

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

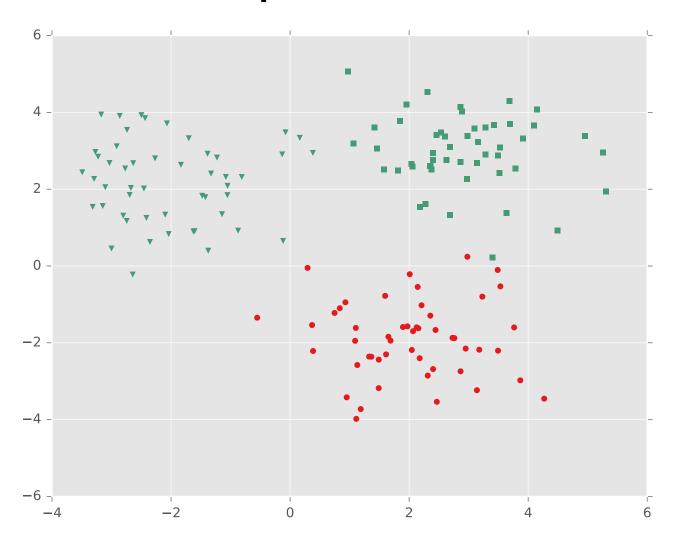
MACHINE LEARNING DEPARTMENT

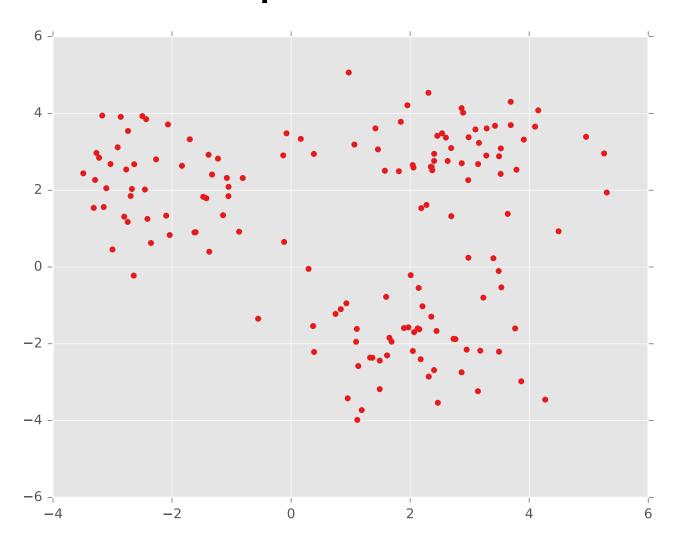
Machine Learning Department School of Computer Science Carnegie Mellon University

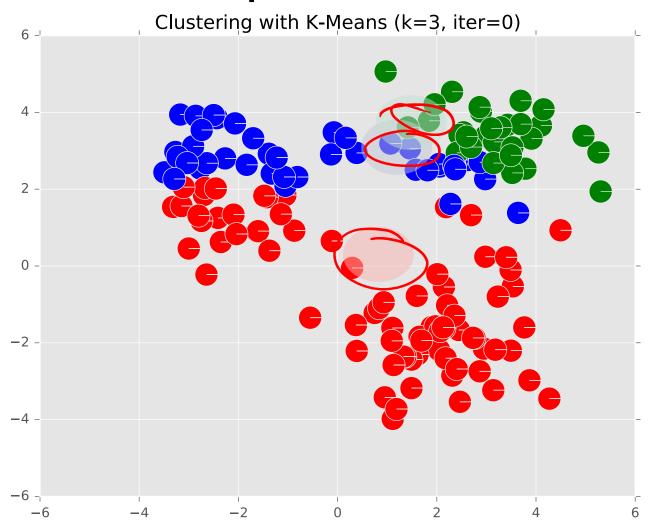
Bayesian Nonparametrics + DP / DPMM

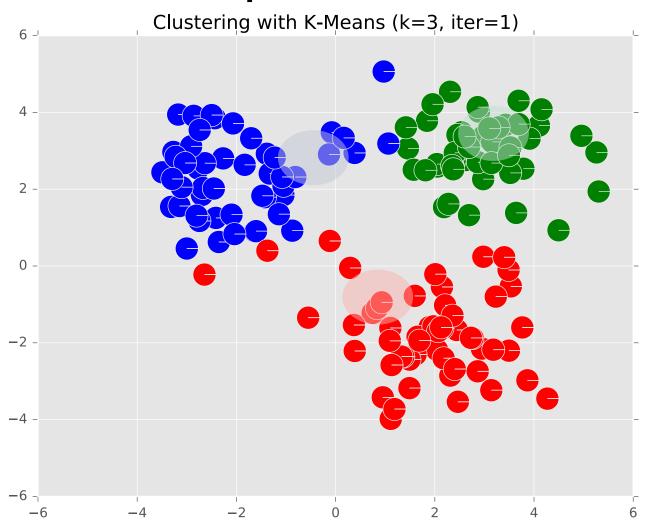
Matt Gormley

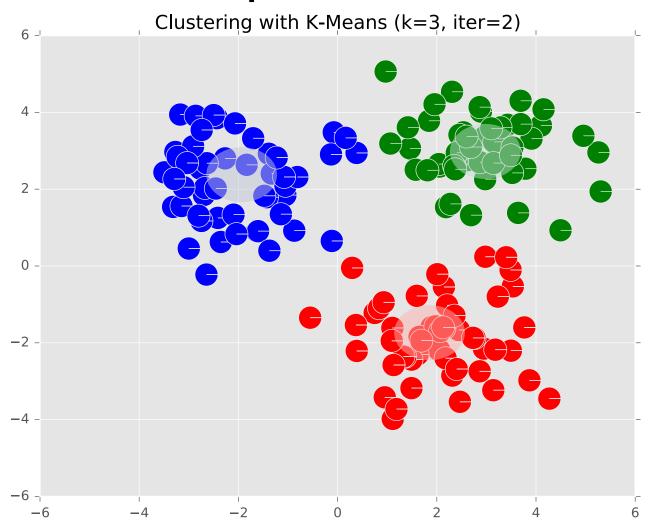
EXAMPLE: K-MEANS & GMM

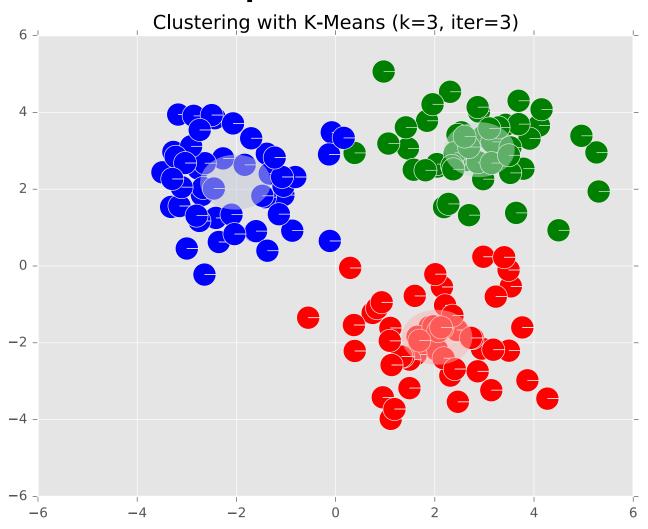


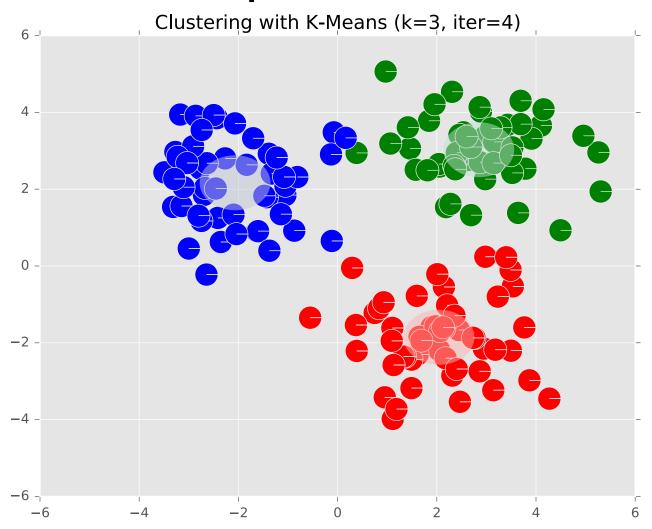


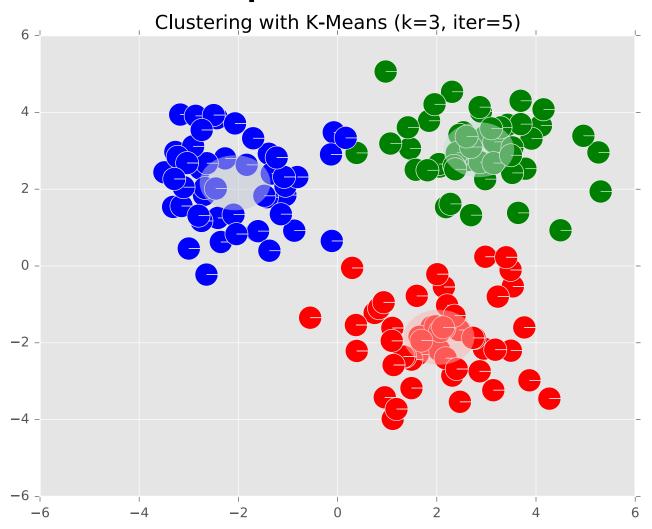


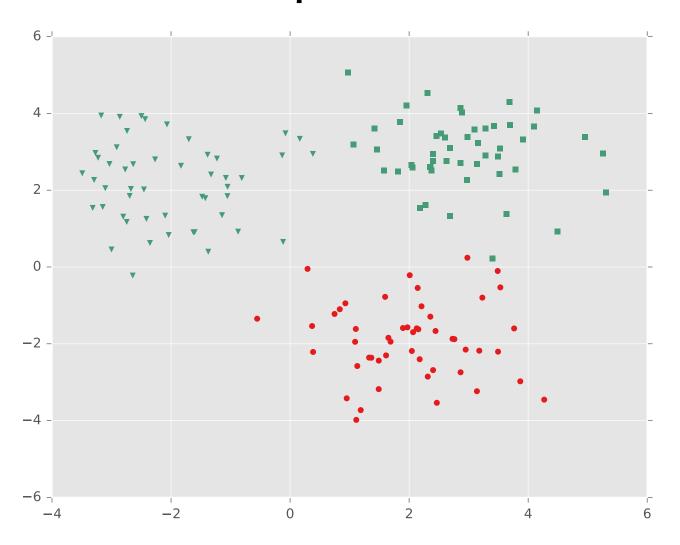


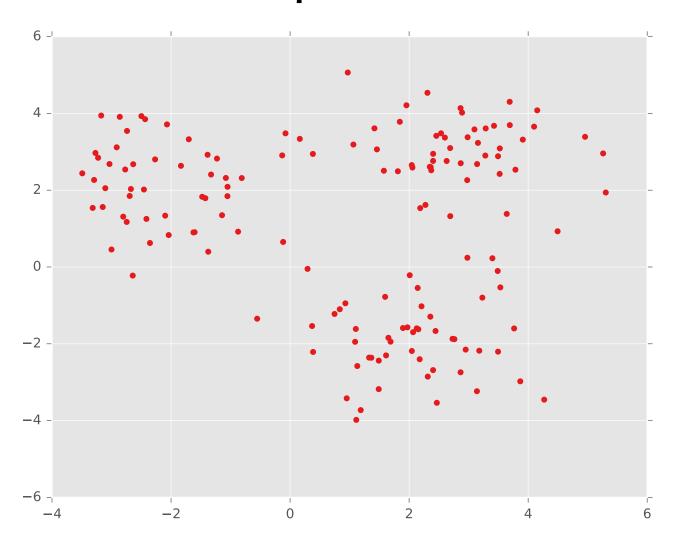


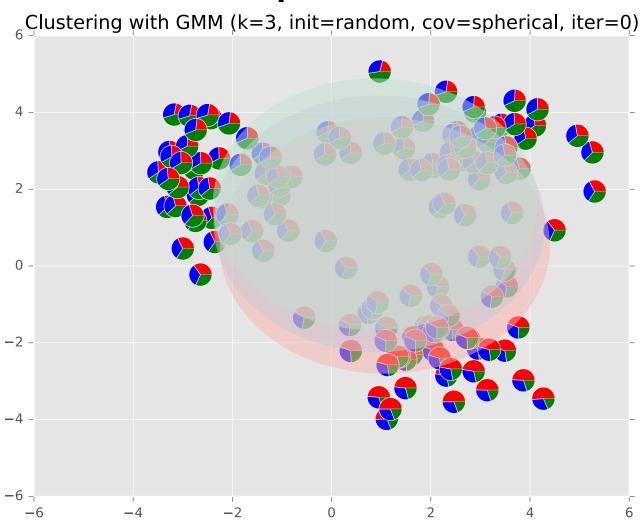


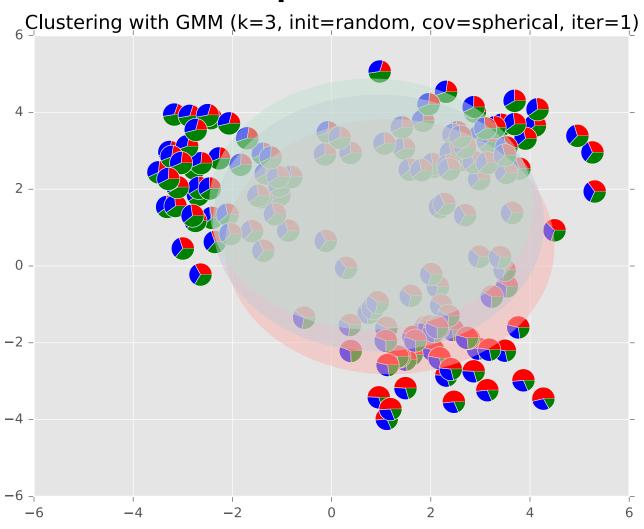


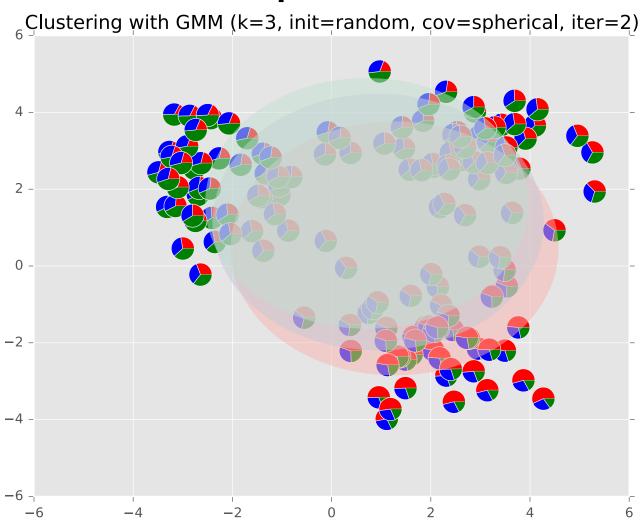


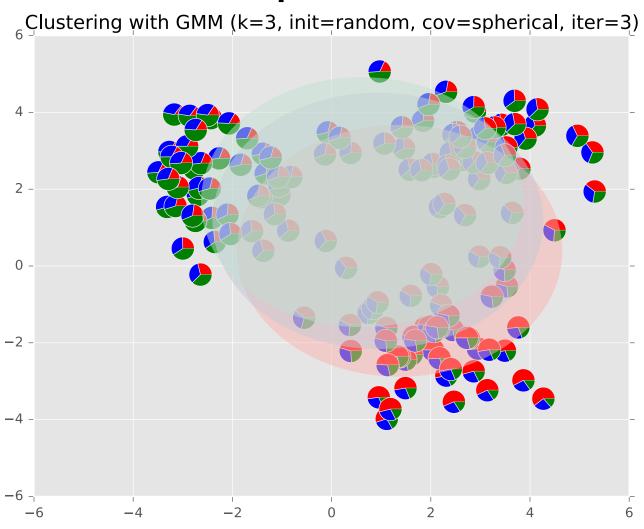


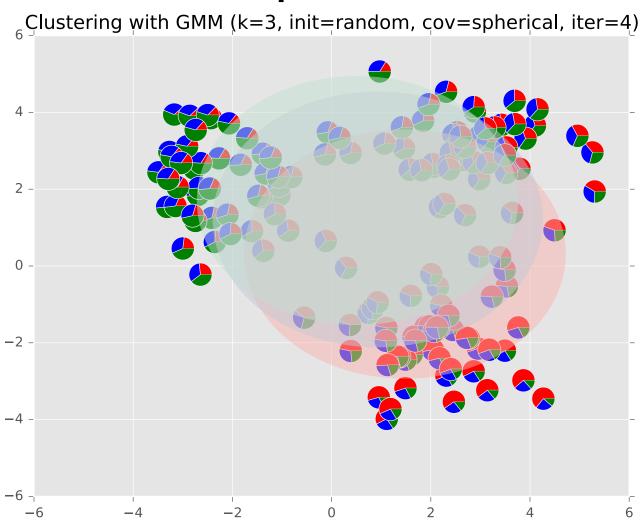


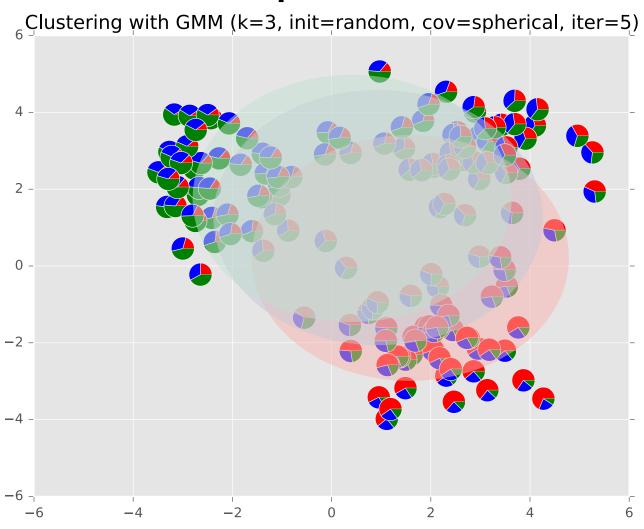


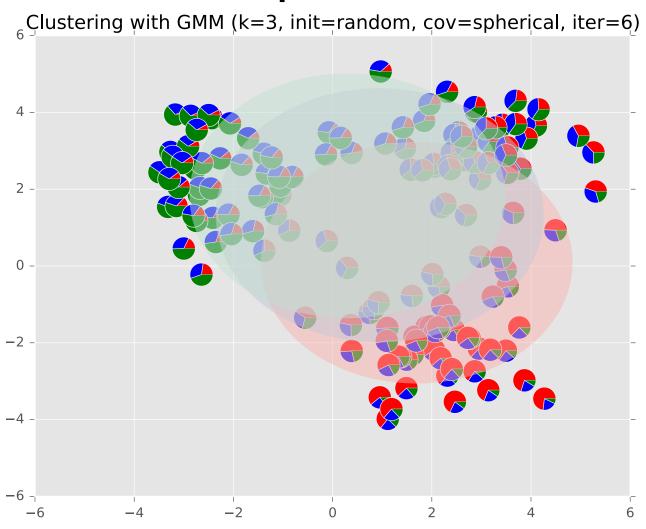


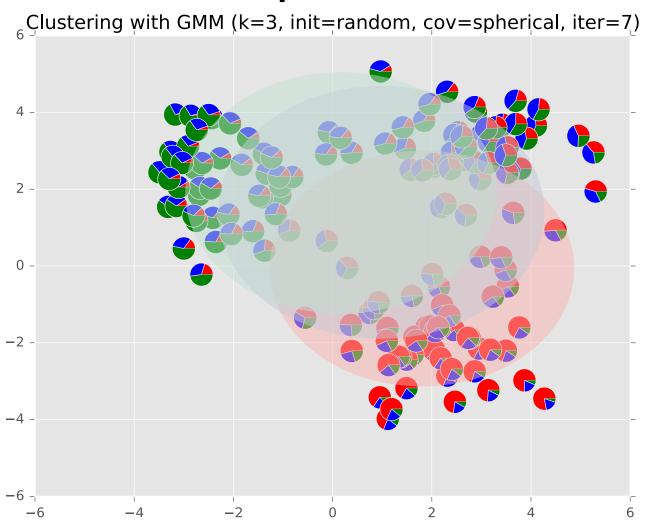


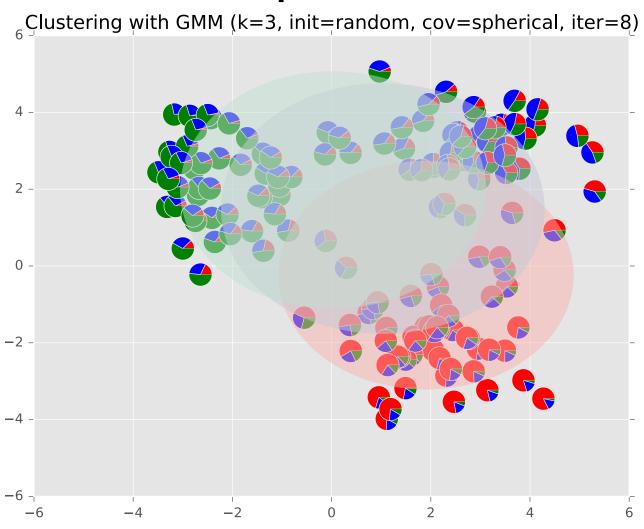


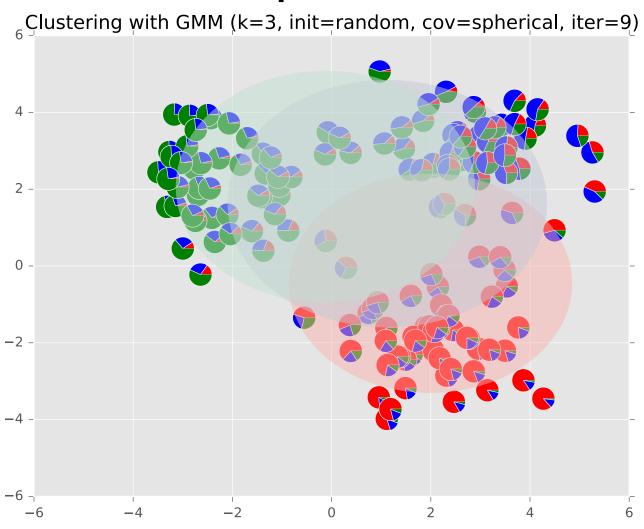


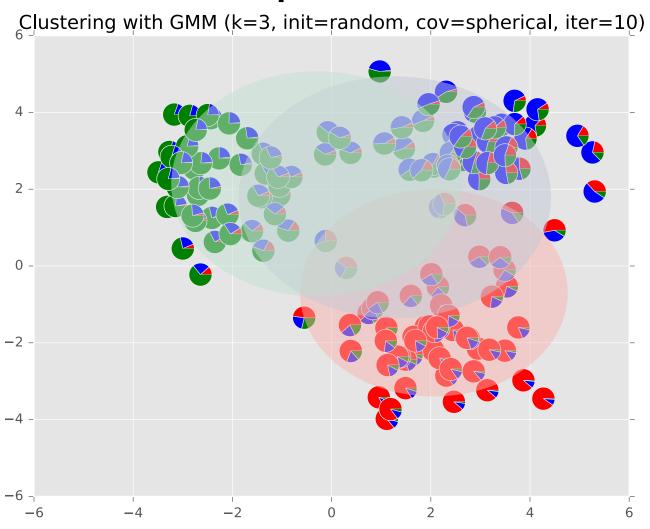


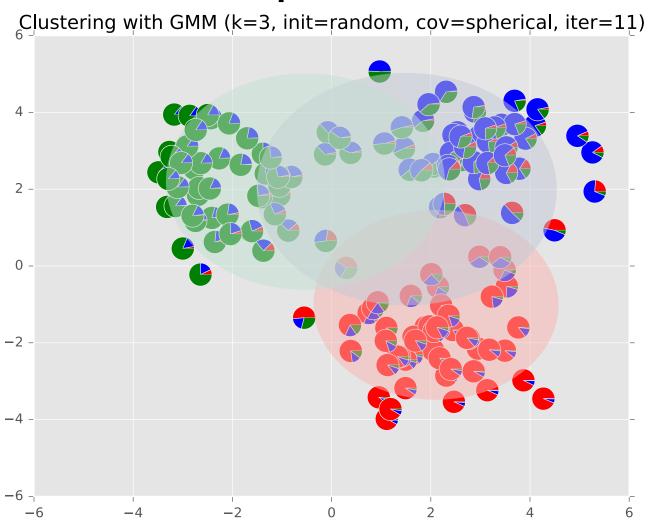


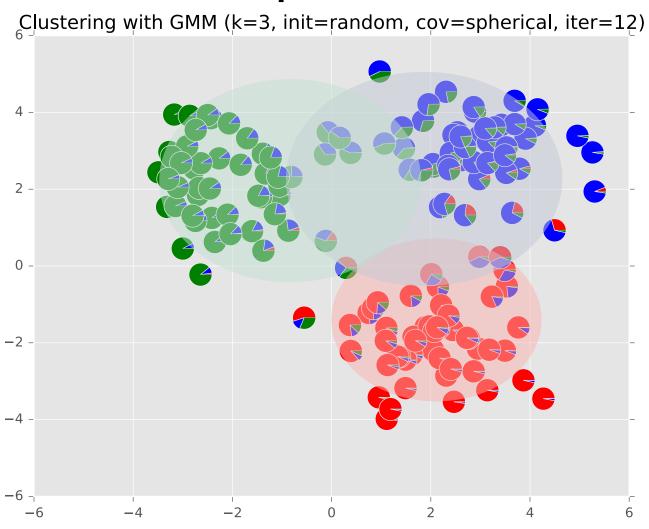


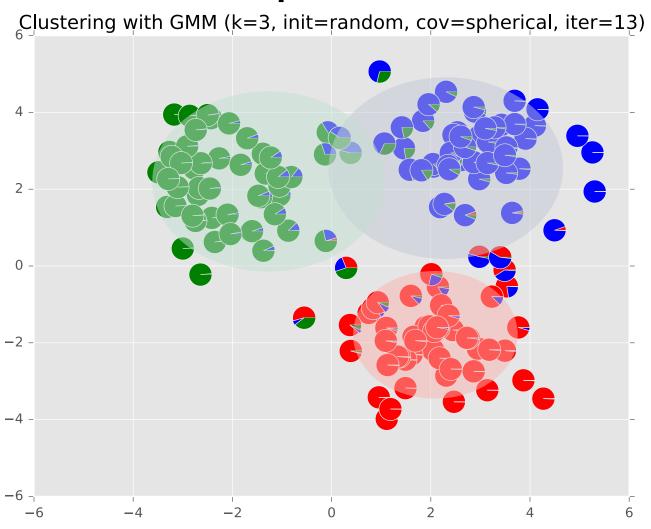


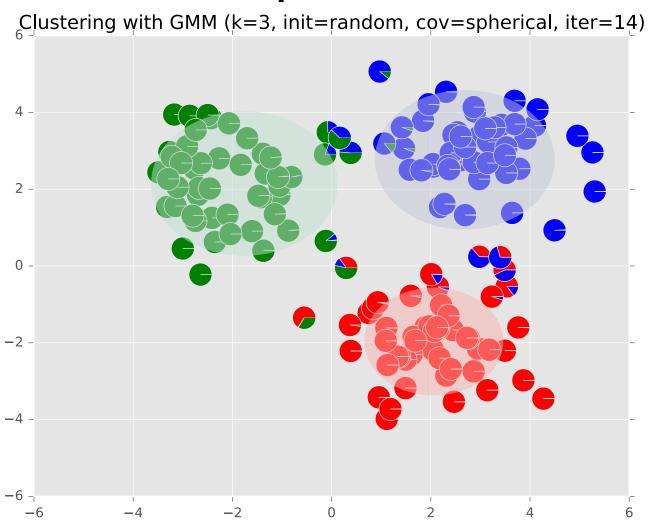


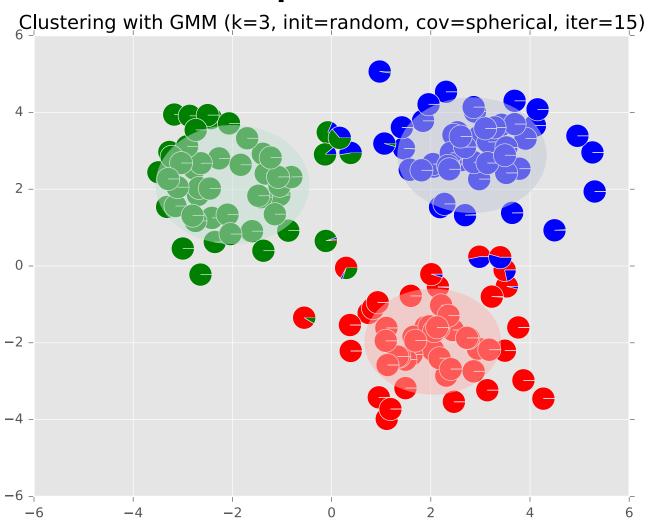


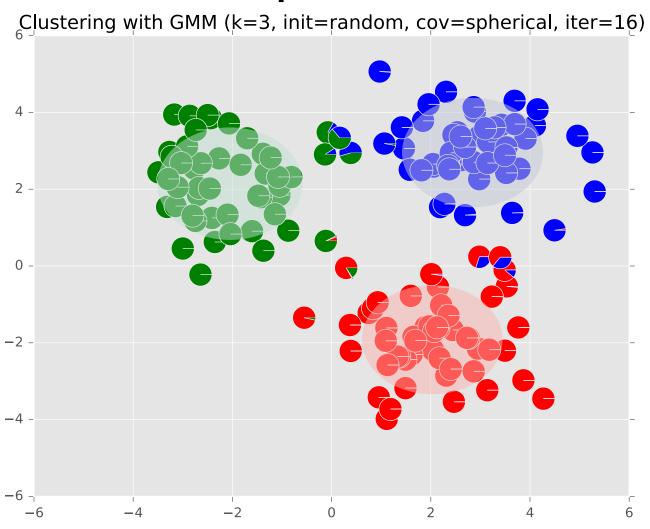


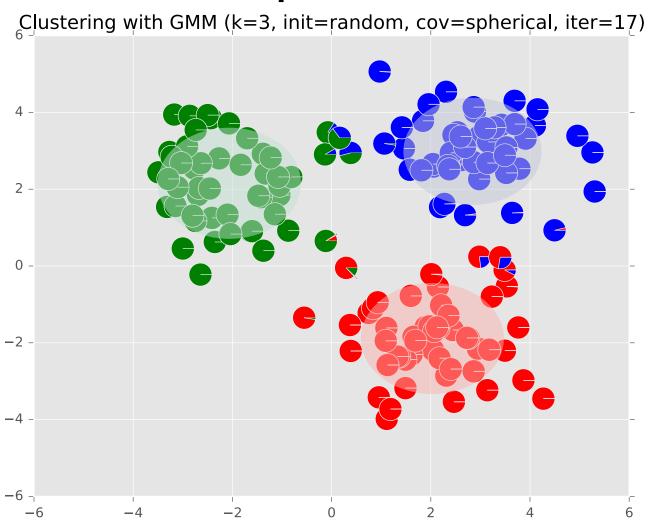


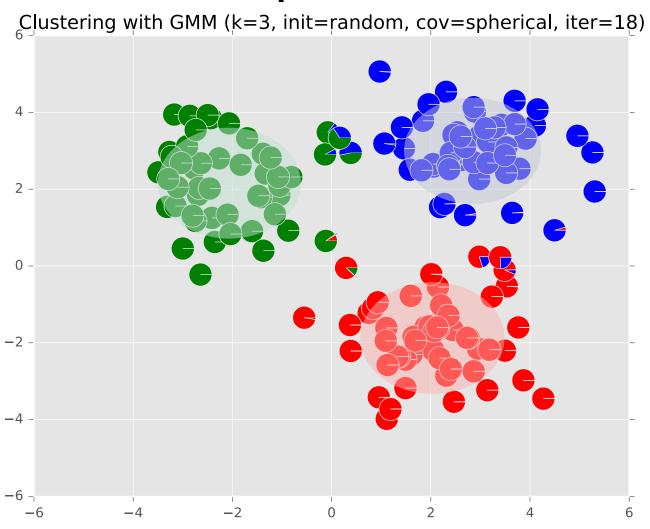


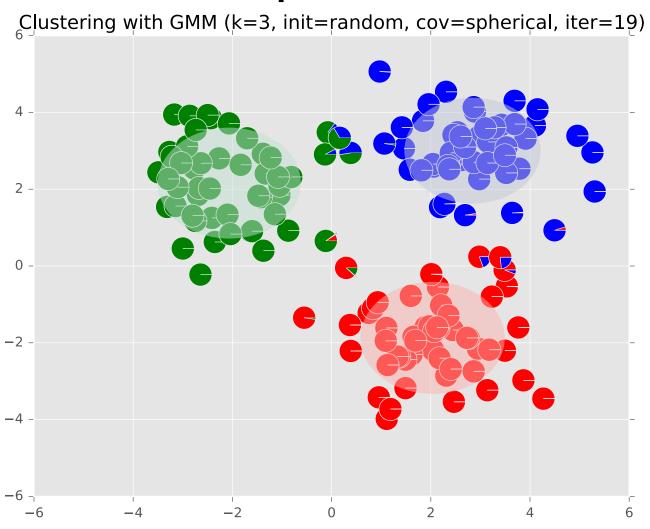






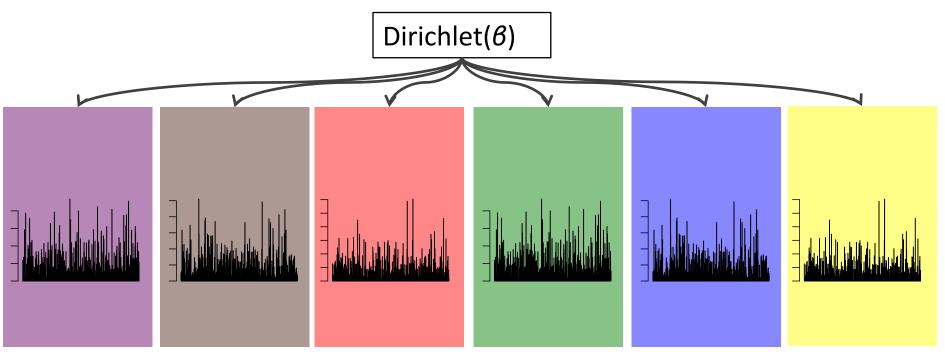






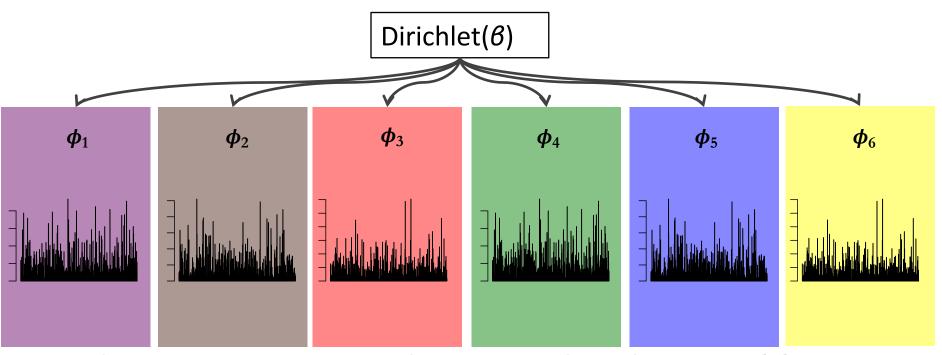
LATENT DIRICHLET ALLOCATION (LDA)

LDA for Topic Modeling



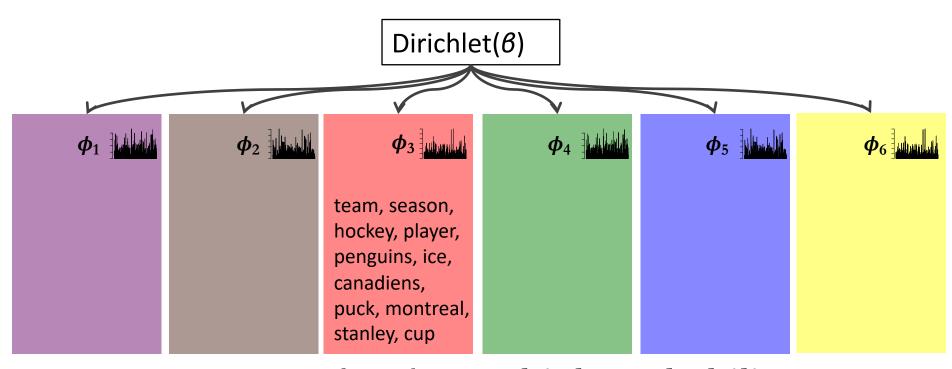
- The generative story begins with only a Dirichlet prior over the topics.
- Each **topic** is defined as a **Multinomial distribution** over the vocabulary, parameterized by $\phi_{\mathbf{k}}$

LDA for Topic Modeling

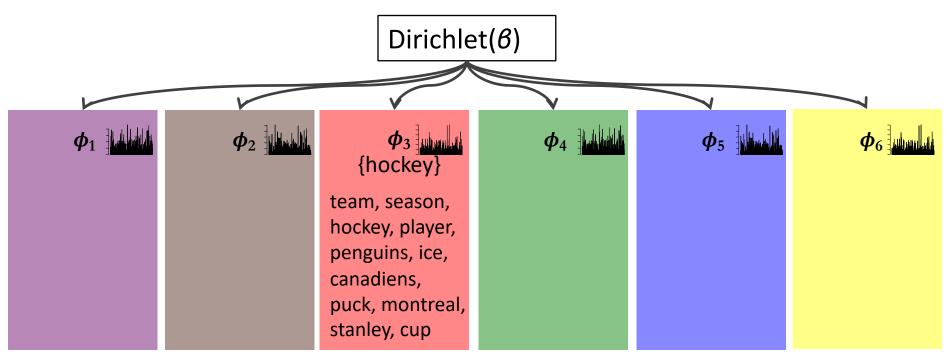


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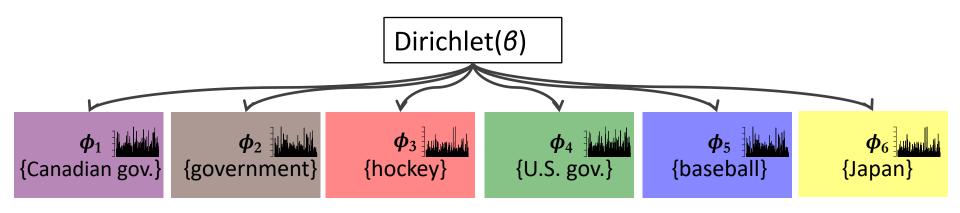
LDA for Topic Modeling



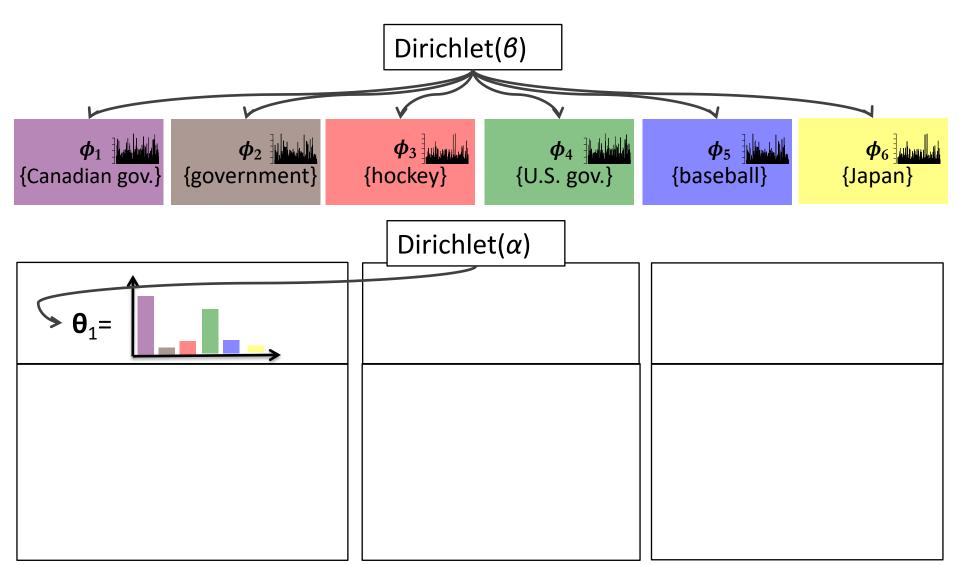
 A topic is visualized as its high probability words.

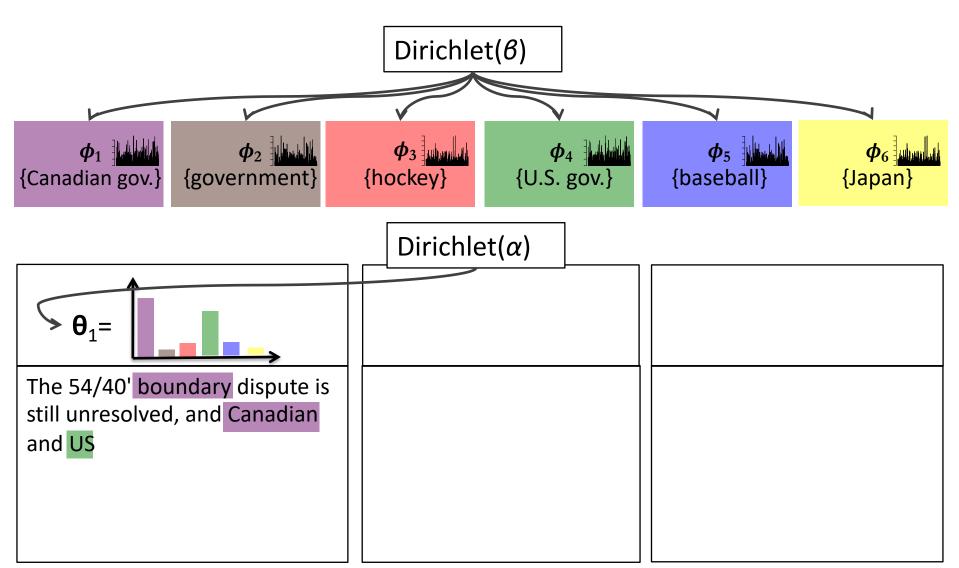


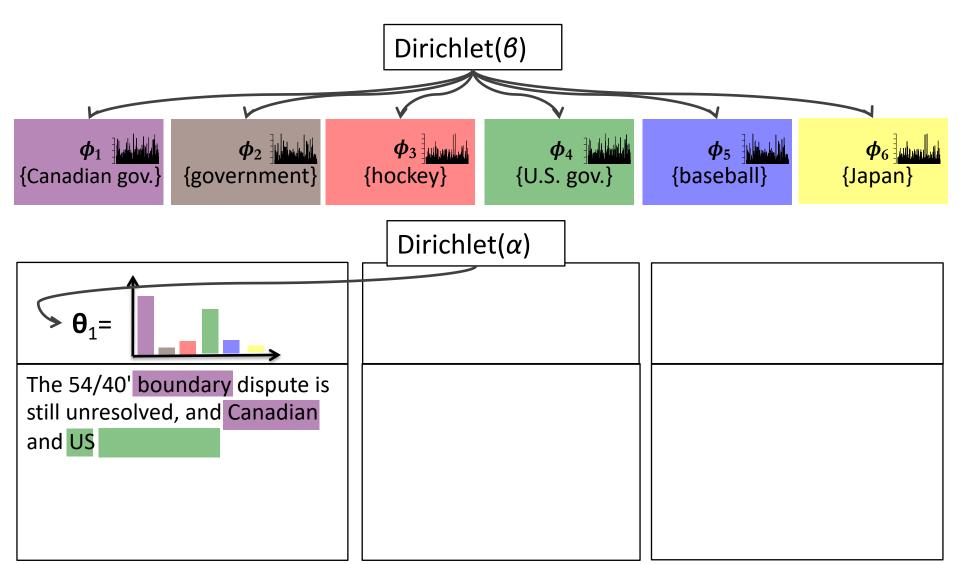
- A topic is visualized as its high probability words.
- A pedagogical label is used to identify the topic.

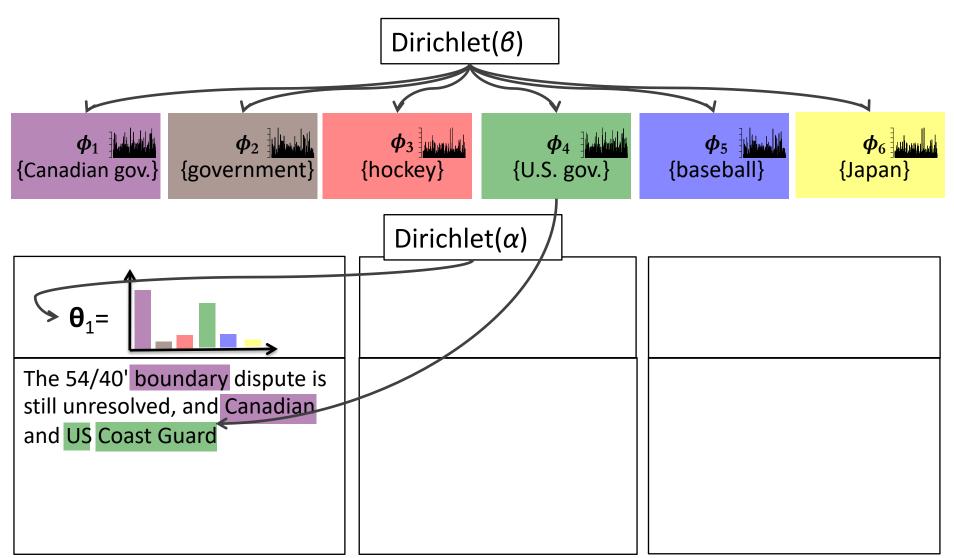


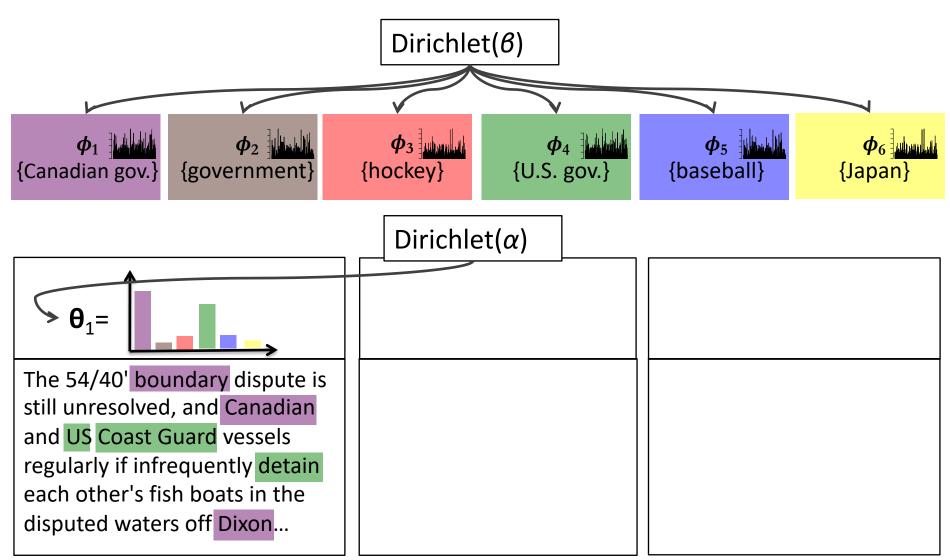
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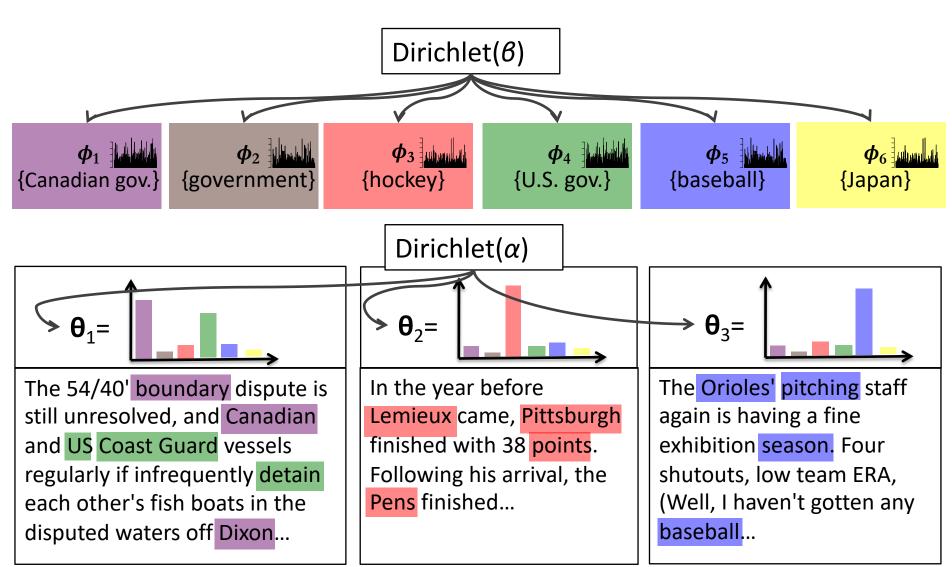


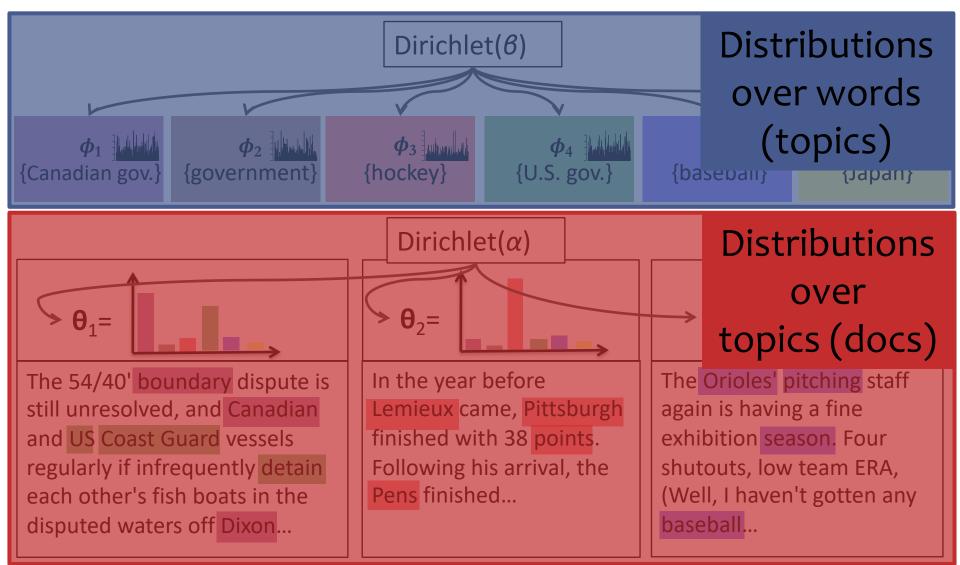


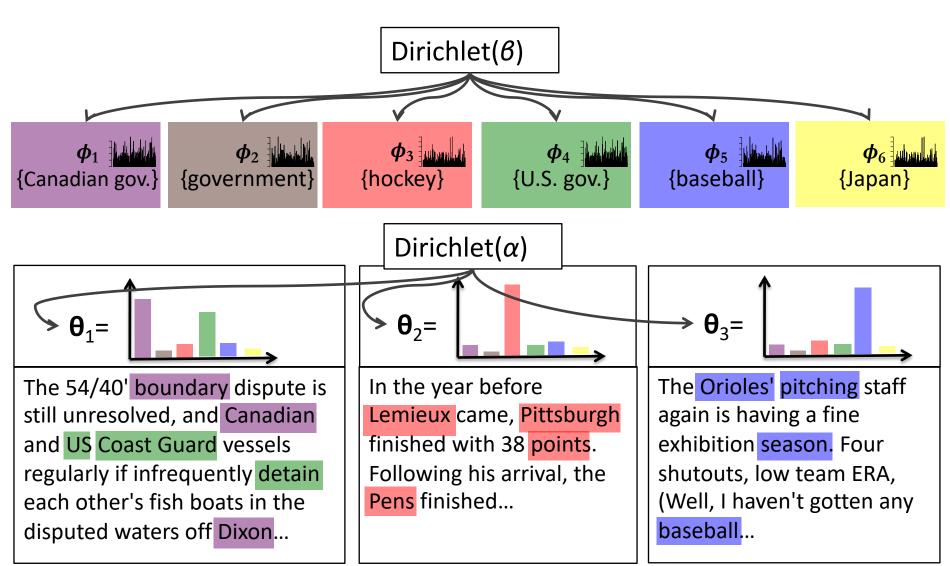












Inference and learning start with only the data

Dirichlet()



$$\phi_2 =$$

$$\phi_3 =$$

$$\phi_4 =$$

$$\phi_5 =$$

$$\phi_6 =$$

Dirichlet()

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...

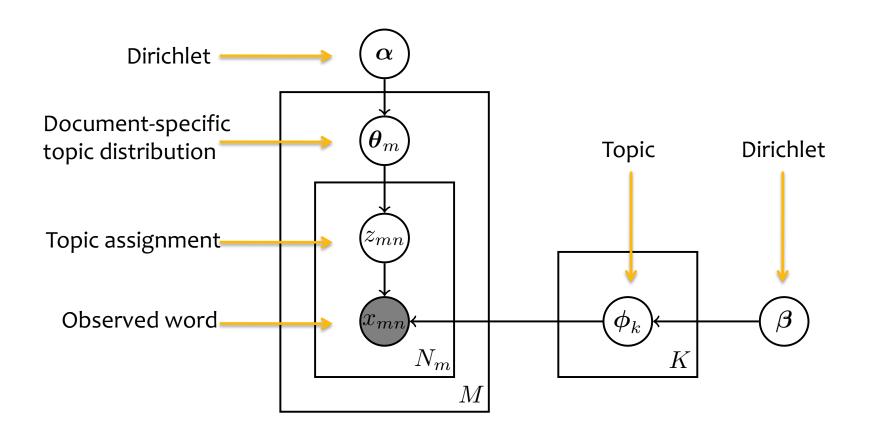
In the year before Lemieux came, Pittsburgh finished with 38 points. Following his arrival, the Pens finished...

$$\rightarrow$$
 θ_3 =

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

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

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 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

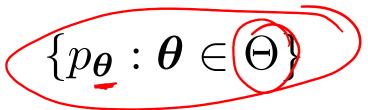
Semiparametric models:

Have a parametric component and a nonparametric component

	Frequentist	Bayesian
Parametric	Logistic regression, ANOVA, Fisher discriminant analysis, ARMA, etc.	Conjugate analysis, hierarchical models, conditional random fields
Semiparametric	Independent component analysis, Cox model, nonmetric MDS, etc.	[Hybrids of the above and below cells]
Nonparametric	Nearest neighbor, kernel methods, boostrap, decision trees, etc.	Gaussian processes, Dirichlet processes, Pitman-Yor processes, etc.

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

Def: a model is a collection of distributions



 parametric model: the parameter vector is finite dimensional

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

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

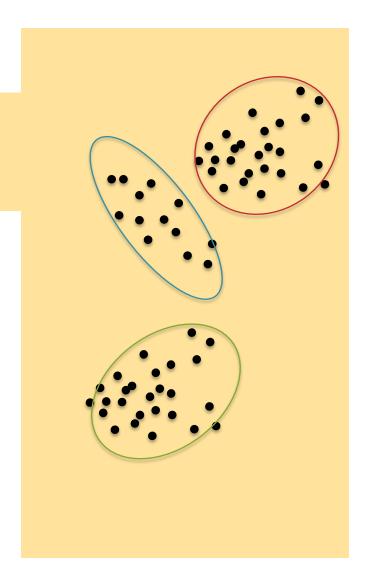
$$\Theta\subset \mathcal{F}$$

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?

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Model Selection

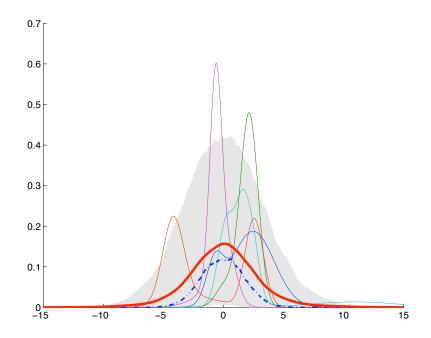
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- 1. Parametric approaches: cross-validation, bootstrap, AIC, BIC, DIC, MDL, Laplace, bridge sampling, etc.
- Nonparametric approach: average of an infinite set of models

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:



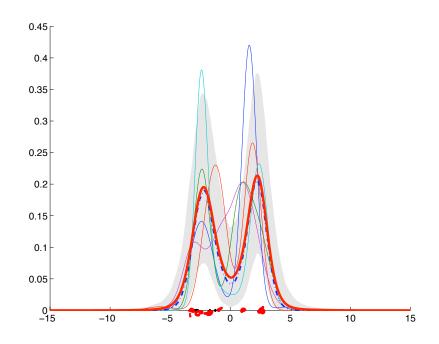
Red: mean density. Blue: median density. Grey: 5-95 quantile.

Others: draws.

Density Estimation

- Given data, estimate a probability density function that best explains it
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Posterior:



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

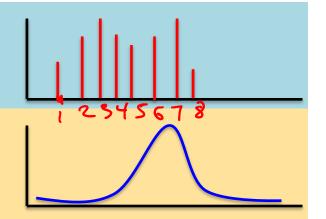
Black: data. Others: draws.

EXCHANGEABILITY AND DE FINETTI'S THEOREM

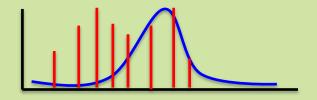
Background

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

- Discrete distribution: 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. Pis 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 $(X_1, X_2, X_3, ...)$ is **exchangeable** if for any finite permutation s of the indices (1, 2, ...n):

$$P(X_1, X_2, ..., X_n) = P(X_{s(1)}, X_{s(2)}, ..., X_{s(n)})$$

Notes:

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

Exchangability and de Finetti's Theorem

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

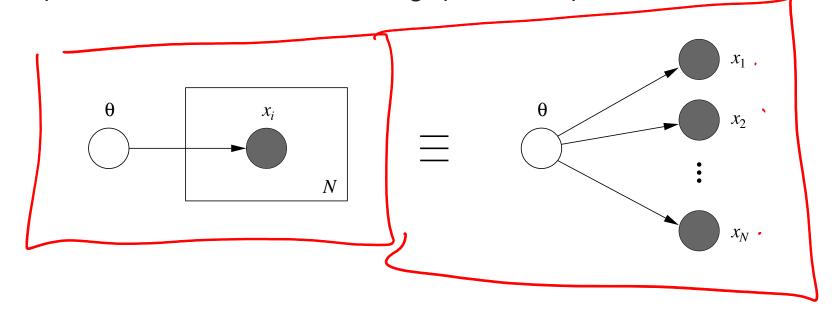
$$p(x_1, x_2, \dots, x_N) = \int \left(\prod_{i=1}^N p(x_i \mid \theta) \right) dP(\theta)$$

for some random variable θ .

- ullet The theorem wouldn't be true if we limited ourselves to parameters heta ranging over Euclidean vector spaces
- In particular, we need to allow θ 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...

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

$$p(x_1, x_2, \dots, x_N) = \int p(\theta) \left(\prod_{i=1}^N p(x_i \mid \theta) \right) d\theta$$

Type of Model	Parametric Example	Nonparametric Example	
		Construction #1	Construction #2
distribution over counts	Dirichlet- Multinomial Model	Dirichlet Process (DP)	
		Chinese Restaurant Process (CRP)	Stick-breaking construction
mixture	Gaussian Mixture Model (GMM)	Dirichlet Process Mixture 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

Chinese Restaurant Process & Stick-breaking Constructions

DIRICHLET PROCESS

Dirichlet Process (Scussin, Beta, Bernoulli

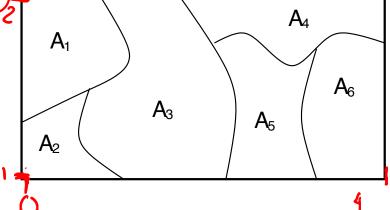
Ferguson Definition

- Parameters of a DP:
 - Base distribution, H, is a probability distribution over Θ
 - Strength parameter, $\alpha \in \mathcal{R}$
- _is a distintation • We say $G \sim DP(\alpha, H)$ if for any partition $A_1 \cup A_2 \cup \ldots \cup A_K = \Theta$ we have:

$$(G(A_1), \ldots, G(A_K)) \sim \underbrace{\operatorname{Dirichlet}(\alpha H(A_1), \ldots, \alpha H(A_K))}_{\text{distribution}}$$

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

A partition of the space Θ



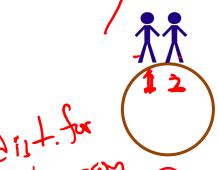
R, [0,1]

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:

 $p(kth \ occupied \ table) \propto n_k$ $p(next unoccupied table) \propto \alpha$

here n_k is the number of people sitting at the table k



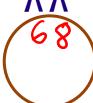
















$$\frac{2}{8+\alpha}$$

$$\frac{1}{2}$$

$$8 + \alpha$$

$$8 + \alpha$$

$$8 + \alpha$$



$$8 + \alpha$$

Chinese Restaurant Process

Properties:

- CRP defines a **distribution over clusterings** (i.e. partitions) of the indices l, ... (n) = # G
 - customer = index
 - table = cluster
 - 2. We write $z_1, z_2, ..., z_n \sim CRP(\alpha)$ to denote a **sequence of cluster indices** drawn from a Chinese Restaurant Process
 - 3. The CRP is an **exchangeable process**
- 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
- 6 Behavior of CRP with α :
 - As α goes to θ , the number of clusters goes to I
 - − As α 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:

we have the following predictive distribution
$$\theta_{n+1} | \theta_1, \dots, \theta_n \sim \frac{1}{\alpha + n} \left(\alpha H + \sum_{i=1}^n \delta_{\theta_i} \right)$$
(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:

$$\mathbb{E}[G(A)] = H(A)$$
 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 $\theta_1, ..., \theta_n$ from G is a DP

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

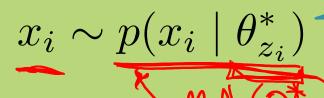
Chinese Restaurant Process & Stick-breaking Constructions

DIRICHLET PROCESS MIXTURE MODEL

• Draw n cluster indices from a CRP:

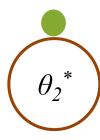
$$z_1, z_2, ..., z_n \sim CRP(\alpha)$$

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



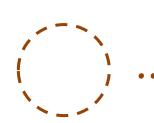
Customer i orders a dish x_i (observation) from a tablespecific distribution over dishes θ_k^* (cluster parameters)









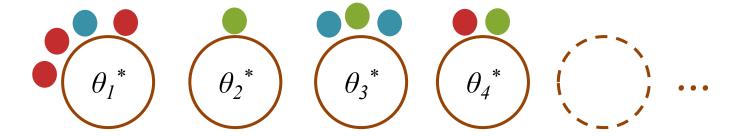


- Draw n cluster indices from a CRP: $z_1, z_2, ..., z_n \sim CRP(\alpha)$
- For each of the resulting K clusters: $\theta_k^* \sim H$ where H is a base distribution
- Draw n observations:

$$x_i \sim p(x_i \mid \theta_{z_i}^*)$$

- 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:

$$z_i \sim p(z_i \mid \mathbf{z}_{-i}, \mathbf{x})$$



Overview of 3 Gibbs Samplers for Conjugate Priors

- Alg. 1: (uncollapsed)
 - Markov chain state: per-customer parameters $\theta_1, ..., \theta_n$
 - For i = 1, ..., n: Draw $\theta_i \sim p(\theta_i \mid \theta_{-i}, x)$
- Alg. 2: (uncollapsed)
 - Markov chain state: per-customer cluster Hall the thetas except θ_i
 - per-cluster parameters θ_{l}^{*} , ..., θ_{k}^{*}
 - For i = 1, ..., n: Draw $z_i \sim p(z_i \mid \boldsymbol{z}_{-i}, \boldsymbol{x}(\boldsymbol{\theta}^*))$
 - Set K = number of clusters in z
 - For k = 1, ..., K: Draw $\theta_k^* \sim p(\theta_k^* | \{x_i : z_i = k\})$
- Alg. 3: (collapsed)
 - Markov chain state: per-customer cluster indices $z_1, ..., z_n$
 - For i = 1, ..., n: Draw $z_i \sim p(z_i \mid z_{-i}, x)$

211-1-12M

- 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

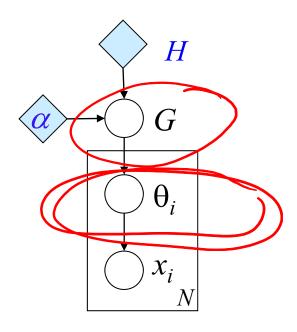
Dirichlet Process: For both the CRP and stickbreaking constructions, if we marginalize out G, we have the following predictive distribution:

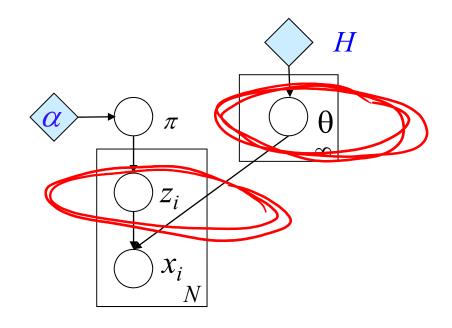
$$\theta_{n+1}|\theta_1,\ldots,\theta_n \sim \frac{1}{\alpha+n} \left(\alpha H + \sum_{i=1}^n \delta_{\theta_i}\right)$$

(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

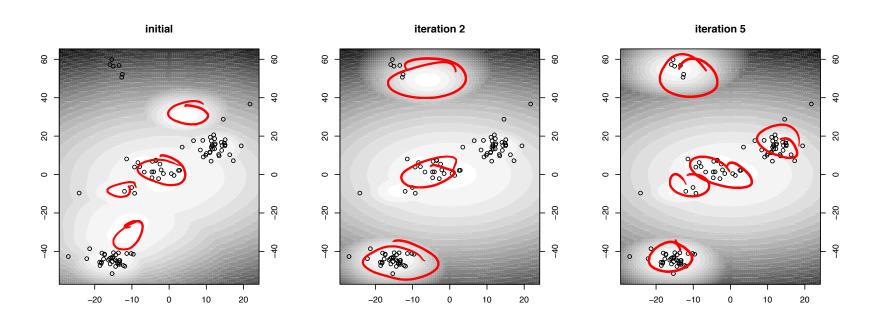


Figure 2: The approximate predictive distribution given by variational inference at different stages of the algorithm. The data are 100 points generated by a Gaussian DP mixture model with fixed diagonal covariance.

Example: DP Gaussian Mixture Model

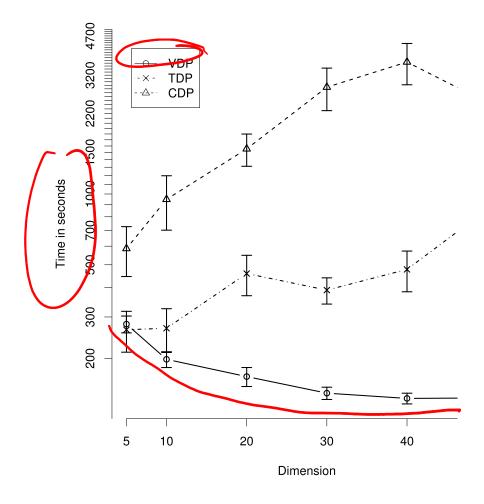


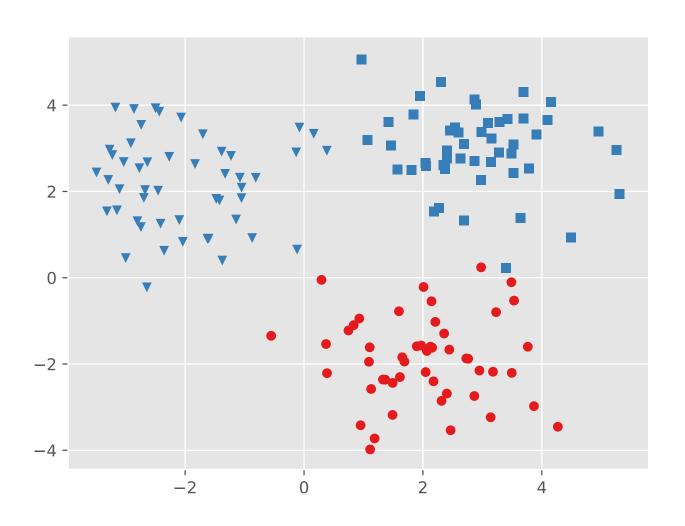
Figure 3: Mean convergence time and standard error across ten data sets per dimension for variational inference, TDP Gibbs sampling, and the collapsed Gibbs sampler.

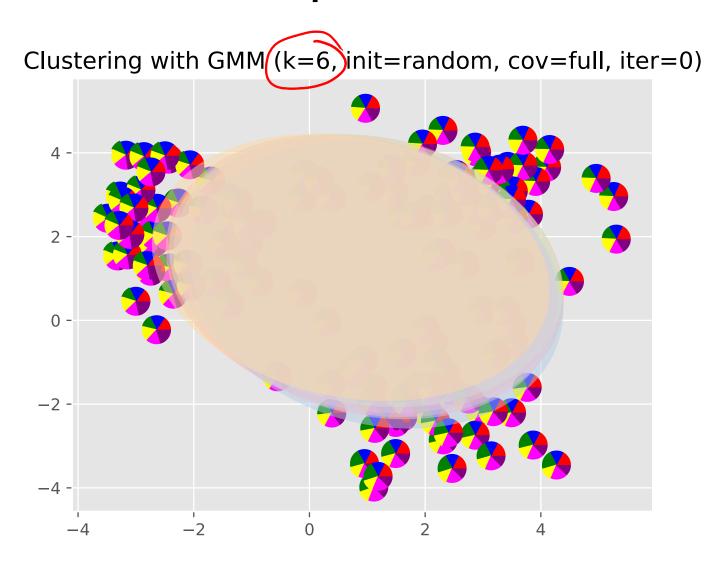
Summary of DP and DP-MM

- 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.

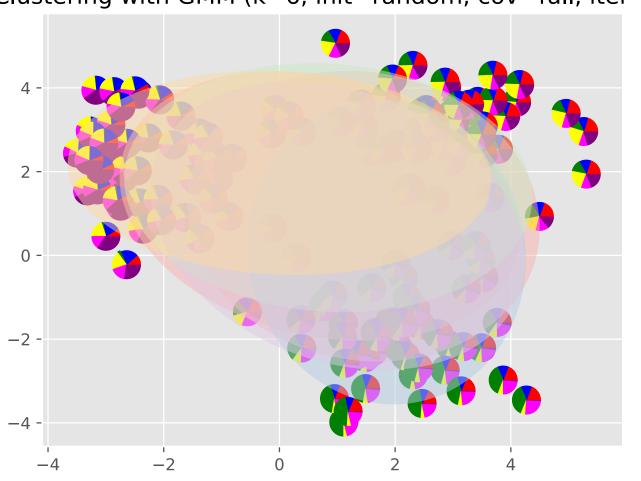
GMM VS. DPMM EXAMPLE

Example: Dataset

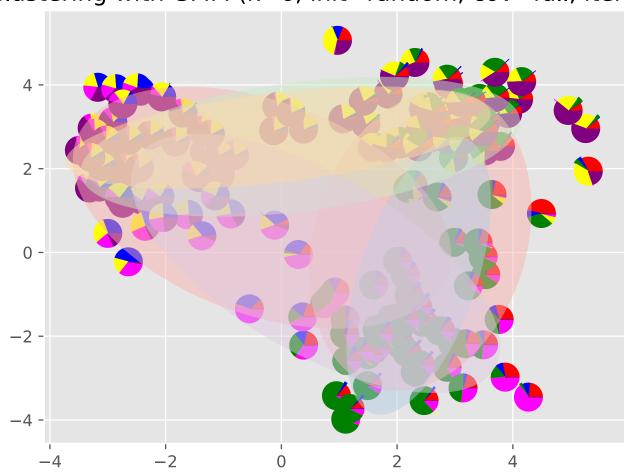




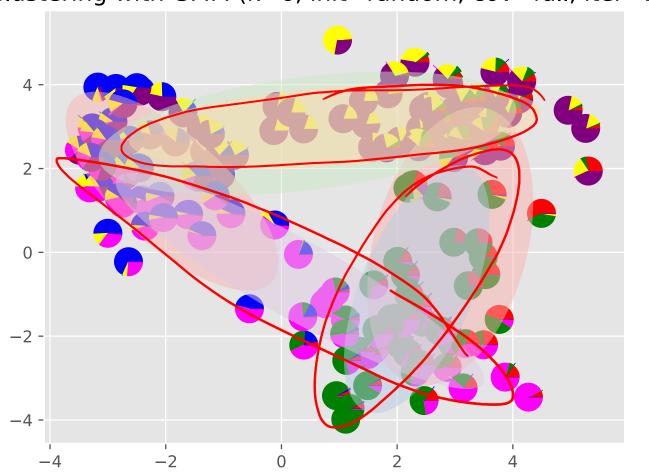
Clustering with GMM (k=6, init=random, cov=full, iter=5)



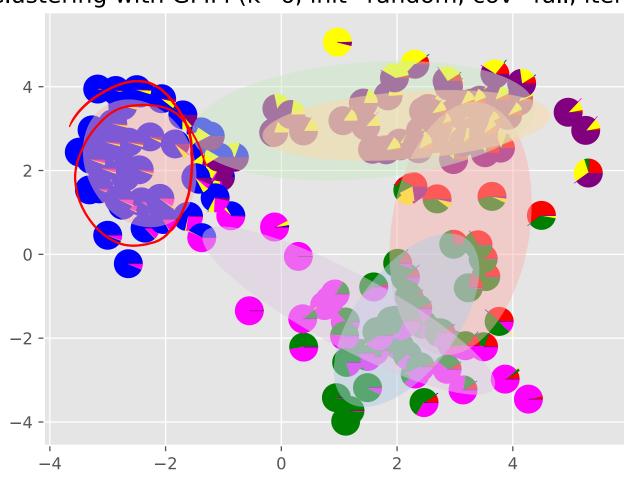
Clustering with GMM (k=6, init=random, cov=full, iter=10)



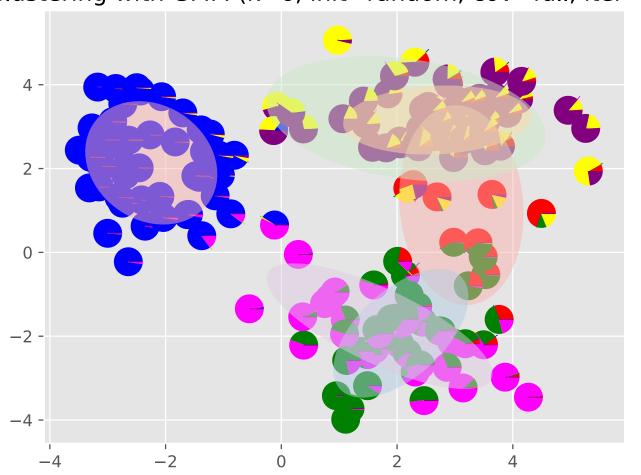
Clustering with GMM (k=6, init=random, cov=full, iter=15)



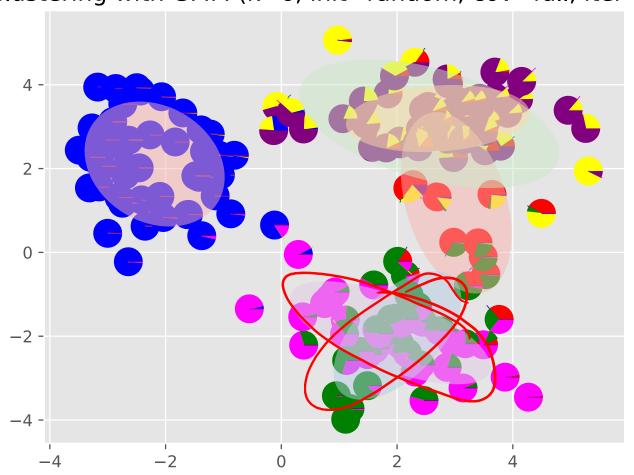
Clustering with GMM (k=6, init=random, cov=full, iter=20)



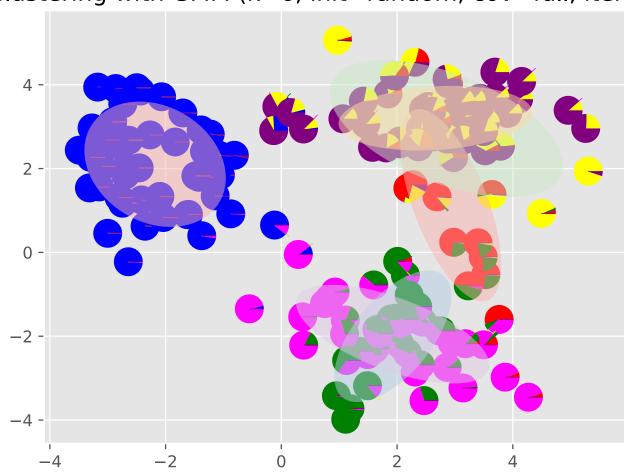
Clustering with GMM (k=6, init=random, cov=full, iter=25)



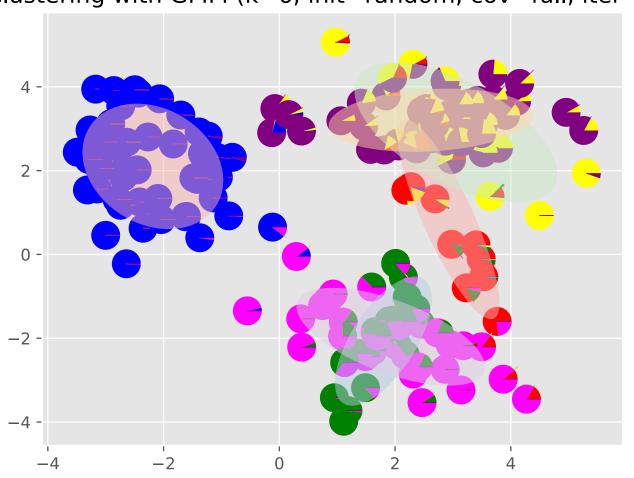
Clustering with GMM (k=6, init=random, cov=full, iter=30)



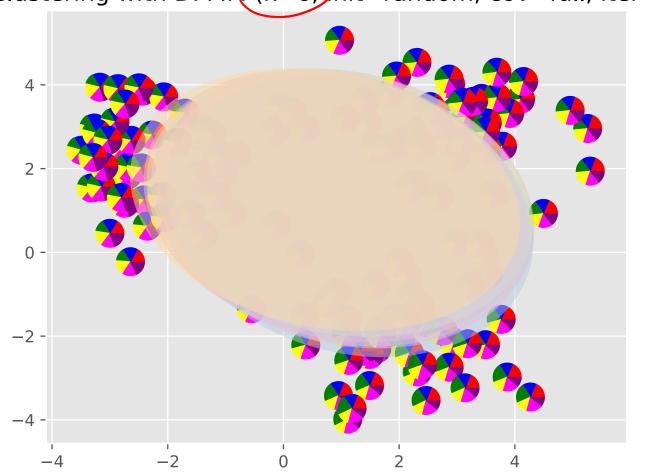
Clustering with GMM (k=6, init=random, cov=full, iter=35)



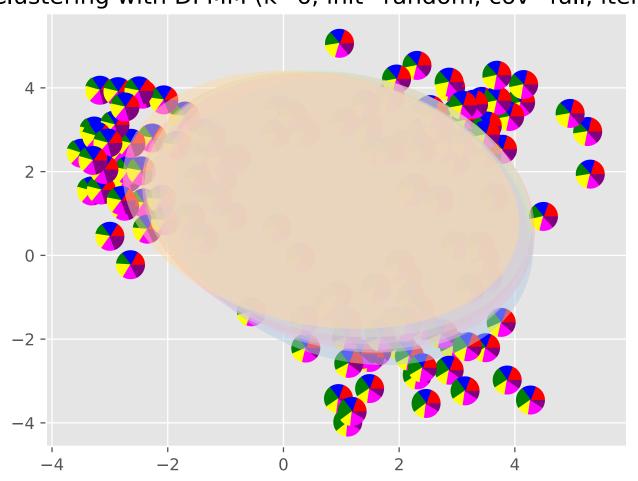
Clustering with GMM (k=6, init=random, cov=full, iter=39)



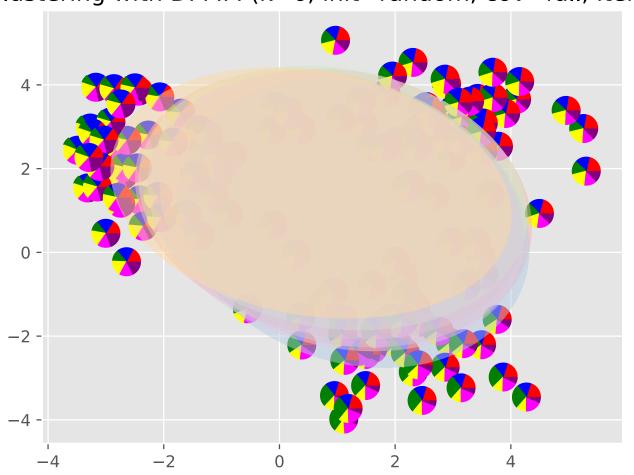
Clustering with DPMM (k=6, init=random, cov=full, iter=0)



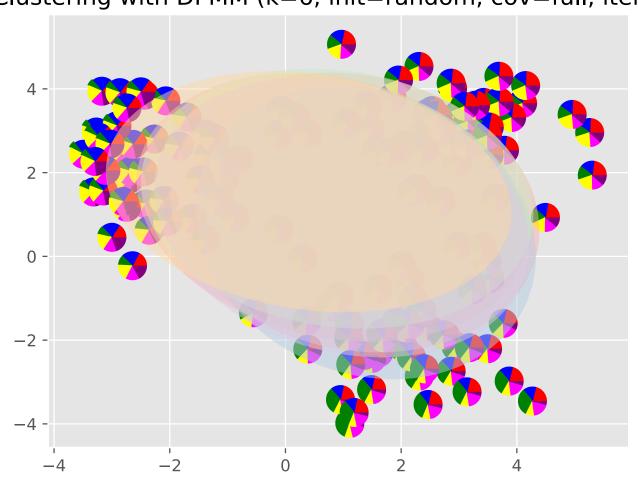
Clustering with DPMM (k=6, init=random, cov=full, iter=1)



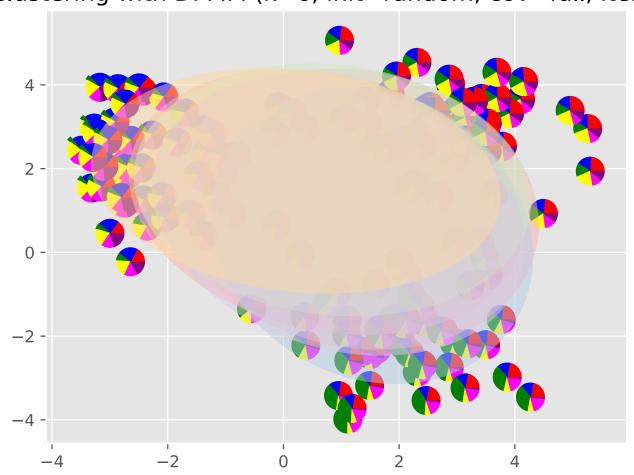
Clustering with DPMM (k=6, init=random, cov=full, iter=2)



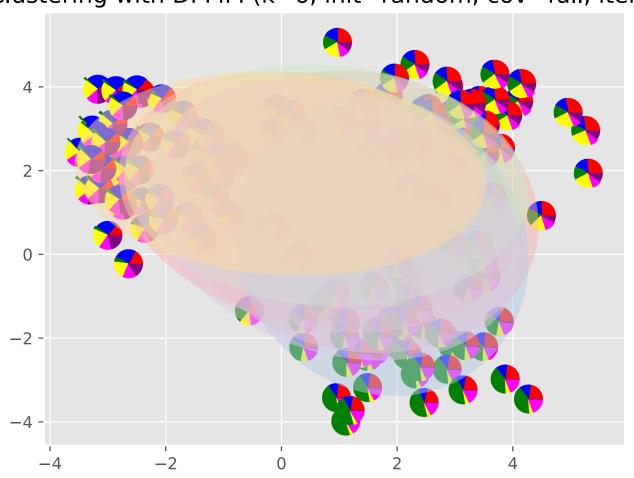
Clustering with DPMM (k=6, init=random, cov=full, iter=3)



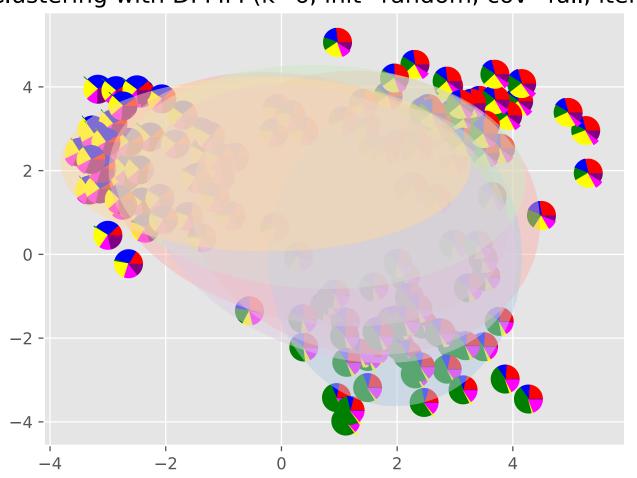
Clustering with DPMM (k=6, init=random, cov=full, iter=4)



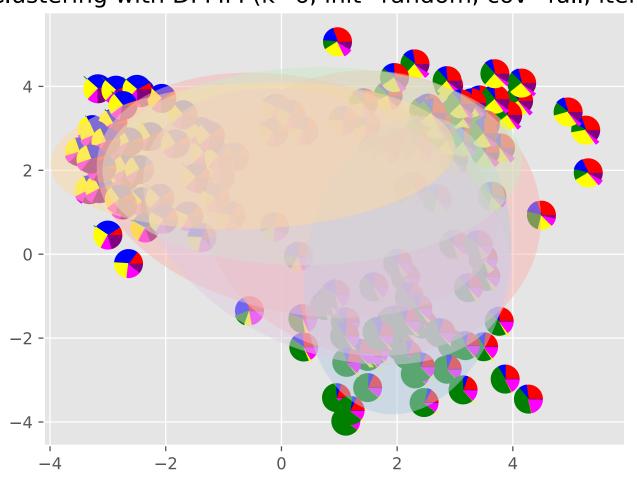
Clustering with DPMM (k=6, init=random, cov=full, iter=5)



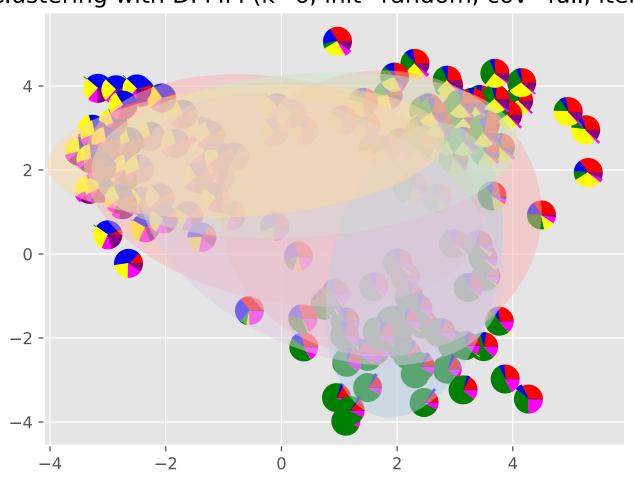
Clustering with DPMM (k=6, init=random, cov=full, iter=6)



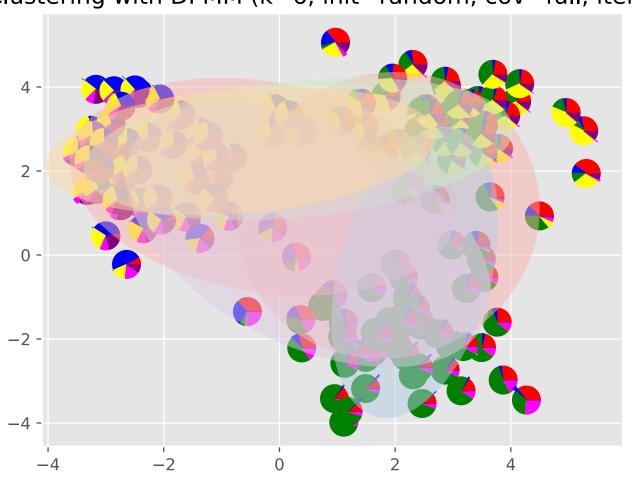
Clustering with DPMM (k=6, init=random, cov=full, iter=7)



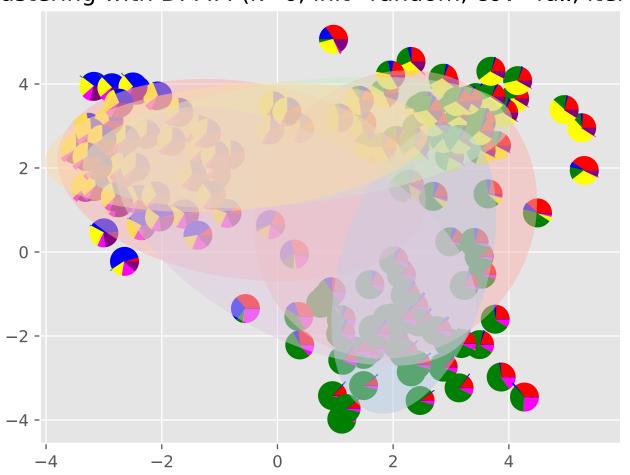
Clustering with DPMM (k=6, init=random, cov=full, iter=8)



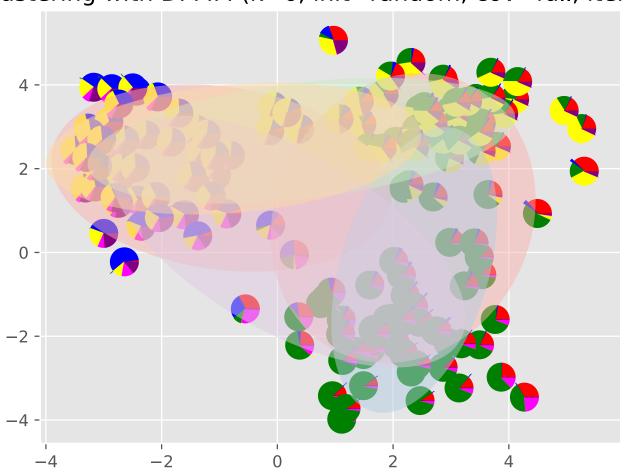
Clustering with DPMM (k=6, init=random, cov=full, iter=9)



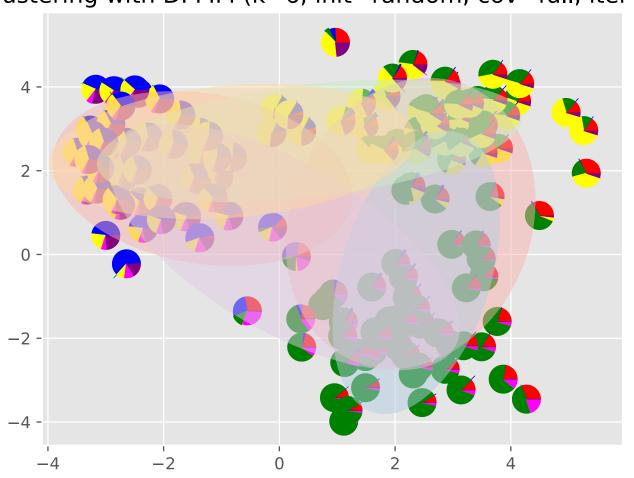
Clustering with DPMM (k=6, init=random, cov=full, iter=10)



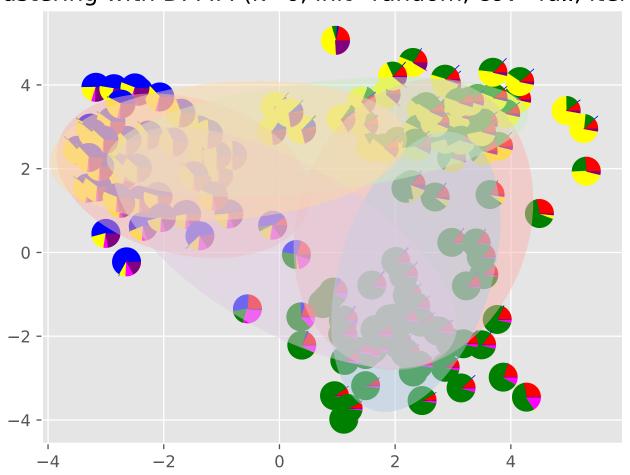
Clustering with DPMM (k=6, init=random, cov=full, iter=11)



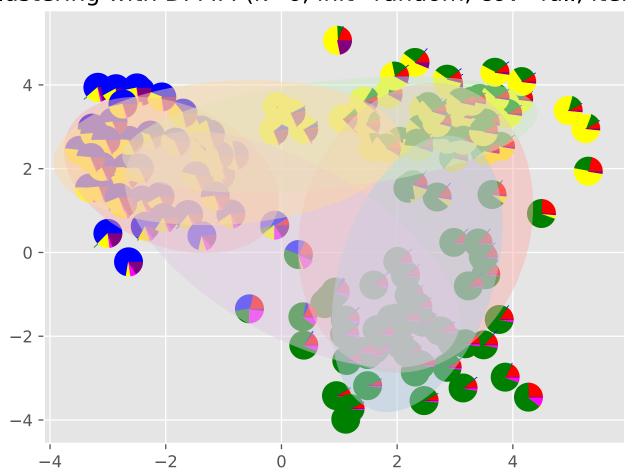
Clustering with DPMM (k=6, init=random, cov=full, iter=12)



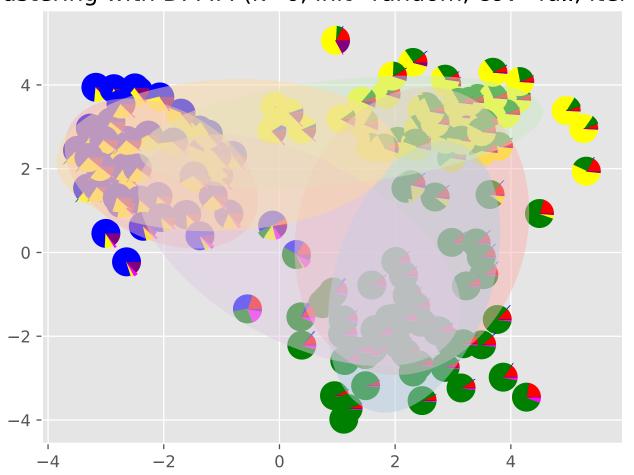
Clustering with DPMM (k=6, init=random, cov=full, iter=13)



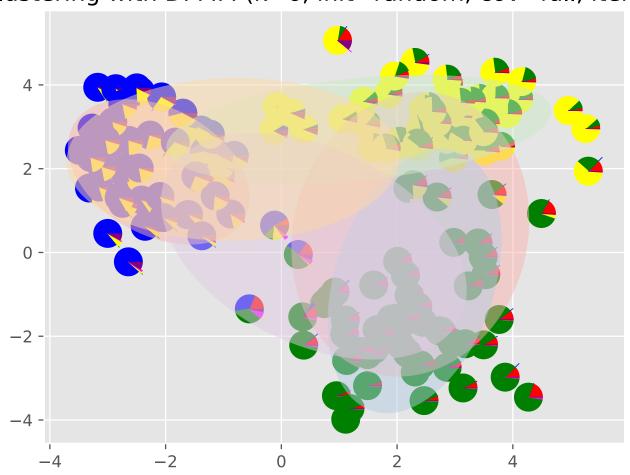
Clustering with DPMM (k=6, init=random, cov=full, iter=14)



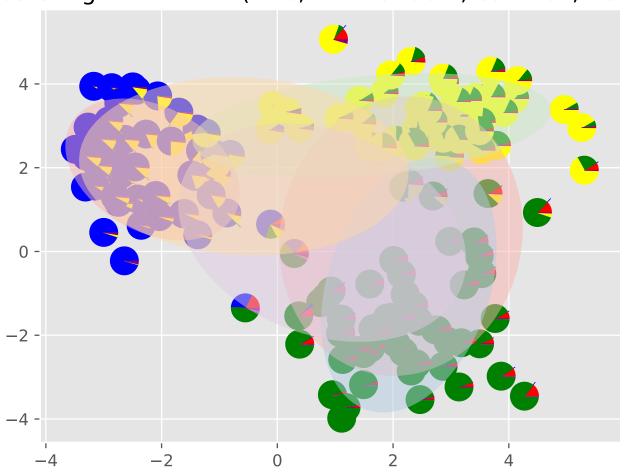
Clustering with DPMM (k=6, init=random, cov=full, iter=15)



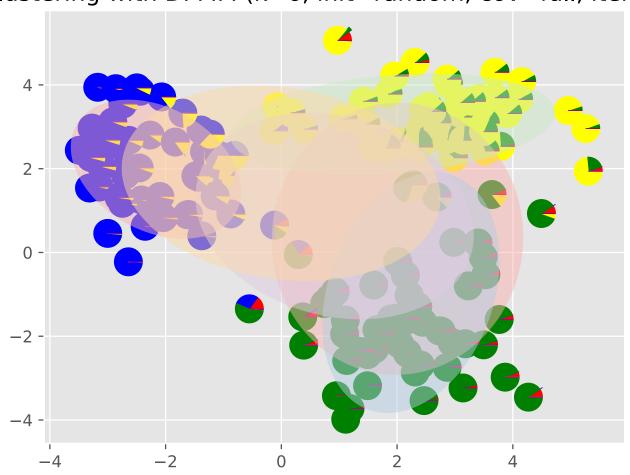
Clustering with DPMM (k=6, init=random, cov=full, iter=16)



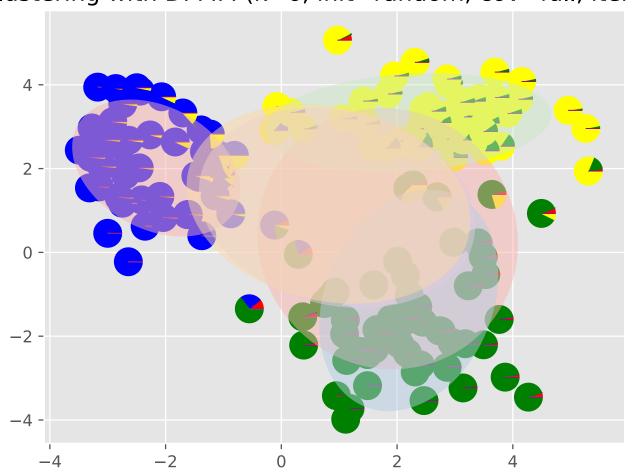
Clustering with DPMM (k=6, init=random, cov=full, iter=17)



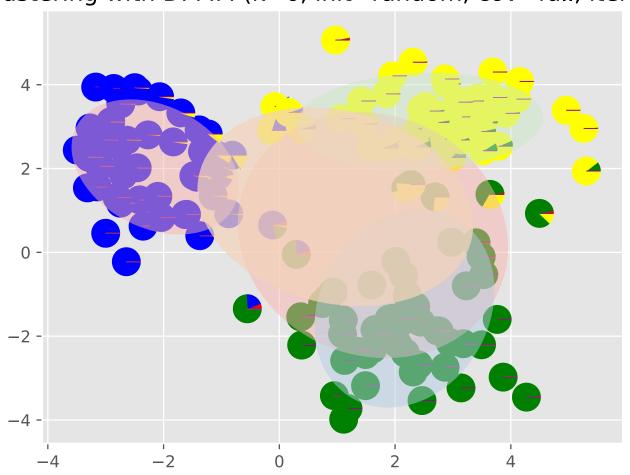
Clustering with DPMM (k=6, init=random, cov=full, iter=18)



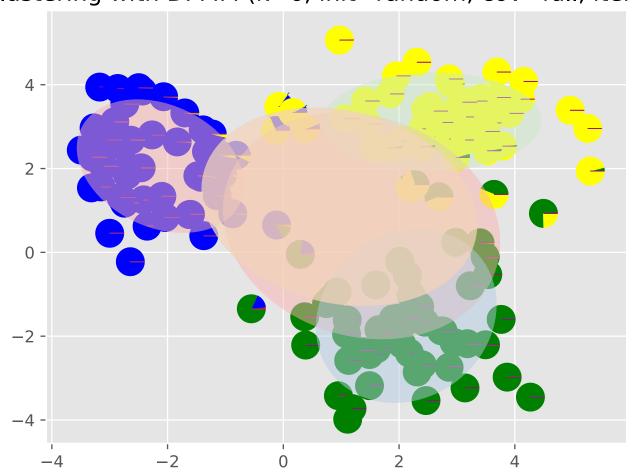
Clustering with DPMM (k=6, init=random, cov=full, iter=19)



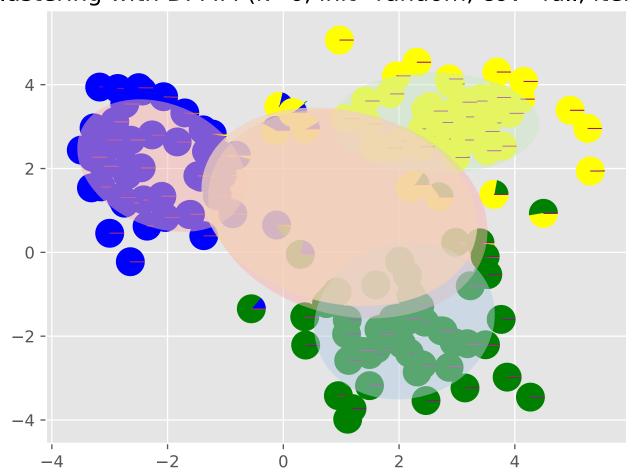
Clustering with DPMM (k=6, init=random, cov=full, iter=20)



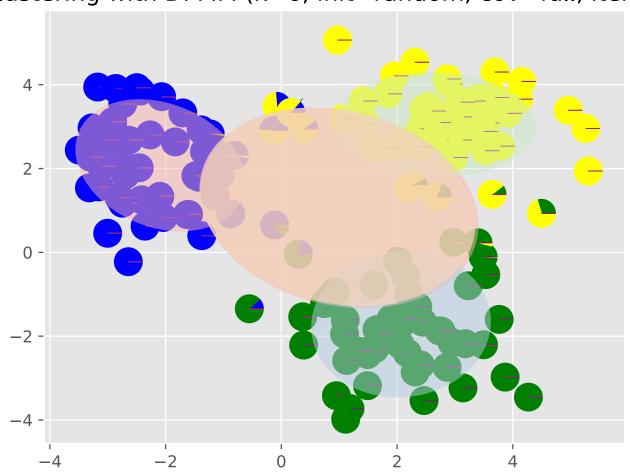
Clustering with DPMM (k=6, init=random, cov=full, iter=21)



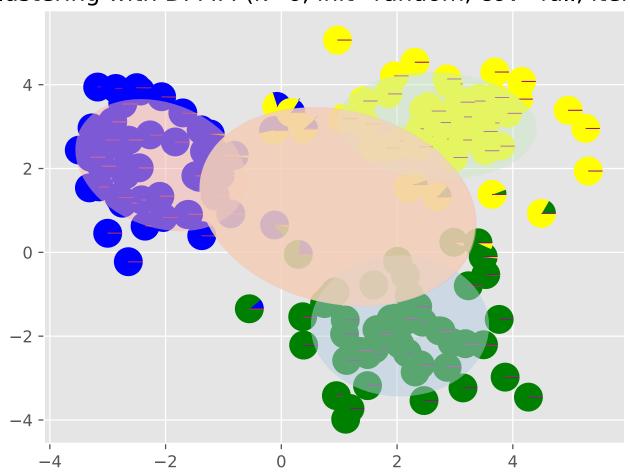
Clustering with DPMM (k=6, init=random, cov=full, iter=22)



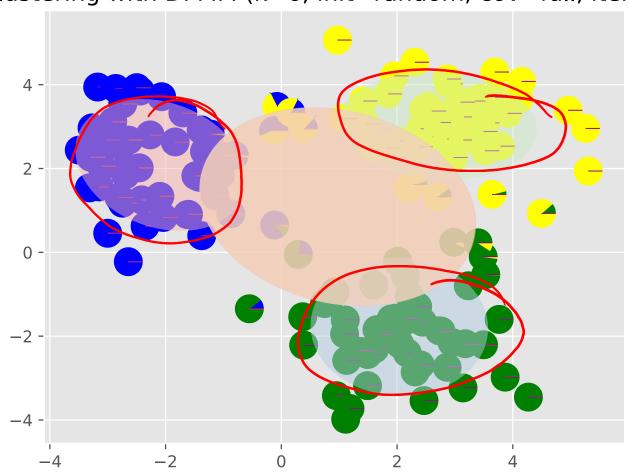
Clustering with DPMM (k=6, init=random, cov=full, iter=23)



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



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



HIERARCHICAL DIRICHLET PROCESS (HDP)

Related Models

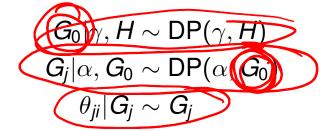
- Hierarchical Dirichlet Process Mixture Model (HDP-MM)
- Infinite HMM
- Infinite PCFG

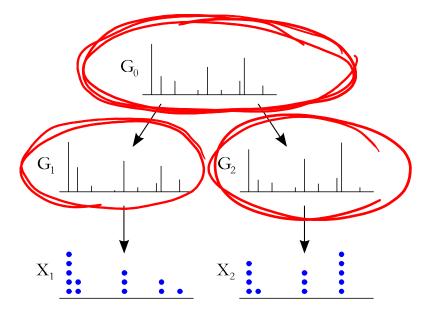
HDP-MM

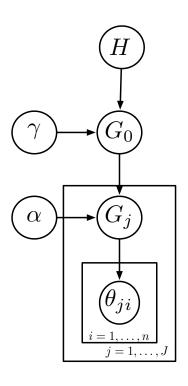
- In LDA, we have *M* independent samples from a Dirichlet distribution.
- The weights are different, but the topics are fixed to be the same.
- If we replace the Dirichlet distributions with Dirichlet processes, each atom of each Dirichlet process will pick a topic *independently* of the other topics.
- 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 $H=\sum_{k=1}^K \alpha_k \delta_{\beta_k} \ \text{then we would have LDA again}.$
- 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

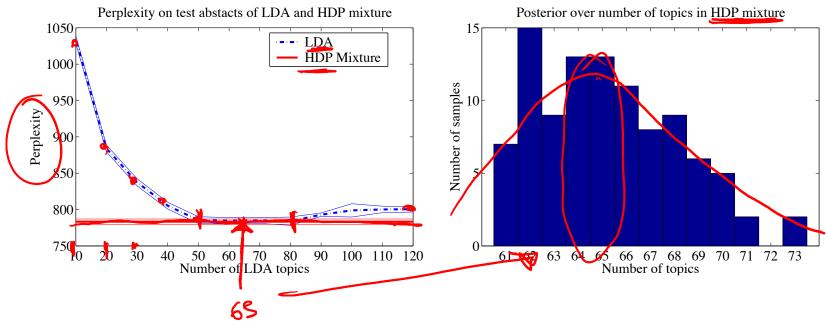


Figure 6: (Left) Comparison of latent Dirichlet allocation and the hierarchical Dirichlet process mixture. Results are averaged over 10 runs; the error bars are one standard error. (Right) Histogram of the number of topics for the hierarchical Dirichlet process mixture over 100 posterior samples.

HDP-HMM (Infinite HMM)

Number of hidden states in Infinite HMM is countably infinite

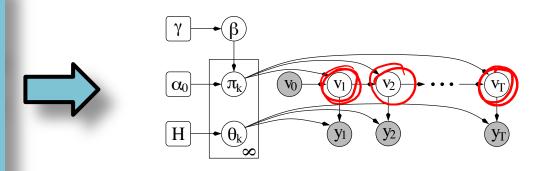


Figure 9: A hierarchical Bayesian model for the infinite hidden Markov model.

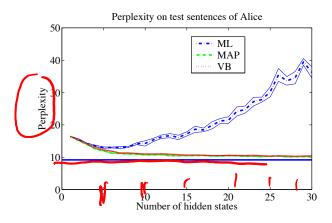
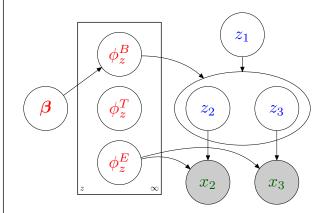


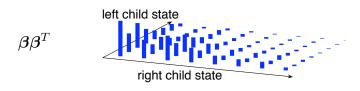
Figure 10: Comparing the infinite hidden Markov model (solid horizontal line) with ML, MAP and VB trained hidden Markov models. The error bars represent one standard error (those for the HDP-HMM are too small to see).

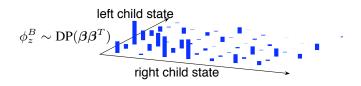
HDP-PCFG (Infinite PCFG)

HDP-PCFG $\beta \sim \text{GEM}(\alpha)$ [draw top-level symbol weights] For each grammar symbol $z \in \{1, 2, \dots\}$: $\phi_z^T \sim \text{Dirichlet}(\alpha^T)$ $\phi_z^E \sim \text{Dirichlet}(\alpha^E)$ $\phi_z^B \sim \text{DP}(\alpha^B, \beta \beta^T)$ [draw rule type parameters] [draw emission parameters] [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 $t_i = BINARY-PRODUCTION$: $(z_{L(i)}, z_{R(i)}) \sim \text{Multinomial}(\phi_{z_s}^B)$ [generate children symbols]









Parametric vs. Nonparametric

Type of Model	Parametric Example	Nonparametric Example	
		Construction #1	Construction #2
distribution over counts	Dirichlet- Multinomial Model	Dirichlet Process (DP)	
		Chinese Restaurant Process (CRP)	Stick-breaking construction
mixture	Gaussian Mixture Model (GMM)	Dirichlet Process Mxture Model (DPMM)	
		CRP Mixture Model	Stick-breaking construction
admixture	Latent Dirichlet Allocation (LDA)	Hierarchical Dirichle Model (H	
		Chinese Restaurant Franchise	Stick-breaking construction

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
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 - Gibbs sampler (stick-breaking)
 - Variational inference (stick-breaking)
 - etc.