STATS 225: Bayesian Analysis
Dirichlet Process Mixture Models

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Dirichlet process

- In this lecture, we are going to introduce Dirichlet process mixture models, which is usually used for nonparametric density estimation and clustering.

- A Dirichlet process, $\mathcal{D}(G_0, \gamma)$, with *base distribution* G_0 and *scale or concentration* parameter γ is a distribution over distributions.

- More formally, we say a random probability measure G is distributed according to $\mathcal{D}(G_0, \gamma)$ if for any finite partition of $(A_1, \ldots, A_n)$ of space Ω, the random vector $(G(A_1), \ldots, G(A_n))$ has a finite dimensional Dirichlet distribution as follows:

$$(G(A_1), \ldots, G(A_n)) \sim \mathrm{Dir}(\gamma G_0(A_1), \ldots, \gamma G_0(A_n)))$$

- Using the Polya urn scheme, Blackwell and MacQueen (1973) showed that the distributions sampled from a Dirichlet process are discrete almost surely.

Dirichlet process

- Ferguson (1973) introduced the Dirichlet process as a class of prior distributions for which the support is large, and the posterior distribution is manageable analytically,

$$G|\theta_1, \ldots, \theta_n \sim \mathcal{D}(\frac{\gamma}{\gamma + n}G_0 + \frac{n}{\gamma + n}P_n, \gamma + n)$$

  where P_n is the empirical distribution.

- Antoniak (1974) proposed the idea of using a Dirichlet process as the prior for the mixing proportions of a simple distribution (e.g., Gaussian).

- First, let's review simple mixture distributions from the Bayesian point of view.

Mixture distributions

- Consider a random sample, $x_1, \ldots, x_n$, drawn independently from some unknown distribution.
- We can use a mixture of simple distributions to model the density of X:

$$P(x_i|\pi, \phi) = \sum_{k=1}^{K} \pi_k P_k(x_i|\phi_k)$$

$$0 \leq \pi_k \leq 1, \quad \sum_{k=1}^{K} \pi_k = 1$$

  Here, π_k are the mixing proportion, and P_k is a simple distribution such as normal with $\phi = (\mu, \sigma)$.

- A common prior for π_k is a symmetric Dirichlet distribution

$$P(\pi_1, ..., \pi_K) \quad = \quad \frac{\Gamma(\gamma)}{\Gamma(\gamma/K)^K} \prod_{k=1}^{K} \pi_k^{(\gamma/K)-1}$$

- ϕ_c are assumed to be independent under the prior with distribution G_0.

Finite mixtures

- For a finite K, we can represent the mixture model as follows:

$$\begin{aligned}
\phi_k &\sim G_0 \\
\pi_1, \ldots, \pi_K &\sim Dirichlet(\gamma/K, \ldots, \gamma/K) \\
z_i|\pi_1, \ldots, \pi_K &\sim Discrete(\pi_1, \ldots, \pi_K) \\
x_i|z_i, \phi &\sim P_k(x_i|\phi_{k_i})
\end{aligned}$$

- By integrating over the Dirichlet prior, we obtain the following conditional distribution for z_i:

$$P(z_i = k|z_1, \ldots, z_{i-1}) = \frac{n_{ik} + \gamma/K}{i - 1 + \gamma}$$

where, n_{ik} represents the number of data points previously (i.e., before the i^{th}) assigned to component k.

Dirichlet process mixture

- We might not know the number of components, K, *a priori*. We can assume $K \to \infty$,

$$\begin{aligned} P(z_i = k | z_1, \ldots, z_{i-1}) &\rightarrow \frac{n_k}{i - 1 + \gamma} \\ P(z_i \neq z_j, \forall j < i | z_1, \ldots, z_{i-1}) &\rightarrow \frac{\gamma}{i - 1 + \gamma} \end{aligned}$$

- Therefore, the successive conditional distribution of θ_i is

$$\theta_i | \theta_1, ..., \theta_{i-1} \sim \frac{1}{i - 1 + \gamma} \sum_{j<i} \delta(\theta_j) + \frac{\gamma}{i - 1 + \gamma} G_0$$

- Because of exchangeability, we can treat i as the last observation so we can use this to write the conditional distribution of θ_i given all other θ's,

$$\theta_i | \theta_{-i} \sim \frac{1}{n - 1 + \gamma} \sum_{j \neq i} \delta(\theta_j) + \frac{\gamma}{n - 1 + \gamma} G_0$$

- The resulting model is equivalent to the Dirichlet process mixture model.

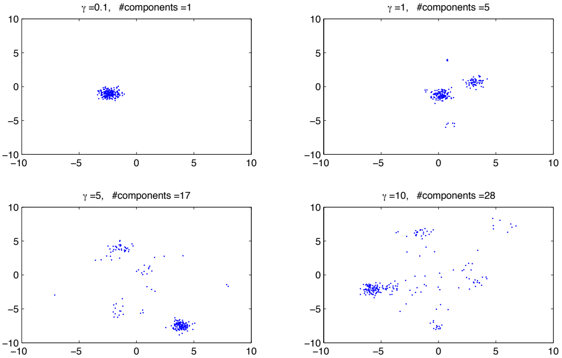
Dirichlet process mixture model

- The idea of using a Dirichlet process as the prior for the mixing proportions of a simple distribution (e.g., Gaussian) was first introduced by Antoniak (1974).
- Suppose we have $x_1, \ldots, x_n$ observations from some unknown distribution.
- We can model the unknown distribution of x as a mixture of simple distributions of the form $F(\theta)$
- We denote the mixing distribution over θ as G and let the prior over G be a Dirichlet process:

$$\begin{aligned} x_i|\theta_i &\sim F(\theta_i) \\ \theta_i|G &\sim G \\ G &\sim \mathcal{D}(G_0, \gamma) \end{aligned}$$

Samples from Dirichlet process mixture prior

- Note that θ's are not unique; we refer to unique values of θ as ϕ.
- Multiple subjects can be mapped to the same ϕ; this creates a clustering of subjects.
- The following graphs shows 4 different datasets ($n = 200$) randomly generated from distributions sampled from Dirichlet process mixture priors with different γ.



Chinese restaurant process

- Dirichlet process is sometimes explained as a "Chinese restaurant" process.
- Consider a restaurant with infinite possibilities, i.e., infinite menu items and infinite number of tables.
- The rule is that people at the same table must order the same food.
- First customer comes and sits anywhere she wants and order whatever she wants. The second customer can sit with the first one (therefore, order the same food), or he can sit by himself and order something different, and so on.
- Note that tables with more customers are more attractive.

Posterior sampling

- Given a finite set of observations, we want to find the posterior distribution of model parameters.
- Using the Chinese restaurant process analogy, we assume that our objective is to cluster customers according to their taste of food.
- We start by randomly allocating customers to a set of tables.
- Them, one-by-one we let them move around and change their table if they want until they find a table that matches their taste.
- When this procedure converges, customers form few clusters.
- Neal (2000) discussed several MCMC algorithms for Ditichlet process mixtures.

Gibbs sampling for conjugate priors

- When conjugate priors are used, the conditional distribution of θ_i becomes

$$\theta_i | \theta_{-i}, x_i \quad \sim \quad \sum_{j \neq i} q_{ij} \delta(\theta_j) + r_i H_i$$

- Here, H_i is the posterior distribution of θ given the conjugate prior G_0 and the single observation x_i.

- Using the likelihood $F(x_i, \theta)$, we obtain q_{ij} and r_i as follows:

$$\begin{aligned} q_{ij} &= bF(x_i, \theta_j) \\ r_i &= b\gamma \int F(x_i, \theta) dG_0(\theta) \end{aligned}$$

such that $\sum_{j \neq i} q_{ij} + r_i = 1$ (we use this to find b).

Gibbs sampling for conjugate priors

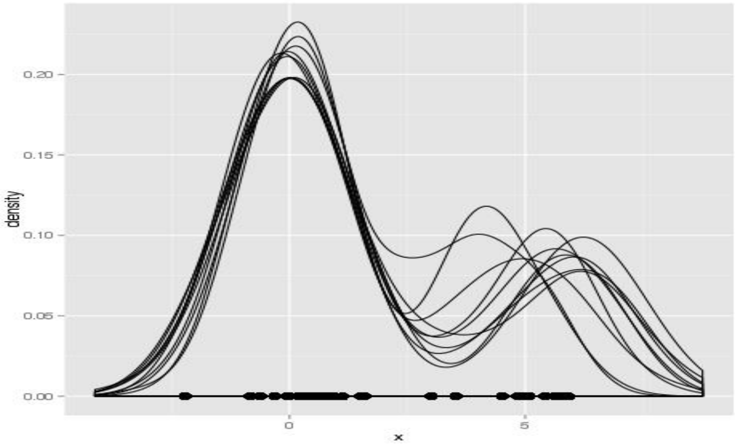
- Given the current state of the Markov chain, $c = \{c_1, \dots, c_n\}$ and $\phi = (\phi_c)$, a simple Gibbs sampling algorithm is as follows (Algorithm 2 in Neal, 2000):
  - For $i = 1, \dots, n$, find n_{-i,c_i}, i.e., the number of observations $j \neq i$ that are assigned to c_i
  - If $n_{-i,c_i} = 0$, remove ϕ_{c_i} from the state
  - Then sample a new value for c_i according to the following conditional probabilities:

$$
\begin{aligned}
P(c_i = c | c_{-i}, x_i, \phi) &= b \frac{n_{-i,c}}{n - 1 + \gamma} F(y_i, \phi_c) \\
P(c_i \neq c_j, \forall j \neq i | c_{-i}, x_i, \phi) &= b \frac{\gamma}{n - 1 + \gamma} \int F(x_i, \theta) dG_0(\theta)
\end{aligned}
$$

  - For all $c = \{c_1, \dots, c_n\}$, sample a new value from $\phi_c | x_i$ such that $c_i = c$

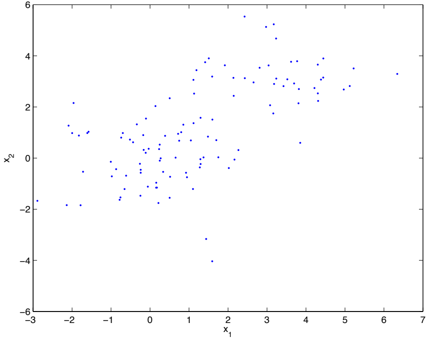
- The last step is called "remixing": after allocating the subjects into clusters with unique ϕ's, we perform draw a new value from $\phi_c | x_i$ given observations with $c_i = c$ only.

DPM of univariate Gaussians



10 Posterior samples using the Gibbs algorithm of Escobar and West (1995), which is Algorithm 1 in Neal (2000).

- In the following movie (click on the figure), data are sampled from two different bivariate normals (i.e., two clusters). A Dirichlet process mixture model (MCMC samples are shown) correctly identifies these two clusters: blue and red.



Non-conjugate priors

- Neal (2000) discusses several algorithms for non-conjugate priors. Here is Algorithm 8:
  - For $i = 1, \ldots, n$, find n_{-i,c_i}
  - If $n_{-i,c_i} \neq 0$ (i.e., i *is not* the only observation in its cluster), let k be the number of unique remaining ϕ's; sample m (e.g., $m = 5$) new ϕ's from G_0 as *auxiliary* components.
  - If $n_{-i,c_i} = 0$ (i.e., i *is* the only observation in its cluster), remove ϕ_{c_i} from the state; let k be the number of unique remaining ϕ's; sample $m - 1$ auxiliary components ϕ's from G_0, and set the m^{th} one to ϕ_{c_i}.
  - Then sample a new value for c_i according to the following conditional probabilities:

$$P(c_i = c | c_{-i}, x_i, \phi) = \begin{cases} b\frac{n_{-i,c}}{n-1+\gamma} F(x_i, \phi_c) & \text{for existing components} \\ b\frac{\gamma/m}{n-1+\gamma} F(x_i, \phi_c) & \text{for auxiliary components} \end{cases}$$

  - Only keep the components that are associated with at least one observation.
  - For all $c = \{c_1, \ldots, c_n\}$, sample a new value from $\phi_c | x_i$ such that $c_i = c$

Sampling the scale parameter

- For the scale parameter γ, we have (Antoniak, 1974)

$$P(k|\gamma) \propto \gamma^k \frac{\Gamma(\gamma)}{\Gamma(\gamma + n)}$$

  where k is the number of unique c_i (or ϕ's).

- Therefore, given k and the prior distribution $P(\gamma)$ we can sample from the posterior distribution of γ using the MH algorithm or the Gibbs sampling method of Escobar and West (1995).