Dirichlet Processes: Tutorial and Practical Course

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Dirichlet Processes

- Dirichlet processes (DPs) are a class of Bayesian nonparametric models.
- Dirichlet processes are used for:
  - Density estimation.
  - Semiparametric modelling.
  - Sidestepping model selection/averaging.
- I will give a tutorial on DPs, followed by a practical course on implementing DP mixture models in MATLAB.
- Prerequisites: understanding of the Bayesian paradigm (graphical models, mixture models, exponential families, Gaussian processes)—you should know these from Zoubin and Carl.
- Other tutorials on DPs:
  - Zoubin Gharamani, UAI 2005.
  - Michael Jordan, NIPS 2005.
  - Volker Tresp, ICML nonparametric Bayes workshop 2006.

Outline

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Function Estimation

- Parametric function estimation (e.g. regression, classification)
  Data: $\mathbf{x} = \{x_1, x_2, \ldots\}, \mathbf{y} = \{y_1, y_2, \ldots\}$
  Model: $y_i = f(x_i|w) + \mathcal{N}(0, \sigma^2)$
- Prior over parameters

$$p(w)$$

- Posterior over parameters

$$p(w|\mathbf{x}, \mathbf{y}) = \frac{p(w)p(\mathbf{y}|\mathbf{x}, w)}{p(\mathbf{y}|\mathbf{x})}$$

- Prediction with posteriors

$$p(y_\star|x_\star, \mathbf{x}, \mathbf{y}) = \int p(y_\star|x_\star, w)p(w|\mathbf{x}, \mathbf{y})\, dw$$

Function Estimation

- Bayesian nonparametric function estimation with Gaussian processes
  Data: $\mathbf{x} = \{x_1, x_2, \ldots\}, \mathbf{y} = \{y_1, y_2, \ldots\}$
  Model: $y_i = f(x_i) + \mathcal{N}(0, \sigma^2)$
- Prior over functions

$$f \sim \mathrm{GP}(\mu, \Sigma)$$

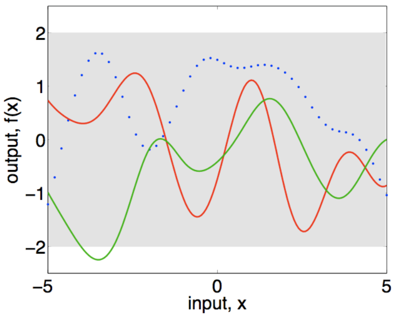
- Posterior over functions

$$p(f|\mathbf{x}, \mathbf{y}) = \frac{p(f)p(\mathbf{y}|\mathbf{x}, f)}{p(\mathbf{y}|\mathbf{x})}$$

- Prediction with posteriors

$$p(y_\star|x_\star, \mathbf{x}, \mathbf{y}) = \int p(y_\star|x_\star, f)p(f|\mathbf{x}, \mathbf{y})\, df$$

Function Estimation



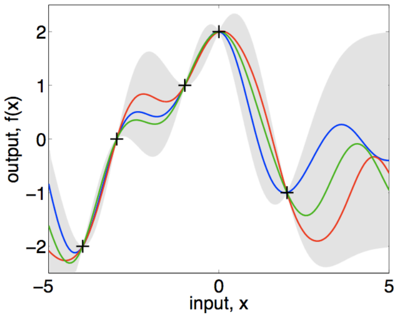


Figure from Carl's lecture.

Density Estimation

- Parametric density estimation (e.g. mixture models)

  Data: $\mathbf{x} = \{x_1, x_2, \ldots\}$

  Model: $x_i | w \sim F(\cdot|w)$

- Prior over parameters

$$p(w)$$

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$$p(w|\mathbf{x}) = \frac{p(w)p(\mathbf{x}|w)}{p(\mathbf{x})}$$

- Prediction with posteriors

$$p(x_\star|\mathbf{x}) = \int p(x_\star|w)p(w|\mathbf{x})\,dw$$

Density Estimation

- Bayesian nonparametric density estimation with Dirichlet processes
  Data: $\mathbf{x} = \{x_1, x_2, \ldots\}$
  Model: $x_i \sim F$
- Prior over distributions

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

- Posterior over distributions

$$p(F|\mathbf{x}) = \frac{p(F)p(\mathbf{x}|F)}{p(\mathbf{x})}$$

- Prediction with posteriors

$$p(x_\star|\mathbf{x}) = \int p(x_\star|F)p(F|\mathbf{x})\,dF = \int F'(x_\star)p(F|\mathbf{x})\,dF$$

- *Not quite correct; see later.*

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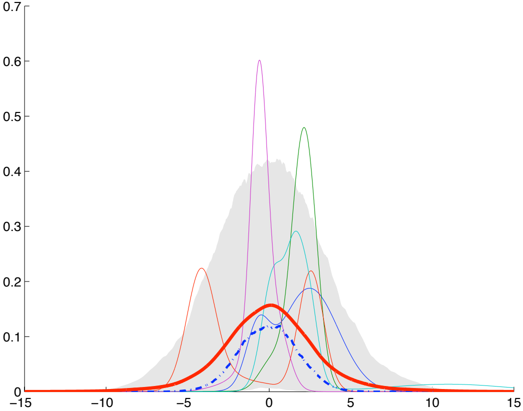
Density Estimation

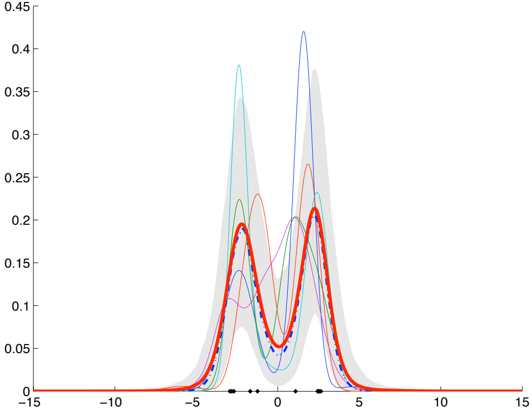
Prior:



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

Density Estimation

Posterior:



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

Semiparametric Modelling

- Linear regression model for inferring effectiveness of new medical treatments.

$$y_{ij} = \beta^\top x_{ij} + b_i^\top z_{ij} + \epsilon_{ij}$$

  y_{ij} is outcome of jth trial on ith subject.

  x_{ij}, z_{ij} are predictors (treatment, dosage, age, health...).

  β are fixed-effects coefficients.

  b_i are random-effects subject-specific coefficients.

  ϵ_{ij} are noise terms.

- Care about inferring β. If x_{ij} is treatment, we want to determine $p(\beta > 0|\mathbf{x}, \mathbf{y})$.

Semiparametric Modelling

$$y_{ij} = \beta^\top x_{ij} + b_i^\top z_{ij} + \epsilon_{ij}$$

- Usually we assume Gaussian noise $\epsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$. Is this a sensible prior? Over-dispersion, skewness,...
- May be better to model noise nonparametrically,

$$\begin{aligned} \epsilon_{ij} &\sim F \\ F &\sim \mathrm{DP} \end{aligned}$$

- Also possible to model subject-specific random effects nonparametrically,

$$\begin{aligned} b_i &\sim G \\ G &\sim \mathrm{DP} \end{aligned}$$

Model Selection/Averaging

- Data: $\mathbf{x} = \{x_1, x_2, \ldots\}$
  Models: $p(\theta_k|M_k)$, $p(\mathbf{x}|\theta_k, M_k)$
- Marginal likelihood

$$p(\mathbf{x}|M_k) = \int p(\mathbf{x}|\theta_k, M_k)p(\theta_k|M_k)\,d\theta_k$$

- Model selection

$$M = \operatorname*{argmax}_{M_k} p(\mathbf{x}|M_k)$$

- Model averaging

$$p(x_\star|\mathbf{x}) = \sum_{M_k} p(x_\star|M_k)p(M_k|\mathbf{x}) = \sum_{M_k} p(x_\star|M_k)\frac{p(\mathbf{x}|M_k)p(M_k)}{p(\mathbf{x})}$$

- *But: is this computationally feasible?*

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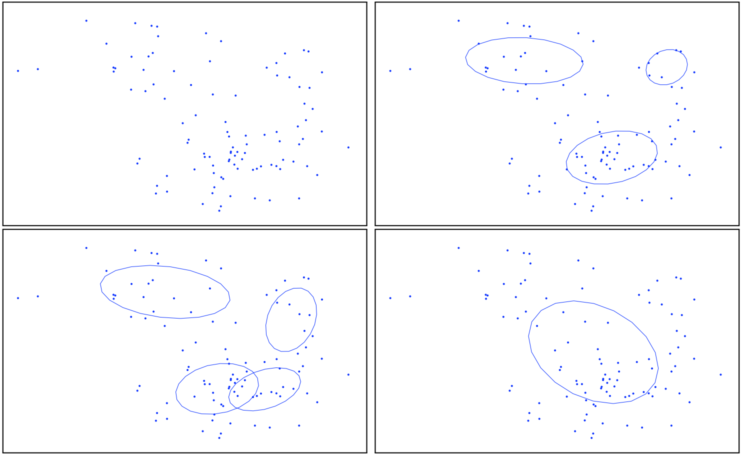
Model Selection/Averaging

- Marginal likelihood is usually extremely hard to compute.

$$p(\mathbf{x}|M_k) = \int p(\mathbf{x}|\theta_k, M_k)p(\theta_k|M_k)\, d\theta_k$$

- Model selection/averaging is to prevent underfitting and overfitting.
- But reasonable and proper Bayesian methods should not overfit [Rasmussen and Ghahramani 2001].
- Use a really large model M_∞ instead, and let the data speak for themselves.

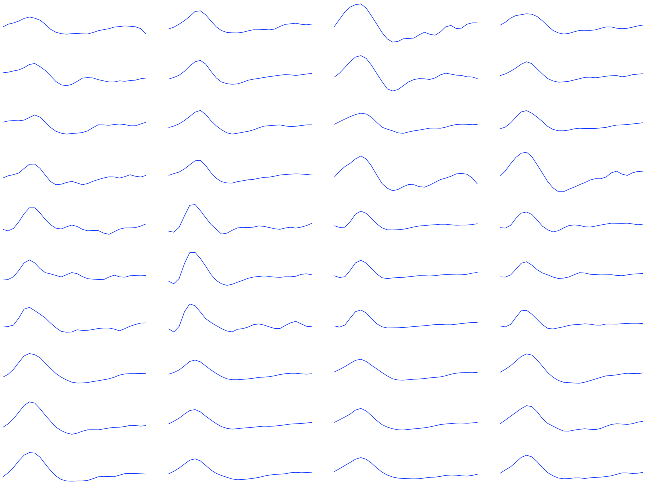
How many clusters are there?



Model Selection/Averaging

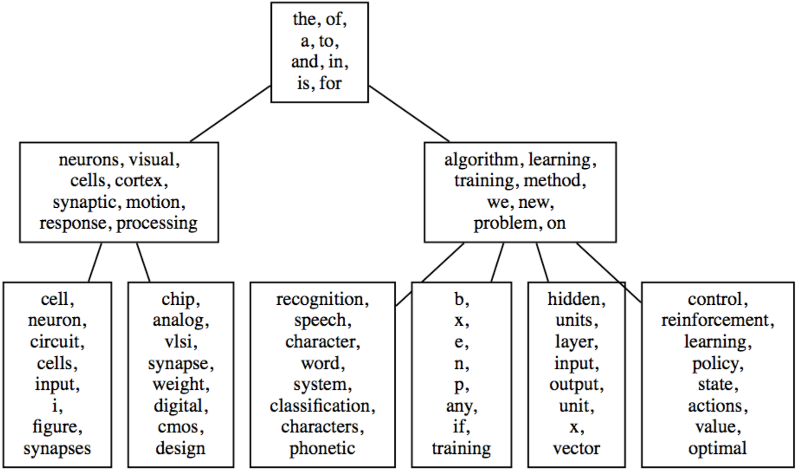
Spike Sorting

How many neurons are there?



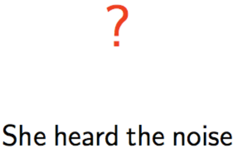
[Görür 2007, Wood et al. 2006]

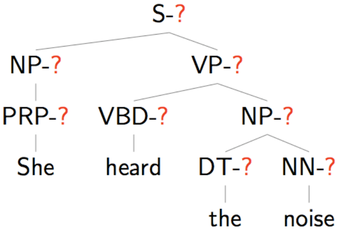
How many topics are there?



[Blei et al. 2004, Teh et al. 2006]

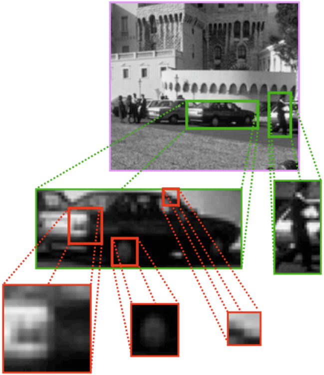
How many grammar symbols are there?





[Liang et al. 2007, Finkel et al. 2007]

How many objects, parts, features?



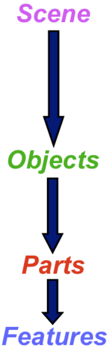


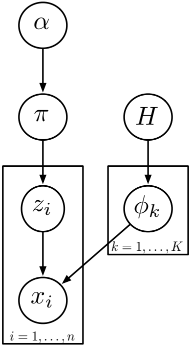
Figure from Sudderth. [Sudderth et al. 2007]

Outline

Finite Mixture Models

- A finite mixture model is defined as follows:

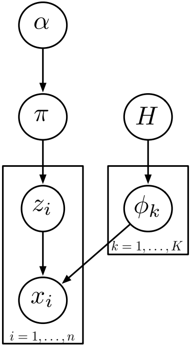
$$\begin{aligned} \phi_k &\sim H \\ \pi &\sim \text{Dirichlet}(\alpha/K, \ldots, \alpha/K) \\ z_i|\pi &\sim \text{Discrete}(\pi) \\ x_i|\phi_{z_i} &\sim F(\cdot|\phi_{z_i}) \end{aligned}$$



- Model selection/averaging over:
  - Hyperparameters in H.
  - Dirichlet parameter α.
  - Number of components K.
- Determining K hardest.

Infinite Mixture Models

- Imagine that $K \gg 0$ is really large.
- If parameters ϕ_k and mixing proportions π integrated out, the number of latent variables left does not grow with K—no overfitting.
- At most n components will be associated with data, aka "active".
- Usually, the number of active components is much less than n.
- This gives an infinite mixture model.
- Demo: dpm_demo2d
- *Issue 1: can we take this limit $K \to \infty$?*
- *Issue 2: what is the corresponding limiting model?*



[Rasmussen 2000]

- A Gaussian process (GP) is a distribution over functions

$$f : \mathbb{X} \mapsto \mathbb{R}$$

- Denote $f \sim \text{GP}$ if f is a GP-distributed random function.
- For any finite set of input points $x_1, \ldots, x_n$, we require $(f(x_1), \ldots, f(x_n))$ to be a multivariate Gaussian.

- The GP is parametrized by its mean $m(x)$ and covariance $c(x, y)$ functions:

$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_n) \end{bmatrix}, \begin{bmatrix} c(x_1, x_1) & \dots & c(x_1, x_n) \\ \vdots & \ddots & \vdots \\ c(x_n, x_1) & \dots & c(x_n, x_n) \end{bmatrix} \right)$$

- The above are finite dimensional marginal distributions of the GP.
- A salient property of these marginal distributions is that they are consistent: integrating out variables preserves the parametric form of the marginal distributions above.

- A sequence of input points $x_1, x_2, x_3, \ldots$ dense in $\mathbb{X}$.
- Draw

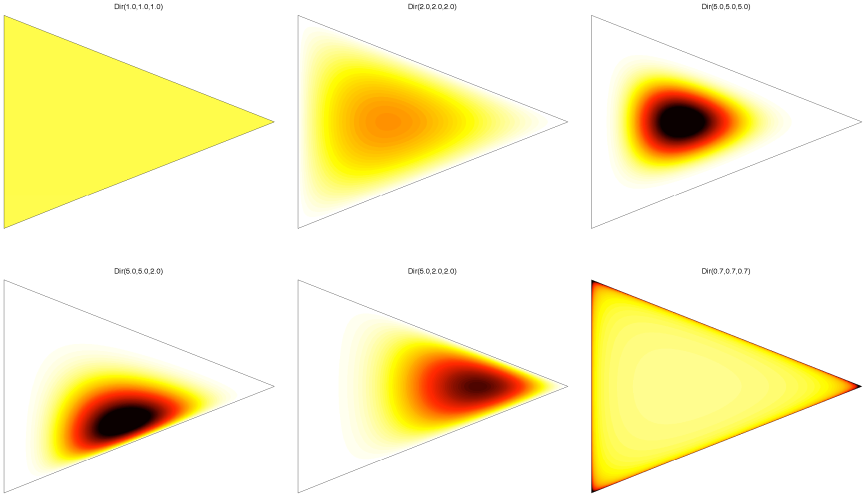
$$\begin{aligned} &f(x_1) \\ &f(x_2) \mid f(x_1) \\ &f(x_3) \mid f(x_1), f(x_2) \\ &\quad\vdots \end{aligned}$$

- Each conditional distribution is Gaussian since $(f(x_1), \ldots, f(x_n))$ is Gaussian.
- Demo: GPgenerate

- A Dirichlet distribution is a distribution over the K-dimensional probability simplex:
$$\Delta_K = \left\{(\pi_1, \ldots, \pi_K) \,:\, \pi_k \geq 0, \textstyle\sum_k \pi_k = 1\right\}$$
- We say $(\pi_1, \ldots, \pi_K)$ is Dirichlet distributed,
$$(\pi_1, \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_K)$$
with parameters $(\alpha_1, \ldots, \alpha_K)$, if
$$p(\pi_1, \ldots, \pi_K) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_{k=1}^{n} \pi_k^{\alpha_k - 1}$$

Dirichlet Processes

Examples of Dirichlet distributions.



Dirichlet Processes

Agglomerative property of Dirichlet distributions.

- Combining entries of probability vectors preserves Dirichlet property, for example:

$$\begin{aligned} & (\pi_1, \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_K) \\ \Rightarrow \qquad & (\pi_1 + \pi_2, \pi_3, \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1 + \alpha_2, \alpha_3, \ldots, \alpha_K) \end{aligned}$$

- Generally, if $(I_1, \ldots, I_j)$ is a partition of $(1, \ldots, n)$:

$$\left(\sum_{i \in I_1} \pi_i, \ldots, \sum_{i \in I_j} \pi_i \right) \sim \text{Dirichlet} \left(\sum_{i \in I_1} \alpha_i, \ldots, \sum_{i \in I_j} \alpha_i \right)$$

- The converse of the agglomerative property is also true, for example if:

$$\begin{aligned}(\pi_1, \ldots, \pi_K) &\sim \text{Dirichlet}(\alpha_1, \ldots, \alpha_K) \\ (\tau_1, \tau_2) &\sim \text{Dirichlet}(\alpha_1\beta_1, \alpha_1\beta_2)\end{aligned}$$

with $\beta_1 + \beta_2 = 1$,

$$\Rightarrow \quad (\pi_1\tau_1, \pi_1\tau_2, \pi_2, \ldots, \pi_K) \sim \text{Dirichlet}(\alpha_1\beta_1, \alpha_2\beta_2, \alpha_2, \ldots, \alpha_K)$$

- A Dirichlet process (DP) is an “infinitely decimated” Dirichlet distribution:

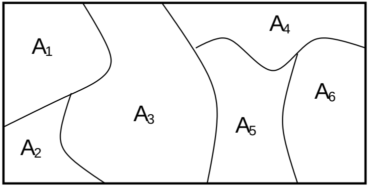
$$
\begin{aligned}
1 &\sim \mathrm{Dirichlet}(\alpha) \\
(\pi_1, \pi_2) &\sim \mathrm{Dirichlet}(\alpha/2, \alpha/2) & \pi_1 + \pi_2 = 1 \\
(\pi_{11}, \pi_{12}, \pi_{21}, \pi_{22}) &\sim \mathrm{Dirichlet}(\alpha/4, \alpha/4, \alpha/4, \alpha/4) & \pi_{i1} + \pi_{i2} = \pi_i \\
&\vdots
\end{aligned}
$$

- Each decimation step involves drawing from a Beta distribution (a Dirichlet with 2 components) and multiplying into the relevant entry.
- Demo: DPgenerate

Dirichlet Processes

A Proper but Non-Constructive Definition

- A probability measure is a function from subsets of a space $\mathbb{X}$ to $[0, 1]$ satisfying certain properties.
- A Dirichlet Process (DP) is a distribution over probability measures.
- Denote $G \sim \text{DP}$ if G is a DP-distributed random probability measure.
- For any finite set of partitions $A_1 \dot\cup \ldots \dot\cup A_K = \mathbb{X}$, we require $(G(A_1), \ldots, G(A_K))$ to be Dirichlet distributed.



- A DP has two parameters:
  - Base distribution H, which is like the *mean* of the DP.
  - Strength parameter α, which is like an *inverse-variance* of the DP.
- We write:

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

if for any partition $(A_1, \ldots, A_K)$ of $\mathbb{X}$:

$$(G(A_1), \ldots, G(A_K)) \sim \mathrm{Dirichlet}(\alpha H(A_1), \ldots, \alpha H(A_K))$$

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- The first two cumulants of the DP:

$$\text{Expectation:} \qquad \mathbb{E}[G(A)] = H(A)$$

$$\text{Variance:} \qquad \mathbb{V}[G(A)] = \frac{H(A)(1 - H(A))}{\alpha + 1}$$

  where A is any measurable subset of $\mathbb{X}$.

- A probability measure is a function from subsets of a space $\mathbb{X}$ to $[0, 1]$ satisfying certain properties.
- A DP is a distribution over probability measures such that marginals on finite partitions are Dirichlet distributed.
- How do we know that such an object exists?!?
- Kolmogorov Consistency Theorem: [Ferguson 1973].
- de Finetti's Theorem: Blackwell-MacQueen urn scheme, Chinese restaurant process, [Blackwell and MacQueen 1973, Aldous 1985].
- Stick-breaking Construction: [Sethuraman 1994].
- Gamma Process: [Ferguson 1973].

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- Suppose $G \sim \mathrm{DP}(\alpha, H)$. G is a (random) probability measure over $\mathbb{X}$. We can treat it as a distribution over $\mathbb{X}$. Let

$$\theta_1, \ldots, \theta_n \sim G$$

  be a random variable with distribution G.

- We saw in the demo that draws from a Dirichlet process seem to be discrete distributions. If so, then:

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

  and there is positive probability that θ_i's can take on the same value θ_k^* for some k, i.e. the θ_i's cluster together.

- In this section we are concerned with representations of Dirichlet processes based upon both the clustering property and the sum of point masses.

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- Suppose G is Dirichlet process distributed:

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

- G is a (random) probability measure over $\mathbb{X}$. We can treat it as a distribution over $\mathbb{X}$. Let

$$\theta \sim G$$

  be a random variable with distribution G.

- We are interested in:

$$p(\theta) = \int p(\theta|G)p(G)\,dG$$

$$p(G|\theta) = \frac{p(\theta|G)p(G)}{p(\theta)}$$

- Consider:

$$(\pi_1, \dots, \pi_K) \sim \text{Dirichlet}(\alpha_1, \dots, \alpha_K)$$
$$z|(\pi_1, \dots, \pi_K) \sim \text{Discrete}(\pi_1, \dots, \pi_K)$$

z is a multinomial variate, taking on value $i \in \{1, \dots, n\}$ with probability π_i.

- Then:

$$z \sim \text{Discrete}\left(\frac{\alpha_1}{\sum_i \alpha_i}, \dots, \frac{\alpha_K}{\sum_i \alpha_i}\right)$$
$$(\pi_1, \dots, \pi_K)|z \sim \text{Dirichlet}(\alpha_1 + \delta_1(z), \dots, \alpha_K + \delta_K(z))$$

where $\delta_i(z) = 1$ if z takes on value i, 0 otherwise.

- Converse also true.

Posterior Dirichlet Processes

- Fix a partition $(A_1, \ldots, A_K)$ of $\mathbb{X}$. Then

$$(G(A_1), \ldots, G(A_K)) \sim \text{Dirichlet}(\alpha H(A_1), \ldots, \alpha H(A_K))$$
$$P(\theta \in A_i | G) = G(A_i)$$

- Using Dirichlet-multinomial conjugacy,

$$P(\theta \in A_i) = H(A_i)$$
$$(G(A_1), \ldots, G(A_K))|\theta \sim \text{Dirichlet}(\alpha H(A_1)+\delta_\theta(A_1), \ldots, \alpha H(A_K)+\delta_\theta(A_K))$$

- The above is true for every finite partition of $\mathbb{X}$. In particular, taking a really fine partition,

$$p(\theta)d\theta = H(d\theta)$$

- Also, the posterior $G|\theta$ is also a Dirichlet process:

$$G|\theta \sim \text{DP}\left(\alpha + 1, \frac{\alpha H + \delta_\theta}{\alpha + 1}\right)$$

Posterior Dirichlet Processes

- Fix a partition $(A_1, \dots, A_K)$ of $\mathbb{X}$. Then

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Posterior Dirichlet Processes

$$\begin{aligned} G &\sim \mathrm{DP}(\alpha, H) \\ \theta | G &\sim G \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} \theta &\sim H \\ G | \theta &\sim \mathrm{DP}\left(\alpha + 1, \tfrac{\alpha H + \delta_\theta}{\alpha + 1}\right) \end{aligned}$$

Blackwell-MacQueen Urn Scheme

- First sample:

$$\begin{aligned} & \theta_1 | G \sim G & & G \sim \mathrm{DP}(\alpha, H) \\ \iff & \theta_1 \sim H & & G|\theta_1 \sim \mathrm{DP}(\alpha + 1, \tfrac{\alpha H + \delta_{\theta_1}}{\alpha + 1}) \end{aligned}$$

- Second sample:

$$\begin{aligned} & \theta_2 | \theta_1, G \sim G & & G|\theta_1 \sim \mathrm{DP}(\alpha + 1, \tfrac{\alpha H + \delta_{\theta_1}}{\alpha + 1}) \\ \iff & \theta_2 | \theta_1 \sim \tfrac{\alpha H + \delta_{\theta_1}}{\alpha + 1} & & G|\theta_1, \theta_2 \sim \mathrm{DP}(\alpha + 2, \tfrac{\alpha H + \delta_{\theta_1} + \delta_{\theta_2}}{\alpha + 2}) \end{aligned}$$

- n^{th} sample

$$\begin{aligned} & \theta_n | \theta_{1:n-1}, G \sim G & & G|\theta_{1:n-1} \sim \mathrm{DP}(\alpha + n - 1, \tfrac{\alpha H + \sum_{i=1}^{n-1} \delta_{\theta_i}}{\alpha + n - 1}) \\ \iff & \theta_n | \theta_{1:n-1} \sim \tfrac{\alpha H + \sum_{i=1}^{n-1} \delta_{\theta_i}}{\alpha + n - 1} & & G|\theta_{1:n} \sim \mathrm{DP}(\alpha + n, \tfrac{\alpha H + \sum_{i=1}^{n} \delta_{\theta_i}}{\alpha + n}) \end{aligned}$$

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$$\iff \qquad \theta_n|\theta_{1:n-1} \sim \tfrac{\alpha H + \sum_{i=1}^{n-1} \delta_{\theta_i}}{\alpha+n-1} \qquad G|\theta_{1:n} \sim \mathrm{DP}(\alpha+n, \tfrac{\alpha H + \sum_{i=1}^{n} \delta_{\theta_i}}{\alpha+n})$$

Blackwell-MacQueen Urn Scheme

- Blackwell-MacQueen urn scheme produces a sequence $\theta_1, \theta_2, \ldots$ with the following conditionals:

$$\theta_n | \theta_{1:n-1} \sim \frac{\alpha H + \sum_{i=1}^{n-1} \delta_{\theta_i}}{\alpha + n - 1}$$

- Picking balls of different colors from an urn:
  - Start with no balls in the urn.
  - with probability $\propto \alpha$, draw $\theta_n \sim H$, and add a ball of that color into the urn.
  - With probability $\propto n - 1$, pick a ball at random from the urn, record θ_n to be its color, return the ball into the urn and place a second ball of same color into urn.
- Blackwell-MacQueen urn scheme is like a "representer" for the DP—a finite projection of an infinite object.

Exchangeability and de Finetti's Theorem

- Starting with a DP, we constructed Blackwell-MacQueen urn scheme.
- The reverse is possible using de Finetti's Theorem.
- Since θ_i are iid $\sim G$, their joint distribution is invariant to permutations, thus $\theta_1, \theta_2, \ldots$ are exchangeable.
- Thus a distribution over measures must exist making them iid.
- This is the DP.

Chinese Restaurant Process

- Draw $\theta_1, \ldots, \theta_n$ from a Blackwell-MacQueen urn scheme.
- They take on $K < n$ distinct values, say $\theta_1^*, \ldots, \theta_K^*$.
- This defines a partition of $1, \ldots, n$ into K clusters, such that if i is in cluster k, then $\theta_i = \theta_k^*$.
- Random draws $\theta_1, \ldots, \theta_n$ from a Blackwell-MacQueen urn scheme induces a random partition of $1, \ldots, n$.
- The induced distribution over partitions is a Chinese restaurant process (CRP).

Chinese Restaurant Process

- Generating from the CRP:
  - First customer sits at the first table.
  - Customer n sits at:
    - Table k with probability $\frac{n_k}{\alpha+n-1}$ where n_k is the number of customers at table k.
    - A new table $K+1$ with probability $\frac{\alpha}{\alpha+n-1}$.
  - Customers $\Leftrightarrow$ integers, tables $\Leftrightarrow$ clusters.
- The CRP exhibits the clustering property of the DP.

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- The CRP exhibits the clustering property of the DP.

Chinese Restaurant Process

- To get back from the CRP to Blackwell-MacQueen urn scheme, simply draw

$$\theta_k^* \sim H$$

for $k = 1, \ldots, K$, then for $i = 1, \ldots, n$ set

$$\theta_i = \theta_{z_i}^*$$

where z_i is the table that customer i sat at.

- The CRP teases apart the clustering property of the DP, from the base distribution.

Stick-breaking Construction

- Returning to the posterior process:

$$\begin{aligned} G &\sim \mathrm{DP}(\alpha, H) \\ \theta &\sim G \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} \theta &\sim H \\ G &\sim \mathrm{DP}(\alpha+1, \tfrac{\alpha H + \delta_\theta}{\alpha+1}) \end{aligned}$$

- Consider a partition $(\theta, \mathbb{X}\backslash\theta)$ of $\mathbb{X}$. We have:

$$\begin{aligned} (G(\theta), G(\mathbb{X}\backslash\theta)) &\sim \mathrm{Dirichlet}((\alpha+1)\tfrac{\alpha H+\delta_\theta}{\alpha+1}(\theta), (\alpha+1)\tfrac{\alpha H+\delta_\theta}{\alpha+1}(\mathbb{X}\backslash\theta)) \\ &= \mathrm{Dirichlet}(1, \alpha) \end{aligned}$$

- G has a point mass located at θ:

$$G = \beta\delta_\theta + (1-\beta)G' \qquad \text{with} \qquad \beta \sim \mathrm{Beta}(1, \alpha)$$

and G' is the (renormalized) probability measure with the point mass removed.

- What is G'?

Stick-breaking Construction

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- Currently, we have:

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- Consider a further partition $(\theta, A_1, \ldots, A_K)$ of $\mathbb{X}$:

$$\begin{aligned} &(G(\theta), G(A_1), \ldots, G(A_K)) \\ =&(\beta, (1-\beta)G'(A_1), \ldots, (1-\beta)G'(A_K)) \end{aligned}$$

- The agglomerative/decimative property of Dirichlet implies:

$$(G'(A_1), \ldots, G'(A_K)) \sim \mathrm{Dirichlet}(\alpha H(A_1), \ldots, \alpha H(A_K))$$
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Stick-breaking Construction

- We have:

$$
\begin{aligned}
G &\sim \mathrm{DP}(\alpha, H) \\
G &= \beta_1 \delta_{\theta_1^*} + (1-\beta_1) G_1 \\
G &= \beta_1 \delta_{\theta_1^*} + (1-\beta_1)(\beta_2 \delta_{\theta_2^*} + (1-\beta_2) G_2) \\
&\vdots \\
G &= \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k^*}
\end{aligned}
$$

where

$$
\pi_k = \beta_k \prod_{i=1}^{k-1} (1-\beta_i) \qquad \beta_k \sim \mathrm{Beta}(1, \alpha) \qquad \theta_k^* \sim H
$$

- This is the stick-breaking construction.
- Demo: SBgenerate

Stick-breaking Construction

- Starting with a DP, we showed that draws from the DP looks like a sum of point masses, with masses drawn from a stick-breaking construction.
- The steps are limited by assumptions of regularity on $\mathbb{X}$ and smoothness on H.
- [Sethuraman 1994] started with the stick-breaking construction, and showed that draws are indeed DP distributed, under very general conditions.

- Posterior Dirichlet process:

$$\begin{aligned} G &\sim \mathrm{DP}(\alpha, H) \\ \theta | G &\sim G \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} \theta &\sim H \\ G|\theta &\sim \mathrm{DP}\left(\alpha + 1, \tfrac{\alpha H + \delta_\theta}{\alpha+1}\right) \end{aligned}$$

- Blackwell-MacQueen urn scheme:

$$\theta_n | \theta_{1:n-1} \sim \frac{\alpha H + \sum_{i=1}^{n-1} \delta_{\theta_i}}{\alpha + n - 1}$$

- Chinese restaurant process:

$$p(\text{customer } n \text{ sat at table } k | \text{past}) = \begin{cases} \frac{n_k}{n-1+\alpha} & \text{if occupied table} \\ \frac{\alpha}{n-1+\alpha} & \text{if new table} \end{cases}$$

- Stick-breaking construction:

$$\pi_k = \beta_k \prod_{i=1}^{k-1} (1 - \beta_i) \qquad \beta_k \sim \mathrm{Beta}(1, \alpha) \qquad \theta_k^* \sim H \qquad G = \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k^*}$$

Outline

Density Estimation

- Recall our approach to density estimation with Dirichlet processes:

$$
\begin{aligned}
G &\sim \mathrm{DP}(\alpha, H) \\
x_i &\sim G
\end{aligned}
$$

- The above does not work. Why?
- Problem: G is a discrete distribution; in particular it has no density!
- Solution: Convolve the DP with a smooth distribution:

$$
\begin{aligned}
G &\sim \mathrm{DP}(\alpha, H) \\
F_x(\cdot) &= \int F(\cdot|\theta) dG(\theta) \\
x_i &\sim F_x
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
G &= \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k^*} \\
F_x(\cdot) &= \sum_{k=1}^{\infty} \pi_k F(\cdot|\theta_k^*) \\
x_i &\sim F_x
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$$\Rightarrow$$

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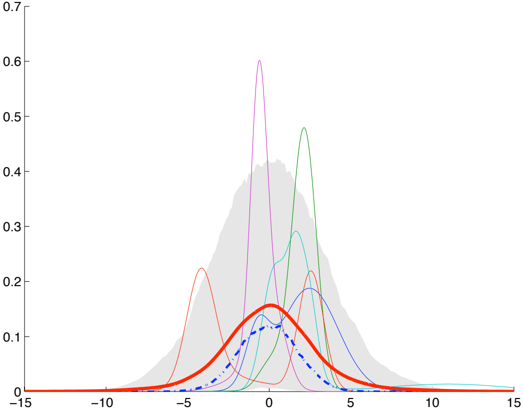
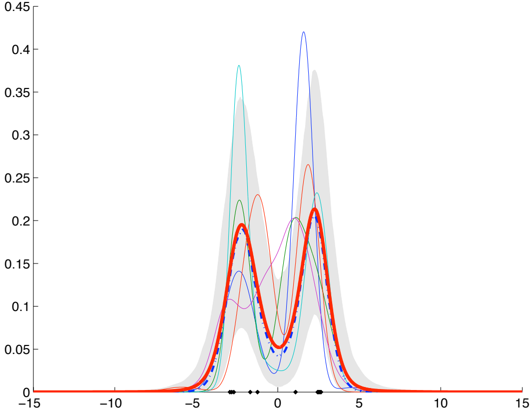
Density Estimation



$F(\cdot|\mu, \Sigma)$ is Gaussian with mean μ, covariance Σ.
$H(\mu, \Sigma)$ is Gaussian-inverse-Wishart conjugate prior.

Density Estimation



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Clustering

- Recall our approach to density estimation:

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\begin{aligned}
G &= \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k^*} \sim \mathrm{DP}(\alpha, H) \\
F_x(\cdot) &= \sum_{k=1}^{\infty} \pi_k F(\cdot|\theta_k^*) \\
x_i &\sim F_x
\end{aligned}
$$

- Above model equivalent to:

$$
\begin{aligned}
z_i &\sim \mathrm{Discrete}(\boldsymbol{\pi}) \\
\theta_i &= \theta_{z_i}^* \\
x_i|z_i &\sim F(\cdot|\theta_i) = F(\cdot|\theta_{z_i}^*)
\end{aligned}
$$

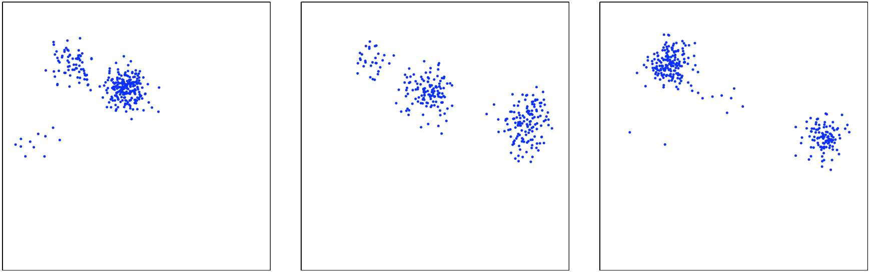
- This is simply a mixture model with an infinite number of components. This is called a DP mixture model.

Clustering

- DP mixture models are used in a variety of clustering applications, where the number of clusters is not known a priori.
- They are also used in applications in which we believe the number of clusters grows without bound as the amount of data grows.
- DPs have also found uses in applications beyond clustering, where the number of latent objects is not known or unbounded.
  - Nonparametric probabilistic context free grammars.
  - Visual scene analysis.
  - Infinite hidden Markov models/trees.
  - Haplotype inference.
  - ...
- In many such applications it is important to be able to model the same set of objects in different contexts.
- This corresponds to the problem of grouped clustering and can be tackled using hierarchical Dirichlet processes.

[Teh et al. 2006]

Grouped Clustering



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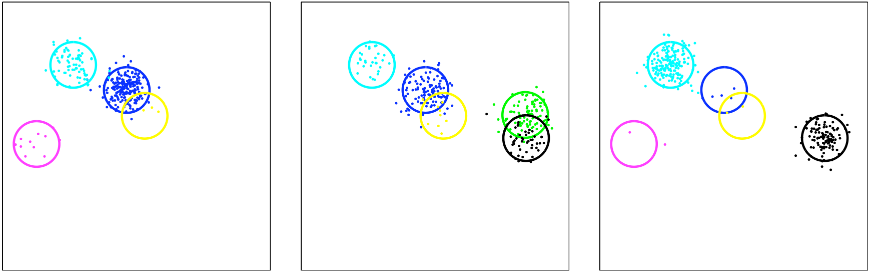
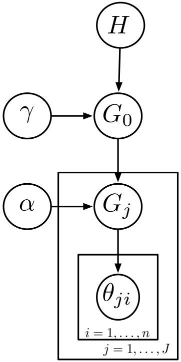


Hierarchical Dirichlet Processes

- Hierarchical Dirichlet process:

$$G_0|\gamma, H \sim \mathrm{DP}(\gamma, H)$$
$$G_j|\alpha, G_0 \sim \mathrm{DP}(\alpha, G_0)$$
$$\theta_{ji}|G_j \sim G_j$$

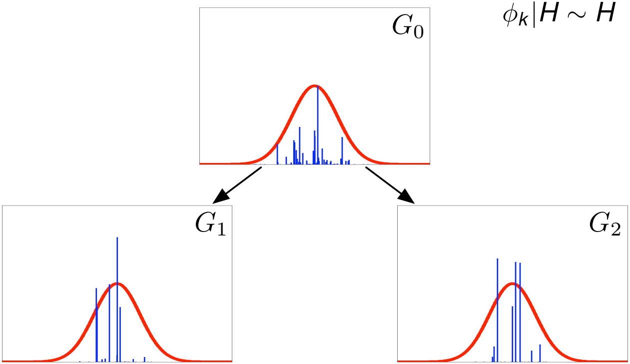


Hierarchical Dirichlet Processes

$$G_0|\gamma, H \sim \mathrm{DP}(\gamma, H) \qquad G_0 = \sum_{k=1}^{\infty} \beta_k \delta_{\phi_k} \qquad \boldsymbol{\beta}|\gamma \sim \mathrm{Stick}(\gamma)$$

$$G_j|\alpha, G_0 \sim \mathrm{DP}(\alpha, G_0) \qquad G_j = \sum_{k=1}^{\infty} \pi_{jk} \delta_{\phi_k} \qquad \boldsymbol{\pi}_j|\alpha, \boldsymbol{\beta} \sim \mathrm{DP}(\alpha, \boldsymbol{\beta})$$

$$\phi_k|H \sim H$$



Summary

- Dirichlet process is “just” a glorified Dirichlet distribution.
- Draws from a DP are probability measures consisting of a weighted sum of point masses.
- Many representations: Blackwell-MacQueen urn scheme, Chinese restaurant process, stick-breaking construction.
- DP mixture models are mixture models with countably infinite number of components.

- I have not delved into:
  - Applications.
  - Generalizations, extensions, other nonparametric processes.
  - Inference: MCMC sampling, variational approximation.
- Also see the tutorial material from Ghaharamani, Jordan and Tresp.

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Bayesian Nonparametrics

- Parametric models can only capture a bounded amount of information from data, since they have bounded complexity.
- Real data is often complex and the parametric assumption is often wrong.
- Nonparametric models allow relaxation of the parametric assumption, bringing significant flexibility to our models of the world.
- Nonparametric models can also often lead to model selection/averaging behaviours without the cost of actually doing model selection/averaging.
- Nonparametric models are gaining popularity, spurred by growth in computational resources and inference algorithms.
- In addition to DPs, HDPs and their generalizations, other nonparametric models include Indian buffet processes, beta processes, tree processes...

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Outline

Exploring the Dirichlet Process

- Before using DPs, it is important to understand its properties, so that we understand what prior assumptions we are imposing on our models.
- In this practical course we shall work towards implementing a DP mixture model to cluster NIPS papers, thus the relevant properties are the clustering properties of the DP.
- Consider the Chinese restaurant process representation of DPs:
  - First customer sits at the first table.
  - Customer n sits at:
    - Table k with probability $\frac{n_k}{\alpha+n-1}$ where n_k is the number of customers at table k.
    - A new table $K+1$ with probability $\frac{\alpha}{\alpha+n-1}$.
- How does number of clusters K scale as a function of α and of n (on average)?
- How does the number n_k of customers sitting around table k depend on k and n (on average)?

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Exploring the Pitman-Yor Process

- Sometimes the assumptions embedded in using DPs to model data are inappropriate.
- The Pitman-Yor process is a generalization of the DP that often has more appropriate properties.
- It has two parameters: d and α with $0 \leq d < 1$ and $\alpha > -d$.

  When $d = 0$ the Pitman-Yor process reduces to a DP.
- It also has a Chinese restaurant process representation:
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Dirichlet Process Mixture Models

- We model a data set $x_1, \ldots, x_n$ using the following model:

$$\begin{aligned} G &\sim \mathrm{DP}(\alpha, H) \\ \theta_i | G &\sim G \\ x_i | \theta_i &\sim F(\cdot | \theta_i) \qquad\qquad \text{for } i = 1, \ldots, n \end{aligned}$$

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- Different representations lead to different inference algorithms for DP mixture models.
- The most common are based on the Chinese restaurant process and on the stick-breaking construction.
- Here we shall work with the Chinese restaurant process representation, which, incidentally, can also be derived as the infinite limit of finite mixture models.
- A finite mixture model is defined as follows:

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\begin{aligned}
\theta_k^* &\sim H && \text{for } k = 1, \ldots, K \\
\pi &\sim \text{Dirichlet}(\alpha/K, \ldots, \alpha/K) \\
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- Assuming H is conjugate to $F(\cdot|\theta)$, we can integrate out both π and θ_k^*'s, leaving us with z_i's only.
- The simplest MCMC algorithm is to Gibbs sample z_i's (collapsed Gibbs sampling):

$$p(z_i = k|\mathbf{z}^{\neg i}, \mathbf{x}) \propto p(z_i = k|\mathbf{z}_{\neg i})p(x_i|\mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i})$$

$$p(x_i|\mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i}) = \int p(x_i|\theta_k^*)p(\theta_k^*|\{x_j : j \neq i, z_j = k\})\, d\theta_k^*$$

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Aside: Markov Chain Monte Carlo Sampling

- Markov chain Monte Carlo sampling is a dominant and diverse family of inference algorithms for probabilistic models. Here we are interested in obtaining samples from the posterior:

$$\mathbf{z}^{(s)} \sim p(\mathbf{z}|\mathbf{x}) = \int p(\mathbf{z}, \theta^*, \pi|\mathbf{x})\, d\theta^* d\pi$$

- The basic idea is to construct a sequence $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots$ so that for large enough t, $\mathbf{z}^{(t)}$ will be an (approximate) sample from the posterior $p(\mathbf{z}|\mathbf{x})$.
- Convergence to the posterior is guaranteed, but (most of the time) there is no convergence diagnostics, only heuristics. Won't worry about this.
- Given the previous state $\mathbf{z}^{(t-1)}$, we construct $\mathbf{z}^{(t)}$ by making a small (stochastic) alteration to $\mathbf{z}^{(t-1)}$ so that $\mathbf{z}^{(t)}$ is "closer" to the posterior.
- In Gibbs sampling, this alteration is achieved by taking an entry, say z_i, and sampling it from the conditional:

$$z_i^{(t)} \sim p(z_i|\mathbf{z}_{\neg i}^{(t-1)}, \mathbf{x}) \qquad \mathbf{z}_{\neg i}^{(t)} = \mathbf{z}_{\neg i}^{(t-1)}$$

[Neal 1993]

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- An exponential family of distributions is parametrized as:

$$\begin{aligned} p(x|\theta) &= \exp\left(t(\theta)^\top s(x) - \phi(x) - \psi(\theta)\right) \\ s(x) &= \text{sufficient statistics vector.} \\ t(\theta) &= \text{natural parameter vector.} \\ \psi(\theta) &= \log \sum_{x'} \exp\left(t(\theta)^\top s(x') - \phi(x')\right) \quad \text{(log normalization)} \end{aligned}$$

- The conjugate prior is an exponential family distribution over θ:

$$p(\theta) = \exp\left(t(\theta)^\top \nu - \eta\psi(\theta) - \xi(\nu, \eta)\right)$$

- The posterior given observations $x_1, \ldots, x_n$ is in the same family:

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$$p(\theta|\mathbf{x}) = \exp\left(t(\theta)^\top (\nu + \textstyle\sum_i s(x_i)) - (\eta + n)\psi(\theta) - \xi(\nu + \textstyle\sum_i s(x_i), \eta + n)\right)$$

- The marginal probability is:

$$p(\mathbf{x}) = \exp\left(\xi(\nu + \textstyle\sum_i s(x_i), \eta + n) - \xi(\nu, \eta) - \textstyle\sum_i \phi(x_i)\right)$$

- Finite mixture model:

$$\begin{aligned} \phi_k &\sim H & \text{for } k = 1, \ldots, K \\ \pi &\sim \text{Dirichlet}(\alpha/K, \ldots, \alpha/K) \\ z_i|\pi &\sim \text{Discrete}(\pi) & \text{for } i = 1, \ldots, n \\ x_i|\phi_{z_i} &\sim F(\phi_{z_i}) \end{aligned}$$

- Integrating out both π and θ_k^*'s, the Gibbs sampling conditional distributions for $\mathbf{z}$ are:

$$p(z_i = k|\mathbf{z}^{\neg i}, \mathbf{x}) \propto (n_k^{\neg i} + \alpha/K) p(x_i|\mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i})$$

$$\begin{aligned} p(x_i|\mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i}) &= \int p(x_i|\theta_k^*) p(\theta_k^*|\{x_j : j \neq i, z_j = k\})\, d\theta_k^* \\ &= \exp\left(\xi(\nu + s(x_i) + \textstyle\sum_{j\neq i: z_j = k} s(x_j), \eta + 1 + n_k^{\neg i}) \right. \\ &\quad \left. - \xi(\nu + \textstyle\sum_{j\neq i: z_j=k} s(x_j), \eta + n_k^{\neg i}) - \phi(x_i)\right) \end{aligned}$$

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- Imagine that $K \gg 0$ is really large.
- Only a few components will be "active" (i.e. with $n_k > 0$), while most are "inactive".

$$p(z_i = k|\mathbf{z}^{\neg i}, \mathbf{x}) \propto \begin{cases} (n_k^{\neg i} + \alpha/K)p(x_i|\mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i}) & \text{if } k \text{ active;} \\ (\alpha/K)p(x_i) & \text{if } k \text{ inactive.} \end{cases}$$

$$\begin{aligned} p(z_i = k \text{ active}|\mathbf{z}^{\neg i}, \mathbf{x}) &\propto (n_k^{\neg i} + \alpha/K)p(x_i|\mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i}) \\ &\approx n_k^{\neg i} p(x_i|\mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i}) \\ p(z_i \text{ inactive}|\mathbf{z}^{\neg i}, \mathbf{x}) &\propto (\alpha(K - K_{\text{active}})/K)p(x_i) \\ &\approx \alpha p(x_i) \end{aligned}$$

- This gives an inference algorithm for DP mixture models in Chinese restaurant process representation.

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- Rearrange mixture component indices so that $1, \ldots, K_{\text{active}}$ are active, and the rest are inactive.

$$p(z_i = k \le K_{\text{active}} | \mathbf{z}^{\neg i}, \mathbf{x}) \propto n_k^{\neg i} p(x_i | \mathbf{z}^{\neg i}, \mathbf{x}_k^{\neg i})$$
$$p(z_i > K_{\text{active}} | \mathbf{z}^{\neg i}, \mathbf{x}) \propto \alpha p(x_i)$$

- If z_i takes on an inactive value, instantiate a new active component, and increment K_{active}.
- If $n_k = 0$ for some k during sampling, delete that active component, and decrement K_{active}.

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Clustering NIPS Papers

- I have prepared a small subset of NIPS papers for you to try clustering them.
- We concentrate on a small subset of papers, and a small subset of "informative" words.
- Each paper is represented as a bag-of-words. Paper i is represented by a vector $\mathbf{x}_i = (x_{i1}, \ldots, x_{iW})$:

$$x_{iw} = c \qquad \text{if word } w \text{ occurs } c \text{ times in paper } i.$$

- Model papers in cluster k using a Multinomial distribution:

$$p(\mathbf{x}_i|\theta_k^*) = \frac{(\sum_w x_{iw})!}{\prod_w x_{iw}!} \prod_w (\theta_{kw}^*)^{x_{iw}}$$

- The conjugate prior for θ_k^* is a Dirichlet:

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Clustering NIPS Papers
Specifying the Priors

- We shall use a symmetric Dirichlet prior for the cluster parameters θ. Specifically $b_w = b/W$ for some $b > 0$.
- The model:

$$\begin{aligned} H &= \text{Dirichlet}(b/W, \ldots, b/W) \\ G &\sim \text{DP}(\alpha, H) \\ \theta_i &\sim G \\ \mathbf{x}_i &\sim \text{Multinomial}(n_i, \theta_i) \end{aligned}$$

- Only two numbers to set: α and b.
- α controls the a priori expected number of clusters.
- b controls the number of words assigned to each cluster.
- What are reasonable values for α and b?

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Sensitivity to Priors

- When building models and making inferences, and one does not "trust" ones prior very much, then it is important to perform sensitivity analysis.
- Sensitivity analysis is about determining how much our inference conclusions depend on the setting of the model priors.
- If our conclusions depend strongly on the priors which we don't trust very much, then we cannot trust our conclusions either.
- If our conclusions do not depend strongly on the priors, then we can more strongly trust our conclusions.
- What part of our model should we worry about?

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Summary

- We explored some properties of the Dirichlet process.
- We implemented a Dirichlet process mixture model.
- We applied a Dirichlet process mixture model to clustering NIPS papers.
- We considered ways of specifying the hyperparameters of the model, and explored the sensitivity to these hyperparameters.

- Dirichlet processes are not that mysterious or hard.

Summary

- We explored some properties of the Dirichlet process.
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