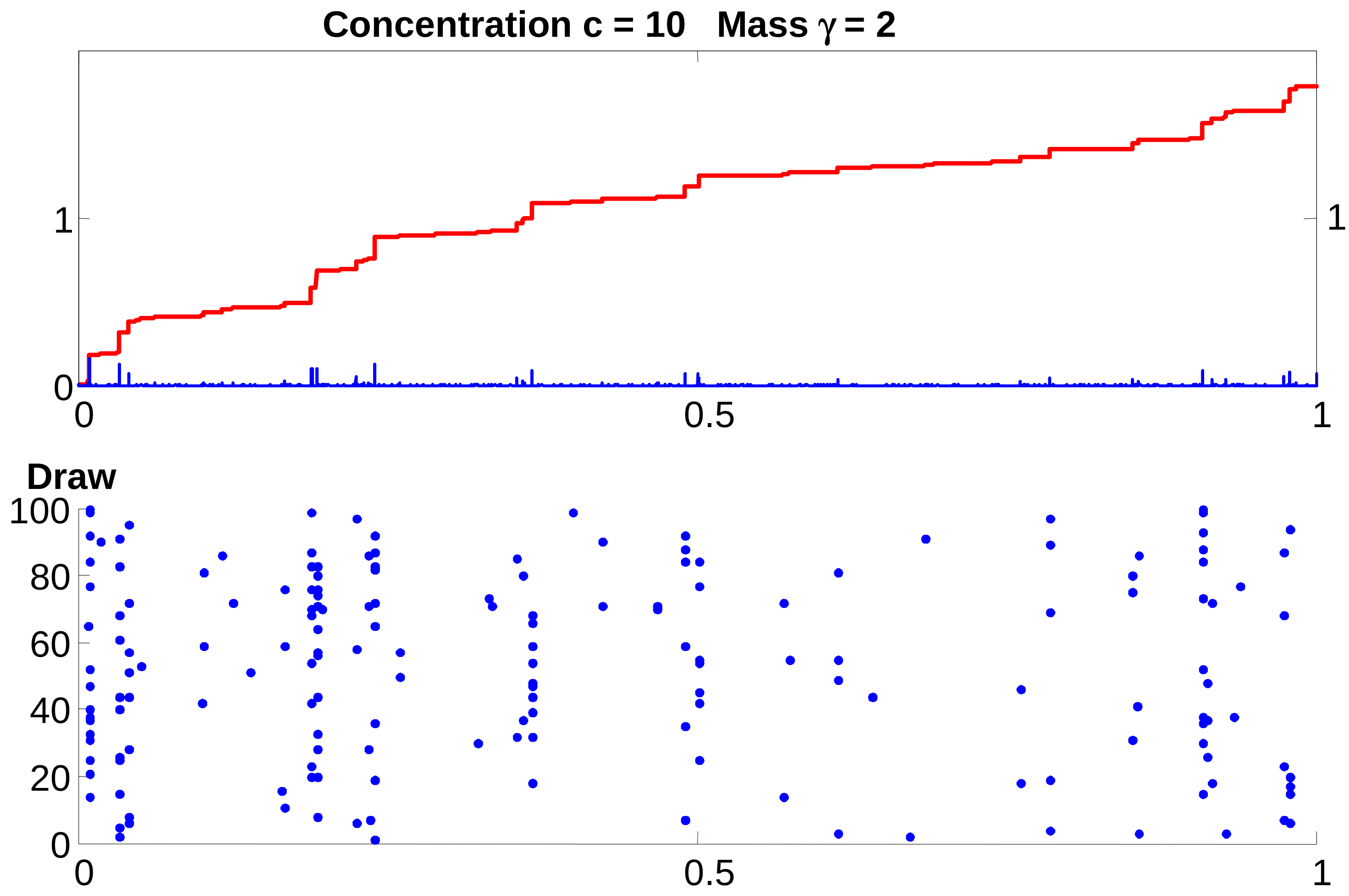
# Beta Processes

- The Dirichlet process yields a multinomial random variable (which table is the customer sitting at?)
- *Problem*: in many problem domains we have a very large (combinatorial) number of possible tables
  - it becomes difficult to control this with the Dirichlet process
- What if instead we want to characterize objects as collections of attributes ("sparse features")?
- Indeed, instead of working with the sample paths of the Dirichlet process, which sum to one, let's instead consider a stochastic process—the beta process—which removes this constraint
- And then we will go on to consider hierarchical beta processes, which will allow features to be shared among multiple related objects

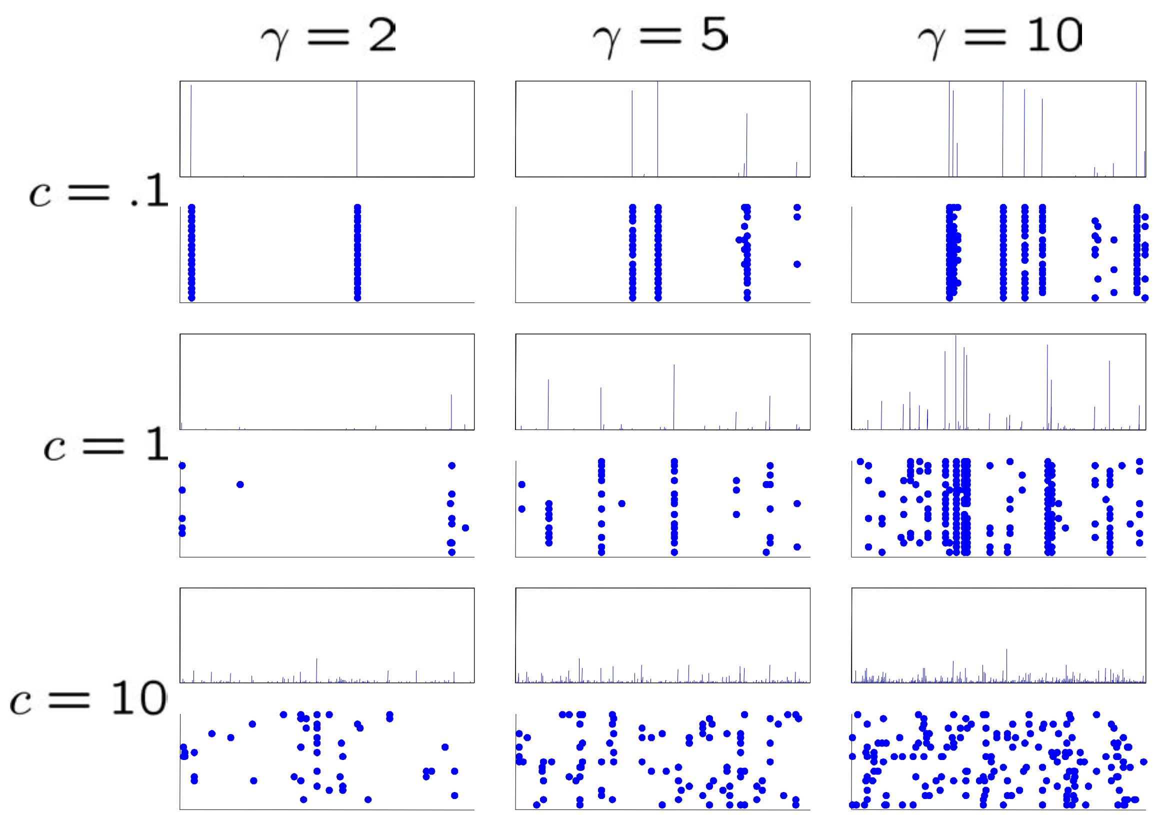
# Completely random processes

- Stochastic processes with independent increments
  - e.g., Gaussian increments (Brownian motion)
  - e.g., gamma increments (gamma processes)
  - in general, (limits of) compound Poisson processes
- The Dirichlet process is not a completely random processes
  - but it's a normalized gamma process
- The beta process assigns beta measure to small regions
- Can then sample to yield (sparse) collections of Bernoulli variables

# Beta Processes



# Examples of Beta Process Sample Paths




- Effect of the two parameters $c$ and $\gamma$ on samples from a beta process.

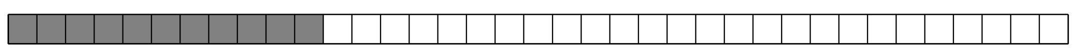
# Beta Processes

- The marginals of the Dirichlet process are characterized by the Chinese restaurant process
- What about the beta process?

# Indian Buffet Process (IBP)

(Griffiths & Ghahramani, 2005; Thibaux & Jordan, 2007)

- Indian restaurant with infinitely many dishes in a buffet line
- $N$ customers serve themselves
  - the first customer samples $\mathrm{Poisson}(\alpha)$ dishes
  - the $i$th customer samples a previously sampled dish with probability $\frac{m_k}{i+1}$ then samples $\mathrm{Poisson}(\frac{\alpha}{i})$ new dishes



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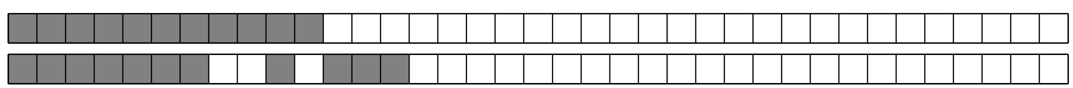

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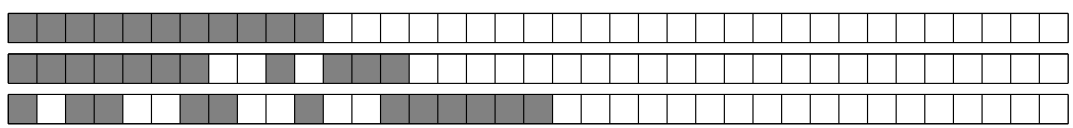

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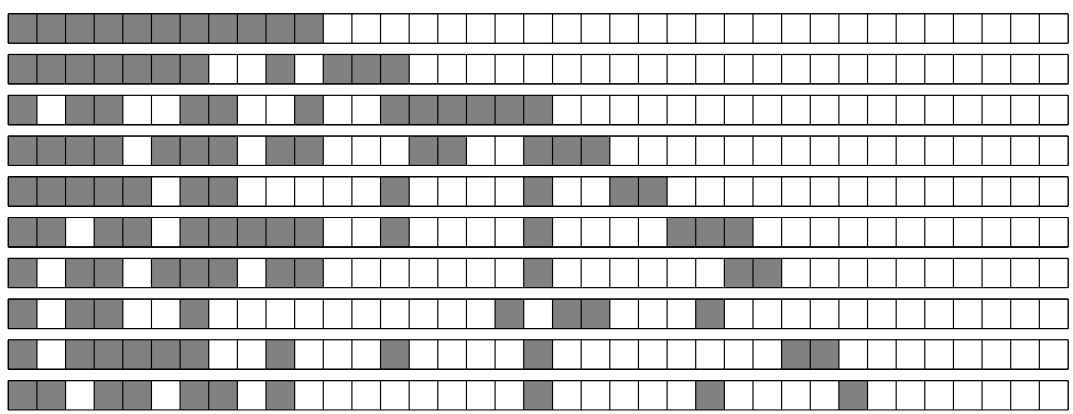
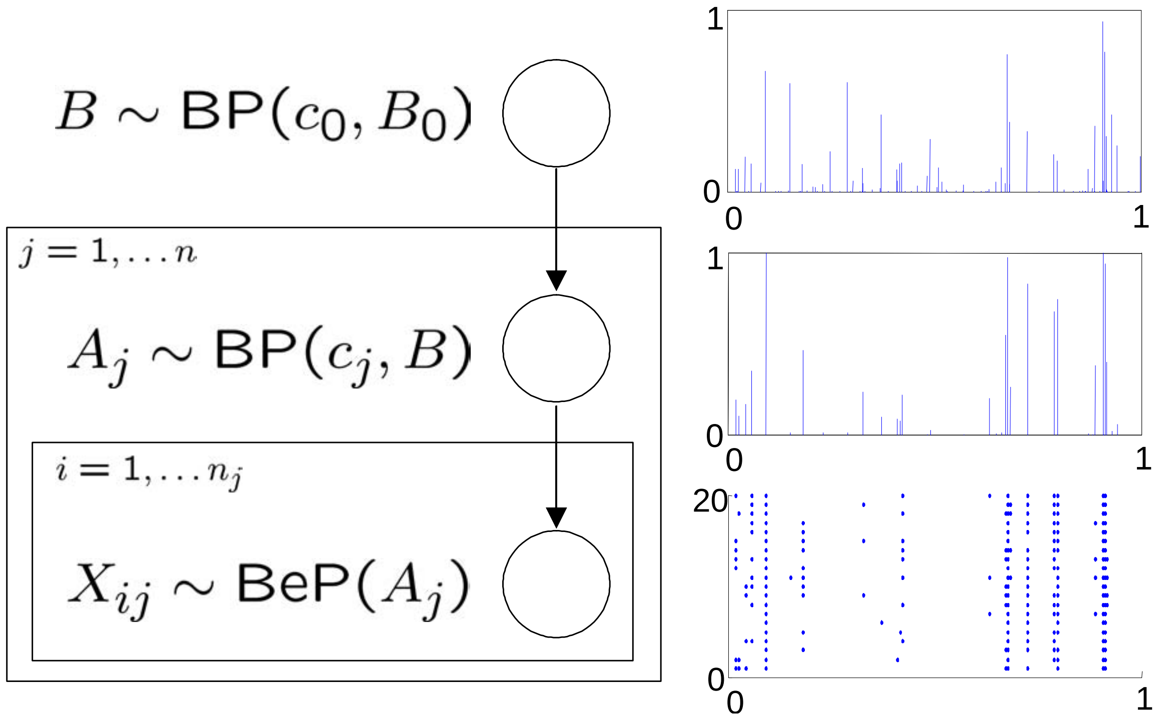


# Hierarchical Beta Process




- A hierarchical beta process is a beta process whose base measure is itself random and drawn from a beta process.

# Conclusions

- Nonparametric Bayesian modeling: flexible data structures meet probabilistic inference
- The underlying theory has to do with exchangeability and partial exchangeability
- We haven't discussed inference algorithms, but many interesting issues and new challenges arise
- For more details, including tutorials:

**http://www.cs.berkeley.edu/~jordan**