S&DS 365 / 665

Intermediate Machine Learning

Approximate Inference: Gibbs Sampling for DP Mixtures

March 2

Yale

Reminders

- Assignment 2 due next Wednesday
- Quiz 2 available starting at 1pm today (CNN, GP, DP)
  - available for 48 hours
  - 30 minutes once started
- Midterm on March 16 in class
  - practice exam next week
  - review week of March 14

For Today

- Recap: Dirichlet process algos and definitions
- Dirichlet process mixtures
- Approximate inference with Gibbs sampling

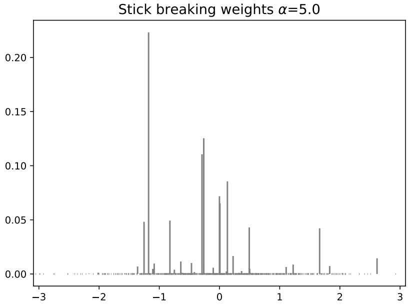
The Dirichlet Process

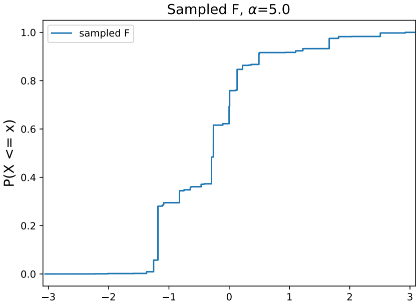
- The Dirichlet process is analogous to the Gaussian process
- Every partition of sample space has a Dirichlet distribution (more precise shortly)
- GPs are tools for regression functions; DPs are tools for distributions and densities

Dirichlet process

Each sample from a Dirichlet process prior has a *random collection of weights*, assigned to a *random selection of data*

Sample from DP prior





Stick breaking process

Stick breaking:

- At each step, break off a fraction $V \sim \text{Beta}(1, \alpha)$

"Imaginary data":

- At each step, sample $X \sim F_0$

Stick breaking process

To draw a single random distribution F from $DP(\alpha, F_0)$:

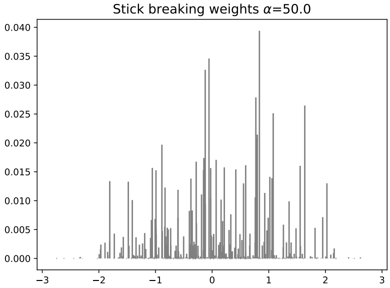
1. Draw $s_1, s_2, \ldots$ independently from F_0.
2. Draw $V_1, V_2, \ldots \sim \text{Beta}(1, \alpha)$ and set $w_j = V_j \prod_{i=1}^{j-1}(1 - V_i)$
3. Let F be the discrete distribution that puts mass w_j at s_j

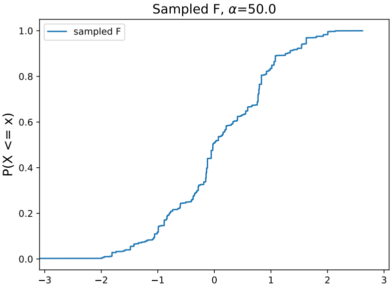
Stick breaking process

The mean of Beta$(1, \alpha)$ is $\frac{1}{1+\alpha}$.

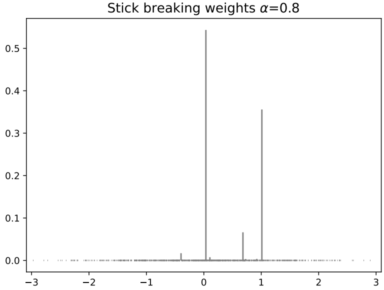
- As α gets larger, the weights get smaller
- Weights always sum to one

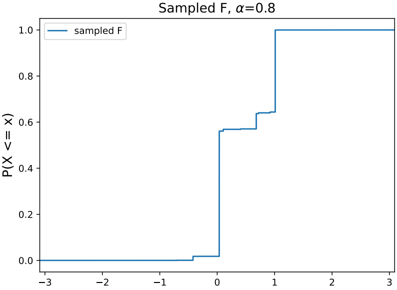
Different α





Different α





Clustering/repeats

Suppose we draw data F from a Dirichlet process, and then sample data from F:

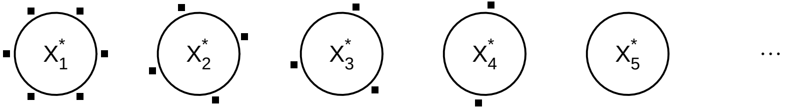
$$F \sim DP(\alpha, F_0)$$

$$X_1, X_2, \ldots, X_n \mid F \sim F$$

Since F is a mixture model (of point masses), the samples X_i are clustered according to which mixture component they are sampled from.

The "Chinese restaurant process" captures this

Chinese restaurant mnemonic



A customer (data point) comes into the restaurant and either

1. sits at an empty table, with probability proportional to α, or
2. sits at an occupied table with probability proportional to number of customers already seated at that table

Chinese restaurant process

1. Draw $X_1 \sim F_0$.
2. Given $X_1, X_2, \ldots, X_n$, sample next point as

$$X_{n+1} \mid X_1, \ldots X_n = \begin{cases} X \sim F_n & \text{with probability } \frac{n}{n+\alpha} \\ \\ X \sim F_0 & \text{with probability } \frac{\alpha}{n+\alpha} \end{cases}$$

   where F_n is the empirical distribution of $X_1, \ldots, X_n$

This allows us to sample from the marginal distribution over X, without explicitly drawing a distribution F from the DP

Chinese restaurant process

Let $X_1^*, X_2^*, \ldots$ denote unique values of $X_1, \ldots, X_n$

Define cluster assignment variables $c_1, \ldots, c_n$ where $c_i = j$ means that X_i takes the value X_j^*

Let $n_j = |\{i : \; c_j = j\}|$. Then

$$X_{n+1} = \begin{cases} X_j^* & \text{with probability } \frac{n_j}{n+\alpha} \\ X \sim F_0 & \text{with probability } \frac{\alpha}{n+\alpha} \end{cases}$$

This allows us to sample from the marginal distribution over X, without explicitly drawing a distribution F from the DP

The posterior distribution

Let $X_1, \ldots, X_n \sim F$ and let F have prior $\pi = DP(\alpha, F_0)$

Then the posterior π for F given $X_1, \ldots, X_n$ is

$$DP\left(\alpha + n, \overline{F}_n\right)$$

where

$$\overline{F}_n = \frac{n}{n+\alpha} F_n + \frac{\alpha}{n+\alpha} F_0.$$

Here F_n is the empirical distribution of $X_1, \ldots, X_n$

This says that the Dirichlet process is conjugate to sampling from the distribution—the posterior is another DP

From DP to DPM

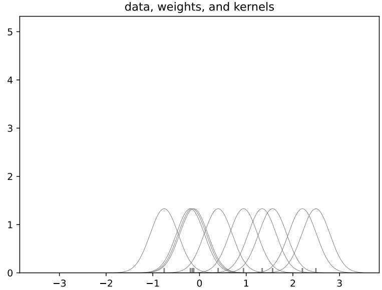
- A DP is a distribution over distributions
- A Dirichlet process mixture is a distribution over mixture models
- DPMs are Bayesian versions of kernel density estimation
- Subject to the curse of dimensionality!
- In stick breaking we replace X_i by θ_i
- In Chinese restaurant process we replace X_i^* by θ_i^*

Recall: KDE

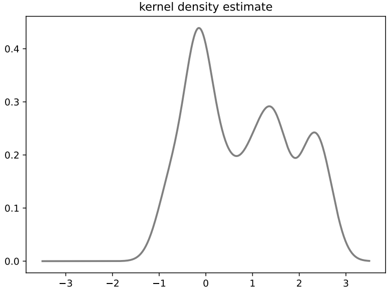
The *kernel density estimate* is the mixture model that places weight $\frac{1}{n}$ on the kernel bump function centered on each data point:

$$\widehat{f}(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right)$$

Recall: KDE

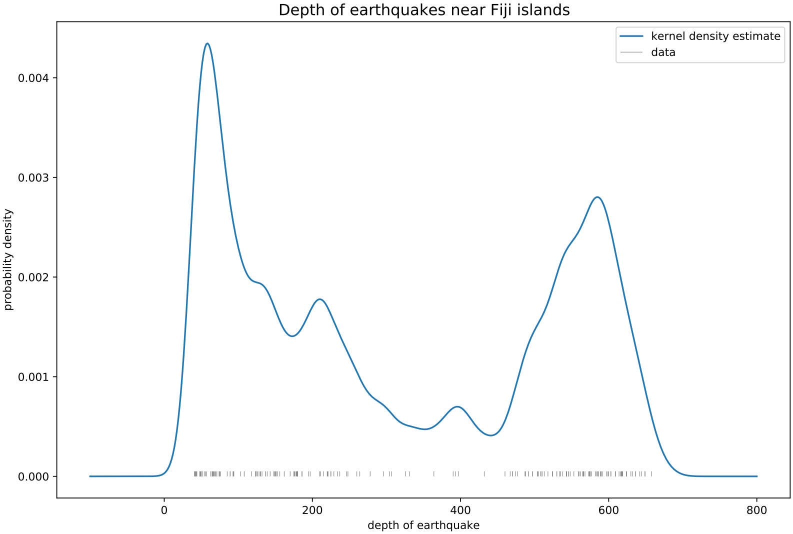


data, weights, and kernels
5
4
3
2
1
0
−3
−2
−1
0
1
2
3



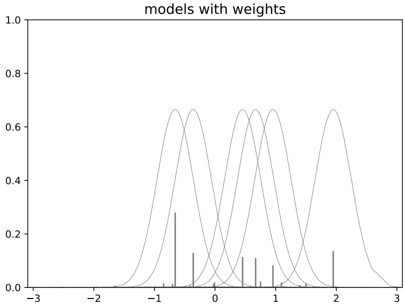
kernel density estimate
0.4
0.3
0.2
0.1
0.0
−3
−2
−1
0
1
2
3

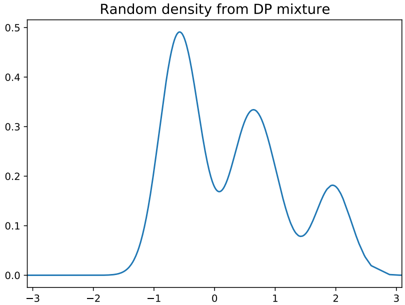
Recall: KDE



Depth of earthquakes near Fiji islands
kernel density estimate
data
probability density
0.004
0.003
0.002
0.001
0.000
0
200
400
600
800
depth of earthquake

Sample from DP mixture





Nonparametric Bayesian mixture model

$$\begin{aligned} F &\sim DP(\alpha, F_0) \\ \theta_1, \ldots, \theta_n \,|\, F &\sim F \\ X_i \,|\, \theta_i &\sim f(x \,|\, \theta_i), \quad i = 1, \ldots, n. \end{aligned}$$

Stick breaking process for DPM

Stick breaking:

- At each step, break off a fraction $V \sim \text{Beta}(1, \alpha)$

Sample model parameters:

- At each step, sample $\theta \sim F_0$

Stick breaking process for DPM

To draw a single random mixture from $DPM(\alpha, F_0)$:

1. Draw $\theta_1, \theta_2, \ldots$ independently from F_0.
2. Draw $V_1, V_2, \ldots \sim \text{Beta}(1, \alpha)$ and set $w_j = V_j \prod_{i=1}^{j-1}(1 - V_i)$
3. Let f be the (infinite) mixture model

$$f(x) = \sum_{j=1}^{\infty} w_j f(x \mid \theta_j)$$

Chinese restaurant process for a DPM

1. Draw $\theta_1 \sim F_0$.
2. Given $\theta_1, \theta_2, \ldots, \theta_n$ sample new model as

$$\theta_{n+1} \,|\, \theta_1, \ldots \theta_{n-1} = \begin{cases} \theta \sim F_n & \text{with probability } \frac{n}{n+\alpha} \\ \\ \theta \sim F_0 & \text{with probability } \frac{\alpha}{n+\alpha} \end{cases}$$

where F_n is the empirical distribution of $\theta_1, \ldots \theta_n$

Chinese restaurant process for a DPM

Let $\theta_1^*, \theta_2^*, \ldots$ denote unique values of $\theta_1, \ldots, \theta_n$

Define cluster assignment variables $c_1, \ldots, c_n$ where $c_i = j$ means that θ_i takes the value θ_j^*

Let $n_j = |\{i : \; c_j = j\}|$. Then

$$\theta_{n+1} = \begin{cases} \theta_j^* & \text{with probability } \frac{n_j}{n+\alpha} \\ \\ \theta \sim F_0 & \text{with probability } \frac{\alpha}{n+\alpha} \end{cases}$$

The posterior for a DPM

- The posterior distribution does not have a closed form — need to approximate it algorithmically
- Two forms of approximations: Gibbs sampling and variational methods — next topic

Gibbs sampling

We'll use the CRP to approximate the DPM posterior

Let's go to the chalk board!

Summary

- A Dirichlet process mixture is a Bayesian version of kernel density estimation
- The posterior distribution cannot be computed explicitly—must be approximated
- Gibbs sampling approximates posterior by iteratively re-clustering the data
- Bayesian nonparametric methods require a lot of conceptual machinery and computation