Bayesian Nonparametrics

+ DP / DPMM

Matt Gormley
EXAMPLE: K-MEANS & GMM
Example: K-Means
Example: K-Means
Example: K-Means

Clustering with K-Means (k=3, iter=1)
Example: K-Means

Clustering with K-Means (k=3, iter=2)
Example: K-Means

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Clustering with K-Means (k=3, iter=4)
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Example: GMM
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Clustering with GMM ($k=3$, init=random, cov=spherical, iter=19)
LATENT DIRICHLET ALLOCATION
(LDA)
LDA for Topic Modeling

• The *generative story* begins with only a Dirichlet prior over the topics.
• Each *topic* is defined as a Multinomial distribution over the vocabulary, parameterized by $\phi_k$.

(Blei, Ng, & Jordan, 2003)
LDA for Topic Modeling

- The generative story begins with only a Dirichlet prior over the topics.
- Each topic is defined as a Multinomial distribution over the vocabulary, parameterized by $\phi_k$
LDA for Topic Modeling

- A topic is visualized as its high probability words.

(Blei, Ng, & Jordan, 2003)
LDA for Topic Modeling

• A topic is visualized as its **high probability words**.

• A pedagogical **label** is used to identify the topic.
LDA for Topic Modeling

- A topic is visualized as its high probability words.
- A pedagogical label is used to identify the topic.

(Blei, Ng, & Jordan, 2003)
LDA for Topic Modeling

\[ \phi_1 \{\text{Canadian gov.}\} \quad \phi_2 \{\text{government}\} \quad \phi_3 \{\text{hockey}\} \quad \phi_4 \{\text{U.S. gov.}\} \quad \phi_5 \{\text{baseball}\} \quad \phi_6 \{\text{Japan}\} \]

Dirichlet(\(\theta\))

Dirichlet(\(\alpha\))

\[ \theta_1 = \]

(Blei, Ng, & Jordan, 2003)
The 54/40' boundary dispute is still unresolved, and Canadian and US
LDA for Topic Modeling

The 54/40' boundary dispute is still unresolved, and Canadian and US government have different perspectives on it.

Dirichlet(θ)

Dirichlet(α)

The 54/40' boundary dispute is still unresolved, and Canadian and US government have different perspectives on it.

Dirichlet(θ)

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The 54/40' boundary dispute is still unresolved, and Canadian and US government have different perspectives on it.

Dirichlet(θ)

Dirichlet(α)

The 54/40' boundary dispute is still unresolved, and Canadian and US government have different perspectives on it.
The 54/40' boundary dispute is still unresolved, and Canadian and US Coast Guard
LDA for Topic Modeling

\[ \theta_1 = \text{Dirichlet}(\beta) \]

\[ \phi_1 = \{\text{Canadian gov.}\} \]
\[ \phi_2 = \{\text{government}\} \]
\[ \phi_3 = \{\text{hockey}\} \]
\[ \phi_4 = \{\text{U.S. gov.}\} \]
\[ \phi_5 = \{\text{baseball}\} \]
\[ \phi_6 = \{\text{Japan}\} \]

The 54/40\(^{\prime}\) boundary dispute is still unresolved, and Canadian and US Coast Guard vessels regularly if infrequently detain each other's fish boats in the disputed waters off Dixon...
The 54/40' boundary dispute is still unresolved, and Canadian and US Coast Guard vessels regularly if infrequently detain each other's fish boats in the disputed waters off Dixon...

In the year before Lemieux came, Pittsburgh finished with 38 points. Following his arrival, the Pens finished...

The Orioles' pitching staff again is having a fine exhibition season. Four shutouts, low team ERA, (Well, I haven't gotten any baseball...
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Latent Dirichlet Allocation

• Plate Diagram

\[\begin{align*}
\alpha \\
\theta^m \\
z^mn \\
x^mn \\
\phi^k \\
\beta
\end{align*}\]

- Document-specific topic distribution
- Topic assignment
- Observed word
- Dirichlet
- Topic
- Dirichlet
Familiar models for unsupervised learning:

1. K-Means
2. Gaussian Mixture Model (GMM)
3. Latent Dirichlet Allocation (LDA)

But without labeled data, how do we know the right number of clusters / topics?
Outline

• Motivation / Applications
• Background
  – de Finetti Theorem
  – Exchangeability
  – Agglomerative and decimative properties of Dirichlet distribution
• CRP and CRP Mixture Model
  – Chinese Restaurant Process (CRP) definition
  – Gibbs sampling for CRP-MM
  – Expected number of clusters
• DP and DP Mixture Model
  – Ferguson definition of Dirichlet process (DP)
  – Stick breaking construction of DP
  – Uncollapsed blocked Gibbs sampler for DP-MM
  – Truncated variational inference for DP-MM
• DP Properties
• Related Models
  – Hierarchical Dirichlet process Mixture Models (HDP-MM)
  – Infinite HMM
  – Infinite PCFG
BAYESIAN NONPARAMETRICS
Parametric vs. Nonparametric

• **Parametric models:**
  – **Finite** and **fixed** number of parameters
  – Number of parameters is **independent of the dataset**

• **Nonparametric models:**
  – **Have** parameters ("**infinite dimensional**" would be a better name)
  – Can be understood as having an **infinite** number of parameters
  – Can be understood as having a **random** number of parameters
  – Number of parameters can **grow with the dataset**

• **Semiparametric models:**
  – Have a **parametric** component and a **nonparametric** component
<table>
<thead>
<tr>
<th></th>
<th>Frequentist</th>
<th>Bayesian</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parametric</td>
<td>Logistic regression, ANOVA, Fisher discriminant analysis, ARMA, etc.</td>
<td>Conjugate analysis, hierarchical models, conditional random fields</td>
</tr>
<tr>
<td>Semiparametric</td>
<td>Independent component analysis, Cox model, nonmetric MDS, etc.</td>
<td>[Hybrids of the above and below cells]</td>
</tr>
<tr>
<td>Nonparametric</td>
<td>Nearest neighbor, kernel methods, boostrap, decision trees, etc.</td>
<td>Gaussian processes, Dirichlet processes, Pitman-Yor processes, etc.</td>
</tr>
</tbody>
</table>
## Parametric vs. Nonparametric Application

<table>
<thead>
<tr>
<th>Application</th>
<th>Parametric</th>
<th>Nonparametric</th>
</tr>
</thead>
<tbody>
<tr>
<td>function</td>
<td>polynomial regression</td>
<td>Gaussian processes</td>
</tr>
<tr>
<td>approximation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>classification</td>
<td>logistic regression</td>
<td>Gaussian process classifiers</td>
</tr>
<tr>
<td>clustering</td>
<td>mixture model, k-means</td>
<td>Dirichlet process mixture model</td>
</tr>
<tr>
<td>time series</td>
<td>hidden Markov model</td>
<td>infinite HMM</td>
</tr>
<tr>
<td>feature discovery</td>
<td>factor analysis, pPCA, PMF</td>
<td>infinite latent factor models</td>
</tr>
</tbody>
</table>
Parametric vs. Nonparametric

• **Def:** a *model* is a collection of distributions

\[ \{p_\theta : \theta \in \Theta\} \]

• *parametric model:* the parameter vector is finite dimensional

\[ \Theta \subset \mathbb{R}^k \]

• *nonparametric model:* the parameters are from a possibly infinite dimensional space, \( \mathcal{F} \)

\[ \Theta \subset \mathcal{F} \]

Table adapted from Jordan ICML 2005
Motivation #1

Model Selection

• For clustering: How many clusters in a mixture model?
• For topic modeling: How many topics in LDA?
• For grammar induction: How many non-terminals in a PCFG?
• For visual scene analysis: How many objects, parts, features?
Motivation #1

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Model Selection

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1. Parametric approaches: cross-validation, bootstrap, AIC, BIC, DIC, MDL, Laplace, bridge sampling, etc.

2. Nonparametric approach: average of an infinite set of models
Motivation #2

Density Estimation

- Given data, estimate a probability density function that best explains it
- A nonparametric prior can be placed over an infinite set of distributions

Prior:

Motivation #2

Density Estimation

- Given data, estimate a probability density function that best explains it
- A nonparametric prior can be placed over an infinite set of distributions

Posterior:

EXCHANGEABILITY AND DE FINETTI’S THEOREM
Background

Suppose we have a random variable $X$ drawn from some distribution $P_{\theta}(X)$ and $X$ ranges over a set $S$.

- **Discrete distribution:**
  $S$ is a countable set.

- **Continuous distribution:**
  $P_{\theta}(X = x) = 0$ for all $x \in S$

- **Mixed distribution:**
  $S$ can be partitioned into two disjoint sets $D$ and $C$ s.t.
  1. $D$ is countable and $0 < P_{\theta}(X \in D) < 1$
  2. $P_{\theta}(X = x) = 0$ for all $x \in C$
Exchangability and de Finetti’s Theorem

Exchangeability:

• **Def #1:** a joint probability distribution is **exchangeable** if it is invariant to permutation

• **Def #2:** The possibly infinite sequence of random variables \((X_1, X_2, X_3, \ldots)\) is **exchangeable** if for any finite permutation \(s\) of the indices \((1, 2, \ldots n)\):

\[
P(X_1, X_2, \ldots, X_n) = P(X_{s(1)}, X_{s(2)}, \ldots, X_{s(n)})
\]

Notes:

• *i.i.d.* and **exchangeable** are not the same!

• the latter says that if our data are reordered it doesn’t matter
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:

\[
p(x_1, x_2, \ldots, x_N) = \int \left( \prod_{i=1}^{N} p(x_i \mid \theta) \right) dP(\theta)
\]

for some random variable \(\theta\).

- The theorem wouldn’t be true if we limited ourselves to parameters \(\theta\) ranging over Euclidean vector spaces

- In particular, we need to allow \(\theta\) to range over measures, in which case \(P(\theta)\) is a measure on measures
  - the Dirichlet process is an example of a measure on measures...

Actually, this is the Hewitt-Savage generalization of the de Finetti theorem. The original version was given for the Bernoulli distribution.
Exchangability and de Finetti’s Theorem

- A *plate* is a “macro” that allows subgraphs to be replicated:

- Note that this is a graphical representation of the De Finetti theorem

\[
p(x_1, x_2, \ldots, x_N) = \int p(\theta) \left( \prod_{i=1}^{N} p(x_i | \theta) \right) d\theta
\]
# Parametric vs. Nonparametric

<table>
<thead>
<tr>
<th>Type of Model</th>
<th>Parametric Example</th>
<th>Nonparametric Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>distribution over counts</td>
<td>Dirichlet-Multinomial Model</td>
<td>Dirichlet Process (DP)</td>
</tr>
<tr>
<td></td>
<td>Chinese Restaurant Process (CRP)</td>
<td>Stick-breaking construction</td>
</tr>
<tr>
<td>mixture</td>
<td>Gaussian Mixture Model (GMM)</td>
<td>Dirichlet Process Mixture Model (DPMM)</td>
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<tr>
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<td>Latent Dirichlet Allocation (LDA)</td>
<td>Hierarchical Dirichlet Process Mixture Model (HDPMM)</td>
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<td>Chinese Restaurant Franchise</td>
<td>Stick-breaking construction</td>
</tr>
</tbody>
</table>
Chinese Restaurant Process & Stick-breaking Constructions

DIRICLHLET PROCESS
Dirichlet Process

Ferguson Definition

- Parameters of a DP:
  1. Base distribution, \( H \), is a probability distribution over \( \Theta \)
  2. Strength parameter, \( \alpha \in \mathcal{R} \)
- We say \( G \sim \text{DP}(\alpha, H) \) if for any partition \( A_1 \cup A_2 \cup \ldots \cup A_K = \Theta \) we have:
  \[
  (G(A_1), \ldots, G(A_K)) \sim \text{Dirichlet}(\alpha H(A_1), \ldots, \alpha H(A_K))
  \]

In English: the DP is a distribution over probability measures s.t. marginals on finite partitions are Dirichlet distributed

A partition of the space \( \Theta \)
Imagine a Chinese restaurant with an infinite number of tables.

Each customer enters and sits down at a table:
- The first customer sits at the first unoccupied table.
- Each subsequent customer chooses a table according to the following probability distribution:

\[ p(k\text{th occupied table}) \propto n_k \]
\[ p(\text{next unoccupied table}) \propto \alpha \]

Where \( n_k \) is the number of people sitting at the table \( k \).
Chinese Restaurant Process

Properties:
1. CRP defines a distribution over clusterings (i.e. partitions) of the indices $1, \ldots, n$.
   - customer = index
   - table = cluster
2. We write $z_1, z_2, \ldots, z_n \sim CRP(\alpha)$ to denote a sequence of cluster indices drawn from a Chinese Restaurant Process.
3. The CRP is an exchangeable process.
4. Expected number of clusters given $n$ customers (i.e. observations) is $O(\alpha \log(n))$.
   - rich-get-richer effect on clusters: popular tables tend to get more crowded.
5. Behavior of CRP with $\alpha$:
   - As $\alpha$ goes to 0, the number of clusters goes to 1.
   - As $\alpha$ goes to $+\infty$, the number of clusters goes to $n$. 

Whiteboard

• Stick-breaking construction of the DP
Dirichlet Process: For both the CRP and stick-breaking constructions, if we marginalize out $G$, we have the following predictive distribution:

$$G \sim \text{DP}(\alpha, H)$$

$$\theta_{n+1} | \theta_1, \ldots, \theta_n \sim \frac{1}{\alpha + n} \left( \alpha H + \sum_{i=1}^{n} \delta_{\theta_i} \right)$$

The Chinese Restaurant Process is just a different construction of the Dirichlet Process where we have marginalized out $G$.
Properties of the DP

1. **Base distribution** is the “mean” of the DP:
   \[ \mathbb{E}[G(A)] = H(A) \text{ for any } A \subset \Theta \]

2. **Strength parameter** is like “inverse variance”
   \[ V[G(A)] = H(A)(1 - H(A))/(\alpha + 1) \]

3. **Samples from a DP** are discrete distributions (stick-breaking construction of \( G \sim \text{DP}(\alpha, H) \) makes this clear)

4. **Posterior distribution** of \( G \sim \text{DP}(\alpha, H) \) given samples \( \theta_1, \ldots, \theta_n \) from \( G \) is a DP
   \[ G|\theta_1, \ldots, \theta_n \sim \text{DP}\left(\alpha + n, \frac{\alpha}{\alpha+n} H + \frac{n}{\alpha+n} \sum_{i=1}^{n} \delta_{\theta_i} \right) \]
Chinese Restaurant Process & Stick-breaking Constructions

DIRICHLET PROCESS MIXTURE MODEL
CRP Mixture Model

- Draw n cluster indices from a CRP:
  \[ z_1, z_2, ..., z_n \sim CRP(\alpha) \]

- For each of the resulting K clusters:
  \[ \theta_k^* \sim H \]
  where \( H \) is a base distribution

- Draw n observations:
  \[ x_i \sim p(x_i \mid \theta_{z_i}^*) \]

Customer \( i \) orders a dish \( x_i \) (observation) from a table-specific distribution over dishes \( \theta_k^* \) (cluster parameters)

(color denotes different values of \( x_i \))
CRP Mixture Model

- Draw \( n \) cluster indices from a CRP: \( z_1, z_2, ..., z_n \sim CRP(\alpha) \)
- For each of the resulting \( K \) clusters: \( \theta_k^* \sim H \)
  where \( H \) is a base distribution
- Draw \( n \) observations: \( x_i \sim p(x_i | \theta_{z_i}^*) \)

- The Gibbs sampler is easy thanks to **exchangeability**
- For each observation, we remove the customer / dish from the restaurant and resample as if they were the **last to enter**
- If we **collapse out the parameters**, the Gibbs sampler draws from the conditionals:
  \[
  z_i \sim p(z_i | z_{-i}, x)
  \]

(color denotes different values of \( x_i \))
CRP Mixture Model

Overview of 3 Gibbs Samplers for Conjugate Priors

- **Alg. 1: (uncollapsed)**
  - Markov chain state: per-customer parameters $\theta_1, \ldots, \theta_n$
  - For $i = 1, \ldots, n$: Draw $\theta_i \sim p(\theta_i | \theta_{-i}, x)$

- **Alg. 2: (uncollapsed)**
  - Markov chain state: per-customer cluster indices $z_1, \ldots, z_n$ and per-cluster parameters $\theta_1^*, \ldots, \theta_k^*$
  - For $i = 1, \ldots, n$: Draw $z_i \sim p(z_i | z_{-i}, x, \theta^*)$
  - Set $K$ = number of clusters in $z$
  - For $k = 1, \ldots, K$: Draw $\theta_k^* \sim p(\theta_k^* | \{x_i : z_i = k\})$

- **Alg. 3: (collapsed)**
  - Markov chain state: per-customer cluster indices $z_1, \ldots, z_n$
  - For $i = 1, \ldots, n$: Draw $z_i \sim p(z_i | z_{-i}, x)$
CRP Mixture Model

• Q: How can the Alg. 2 Gibbs samplers permit an infinite set of clusters in finite space?

• A: Easy!
  – We are only representing a finite number of clusters at a time – those to which the data have been assigned
  – We can always bring back the parameters for the “next unoccupied table” if we need them
Whiteboard

• Dirichlet Process Mixture Model (stick-breaking version)
CRP-MM vs. DP-MM

Dirichlet Process: For both the CRP and stick-breaking constructions, if we marginalize out $G$, we have the following predictive distribution:

$$
\theta_{n+1}|\theta_1, \ldots, \theta_n \sim \frac{1}{\alpha + n} \left( \alpha H + \sum_{i=1}^{n} \delta_{\theta_i} \right)
$$

(Blackwell-MacQueen Urn Scheme)

The Chinese Restaurant Process Mixture Model is just a different construction of the Dirichlet Process Mixture Model where we have marginalized out $G$. 
Graphical Models for DPMMs

The Pólya urn construction

The Stick-breaking construction

Equivalent
Example: DP Gaussian Mixture Model

Figure 2: The approximate predictive distribution given by variational inference at different stages of the algorithm. The data are 100 points generated by a Gaussian DP mixture model with fixed diagonal covariance.
Example: DP Gaussian Mixture Model

Figure 3: Mean convergence time and standard error across ten data sets per dimension for variational inference, TDP Gibbs sampling, and the collapsed Gibbs sampler.
Summary of DP and DP-MM

• **DP** has many **different representations:**
  – Chinese Restaurant Process
  – Stick-breaking construction
  – Blackwell-MacQueen Urn Scheme
  – Limit of finite mixtures
  – etc.

• These representations give rise to a variety of **inference techniques** for the **DP-MM** and related models
  – Gibbs sampler (CRP)
  – Gibbs sampler (stick-breaking)
  – Variational inference (stick-breaking)
  – etc.
GMM VS. DPMM EXAMPLE
Example: GMM

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Clustering with DPMM (k=6, init=random, cov=full, iter=25)
HIERARCHICAL DIRICHLET PROCESS (HDP)
Related Models

• Hierarchical Dirichlet Process Mixture Model (HDP-MM)
• Infinite HMM
• Infinite PCFG
HDP-MM

- In LDA, we have \( M \) independent samples from a Dirichlet distribution.
- The weights are different, but the topics are fixed to be the same.
- If we replace the Dirichlet distributions with Dirichlet processes, each atom of each Dirichlet process will pick a topic \textit{independently} of the other topics.
- Because the base measure is \textit{continuous}, we have zero probability of picking the same topic twice.
- If we want to pick the same topic twice, we need to use a \textit{discrete} base measure.
- For example, if we chose the base measure to be

\[
H = \sum_{k=1}^{K} \alpha_k \delta_{\beta_k}
\]

then we would have LDA again.

- We want there to be an infinite number of topics, so we want an \textit{infinite}, \textit{discrete} base measure.
- We want the location of the topics to be random, so we want an \textit{infinite}, \textit{discrete}, \textit{random} base measure.
Hierarchical Dirichlet process:

\[ G_0 \mid \gamma, H \sim \text{DP}(\gamma, H) \]

\[ G_j \mid \alpha, G_0 \sim \text{DP}(\alpha, G_0) \]

\[ \theta_{ji} \mid G_j \sim G_j \]

Because the base measure is continuous, we have zero probability of picking the same topic twice. If we want to pick the same topic twice, we need to use a discrete base measure. For example, if we chose the base measure to be \( \text{DP}(\alpha, G_0) \), we would have LDA again. We want there to be an infinite number of topics, so we want an infinite, discrete base measure. We want the location of the topics to be random, so we want an infinite, discrete, random base measure.
Figure 6: (Left) Comparison of latent Dirichlet allocation and the hierarchical Dirichlet process mixture. Results are averaged over 10 runs; the error bars are one standard error. (Right) Histogram of the number of topics for the hierarchical Dirichlet process mixture over 100 posterior samples.
HDP-HMM (Infinite HMM)

Number of hidden states in Infinite HMM is countably infinite

Figure 9: A hierarchical Bayesian model for the infinite hidden Markov model.

Figure 10: Comparing the infinite hidden Markov model (solid horizontal line) with ML, MAP and VB trained hidden Markov models. The error bars represent one standard error (those for the HDP-HMM are too small to see).
HDP-PCFG (Infinite PCFG)

**HDP-PCFG**

\[ \beta \sim \text{GEM}(\alpha) \]  
[draw top-level symbol weights]

For each grammar symbol \( z \in \{1, 2, \ldots \} \):
- \( \phi_z^T \sim \text{Dirichlet}(\alpha_T^T) \)  
  [draw rule type parameters]
- \( \phi_z^E \sim \text{Dirichlet}(\alpha_E^E) \)  
  [draw emission parameters]
- \( \phi_z^B \sim \text{DP}(\alpha_B^B, \beta^\beta_T) \)  
  [draw binary production parameters]

For each node \( i \) in the parse tree:
- \( t_i \sim \text{Multinomial}(\phi_{z_i}^T) \)  
  [choose rule type]
- If \( t_i = \text{EMISSION} \):
  - \( x_i \sim \text{Multinomial}(\phi_{z_i}^E) \)  
    [emit terminal symbol]
- If \( t_i = \text{BINARY-PRODUCTION} \):
  - \( (z_{L(i)}, z_{R(i)}) \sim \text{Multinomial}(\phi_{z_i}^B) \)  
    [generate children symbols]
# Parametric vs. Nonparametric

<table>
<thead>
<tr>
<th>Type of Model</th>
<th>Parametric Example</th>
<th>Nonparametric Example</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Construction #1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Construction #2</td>
</tr>
<tr>
<td>distribution over</td>
<td>Dirichlet-Multinomial Model</td>
<td>Dirichlet Process (DP)</td>
</tr>
<tr>
<td>counts</td>
<td></td>
<td>Chinese Restaurant Process (CRP)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Stick-breaking construction</td>
</tr>
<tr>
<td>mixture</td>
<td>Gaussian Mixture Model (GMM)</td>
<td>Dirichlet Process Mixture Model (DPMM)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CRP Mixture Model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Stick-breaking construction</td>
</tr>
<tr>
<td>admixture</td>
<td>Latent Dirichlet Allocation (LDA)</td>
<td>Hierarchical Dirichlet Process Mixture Model (HDPMM)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Chinese Restaurant Franchise</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Stick-breaking construction</td>
</tr>
</tbody>
</table>
Summary of DP and DP-MM

• **DP** has many **different representations:**
  – Chinese Restaurant Process
  – Stick-breaking construction
  – Blackwell-MacQueen Urn Scheme
  – Limit of finite mixtures
  – etc.

• These representations give rise to a variety of **inference techniques** for the **DP-MM** and related models
  – Gibbs sampler (CRP)
  – Gibbs sampler (stick-breaking)
  – Variational inference (stick-breaking)
  – etc.