# 10-418 / 10-618 Machine Learning for Structured Data 

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## Bayesian Nonparametrics

$$
\stackrel{+}{\text { DP / DPMM }}
$$

Matt Gormley

## EXAMPLE: K-MEANS \& GMM

## Example: K-Means



## Example: K-Means



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## Example: K-Means



## Example: K-Means



## Example: K-Means



## Example: K-Means



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM



## Example: GMM

Clustering with GMM ( $k=3$, init=random, cov=spherical, iter=10)


## Example: GMM

Clustering with GMM ( $k=3$, init=random, cov=spherical, iter=11)


## Example: GMM

Clustering with GMM ( $k=3$, init=random, cov=spherical, iter=12)


## Example: GMM

Clustering with GMM ( $\mathrm{k}=3$, init=random, cov=spherical, iter=13)


## Example: GMM

Clustering with GMM ( $k=3$, init=random, cov=spherical, iter=14)


## Example: GMM

Clustering with GMM ( $\mathrm{k}=3$, init=random, cov=spherical, iter=15)


## Example: GMM

Clustering with GMM ( $k=3$, init=random, cov=spherical, iter=16)


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Clustering with GMM ( $\mathrm{k}=3$, init=random, cov=spherical, iter=17)


## Example: GMM

Clustering with GMM ( $k=3$, init=random, cov=spherical, iter=18)


## Example: GMM

Clustering with GMM ( $\mathrm{k}=3$, 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 $\boldsymbol{\phi}_{\mathrm{k}}$


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## LDA for Topic Modeling



- A topic is visualized as its high probability words.


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## LDA for Topic Modeling

Inference and learning start with only the data


## Latent Dirichlet Allocation

- Plate Diagram


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
- Aglommerative and decimative properties of Dirichlet distribution
$\square$ ERP 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


## Parametric vs. Nonparametric



## Parametric vs. Nonparametric

| Application | Parametric | Nonparametric |
| :--- | :--- | :--- |
| function <br> approximation | polynomial regression | Gaussian processes |
| classification | logistic regression | Gaussian process <br> classifiers |
| clustering | mixture model, k- <br> means | Dirichlet process <br> mixture model |
| time series | hidden Markov model | infinite HMM |
| feature discovery | factor analysis, pPCA, <br> PMF | infinite latent factor <br> models |

## Parametric vs. Nonparametric

- Def: a model is a collection of distributions

$$
\left\{p_{\boldsymbol{\theta}}: \boldsymbol{\theta} \in \widehat{\Theta}\right\}
$$

- parametric model: the parameter vector is finite dimensional

$$
\underline{\Theta} \subset \mathcal{R}^{k}
$$

- nonparametric model: the parameters are from a possibly infinite dimensional space, $\mathcal{F}$

$$
\Theta \subset \mathcal{F}
$$

## 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 nonterminals in a PCFG?

- For visual scene analysis:

How many objects, parts, features?

## Motivation \#1

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## 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 nonterminals in a PCFG?
- For visual scene analysis: How many objects, parts, features?

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:


Red: mean density. Blue: median density. Grey: 5-95 quantile. Others: draws.

## 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:


Red: mean density. Blue: median density. Grey: 5-95 quantile. Black: data. Others: draws.

## 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 $\mathcal{S}$.

- Discrete distribution: $\mathcal{S}$ is a countable set.
- Continuous distribution: $P_{\theta}(X=x)=0$ for all $x \in \mathcal{S}$

- Mixed distribution:
$\mathcal{S}$ can be partitioned into two disjoint sets $\mathcal{D}$ and $\mathcal{C}$ s.t.

1. is countable and $0<P_{\theta}(X \in D)<1$
2. $P_{\theta}(X=x)=0$ for all $x \in \mathcal{C}$


## 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 ( $X_{l}, X_{2}, X_{3}, \ldots$ ) is exchangeable if for any finite permutation $s$ of the indices $(1,2, \ldots n)$ :

$$
P\left(X_{1}, X_{2}, \ldots, X_{n}\right)=P\left(X_{s(1)}, X_{s(2)}, \ldots, X_{s(n)}\right)
$$

## Notes:

- i.i.d. and exchangeable are not the same!
- the latter says that if our data are reordered it doesn't matter


## Exchangability and de Finetti's Theorem

Slide from Jordan

Theorem (De Finetti, 1935). If $\left(x_{1}, x_{2}, \ldots\right)$ are infinitely exchangeable, then the joint probability $p\left(x_{1}, x_{2}, \ldots, x_{N}\right)$ has a representation as a mixture:

$$
p\left(x_{1}, x_{2}, \ldots, x_{N}\right)=\int\left(\prod_{i=1}^{N} p\left(x_{i} \mid \theta\right)\right) d P(\theta)
$$

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

Slide from Jordan

- A plate is a "macro" that allows subgraphs to be replicated:

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

$$
p\left(x_{1}, x_{2}, \ldots, x_{N}\right)=\int p(\theta)\left(\prod_{i=1}^{N} p\left(x_{i} \mid \theta\right)\right) d \theta
$$

## Parametric vs. Nonparametric

| Type of Model | Parametric <br> Example | Nonparametric Example |  |
| :---: | :---: | :---: | :---: |
|  |  | Construction \#1 | Construction \#2 |
| distribution over counts | Dirichlet- <br> Multinomial Model | Dirichlet Process (DP) |  |
|  |  | Chinese Restaurant Process (CRP) | Stick-breaking construction |
| mixture | Gaussian Mixture <br> Model (GMM) | Dirichlet Process Mixture Model (DPMM) |  |
|  |  | CRP Mixture Model | Stick-breaking construction |
| admixture | Latent Dirichlet <br> Allocation (LDA) | Hierarchical Dirichlet Process Mixture Model (HDPMM) |  |
|  |  | Chinese Restaurant Franchise | Stick-breaking construction |

Chinese Restaurant Process \& Stick-breaking Constructions

## DIRICHLET PROCESS

## Dirichlet Process



- Parameters of a DP:

1. Base distribution, $H$, is a probability distribution over $\Theta$
2. Strength parameter, $\alpha \in \mathcal{R}$

- We say $G \sim \operatorname{DP}(\alpha, \bar{H}), \alpha \in \mathcal{R}$ is a distinbotron
if for any partition $\underline{A_{1}} \cup A_{2} \cup \ldots \cup A_{K}=\Theta$
we have:

$$
\frac{\left(G\left(A_{1}\right)\right.}{\pi_{1}}, \ldots, \frac{G\left(A_{K}\right)}{\pi_{2}} \cdots \frac{\text { Dirichlet }}{2}\left(\alpha, \alpha H\left(A_{1}\right), \ldots, \alpha H\left(A_{K}\right)\right)
$$

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

A partition of the space $\Theta$


## Chinese Restaurant Process

- 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:
$p\left(k t h\right.$ occupied table) $\propto n_{k}$ $p$ (next unoccupied table) $\alpha \alpha$
there $n_{k}$ is the number of people sitting at the table $k$
continous
aist.for

mixed


## Chinese Restaurant Process

## Properties:

1. CRP defines a distribution over clusterings (i.e. partitions) of the indices $1, \ldots . \pi=\#$ af customers

- customer = index
- table = cluster

2. We write $z_{1}, z_{2}, \ldots, z_{n} \sim C R P(\alpha)$ 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


## CRP vs. DP

Dirichlet Process: For both the CRP and stickbreaking constructions, if we marginalize out $G$, we have the following predictive distribution:
$G \sim D P(x, t)$
$\sigma_{0}, \phi_{2}, \ldots \phi_{n} \sim \mathcal{G}^{\theta_{n+1} \mid \theta_{1}, \ldots, \theta_{n} \sim \frac{1}{\alpha+n}\left(\alpha H+\sum_{i=1}^{n} \delta_{\theta_{i}}\right)}$
(Blackwell-MacQueen Urn Scheme)
The Chinese Restaurant Process 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 $G \sim \mathrm{DP}(\alpha, H)$ makes this clear)
4. Posterior distribution of $G \sim \mathrm{DP}(\alpha, H)$ given samples $\theta_{l}, \ldots, \theta_{n}$ from $G$ is a DP

$$
G \mid \theta_{1}, \ldots, \theta_{n} \sim \mathrm{DP}\left(\alpha+n, \frac{\alpha}{\alpha+n} H+\frac{n}{\alpha+n} \frac{\sum_{i=1}^{n} \delta_{\theta_{i}}}{n}\right)
$$

## DIRICHLET PROCESS MIXTURE MODEL

## CRP Mixture Model

- Draw n cluster indices from a CRP:

$$
z_{1}, z_{2}, \ldots, z_{n} \sim \operatorname{CRP}(\alpha)
$$

- For each of the resulting $K$ clusters:


## $\theta_{k}{ }^{*} \sim H$ <br> 

$\Rightarrow \vec{\theta}_{k}^{*}$ sumsto 1

## where $H$ is a base đistribution

- Draw n observations:

Customer $i$ orders a dish $x_{i}$
$x_{i} \sim p\left(x_{i} \mid \theta_{z_{i}}^{*}\right) \quad{ }_{\text {specific }}^{\text {(observait) from a table- }}$ specific distribution over dishes $\theta_{k}{ }^{*}$ (cluster parameters)


## CRP Mixture Model

- Draw n cluster indices from a CRP:

$$
z_{1}, z_{2}, \ldots, z_{n} \sim C R P(\alpha)
$$

- For each of the resulting $K$ clusters:
$\theta_{k}{ }^{*} \sim H$
where $H$ is a base distribution
- Draw n observations:

$$
x_{i} \sim p\left(x_{i} \mid \theta_{z_{i}}^{*}\right)
$$

- 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:

```
\mp@subsup{z}{i}{}~p(\mp@subsup{z}{i}{}|\mp@subsup{\boldsymbol{z}}{-i}{},\boldsymbol{x})
```



## 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 $\theta_{i} \sim p\left(\theta_{i} \mid \boldsymbol{\theta}_{-i}, \boldsymbol{x}\right)$
- Alg. 2: (uncollapsed)
- Markov chain state: per-customer cluster All the thetas except $\theta_{i}$ per-cluster parameters $\theta_{1}^{*}, \ldots, \theta_{k}^{*}$
- For $i=1, \ldots, n$ : $\operatorname{Draw} z_{i} \sim p\left(z_{i} \mid \boldsymbol{z}_{-i}, \boldsymbol{x}, \boldsymbol{\theta}^{*}\right)$

$$
z_{1}, \ldots, z_{n}
$$

- Set $K=$ number of clusters in $z$
- For $k=1, \ldots, K$ : Draw $\theta_{k}{ }^{*} \sim p\left(\theta_{k}{ }^{*} \mid \underline{\left\{x_{i}: z_{i}=k\right\}}\right)$
- Alg. 3: (collapsed)
- Markov chain state: per-customer cluster indices $z_{1}, \ldots, z_{n}$
- For $i=1, \ldots, n$ : Draw $z_{i} \sim p\left(z_{i} \mid \boldsymbol{z}_{-i}, \boldsymbol{x}\right)$


## 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 stickbreaking constructions, if we marginalize out $G$, we have the following predictive distribution:

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

(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


## 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: Dataset



## Example: GMM

Clustering with $G M M(k=6$, init=random, cov=full, iter=0)

## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=5)


## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=10)


## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=15)


## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=20)


## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=25)


## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=30)


## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=35)


## Example: GMM

Clustering with GMM ( $k=6$, init=random, cov=full, iter=39)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=0)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=1)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=2)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=3)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=4)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=5)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=6)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=7)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=8)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=9)


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Clustering with DPMM ( $k=6$, init=random, cov=full, iter=16)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=17)


## Example: DPMM

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## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=19)


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Clustering with DPMM ( $k=6$, init=random, cov=full, iter=23)


## Example: DPMM

Clustering with DPMM ( $k=6$, init=random, cov=full, iter=24)


## Example: DPMM

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 independently of the other topics.
- 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
$H=\sum_{k=1}^{K} \alpha_{k} \delta_{\beta_{k}}$ then we would have LDA again.
- We want there to be an infinite number of topics, so we want an infinite, discrete base measure.
- We want the location of the topics to be random, so we want an infinite, discrete, random base measure.


## HDP-MM

Hierarchical Dirichlet process:


## HDP-MM



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

$\boldsymbol{\beta} \sim \operatorname{GEM}(\alpha) \quad$ [draw top-level symbol weights]
For each grammar symbol $z \in\{1,2, \ldots\}$ :

$$
\begin{aligned}
\phi_{z}^{T} & \sim \operatorname{Dirichlet}\left(\alpha^{T}\right) \\
\phi_{z}^{E} & \sim \operatorname{Dirichlet}\left(\alpha^{E}\right) \\
\phi_{z}^{B} & \sim \operatorname{DP}\left(\alpha^{B}, \boldsymbol{\beta} \boldsymbol{\beta}^{T}\right)
\end{aligned}
$$

[draw rule type parameters] [draw emission parameters] [draw binary production parameters]
For each node $i$ in the parse tree:
$t_{i} \sim \operatorname{Multinomial}\left(\phi_{z_{i}}^{T}\right)$
If $t_{i}=$ Emission:
$x_{i} \sim \operatorname{Multinomial}\left(\phi_{z_{i}}^{E}\right)$
[choose rule type]
If $t_{i}=$ BinARY-PRODUCTION:
$\left(z_{L(i)}, z_{R(i)}\right) \sim \operatorname{Multinomial}\left(\phi_{z_{i}}^{B}\right) \quad$ [generate children symbols]
$\beta \sim \operatorname{GEM}(\alpha) \xrightarrow[\text { state }]{|\quad| \quad|\quad| \quad, \quad}$
$\boldsymbol{\beta}^{T} \underbrace{\text { left child state }}_{\text {light child state }}$



## Parametric vs. Nonparametric

| Type of Model | Parametric <br> Example | Nonparametric Example |  |
| :---: | :---: | :---: | :---: |
|  |  | Construction \#1 | Construction \#2 |
| distribution over counts | Dirichlet- <br> Multinomial Model | Diricilet Process (DP) |  |
|  |  | Chinese Restaurant Process (CRP) | Stick-breaking construction |
| mixture | Gaussian Mixture <br> Model (GMM) | Dirichlet Process M x xture Model (DPMM) |  |
|  |  | CRP Mixture Model | Stick-breaking construction |
| admixture | Latent Dirichlet Allocation (LDA) | Hierarchical Dirichlet Process Mixture Model (HDPMM) |  |
|  |  | Chinese Restaurant Franchise | Stick-breaking construction |

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