

Machine Learning: Jordan Boyd-Graber University of Maryland

Clustering as Probabilistic Inference

- GMM is a probabilistic model (unlike *K*-means)
- There are several latent variables:
 - Means
 - Assignments
 - (Variances)

Clustering as Probabilistic Inference

- GMM is a probabilistic model (unlike K-means)
- There are several latent variables:
 - Means
 - Assignments
 - (Variances)
- Before, we were doing EM

Clustering as Probabilistic Inference

- GMM is a probabilistic model (unlike K-means)
- There are several latent variables:
 - Means
 - Assignments
 - (Variances)
- Before, we were doing EM
- Today, new models and new methods

Nonparametric Clustering

- What if the number of clusters is not fixed?
- Nonparametric: can grow if data need it
- Probabilistic distribution over number of clusters

- Distribution over distributions
- Parameterized by: α, G

- Distribution over distributions
- Parameterized by: α , G
- Concentration parameter

- Distribution over distributions
- Parameterized by: α, G
- Concentration parameter
- Base distribution

- Distribution over distributions
- Parameterized by: α, G
- Concentration parameter
- Base distribution
- You can then draw observations from $x \sim DP(\alpha, G)$.

Defining a DP

Break off sticks

$$V_1, V_2, \ldots \sim_{ ext{iid}} \operatorname{Beta}(1, lpha) \qquad ext{ and } \qquad C_k := V_k \prod_{j=1}^{k-1} (1 - V_k)$$

Defining a DP

Break off sticks

$$V_1, V_2, \ldots \sim_{ ext{iid}} \operatorname{Beta}(1, lpha) \qquad ext{ and } \qquad C_k := V_k \prod_{j=1}^{k-1} (1 - V_k)$$

Draw atoms

$$\Phi_1, \Phi_2, \ldots \sim_{\mathrm{iid}} G$$

Defining a DP

Break off sticks

$$V_1, V_2, \ldots \sim_{ ext{iid}} \operatorname{Beta}(1, lpha) \qquad ext{ and } \qquad C_k := V_k \prod_{j=1}^{k-1} (1 - V_k)$$

Draw atoms

$$\Phi_1, \Phi_2, \ldots \sim_{\text{iid}} G$$

Merge into complete distribution

$$\Theta = \sum_{k \in \mathbb{N}} C_k \delta_{\Phi_k}$$

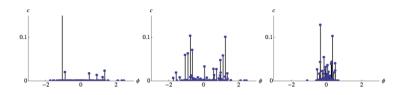
Properties of a DPMM

Expected value is the same as base distribution

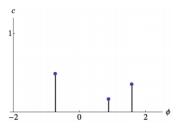
$$\mathbb{E}_{\mathsf{DP}(\alpha,G)}[x] = \mathbb{E}_G[x] \tag{1}$$

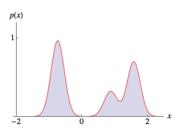
- As $\alpha \to \infty$, $DP(\alpha, G) = G$
- Number of components unbounded
- Impossible to represent fully on computer (truncation)
- You can nest DPs

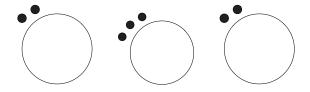
Effect of scaling parameter α

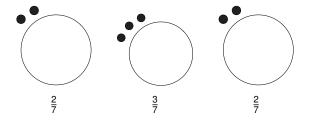


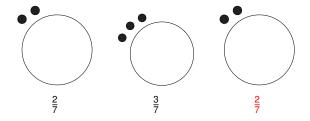
DP as mixture Model

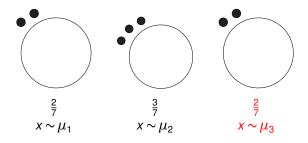




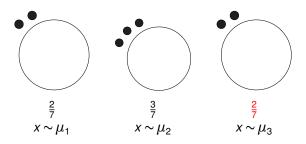








To generate an observation, you first sit down at a table. You sit down at a table proportional to the number of people sitting at the table.



But this is just Maximum Likelihood

Why are we talking about Chinese Restaurants?

Always can squeeze in one more table ...

- The posterior of a DP is CRP
- A new observation has a new table / cluster with probability proportional to α
- But this must be balanced against the probability of an observation given a cluster

$$\Theta = \sum_{k \in \mathbb{N}} C_k \delta_{\Phi_k}$$

- We want to know the cluster assignment of each observation
- Take a random guess initially

- We want to know the cluster assignment of each observation
- Take a random guess initially
- This provides a mean for each cluster

- We want to know the cluster assignment of each observation
- Take a random guess initially
- This provides a mean for each cluster
- Let the number of clusters grow

- We want to know the cluster assignment of each observation (tables)
- Take a random guess initially
- This provides a mean for each cluster
- Let the number of clusters grow

- We want to know Z
- Compute $p(z_i | z_1 ... z_{i-1}, z_{i+1}, ... z_m, x, \alpha, G)$
- Update z_i by sampling from that distribution
- Keep going . . .

- We want to know →
- Compute $p(z_i | z_1 ... z_{i-1}, z_{i+1}, ... z_m, x, \alpha, G)$
- Update z_i by sampling from that distribution
- Keep going . . .

Notation

$$p(z_i = k | z_{-i}) \equiv p(z_i | z_1 \dots z_{i-1}, z_{i+1}, \dots z_m)$$
 (2)

$$\rho(z_i = k \mid \vec{z}_{-i}, \vec{x}, \{\theta_k\}, \alpha)$$
 (3)

(4)

$$p(z_i = k \mid \vec{z}_{-i}, \vec{x}, \{\theta_k\}, \alpha)$$
(3)

$$=p(z_i=k\,|\,\vec{z}_{-i},x_i,\vec{x},\theta_k,\alpha) \tag{4}$$

(5)

Dropping irrelevant terms

$$p(z_i = k \mid \vec{z}_{-i}, \vec{x}, \{\theta_k\}, \alpha) \tag{3}$$

$$= p(z_i = k \mid \vec{z}_{-i}, x_i, \vec{x}, \theta_k, \alpha)$$
 (4)

$$= p(z_i = k \mid \vec{z}_{-i}, \alpha) p(x_i \mid \theta_k, \vec{x})$$
 (5)

(6)

Chain rule

$$p(z_i = k \mid \vec{z}_{-i}, \vec{x}, \{\theta_k\}, \alpha)$$
(3)

$$= p(z_i = k \mid \vec{z}_{-i}, x_i, \vec{x}, \theta_k, \alpha) \tag{4}$$

$$= p(z_i = k \mid \vec{z}_{-i}, \alpha) p(x_i \mid \theta_k, \vec{x})$$
 (5)

$$= \begin{cases} \left(\frac{n_k}{n.+\alpha}\right) \int_{\theta} p(x_i \mid \theta) p(\theta \mid G, \vec{x}) & \text{existing} \\ \frac{\alpha}{n.+\alpha} \int_{\theta} p(x_i \mid \theta) p(\theta \mid G) & \text{new} \end{cases}$$
 (6)

(7)

Applying CRP

$$p(z_i = k \mid \vec{z}_{-i}, \vec{x}, \{\theta_k\}, \alpha)$$
(3)

$$= p(z_i = k \mid \vec{z}_{-i}, x_i, \vec{x}, \theta_k, \alpha) \tag{4}$$

$$= p(z_i = k \mid \vec{z}_{-i}, \alpha) p(x_i \mid \theta_k, \vec{x})$$
 (5)

$$= \begin{cases} \left(\frac{n_k}{n + \alpha}\right) \int_{\theta} p(x_i | \theta) p(\theta | G, \vec{x}) & \text{existing} \\ \frac{\alpha}{n + \alpha} \int_{\theta} p(x_i | \theta) p(\theta | G) & \text{new} \end{cases}$$
 (6)

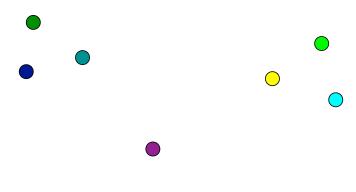
$$= \begin{cases} \left(\frac{n_k}{n.+\alpha}\right) \mathcal{N}\left(x, \frac{n\bar{x}}{n+1}, 1\right) & \text{existing} \\ \frac{\alpha}{n.+\alpha} \mathcal{N}\left(x, 0, 1\right) & \text{new} \end{cases}$$
 (7)

Scary integrals assuming G is normal distribution with mean zero and unit variance. (Derived in optional reading.)

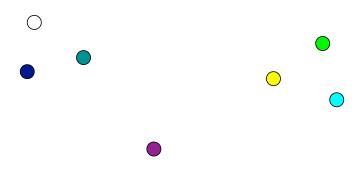
Algorithm for Gibbs Sampling

- Random initial assignment to clusters
- 2. For iteration *i*:
 - 2.1 "Unassign" observation n
 - 2.2 Choose new cluster for that observation

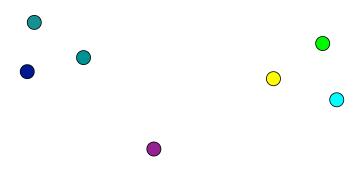
Toy Example

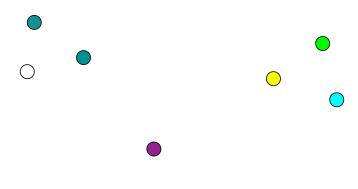


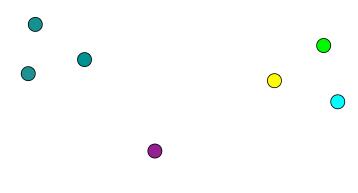
Toy Example

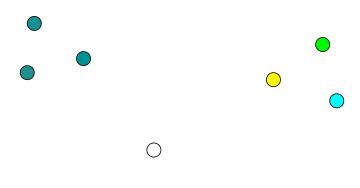


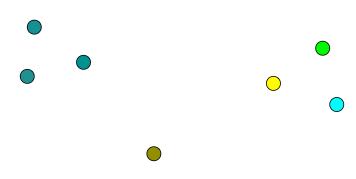
Toy Example



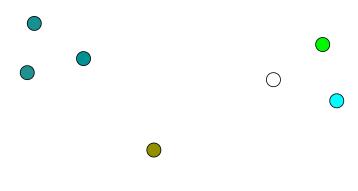


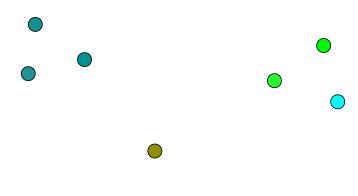


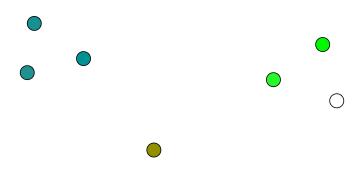


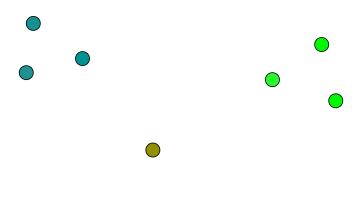


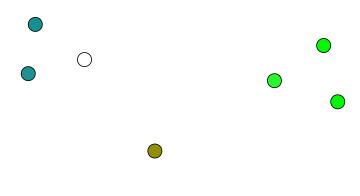
New cluster created!

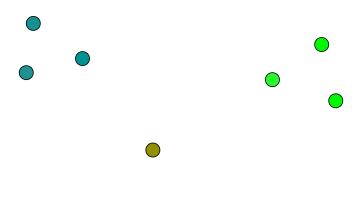


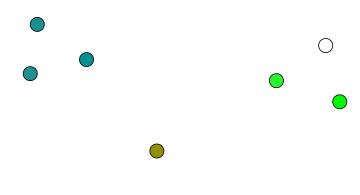


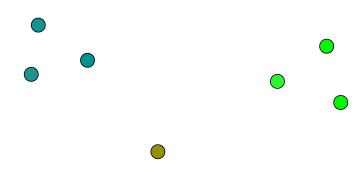












And repeat ...

Differences between EM and Gibbs

- Gibbs often faster to implement
- EM easier to diagnose convergence
- EM can be parallelized
- Gibbs is more widely applicable

In class and next week

- Walking through DPMM clustering
- Clustering discrete data with more than one cluster per observation