Bayesian Mixture Models and Expectation Maximization

STATS 305C: Applied Statistics

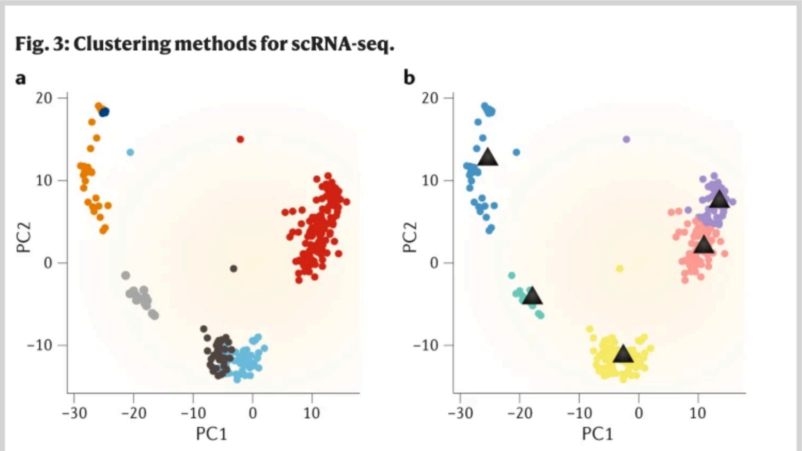
Scott Linderman

April 20, 2022

Outline

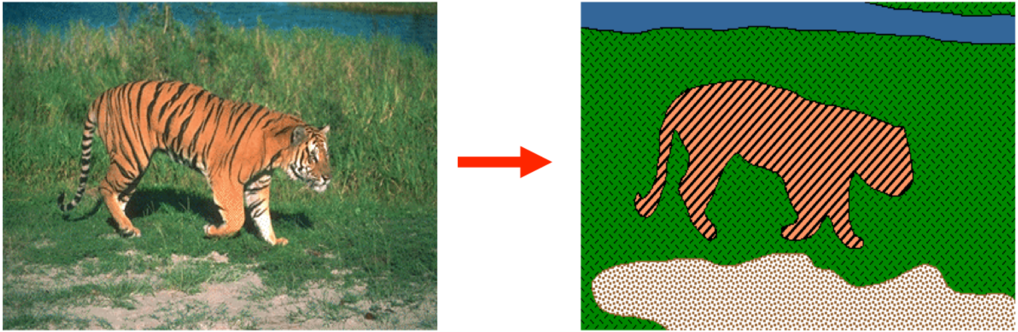
- Model: Bayesian mixture models
- Algorithm: MAP Estimation / K-Means

Motivation: Clustering scRNA-seq data



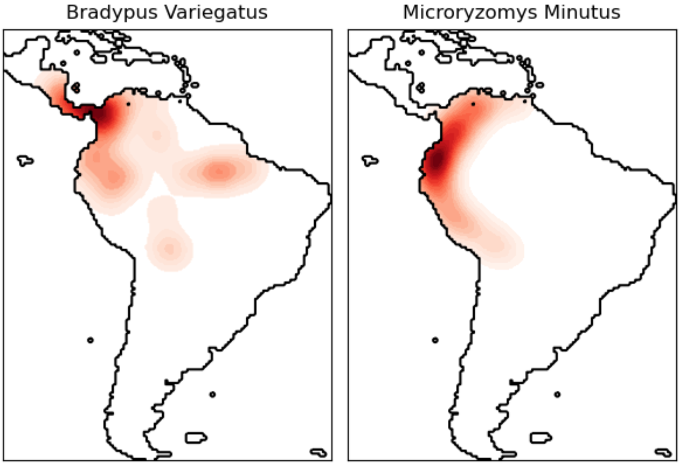
From Kiselev et al. [2019]

Motivation: Foreground/background segmentation



https://ai.stanford.edu/~syyeung/cvweb/tutorial3.html

Motivation: Density estimation



https://scikit-learn.org/stable/auto_examples/neighbors/plot_species_kde.html

Notation

Constants: Let

- N denote the number of data points.
- K denote the number of mixture components (i.e. clusters)

Data: Let

- $\boldsymbol{x}_n \in \mathbb{R}^D$ denote the n-th data point.

Latent Variables: Let

- $z_n \in \{1, \ldots, K\}$ denote the *assignment* of the n-th data point.

Notation II

Parameters: Let

- $\boldsymbol{\theta}_k$ denote the *natural parameters* of component k
- $\boldsymbol{\pi} \in \Delta_{K-1}$ denote the component *proportions* (i.e. probabilities).

Hyperparameters: Let

- $\boldsymbol{\phi}, \nu$ denote hyperparameters of the prior on $\boldsymbol{\theta}$
- $\boldsymbol{\alpha} \in \mathbb{R}_+^K$ denote the concentration of the prior on proportions.

Generative Model

1. Sample the proportions from a Dirichlet prior:

$$\pi \sim \mathrm{Dir}(\boldsymbol{\alpha}) \tag{1}$$

The beta distribution

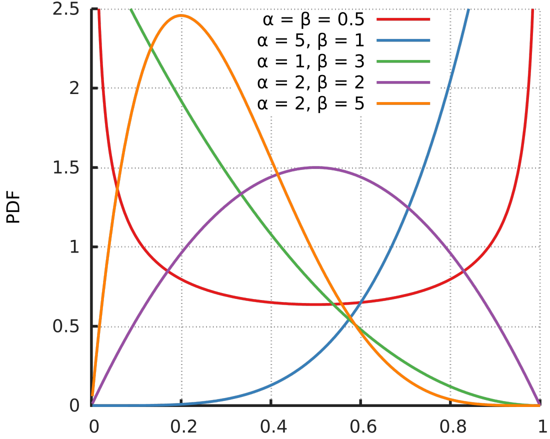


Figure: The beta distribution over $\pi \in [0, 1]$ is a special case of the Dirichlet distribution.
`https://en.wikipedia.org/wiki/Beta_distribution`

The Dirichlet distribution

If the beta distribution generates weighted coins, the Dirichlet generates weighted dice.

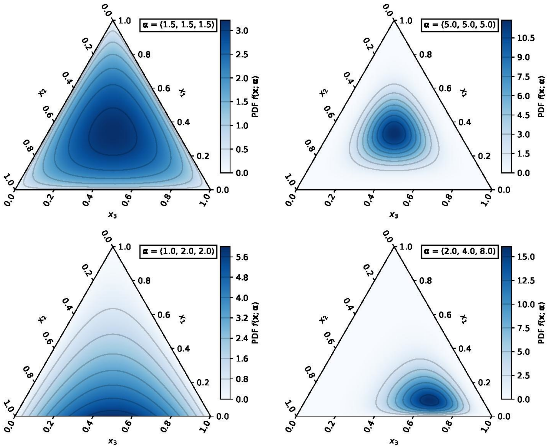


Figure: The Dirichlet distribution over $\pi \in \Delta_2$; i.e. distributions over $K = 3$ outcomes. From `https://en.wikipedia.org/wiki/Dirichlet_distribution`

Generative Model

1. Sample the proportions from a Dirichlet prior:

$$\boldsymbol{\pi} \sim \mathrm{Dir}(\boldsymbol{\alpha}) \tag{2}$$

2. Sample the parameters for each component:

$$\boldsymbol{\theta}_k \overset{\text{iid}}{\sim} p(\boldsymbol{\theta} \mid \boldsymbol{\phi}, \nu) \qquad \text{for } k = 1, \ldots, K \tag{3}$$

3. Sample the assignment of each data point:

$$z_n \overset{\text{iid}}{\sim} \boldsymbol{\pi} \qquad \text{for } n = 1, \ldots, N \tag{4}$$

4. Sample data points given their assignments:

$$\boldsymbol{x}_n \sim p(\boldsymbol{x} \mid \boldsymbol{\theta}_{z_n}) \qquad \text{for } n = 1, \ldots, N \tag{5}$$

Joint distribution

- This generative model corresponds to the following factorization of the joint distribution,

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = p(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N p(z_n \mid \pi)\, p(\boldsymbol{x}_n \mid \boldsymbol{z}_n, \{\boldsymbol{\theta}_k\}_{k=1}^K) \tag{6}$$

- Equivalently,

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = p(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N \prod_{k=1}^K \left[\Pr(z_n = k \mid \pi)\, p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k)\right]^{\mathbb{I}[z_n = k]} \tag{7}$$

- Substituting in the assumed forms

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = \mathrm{Dir}(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N \prod_{k=1}^K \left[\pi_k\, p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k)\right]^{\mathbb{I}[z_n = k]} \tag{8}$$

Joint distribution

- This generative model corresponds to the following factorization of the joint distribution,

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = p(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N p(z_n \mid \pi)\, p(\boldsymbol{x}_n \mid \boldsymbol{z}_n, \{\boldsymbol{\theta}_k\}_{k=1}^K) \tag{6}$$

- Equivalently,

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = p(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N \prod_{k=1}^K \left[\Pr(z_n = k \mid \pi)\, p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k)\right]^{\mathbb{I}[z_n = k]} \tag{7}$$

- Substituting in the assumed forms

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = \mathrm{Dir}(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N \prod_{k=1}^K \left[\pi_k\, p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k)\right]^{\mathbb{I}[z_n = k]} \tag{8}$$

Joint distribution

- This generative model corresponds to the following factorization of the joint distribution,

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = p(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N p(z_n \mid \pi)\, p(\boldsymbol{x}_n \mid \boldsymbol{z}_n, \{\boldsymbol{\theta}_k\}_{k=1}^K) \tag{6}$$

- Equivalently,

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = \\ p(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N \prod_{k=1}^K \left[\Pr(z_n = k \mid \pi)\, p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k)\right]^{\mathbb{I}[z_n=k]} \tag{7}$$

- Substituting in the assumed forms

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) = \mathrm{Dir}(\pi \mid \boldsymbol{\alpha}) \prod_{k=1}^K p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \prod_{n=1}^N \prod_{k=1}^K \left[\pi_k\, p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k)\right]^{\mathbb{I}[z_n=k]} \tag{8}$$

Exponential family mixture models

What about $p(\boldsymbol{x} \mid \boldsymbol{\theta}_k)$ and $p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu)$?

Let's assume an **exponential family** likelihood,

$$p(\boldsymbol{x} \mid \boldsymbol{\theta}_k) = h(\boldsymbol{x}_n) \exp\left\{\langle t(\boldsymbol{x}_n), \boldsymbol{\theta}_k\rangle - A(\boldsymbol{\theta}_k)\right\}. \tag{9}$$

Then assume a **conjugate prior**,

$$p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) \propto \exp\left\{\langle \boldsymbol{\phi}, \boldsymbol{\theta}_k\rangle - \nu A(\boldsymbol{\theta}_k)\right\}. \tag{10}$$

The hyperparmeters $\boldsymbol{\phi}$ are **pseudo-observations** of the sufficient statistics (like statistics from fake data points) and ν is a **pseudo-count** (like the number of fake data points).

Note that the product of prior and likelihood remains in the same family as the prior. That's why we call it conjugate.

Example: Gaussian mixture model

Assume the conditional distribution of $\boldsymbol{x}_n$ is a Gaussian with mean $\boldsymbol{\theta}_k \in \mathbb{R}^D$ and identity covariance,

$$
\begin{aligned}
p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k) &= \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k, \boldsymbol{I}) && (11)\\
&= (2\pi)^{-D/2} \exp\left\{-\tfrac{1}{2}(\boldsymbol{x}_n - \boldsymbol{\theta}_k)^\top (\boldsymbol{x}_n - \boldsymbol{\theta}_k)\right\} && (12)\\
&= (2\pi)^{-D/2} \exp\left\{-\tfrac{1}{2}\boldsymbol{x}_n^\top \boldsymbol{x}_n + \boldsymbol{x}_n^\top \boldsymbol{\theta}_k - \tfrac{1}{2}\boldsymbol{\theta}_k^\top \boldsymbol{\theta}_k\right\}, && (13)
\end{aligned}
$$

which is an exponential family distribution with base measure $h(\boldsymbol{x}_n) = (2\pi)^{-D/2} e^{-\frac{1}{2}\boldsymbol{x}_n^\top \boldsymbol{x}_n}$, sufficient statistics $t(\boldsymbol{x}_n) = \boldsymbol{x}_n$, and log normalizer $A(\boldsymbol{\theta}_k) = \frac{1}{2}\boldsymbol{\theta}_k^\top \boldsymbol{\theta}_k$.

The conjugate prior is a Gaussian prior on the mean,

$$
p(\boldsymbol{\theta}_k \mid \boldsymbol{\phi}, \nu) = \mathcal{N}(\nu^{-1}\boldsymbol{\phi}, \nu^{-1}\boldsymbol{I}) \propto \exp\left\{\boldsymbol{\phi}^\top \boldsymbol{\theta}_k - \tfrac{\nu}{2}\boldsymbol{\theta}_k^\top \boldsymbol{\theta}_k\right\} = \exp\left\{\boldsymbol{\phi}^\top \boldsymbol{\theta}_k - \nu A(\boldsymbol{\theta}_k)\right\}. \qquad (14)
$$

Note that $\boldsymbol{\phi}$ sets the location and ν sets the precision (i.e. inverse variance).

Outline

- Model: Bayesian mixture models
- **Algorithm: MAP Estimation / K-Means**

MAP inference via coordinate ascent

Let's first consider **maximum a posteriori (MAP) inference**.

Idea: find the mode of $p(\boldsymbol{\pi}, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{z_n\}_{n=1}^N \mid \{\boldsymbol{x}_n\}_{n=1}^N, \boldsymbol{\phi}, \nu, \boldsymbol{\alpha})$ by **coordinate ascent**.

For now, set $\boldsymbol{\phi} = \mathbf{0}$, and $\nu = 0$ so that the prior is an (improper) uniform distribution. Then maximizing the posterior is equivalent to maximizing the likelihood.

While we're simplifying, let's even fix $\boldsymbol{\pi} = \frac{1}{K}\mathbf{1}_K$.

Coordinate ascent in the Gaussian mixture model

For the Gaussian mixture model (with uniform prior and $\boldsymbol{\pi} = \frac{1}{K}\mathbf{1}_K$), coordinate ascent amounts to:

1. For each $n = 1, \ldots, N$, fix all variables but z_n and find $z_n^\star$ that maximizes

$$p(\boldsymbol{\pi}, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) \propto p(\boldsymbol{x}_n \mid z_n, \{\boldsymbol{\theta}_k\}_{k=1}^K) = \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\theta}_{z_n}, \boldsymbol{I}) \tag{15}$$

The cluster assignment that maximizes the likelihood is the one with the closest mean to $\boldsymbol{x}_n$, so set

$$z_n^\star = \underset{k \in \{1,\ldots,K\}}{\arg\min} \|\boldsymbol{x}_n - \boldsymbol{\theta}_k\|_2. \tag{16}$$

Coordinate ascent in the Gaussian mixture model II

2 For each $k = 1, \ldots, K$, fix all variables but $\boldsymbol{\theta}_k$ and find $\boldsymbol{\theta}_k^\star$ that maximizes,

$$p(\pi, \{\boldsymbol{\theta}_k\}_{k=1}^K, \{(z_n, \boldsymbol{x}_n)\}_{n=1}^N \mid \boldsymbol{\phi}, \nu, \boldsymbol{\alpha}) \propto \prod_{n=1}^N p(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k)^{\mathbb{I}[z_n=k]} \tag{17}$$

$$\propto \exp\left\{\sum_{n=1}^N \mathbb{I}[z_n = k]\left(\boldsymbol{x}_n^\top \boldsymbol{\theta}_k - \tfrac{1}{2}\boldsymbol{\theta}_k^\top \boldsymbol{\theta}_k\right)\right\} \tag{18}$$

Taking the derivative of the log and setting to zero yields,

$$\boldsymbol{\theta}_k^\star = \frac{1}{N_k}\sum_{n=1}^K \mathbb{I}[z_n = k]\boldsymbol{x}_n, \tag{19}$$

where $N_k = \sum_{n=1}^N \mathbb{I}[z_n = k]$.

This is the **k-means algorithm**!

EM in the Gaussian mixture model

K-Means made **hard assignments** of data points to clusters in each iteration. What if we used **soft assignments** instead?

Instead of assigning $z_n^\star$ to the closest cluster, we compute *responsibilities* for each cluster:

1. For each data point n and component k, set the *responsibility* to,

$$\omega_{nk} = \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\theta}_k, \boldsymbol{I})}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\theta}_j, \boldsymbol{I})}. \tag{20}$$

2. For each component k, set the new mean to

$$\boldsymbol{\theta}_k^\star = \frac{1}{N_k} \sum_{n=1}^{K} \omega_{nk} \boldsymbol{x}_n, \tag{21}$$

where $N_k = \sum_{n=1}^{N} \omega_{nk}$.

This is called the **expectation maximization (EM)** algorithm.

References I

Vladimir Yu Kiselev, Tallulah S Andrews, and Martin Hemberg. Challenges in unsupervised clustering of single-cell RNA-seq data. *Nat. Rev. Genet.*, 20(5):273–282, May 2019.