Module 3: Bayesian Nonparametrics

Infinite Mixture Models

1st finite MM recap

STAT/BIOSTAT 527, University of Washington

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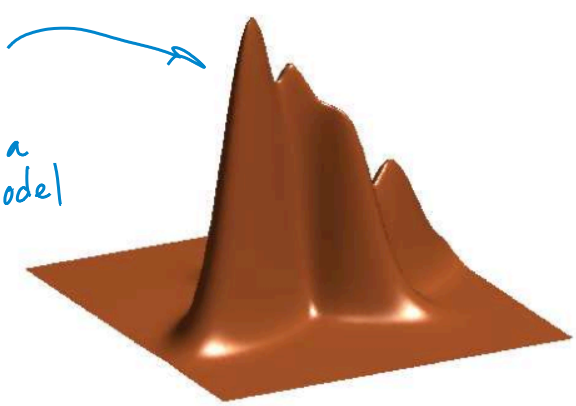
Density Estimation

- Estimate a density based on $x_1,\dots,x_N$

$x_1,\dots,x_N \sim P$

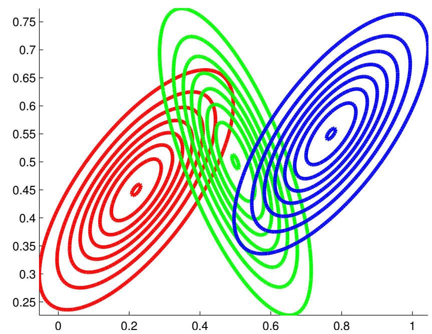
Let's consider a parametric model



Density as Mixture of Gaussians

- Approximate density with a mixture of Gaussians

Mixture of 3 Gaussians



K=3

p =

$$p(x_i \mid \pi, \mu, \Sigma) = \sum_{k=1}^{K} \pi_k N(x_i \mid \mu_k, \Sigma_k)$$

$= [\pi_1, \dots, \pi_K]$, $\{\mu_k, \Sigma_k\}$

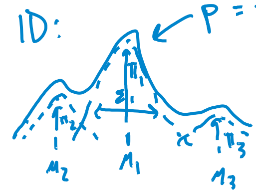
# of mix comp.

mix. weights

shape params

Gauss. kernel, just like in KDE, but not centered at obs.

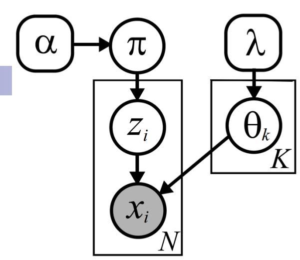
In 1D:



p = target density

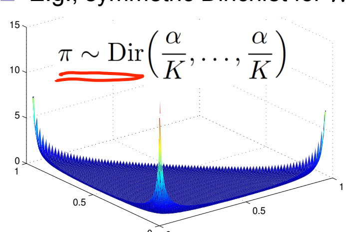
$\sum \pi_k = 1$

Model Summary



- Prior on model parameters
  - E.g., symmetric Dirichlet for π

$$\pi \sim \mathrm{Dir}\left(\frac{\alpha}{K}, \dots, \frac{\alpha}{K}\right)$$



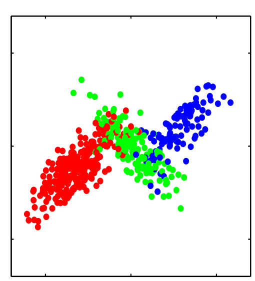
  - Normal inverse Wishart prior for $\theta_k = \{\mu_k, \Sigma_k\}$

$\{1, \dots, K\}$

- Sample observations as

$$z_i \sim \pi$$ choose a cluster

$$x_i \mid z_i \sim N(\mu_{z_i}, \Sigma_{z_i})$$ sim obs. from selected Gauss.

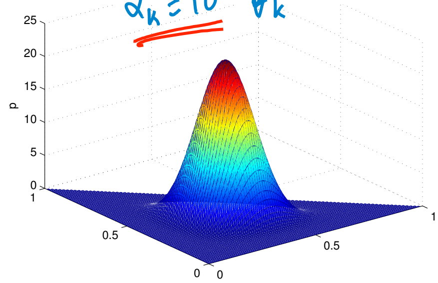


Dirichlet Distributions

- The Dirichlet distribution is defined on the simplex

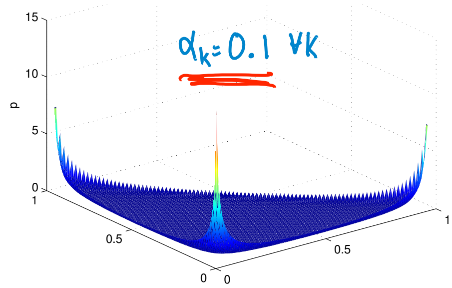
$\pi \sim \mathrm{Dir}(\alpha_1, \ldots, \alpha_K)$
$\Rightarrow \sum \pi_k = 1$

$\alpha_k = 10 \ \forall k$



$$p(\pi \mid \alpha) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1}$$

$\alpha_k = 0.1 \ \forall k$



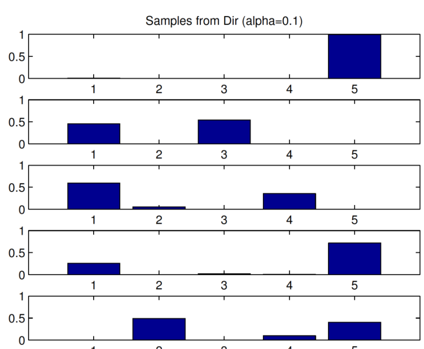
Moments: $\mathbb{E}_\alpha[\pi_k] = \frac{\alpha_k}{\alpha_0}$

$$\mathrm{Var}_\alpha[\pi_k] = \frac{K-1}{K^2(\alpha_0 + 1)}$$

Dirichlet Samples

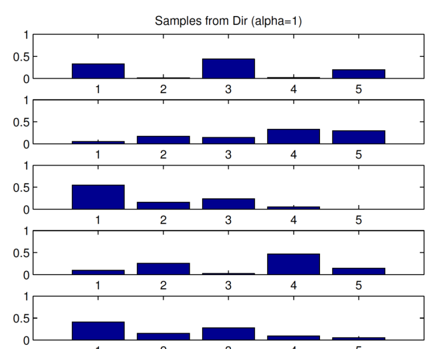
$$\mathbb{E}_\alpha[\pi_k] = \frac{\alpha_k}{\alpha_0}$$

- Samples are ***sparse*** for small values of α_i



$\mathrm{Dir}(\pi \mid 0.1, 0.1, 0.1, 0.1, 0.1)$

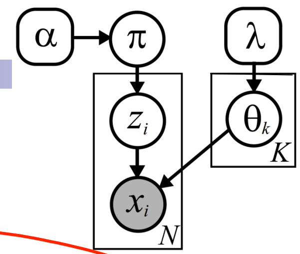
puts mass @ corners



$\mathrm{Dir}(\pi \mid 1.0, 1.0, 1.0, 1.0, 1.0)$

uniform

Model In Pictures



- Mixture weights

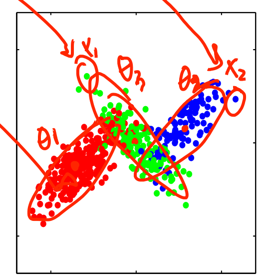
π

$z_2 = 2$

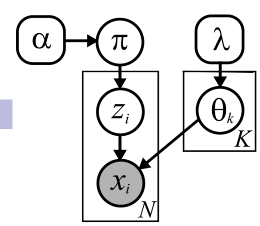
$z_1 = 3$

- For each observation,

$$z_i \sim \pi$$
$$x_i \mid z_i \sim N(\mu_{z_i}, \Sigma_{z_i})$$



GMM Sampler



- Recall model
  - Observations: $x_1, \dots, x_N$
  - Cluster indicators: $z_1, \dots, z_N$
  - Parameters: π, θ_k $\quad \pi = [\pi_1, \dots, \pi_K]$ $\quad \theta_k = \{\mu_k, \Sigma_k\}$
  - Generative model:

want these

$$\pi \sim \text{Dir}(\alpha_1, \dots, \alpha_K) \qquad z_i \sim \pi$$
$$\{\mu_k, \Sigma_k\} \sim \text{NIW}(\lambda) \qquad x_i \mid z_i, \{\theta_k\} \sim N(\mu_{z_i}, \Sigma_{z_i})$$

- Iteratively sample

$z_i \mid \pi, \{\theta_k\}, \{x_i\}$ $\quad i=1,\dots,N$

$\pi \mid \{z_i\}, \cancel{\{\theta_k\}}, \cancel{\{x_i\}}$

$\theta_k \mid \cancel{\pi}, \{z_i\}, \{x_i\}$ $\quad k=1,\dots,K$

Standard Finite Mixture Sampler

Given mixture weights $\pi^{(t-1)}$ and cluster parameters $\{\theta_k^{(t-1)}\}_{k=1}^K$ from the previous iteration, sample a new set of mixture parameters as follows:

1. Independently assign each of the N data points x_i to one of the K clusters by sampling the indicator variables $z = \{z_i\}_{i=1}^N$ from the following multinomial distributions:

$$z_i^{(t)} \sim \frac{1}{Z_i} \sum_{k=1}^K \pi_k^{(t-1)} f(x_i \mid \theta_k^{(t-1)})\, \delta(z_i, k) \qquad Z_i = \sum_{k=1}^K \pi_k^{(t-1)} f(x_i \mid \theta_k^{(t-1)})$$

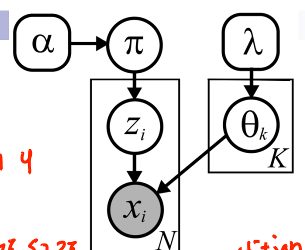
2. Sample new mixture weights according to the following Dirichlet distribution:

$$\pi^{(t)} \sim \mathrm{Dir}(\underline{N_1} + \alpha/K, \ldots, \underline{N_K} + \alpha/K) \qquad N_k = \sum_{i=1}^N \delta(z_i^{(t)}, k)$$

3. For each of the K clusters, independently sample new parameters from the conditional distribution implied by those observations currently assigned to that cluster:

$$\theta_k^{(t)} \sim p(\theta_k \mid \{x_i \mid z_i^{(t)} = k\}, \lambda)$$

Mixtures Induce Partitions



- If our goal is clustering, the output grouping is defined by assignment *indicator variables:*

$$z_i \sim \pi$$

$z_1, \ldots, z_N$

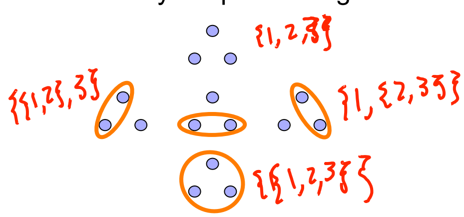
1 5 5 3 2 1 1 4

$\downarrow$

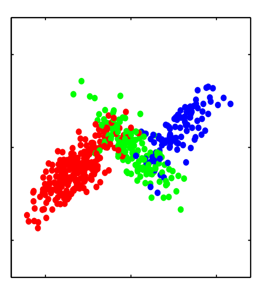
$\{\{1,6,7\},\{2,3\},4,5,8\}$ partition

- The number of ways of assigning N data points to K mixture components is K^N

- If $K \geq N$ this is much larger than the number of ways of partitioning that data:



N=3: 5 partitions versus $3^3 = 27$



Mixtures Induce Partitions

- If our goal is clustering, the output grouping is defined by assignment *indicator variables:*

$$z_i \sim \pi$$

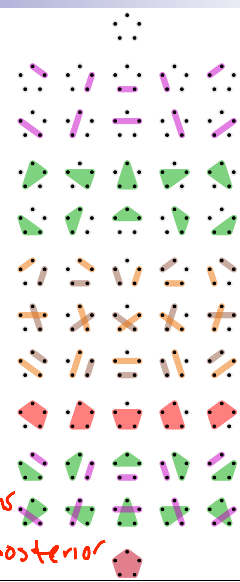
- The number of ways of assigning *N* data points to *K* mixture components is K^N
- If $K \geq N$ this is much larger than the number of ways of partitioning that data:

For any clustering, there is a unique partition, but many ways to label that partition's blocks.

Note: sampler can switch between eq. partitions

N=5: 52 partitions versus $5^5 = 3125$

If prior sym., then eq. under posterior



Courtesy Wikipedia

Module 3: Bayesian Nonparametrics

Infinite Mixture Models

going infinite ...

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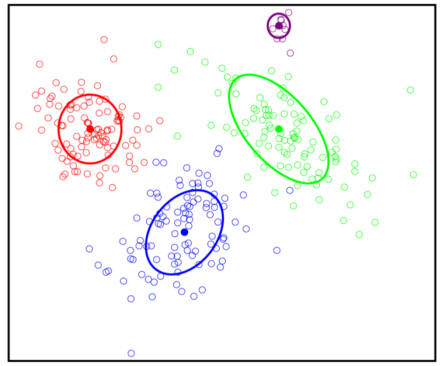
Motivating Nonparametric GMM

- What if current model doesn't fit new data?
- Bayesian nonparametric approach: $K \to \infty$
  - Allows infinite # clusters
  - Uses sparse subset
  - Model ***complexity adapts*** to observations

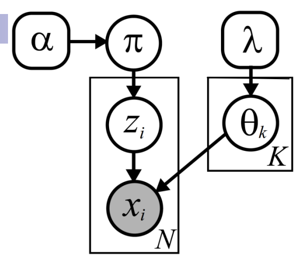


Mixture of Gaussians

← allows us to add in new model comp.

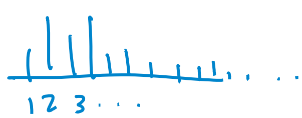
$\theta_1 \quad \theta_2 \quad \theta_3 \quad \theta_4 \quad \theta_5 \quad \theta_6 \quad \theta_7 \quad \cdots$

Nonparam. Model In Pictures



- Mixture weights

π

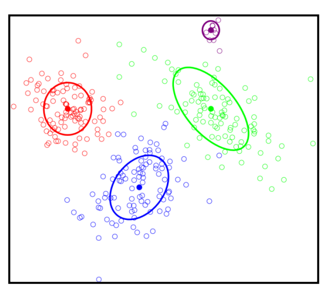


$\{\theta_k\} \quad k=1,2,\ldots$

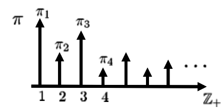
- For each observation, draw

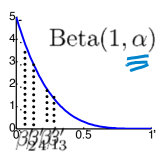
$$z_i \sim \pi$$
$$x_i \mid z_i \sim N(\mu_{z_i}, \Sigma_{z_i})$$

How to define π?



Stick-Breaking Process





Stick of unit probability mass

- Start with stick of unit probability mass
- Repeatedly break portions of the remaining stick

$\beta_k \sim \text{Beta}(1,\alpha)$

$\pi_1 = \beta_1$

$\pi_2 = \beta_2(1-\beta_1)$

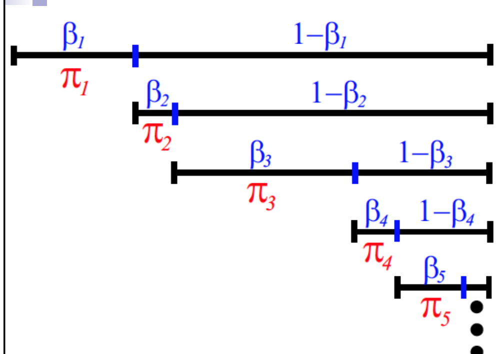
$\vdots$

$\pi_k = \beta_k \prod_{\ell=1}^{k-1}(1-\beta_\ell)$

$\vdots$

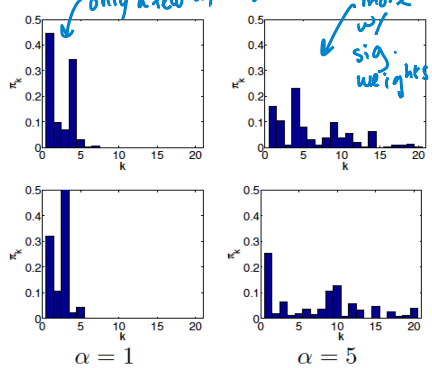
$\boxed{\pi \sim \text{Stick}(\alpha)}$

Stick-Breaking Process Summary



only a few w/ large weights

more w/ sig. weights



$$\pi_k = \beta_k \prod_{\ell=1}^{k-1}(1-\beta_\ell) = \beta_k\left(1 - \sum_{\ell=1}^{k-1}\pi_\ell\right)$$

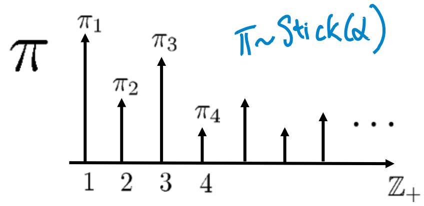
$$\beta_k \sim \text{Beta}(1,\alpha)$$

$$\mathbb{E}[\beta_k] = \frac{1}{1+\alpha}$$

For large α, breaking small portions

Stick Breaks + Dirichlet Process

$\pi \sim \mathrm{Stick}(\alpha)$



$\{\theta_k\}$

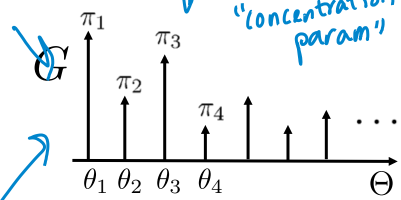
$\theta_k \sim H$ (e.g. NIW)

$G \sim DP(\alpha, H)$

wpl

"concentration param"

base msr



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

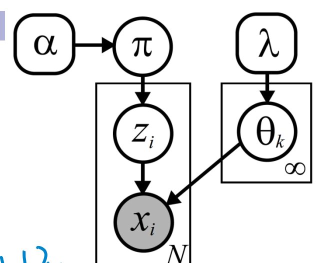
Dirichlet Process Mixture Model

- Place Dirichlet process prior on weights and mixture parameters:

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

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

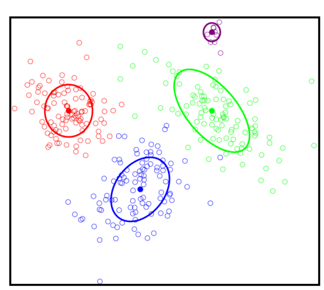
ind. $\begin{cases} \pi \sim \mathrm{stick}(\alpha) \\ \theta_k \overset{iid}{\sim} H \quad \text{(e.g. NIW)} \quad k=1,2,\ldots \end{cases}$



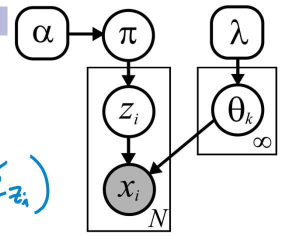
- For each observation, draw

$$z_i \sim \pi$$

$$x_i \mid z_i \sim N(\mu_{z_i}, \Sigma_{z_i})$$



Finite versus DP Mixtures



Finite Mixture

$$\pi \sim \mathrm{Dir}\left(\frac{\alpha}{K}, \ldots, \frac{\alpha}{K}\right)$$

sym.

DP Mixture

$$\pi \sim \mathrm{Stick}(\alpha)$$

$$z_i \sim \pi$$
$$x_i \sim F(\theta_{z_i})$$

e.g. $N(\mu_{z_i}, \Sigma_{z_i})$

THEOREM: For any measureable function *f*, as $K \to \infty$

$$\int_\Theta f(\theta)\, dG^K(\theta) \xrightarrow[K\to\infty]{\mathcal{D}} \int_\Theta f(\theta)\, dG(\theta)$$

$$G^K(\theta) = \sum_{k=1}^{K} \pi_k^K \delta_{\theta_k}(\theta) \qquad G \sim \mathrm{DP}(\alpha, H)$$

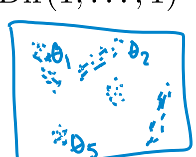
$$\pi^K \sim \mathrm{Dir}\left(\frac{\alpha}{K}, \ldots, \frac{\alpha}{K}\right)$$

Induced Partitions

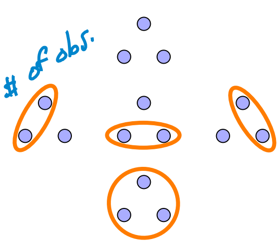
- Recall that mixture models induce partitions of the data

$$z_i \sim \pi$$

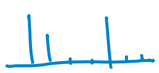
- For a given prior on mixture weights, some partitions are more likely than others apriori
  - Example 1: $\pi \sim \mathrm{Dir}(1, \ldots, 1)$ uniform

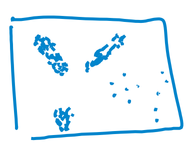


expect roughly the same # of obs. in each cluster



  - Example 2: $\pi \sim \mathrm{Dir}(0.01, \ldots, 0.01)$



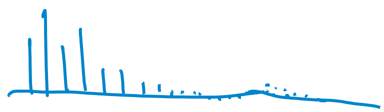


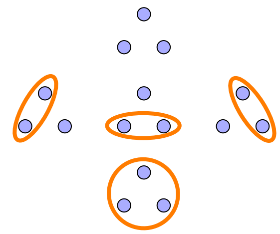
Induced Partitions

- Recall that mixture models induce partitions of the data

$$z_i \sim \pi$$

- For a given prior on mixture weights, some partitions are more likely than others apriori
  - Example 3 (DP mix): $\pi \sim \text{Stick}(\alpha)$





only a few w/ sig. mass

∞-ly many tiny weights

- What is the induced distribution on $z_1, \ldots, z_N$?
  - Do we expect many unique clusters?

Answer: Chinese restaurant process

Chinese Restaurant Process (CRP)

- Distribution on induced partitions described via the CRP
- Visualize clustering as a sequential process of customers sitting at tables in an (infinitely large) restaurant:

customers ⟷ *observed data to be clustered* X_i

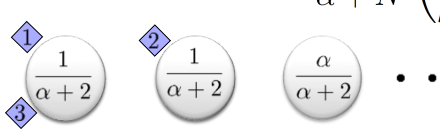
tables ⟷ *distinct clusters* each serving unique dish θ_k

- The first customer sits at a table. Subsequent customers randomly select a table according to:

norm.

\# of unique clusters in $z_{1:N}$

$$p(z_{N+1} = z \mid z_1, \ldots, z_N, \alpha) = \frac{1}{\alpha + N}\left(\sum_{k=1}^{K} N_k \delta(z, k) + \alpha \delta(z, \bar{k})\right)$$

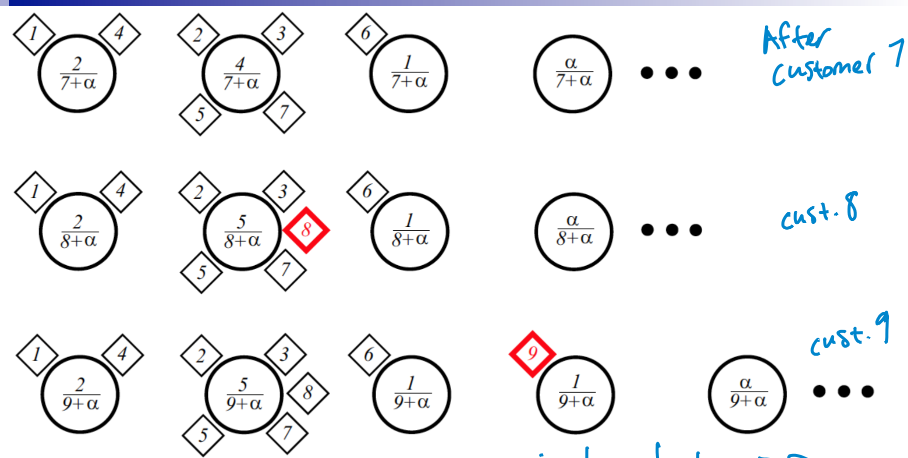


\# z_i already at table k

weight on new cluster

new cluster index

Chinese Restaurant Process (CRP)



clustering / reinforcement induced by DP

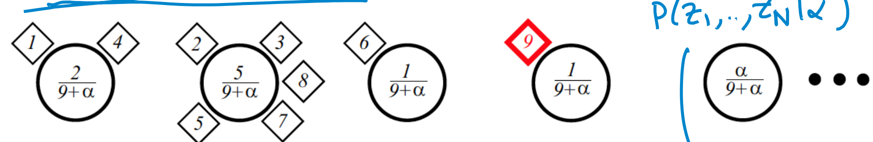
"rich get richer"

CRPs & Exchangeable Partitions

$$p(z_{N+1} = z \mid z_1, \ldots, z_N, \alpha) = \frac{1}{\alpha + N}\left(\sum_{k=1}^{K} N_k \delta(z,k) + \alpha\delta(z,\bar{k})\right)$$

- The probability of a seating arrangement of N customers is *independent* of the order they enter the restaurant:

$p(z_1, .., z_N | \alpha)$



$p(z_1)p(z_2|z_1) \cdots p(z_N|z_{1:N-1})$

- Denominator terms:

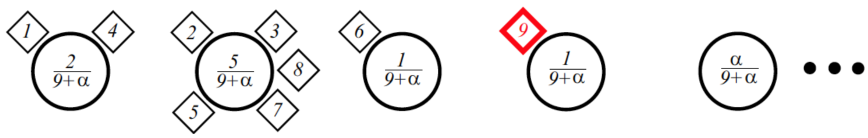
$$1 \cdot \frac{1}{1+\alpha} \cdot \frac{1}{2+\alpha} \cdots \frac{1}{N-1+\alpha} = \frac{\Gamma(\alpha)}{\Gamma(N+\alpha)}$$

$\uparrow$ 2nd cust. $\uparrow$ 3rd cust.

CRPs & Exchangeable Partitions

$$p(z_{N+1} = z \mid z_1, \ldots, z_N, \alpha) = \frac{1}{\alpha + N}\left(\sum_{k=1}^{K} N_k \delta(z, k) + \alpha\delta(z, \bar{k})\right)$$

- The probability of a seating arrangement of *N* customers is *independent* of the order they enter the restaurant:

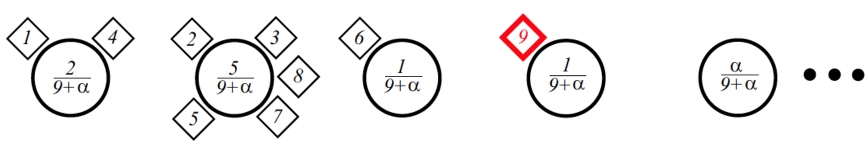


  - Denominator terms: $\frac{1}{1+\alpha} \cdot \frac{1}{2+\alpha} \cdots \frac{1}{N-1+\alpha} = \frac{\Gamma(\alpha)}{\Gamma(N+\alpha)}$
  - Number of new tables: K
    Numerator term for each new table: α
    Combined: α^K

CRPs & Exchangeable Partitions

$$p(z_{N+1} = z \mid z_1, \ldots, z_N, \alpha) = \frac{1}{\alpha + N}\left(\sum_{k=1}^{K} N_k \delta(z, k) + \alpha\delta(z, \bar{k})\right)$$

- The probability of a seating arrangement of *N* customers is *independent* of the order they enter the restaurant:



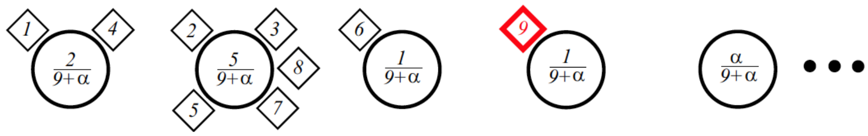
  - Denominator terms: $\frac{1}{1+\alpha} \cdot \frac{1}{2+\alpha} \cdots \frac{1}{N-1+\alpha} = \frac{\Gamma(\alpha)}{\Gamma(N+\alpha)}$
  - New table numerator terms: α^K
  - Customers joining k^{th} occupied table: $1 \cdot 2 \cdots (N_k - 1) = (N_k - 1)! = \Gamma(N_k)$

↑ already 1 person sitting @ k^{th} table

CRPs & Exchangeable Partitions

$$p(z_{N+1} = z \mid z_1, \ldots, z_N, \alpha) = \frac{1}{\alpha + N}\left(\sum_{k=1}^{K} N_k \delta(z, k) + \alpha \delta(z, \bar{k})\right)$$

- The probability of a seating arrangement of *N* customers is *independent* of the order they enter the restaurant:



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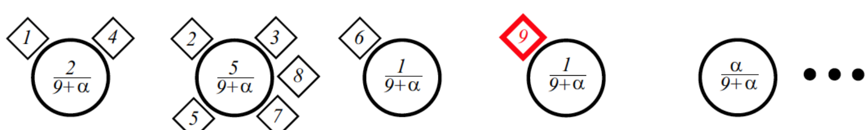
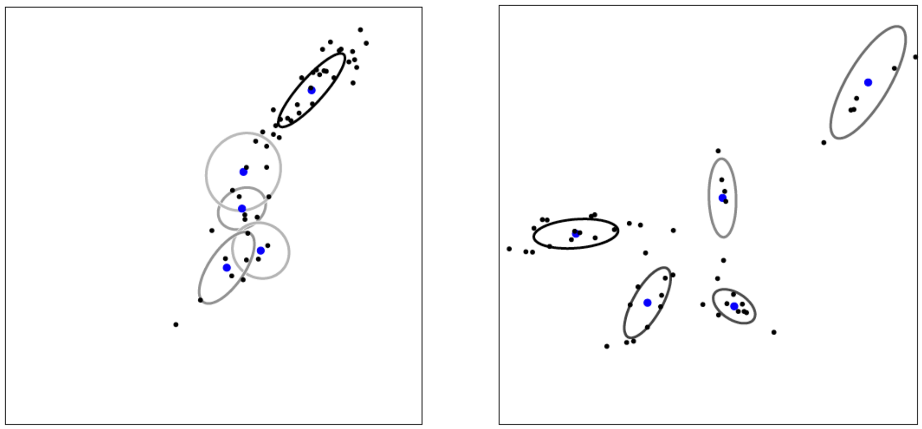


$$\boxed{p(z_1, \ldots, z_N \mid \alpha) = \frac{\Gamma(\alpha)}{\Gamma(N+\alpha)} \alpha^K \prod_{k=1}^{K} \Gamma(N_k)}$$

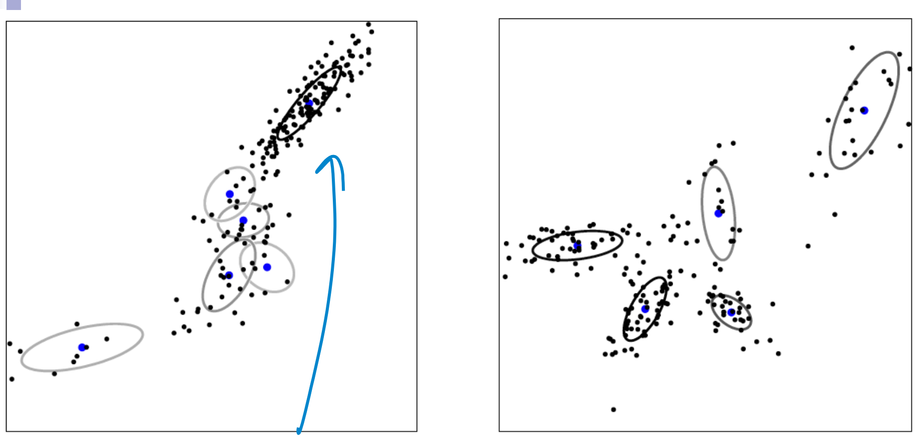
- Thus, the CRP is a prior on an *infinitely exchangeable* sequence

Samples from DP Mixture Priors



N=50

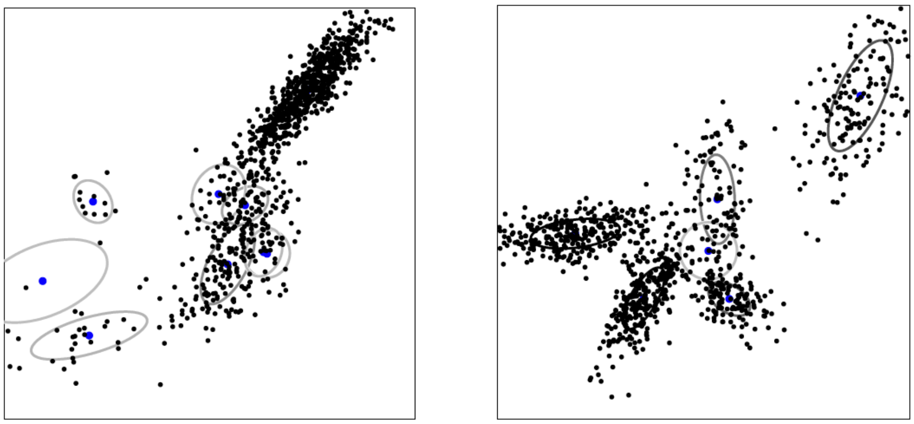
Samples from DP Mixture Priors



"rich get richer"

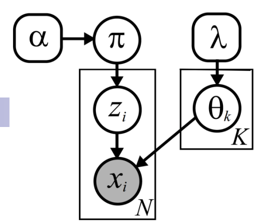
N=200

Samples from DP Mixture Priors



N=1000

Finite GMM Sampler



- Recall model
  - Observations: $x_1, \ldots, x_N$
  - Cluster indicators: $z_1, \ldots, z_N$
  - Parameters: π, θ_k

want these

$\pi = [\pi_1, \ldots, \pi_K]$

$\theta_k = \{\mu_k, \Sigma_k\}$

  - Generative model:

$$\pi \sim \mathrm{Dir}(\alpha_1, \ldots, \alpha_K) \qquad z_i \sim \pi$$

$$\{\mu_k, \Sigma_k\} \sim \mathrm{NIW}(\lambda) \qquad x_i \mid z_i, \{\theta_k\} \sim N(\mu_{z_i}, \Sigma_{z_i})$$

- Iteratively sample

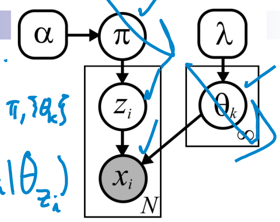
$z_i \mid \pi, \{\theta_k\}, \{x_i\}$ $\quad i=1,\ldots,N$

$\pi \mid \{z_i\}, \cancel{\{\theta_k\}}, \cancel{\{x_i\}}$

$\theta_k \mid \cancel{\pi}, \{z_i\}, \{x_i\}$ $\quad k=1,\ldots K$

Collapsed DP Mixture Sampler

- Can't sample π directly
- Integrate out all infinite-dimensional params $\pi, \{\theta_k\}$



$$p(z_{1:N}, x_{1:N}) = \int_{\pi} \int_{\theta_1, \theta_2, \dots} p(\pi \mid \alpha) \prod_{k=1}^{\infty} p(\theta_k \mid \lambda) \prod_{i=1}^{N} p(z_i \mid \pi)\, p(x_i \mid \theta_{z_i})$$

$$= \underbrace{p(z_1, \dots, z_N \mid \alpha)}_{\text{CRP}} \prod_{k=1}^{\infty} \underbrace{p(\{x_i : z_i = k\} \mid \lambda)}_{\text{"likelihood"}}$$

"likelihood"

- Iteratively sample the cluster indicators

treat as last obs. in CRP

$$z_i^{(t)} \sim \underbrace{p(z_i = k \mid z_{\setminus i}^{(t-1)}, \alpha)}_{\text{"prior"}}\; p(x_i \mid \{x_j : z_j = k,\ i \neq j\})$$

all other indicators

all other obs. assigned to k^{th} cluster

Collapsed Sampler Intuition

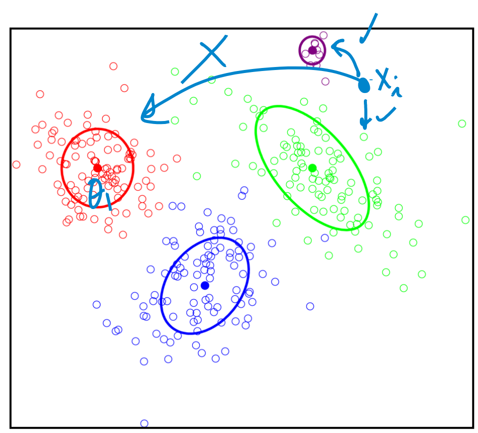
- Previously, $p(z_i = k \mid x_i, \pi, \theta) \propto \pi_k p(x_i \mid \theta_k)$
- If you're not told π, θ_k

Approx π by CRP

→ "prior" is based on cluster occupancy

Approx θ_k

→ "likelihood" based on obs. already assigned to cluster



Predictive Likelihood Term

- Recall NIW prior…Let's consider 1D example → N-IG

$$\mu_k \mid \sigma_k^2 \sim N(0, \gamma\sigma_k^2) \quad \sigma_k^2 \sim \text{IG}\left(\frac{\nu_0}{2}, \frac{\nu_0 S_0}{2}\right)$$

- Normal inverse gamma posterior
  → Student t predictive likelihood

normal likelihood

NIW posterior

$$p(x_i \mid \{x_j : z_j = k, j \neq i\}) = \int p(x_i \mid \theta_k)\, p(\theta_k \mid \{x_j : z_j = k, j \neq i\})\, d\theta_k$$

$$p(x \mid \{x_j | z_j = k, j \neq i\}) = t_{\nu_0 + N_k^{-i}}\Bigg(\frac{1}{\gamma^{-1} + N_k^{-i}} \sum_{j:z_j=k,j\neq i} x_j,$$

$$\frac{N_k^{-i} + \gamma^{-1} + 1}{(N_k^{-i} + \gamma^{-1})(\nu_0 + N_k^{-i})}\left(\nu_0 S_0 + \sum_{j:z_j=k,j\neq i} x_j^2 - (N_k + \gamma^{-1})^{-1}\Big(\sum_{j:z_j=k,j\neq i} x_j\Big)^2\right)\Bigg)$$

  - Conjugacy: This integral is **tractable**

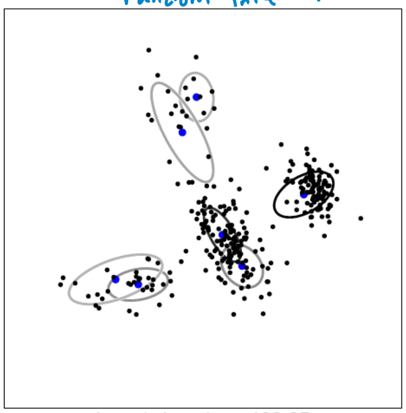
Collapsed DP Mixture Sampler

1. Sample a random permutation $\tau(\cdot)$ of the integers $\{1, \ldots, N\}$.
2. Set $\alpha = \alpha^{(t-1)}$ and $z = z^{(t-1)}$. For each $i \in \{\tau(1), \ldots, \tau(N)\}$, resample z_i as follows:
   (a) For each of the K existing clusters, determine the predictive likelihood
   $$f_k(x_i) = p(x_i \mid \{x_j \mid z_j = k, j \neq i\}, \lambda)$$
   Also determine the likelihood $f_{\bar{k}}(x_i)$ of a potential new cluster $\bar{k}$
   $$p(x_i \mid \lambda) = \int_\Theta f(x_i \mid \theta)\, h(\theta \mid \lambda)\, d\theta$$
   (b) Sample a new cluster assignment z_i from the following $(K+1)$–dim. multinomial:
   $$z_i \sim \frac{1}{Z_i}\left(\alpha f_{\bar{k}}(x_i)\delta(z_i, \bar{k}) + \sum_{k=1}^{K} N_k^{-i} f_k(x_i)\delta(z_i, k)\right) \qquad Z_i = \alpha f_{\bar{k}}(x_i) + \sum_{k=1}^{K} N_k^{-i} f_k(x_i)$$
   N_k^{-i} is the number of other observations currently assigned to cluster k.
   (c) Update cached sufficient statistics to reflect the assignment of x_i to cluster z_i. If $z_i = \bar{k}$, create a new cluster and increment K.
3. Set $z^{(t)} = z$.
4. If any current clusters are empty ($N_k = 0$), remove them and decrement K accordingly.

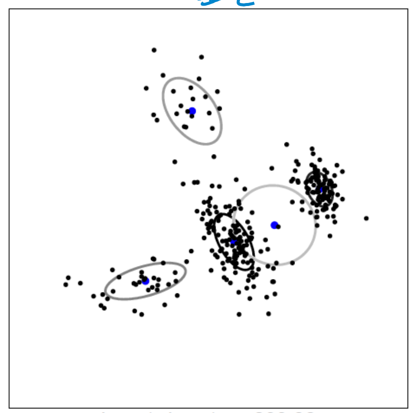
Collapsed DP Sampler: 2 Iterations

random init #1

#2

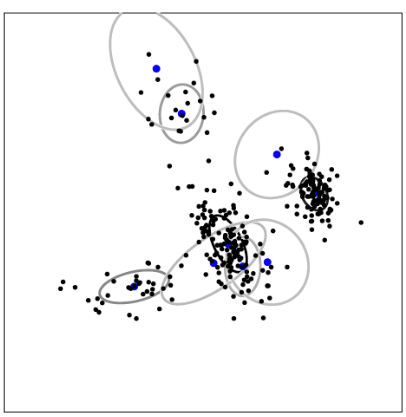


log p(x | π, θ) = –462.25

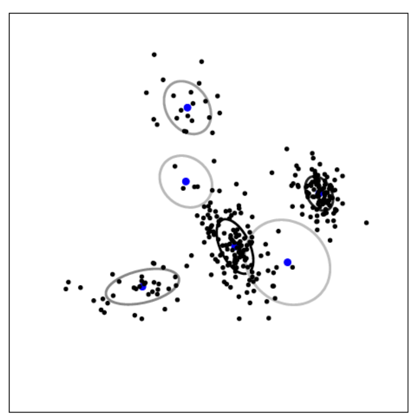


log p(x | π, θ) = –399.82

Collapsed DP Sampler: 10 Iterations

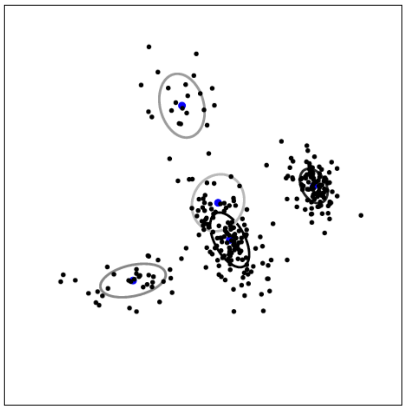


log p(x | π, θ) = –398.32

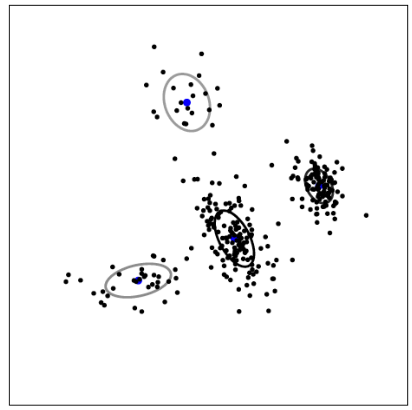


log p(x | π, θ) = –399.08

Collapsed DP Sampler: 50 Iterations

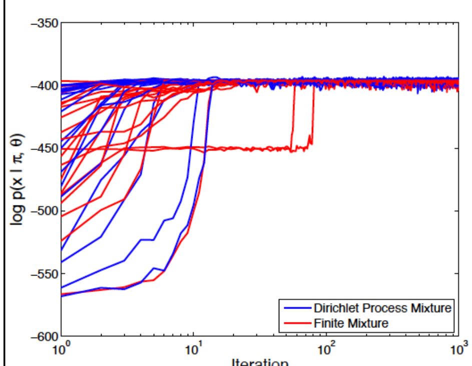


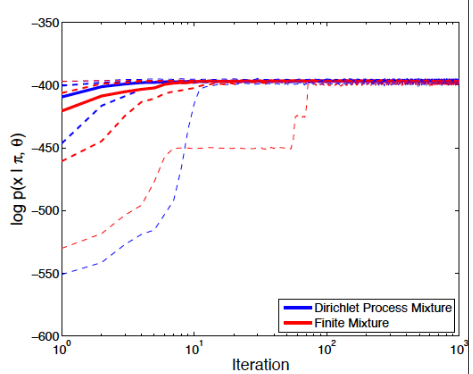
log p(x | π, θ) = –397.67



log p(x | π, θ) = –396.71

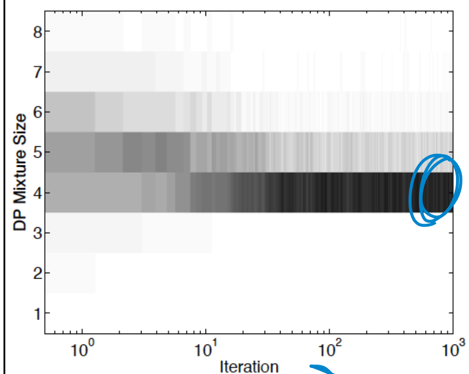
DP vs. Finite Mixture Samplers

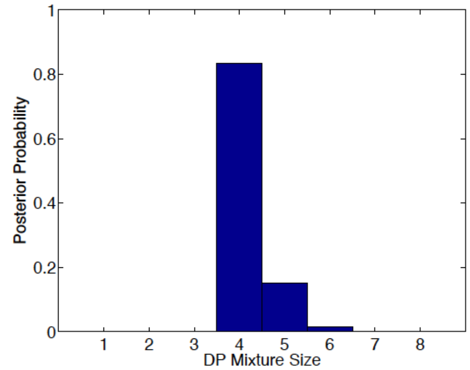




pretty competitive

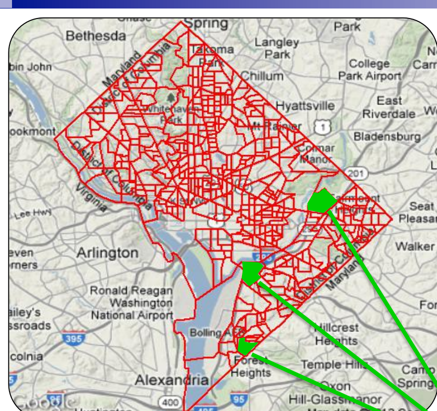
DP Posterior Number of Clusters



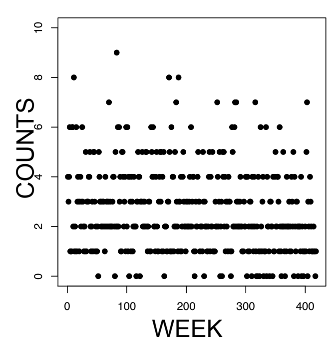


Asy. consistency results for density est.
(assuming light tails on target density)
Not asy. consistent on # of comp.

DC Violent Crime Data



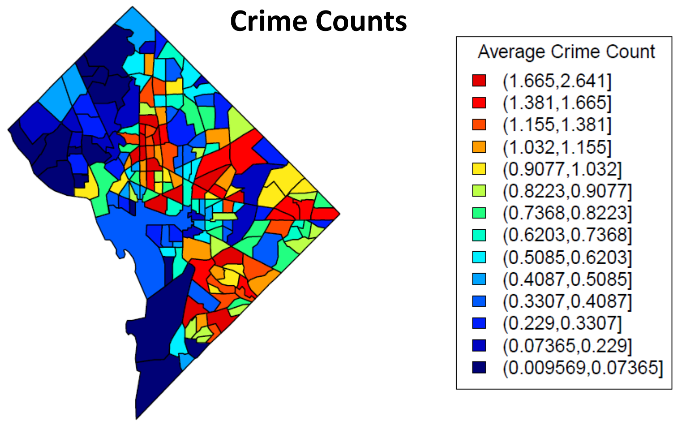
- 188 census tracts
- Weekly crime counts from 2001-2008
- Violent crime types:
  - ADW, arson, robbery, rape



Time series = crime counts

DC Violent Crime Data

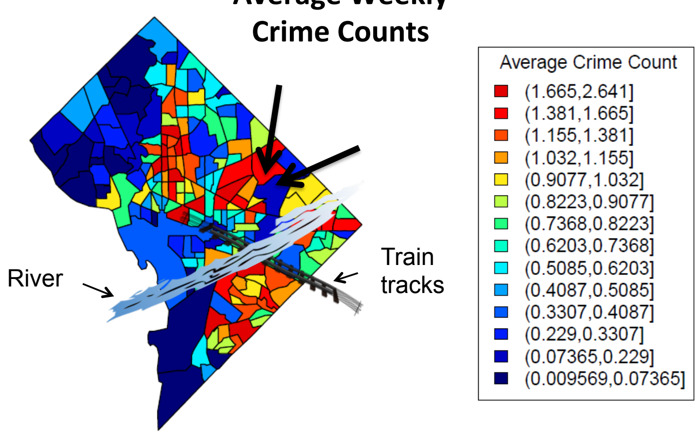
Average Weekly Crime Counts



Goal: Forecast next week's map

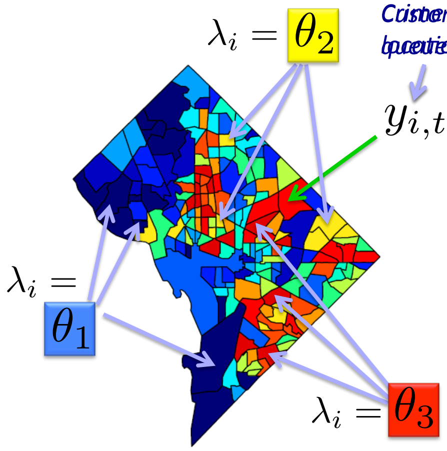
DC Violent Crime Data

Average Weekly Crime Counts



Similar behavior in spatially disjoint tracts
→ Cluster census tracts

Poisson Integer-Valued Autoregressions



Crime counts in location i at time t / *Customers in queue at time t*

Poisson new customers

$$y_{i,t} = \alpha \odot y_{i,t-1} + \epsilon_{i,t}(\lambda_i)$$

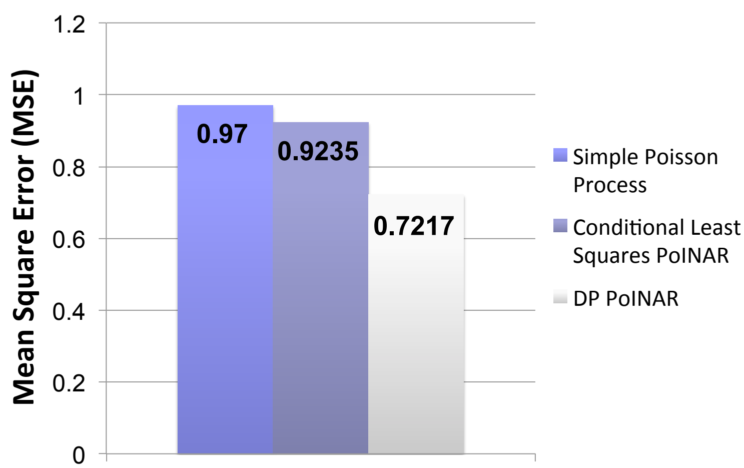
Thinning of customers previously in queue

Rate of arrivals in location i

- Cluster regions based on *rate of arriving crimes*
- Pool info within clusters
- Unknown number of clusters → *Dirichlet process*

Aldor-Noiman, Brown, Fox, and Stine, *arXiv:1304.5642*, April 2013

Prediction Results



Aldor-Noiman, Brown, Fox, and Stine, *arXiv:1304.5642*, April 2013

Acknowledgements

Slides based on parts of the lecture notes of Erik Sudderth for "Applied Bayesian Nonparametrics" at Brown University