RWTH AACHEN UNIVERSITY

Advanced Machine Learning
Lecture 10

Mixture Models II

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Announcement

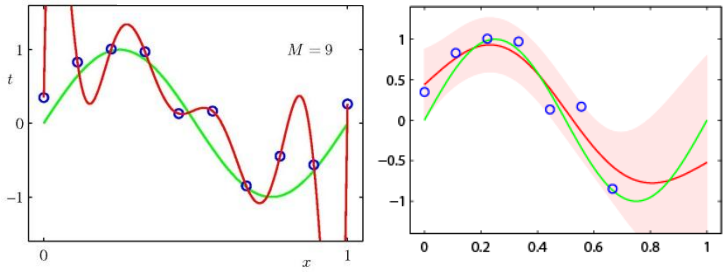
- Exercise sheet 2 online
  - Sampling
  - Rejection Sampling
  - Importance Sampling
  - Metropolis-Hastings
  - EM
  - Mixtures of Bernoulli distributions [today's topic]
  - Exercise will be on Monday, 03.12.

  ⇒ *Please submit your results until 02.12. midnight.*

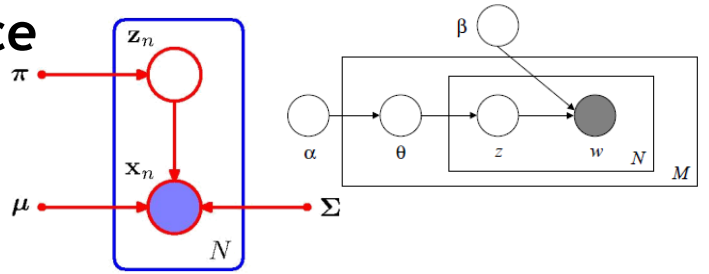
This Lecture: *Advanced Machine Learning*

- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

$$f : \mathcal{X} \rightarrow \mathbb{R}$$



- Bayesian Estimation & Bayesian Non-Parametrics
  - Prob. Distributions, Approx. Inference
  - Mixture Models & EM
  - Dirichlet Processes
  - Latent Factor Models
  - Beta Processes



- SVMs and Structured Output Learning
  - SV Regression, SVDD
  - Large-margin Learning

$$f : \mathcal{X} \rightarrow \mathcal{Y}$$

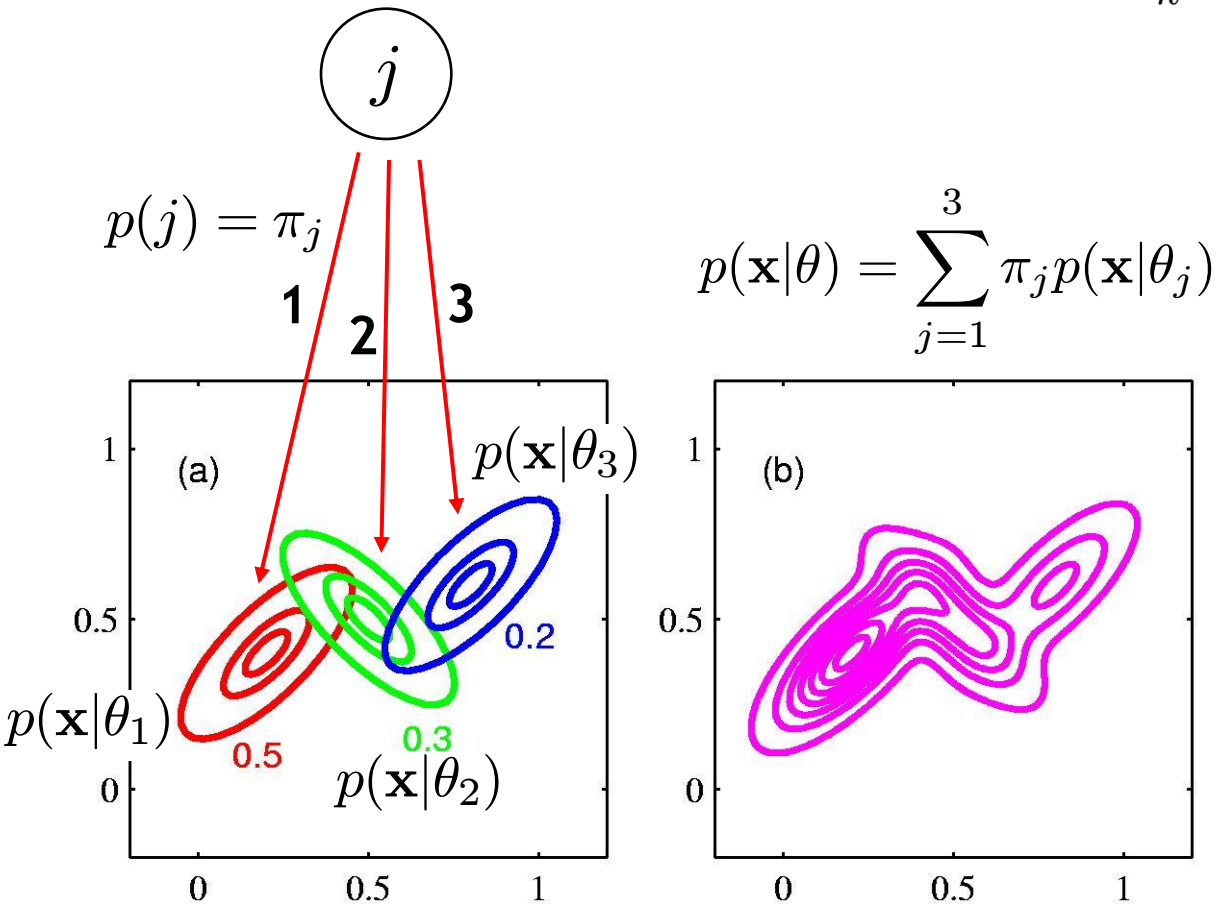
Topics of This Lecture

- The EM algorithm in general
  - Recap: General EM
  - Example: Mixtures of Bernoulli distributions
  - Monte Carlo EM
- Bayesian Mixture Models
  - Towards a full Bayesian treatment
  - Dirichlet priors
  - Finite mixtures
  - Infinite mixtures
  - Approximate inference
- Outlook: Dirichlet Processes

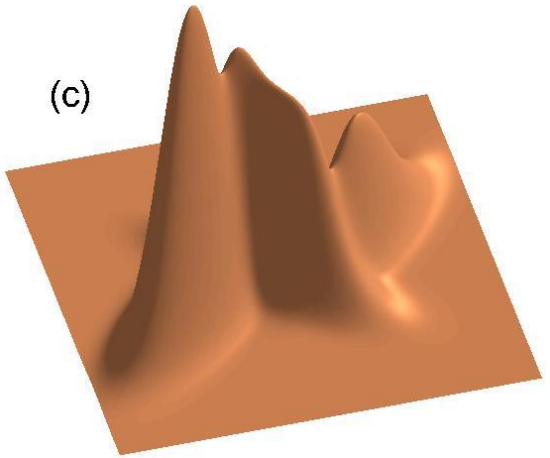
Recap: Mixture of Gaussians

- "Generative model"

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$



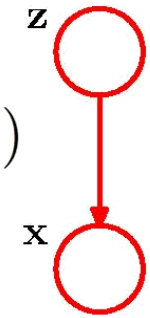
$$p(\mathbf{x}|\theta) = \sum_{j=1}^{3} \pi_j p(\mathbf{x}|\theta_j)$$



Recap: GMMs as Latent Variable Models

- Write GMMs in terms of latent variables $\mathbf{z}$
  - Marginal distribution of $\mathbf{x}$

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

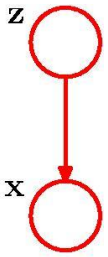


- Advantage of this formulation
  - We have represented the marginal distribution in terms of latent variables $\mathbf{z}$.
  - Since $p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z})$, there is a corresponding latent variable $\mathbf{z}_n$ for each data point $\mathbf{x}_n$.
  - We are now able to work with the joint distribution $p(\mathbf{x}, \mathbf{z})$ instead of the marginal distribution $p(\mathbf{x})$.

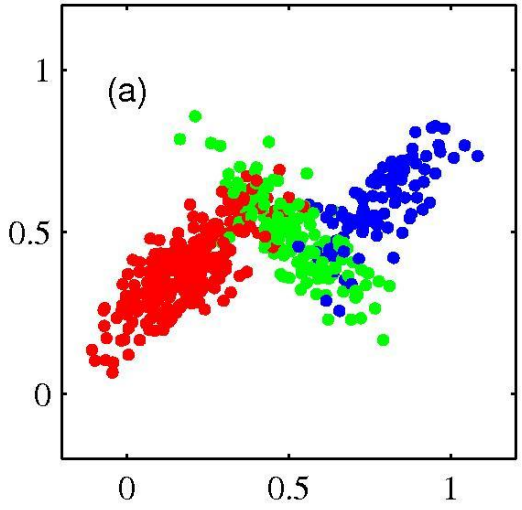
$\Rightarrow$ This will lead to significant simplifications…

Recap: Sampling from a Gaussian Mixture

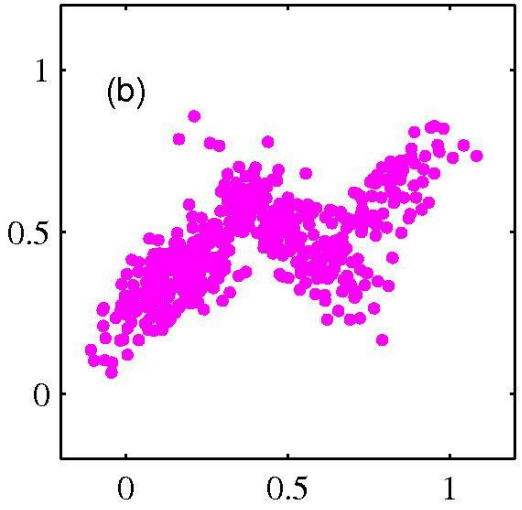
- MoG Sampling
  - We can use ancestral sampling to generate random samples from a Gaussian mixture model.
    1. Generate a value $\hat{\mathbf{z}}$ from the marginal distribution $p(\mathbf{z})$.
    2. Generate a value $\hat{\mathbf{x}}$ from the conditional distribution $p(\mathbf{x}|\hat{\mathbf{z}})$.



Samples from the joint $p(\mathbf{x}, \mathbf{z})$



Samples from the marginal $p(\mathbf{x})$



Evaluating the responsibilities $\gamma(z_{nk})$

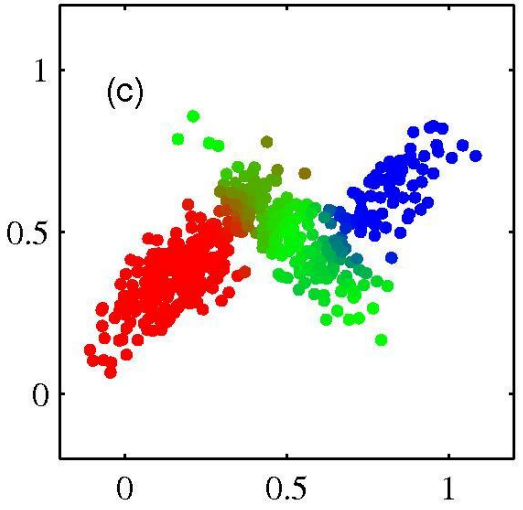
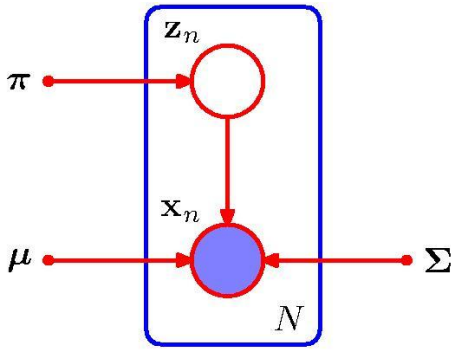


Image source: C.M. Bishop, 2006

Recap: Gaussian Mixtures Revisited

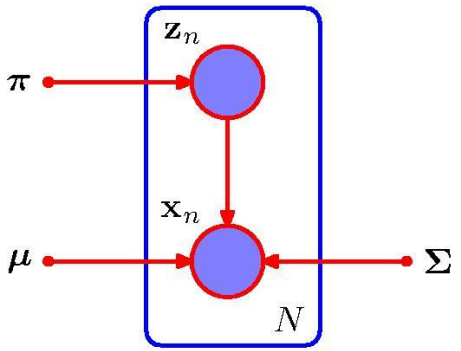
- Applying the latent variable view of EM
  - Goal is to maximize the log-likelihood using the observed data $\mathbf{X}$

$$\log p(\mathbf{X}|\boldsymbol{\theta}) = \log \left\{ \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) \right\}$$



  - Corresponding graphical model:

  - Suppose we are additionally given the values of the latent variables $\mathbf{Z}$.
  - The corresponding graphical model for the complete data now looks like this:



$\Rightarrow$ Straightforward to marginalize…

Image source: C.M. Bishop, 2006

Recap: Alternative View of EM

- In practice, however,…
  - We are not given the complete data set $\{\mathbf{X},\mathbf{Z}\}$, but only the incomplete data $\mathbf{X}$. All we can compute about $\mathbf{Z}$ is the posterior distribution $p(\mathbf{Z}|\mathbf{X},\boldsymbol{\theta})$.
  - Since we cannot use the complete-data log-likelihood, we consider instead its expected value under the posterior distribution of the latent variable:

$$\mathcal{Q}(\boldsymbol{\theta},\boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\boldsymbol{\theta}^{\text{old}}) \log p(\mathbf{X},\mathbf{Z}|\boldsymbol{\theta})$$

  - This corresponds to the E-step of the EM algorithm.
  - In the subsequent M-step, we then maximize the expectation to obtain the revised parameter set $\boldsymbol{\theta}^{\text{new}}$.

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta},\boldsymbol{\theta}^{\text{old}})$$

Recap: General EM Algorithm

- Algorithm
  1. Choose an initial setting for the parameters $\boldsymbol{\theta}^{\text{old}}$
  2. E-step: Evaluate $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$
  3. M-step: Evaluate $\boldsymbol{\theta}^{\text{new}}$ given by

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$$

     where

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$$

  4. While not converged, let $\boldsymbol{\theta}^{\text{old}} \leftarrow \boldsymbol{\theta}^{\text{new}}$ and return to step 2.

Recap: MAP-EM

- Modification for MAP
  - The EM algorithm can be adapted to find MAP solutions for models for which a prior $p(\boldsymbol{\theta})$ is defined over the parameters.
  - Only changes needed:

2. **E-step**: Evaluate $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$

3. **M-step**: Evaluate $\boldsymbol{\theta}^{\text{new}}$ given by

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) + \log p(\boldsymbol{\theta})$$

$\Rightarrow$ Suitable choices for the prior will remove the ML singularities!

Summary So Far

- We have now seen a generalized EM algorithm
  - Applicable to general estimation problems with latent variables
  - In particular, also applicable to mixtures of other base distributions
  - In order to get some familiarity with the general EM algorithm, let's apply it to a different class of distributions…

Topics of This Lecture

- **The EM algorithm in general**
  - Recap: General EM
  - Example: Mixtures of Bernoulli distributions
  - Monte Carlo EM
- Bayesian Mixture Models
  - Towards a full Bayesian treatment
  - Dirichlet priors
  - Finite mixtures
  - Infinite mixtures
  - Approximate inference
- Outlook: Dirichlet Processes

Mixtures of Bernoulli Distributions

- **Discrete binary variables**
  - Consider D binary variables $\mathbf{x} = (x_1,\ldots,x_D)^T$, each of them described by a Bernoulli distribution with parameter μ_i, so that

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{i=1}^{D} \mu_i^{x_i}(1-\mu_i)^{(1-x_i)}$$

  - Mean and covariance are given by

$$\begin{aligned} \mathbb{E}[\mathbf{x}] &= \boldsymbol{\mu} \\ \mathrm{cov}[\mathbf{x}] &= \mathrm{diag}\{\boldsymbol{\mu}(1-\boldsymbol{\mu})\} \end{aligned}$$

Diagonal covariance ⇒ variables independently modeled

Mixtures of Bernoulli Distributions

- Mixtures of discrete binary variables
  - Now, consider a finite mixture of those distributions

$$p(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\pi}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k)$$

$$= \sum_{k=1}^{K} \pi_k \prod_{i=1}^{D} \mu_{ki}^{x_i}(1-\mu_{ki})^{(1-x_i)}$$

  - Mean and covariance of the mixture are given by

$$\mathbb{E}[\mathbf{x}] = \sum_{k=1}^{K} \pi_k \boldsymbol{\mu}_k$$

$$\mathrm{cov}[\mathbf{x}] = \sum_{k=1}^{K} \pi_k \left\{\boldsymbol{\Sigma}_k + \boldsymbol{\mu}_k \boldsymbol{\mu}_k^T\right\} - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{x}]^T$$

where $\boldsymbol{\Sigma}_k = \mathrm{diag}\{\mu_{ki}(1 - \mu_{ki})\}$.

Covariance not diagonal
⇒ Model can capture dependencies between variables

Mixtures of Bernoulli Distributions

- **Log-likelihood for the model**
  - Given a data set $\mathbf{X} = \{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$,

$$\log p(\mathbf{X}|\boldsymbol{\mu},\boldsymbol{\pi}) = \sum_{n=1}^{N} \log \left\{ \sum_{k=1}^{K} \pi_k p(\mathbf{x}_n|\boldsymbol{\mu}_k) \right\}$$

  - Again observation: summation inside logarithm ⇒ difficult.
  - In the following, we will derive the EM algorithm for mixtures of Bernoulli distributions.
    - This will show how we can derive EM algorithms in the general case…

EM for Bernoulli Mixtures

- Latent variable formulation
  - Introduce latent variable $\mathbf{z} = (z_1,\ldots,z_K)^T$ with 1-of-K coding.
  - Conditional distribution of $\mathbf{x}$:

$$p(\mathbf{x}|\mathbf{z},\boldsymbol{\mu}) = \prod_{k=1}^{K} p(\mathbf{x}|\boldsymbol{\mu}_k)^{z_k}$$

  - Prior distribution for the latent variables

$$p(\mathbf{z}|\boldsymbol{\pi}) = \prod_{k=1}^{K} \pi_k^{z_k}$$

  - Again, we can verify that

$$p(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\pi}) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z},\boldsymbol{\mu})p(\mathbf{z}|\boldsymbol{\pi}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k)$$

Recap: General EM Algorithm

- Algorithm
  1. Choose an initial setting for the parameters $\boldsymbol{\theta}^{\text{old}}$
  2. **E-step**: Evaluate $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$
  3. **M-step**: Evaluate $\boldsymbol{\theta}^{\text{new}}$ given by

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$$

     where

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$$

  4. While not converged, let $\boldsymbol{\theta}^{\text{old}} \leftarrow \boldsymbol{\theta}^{\text{new}}$ and return to step 2.

EM for Bernoulli Mixtures: E-Step

- **Complete-data likelihood**

$$p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\pi}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \left[\pi_k p(\mathbf{x}_n|\boldsymbol{\mu}_k)\right]^{z_{nk}}$$

$$= \prod_{n=1}^{N} \prod_{k=1}^{K} \left\{ \pi_k \prod_{i=1}^{D} \mu_{ki}^{x_{ni}} (1-\mu_{ki})^{(1-x_{ni})} \right\}^{z_{nk}}$$

- **Posterior distribution of the latent variables $\mathbf{Z}$**

$$p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\pi}) = \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\pi})}{p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\pi})}$$

$$= \prod_{n=1}^{N} \prod_{k=1}^{K} \frac{\left[\pi_k p(\mathbf{x}_n|\boldsymbol{\mu}_k)\right]^{z_{nk}}}{\sum_{j=1}^{K} \pi_j p(\mathbf{x}_n|\boldsymbol{\mu}_j)}$$

EM for Bernoulli Mixtures: E-Step

- **E-Step**
  - **Evaluate the responsibilities**

$$\gamma(z_{nk}) = \mathbb{E}[z_{nk}] = \sum_{z_{nk}} z_{nk} \frac{[\pi_k p(\mathbf{x}_n|\boldsymbol{\mu}_k)]^{z_{nk}}}{\sum_{j=1}^{K} \pi_j p(\mathbf{x}_n|\boldsymbol{\mu}_j)}$$

$$= \frac{\pi_k p(\mathbf{x}_n|\boldsymbol{\mu}_k)}{\sum_{j=1}^{K} \pi_j p(\mathbf{x}_n|\boldsymbol{\mu}_j)}$$

  - **Note: we again get the same form as for Gaussian mixtures**

$$\gamma_j(\mathbf{x}_n) \leftarrow \frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_{k=1}^{N} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}$$

Recap: General EM Algorithm

- Algorithm
  1. Choose an initial setting for the parameters $\boldsymbol{\theta}^{\text{old}}$
  2. E-step: Evaluate $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$
  3. M-step: Evaluate $\boldsymbol{\theta}^{\text{new}}$ given by

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$$

where

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$$

  4. While not converged, let $\boldsymbol{\theta}^{\text{old}} \leftarrow \boldsymbol{\theta}^{\text{new}}$ and return to step 2.

EM for Bernoulli Mixtures: M-Step

- **Complete-data log-likelihood**

$$\log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\pi}) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} \left\{\log \pi_k + \sum_{i=1}^{D} [x_{ni} \log \mu_{ki} + (1 - x_{ni}) \log(1 - \mu_{ki})]\right\}$$

- **Expectation w.r.t. the posterior distribution of $\mathbf{Z}$**

$$\underbrace{\mathbb{E}_{\mathbf{Z}}[\log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\pi})]}_{\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})} = \sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(z_{nk}) \left\{\log \pi_k + \sum_{i=1}^{D} [x_{ni} \log \mu_{ki} + (1 - x_{ni}) \log(1 - \mu_{ki})]\right\}$$

where $\gamma(z_{nk}) = \mathbb{E}[z_{nk}]$ are again the responsibilities for each $\mathbf{x}_n$.

EM for Bernoulli Mixtures: M-Step

- **Remark**
  - The $\gamma(z_{nk})$ only occur in two forms in the expectation:

$$N_k = \sum_{n=1}^{N} \gamma(z_{nk})$$

$$\bar{\mathbf{x}}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

- **Interpretation**
  - N_k is the effective number of data points associated with component k.
  - $\bar{\mathbf{x}}_k$ is the responsibility-weighted mean of the data points softly assigned to component k.

EM for Bernoulli Mixtures: M-Step

- **M-Step**
  - Maximize the expected complete-data log-likelihood w.r.t the parameter $\boldsymbol{\mu}_k$.

$$\frac{\partial}{\partial \boldsymbol{\mu}_k}\mathbb{E}_{\mathbf{Z}}[p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\pi})]$$

$$= \frac{\partial}{\partial \boldsymbol{\mu}_k}\sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\left\{\log \pi_k + [\mathbf{x}_n \log \boldsymbol{\mu}_k + (1-\mathbf{x}_n)\log(1-\boldsymbol{\mu}_k)]\right\}$$

$$= \frac{1}{\boldsymbol{\mu}_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n - \frac{1}{1-\boldsymbol{\mu}_k}\sum_{n=1}^{N}\gamma(z_{nk})(1-\mathbf{x}_n) \stackrel{!}{=} 0$$

$$\vdots$$

$$\boldsymbol{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n = \bar{\mathbf{x}}_k$$

EM for Bernoulli Mixtures: M-Step

- M-Step
  - Maximize the expected complete-data log-likelihood w.r.t the parameter π_k under the constraint $\sum_k \pi_k = 1$.
  - Solution with Lagrange multiplier λ

$$\arg\max_{\pi_k} \mathbb{E}_{\mathbf{Z}}[p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\pi})] + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right)$$

$$\vdots$$

$$\pi_k = \frac{N_k}{N}$$

Discussion

- Comparison with Gaussian mixtures
  - In contrast to Gaussian mixtures, there are no singularities in which the likelihood goes to infinity.
  - This follows from the property of Bernoulli distributions that

$$0 \leq p(\mathbf{x}_n|\boldsymbol{\mu}_k) \leq 1$$

  - However, there are still problem cases when μ_{ki} becomes 0 or 1

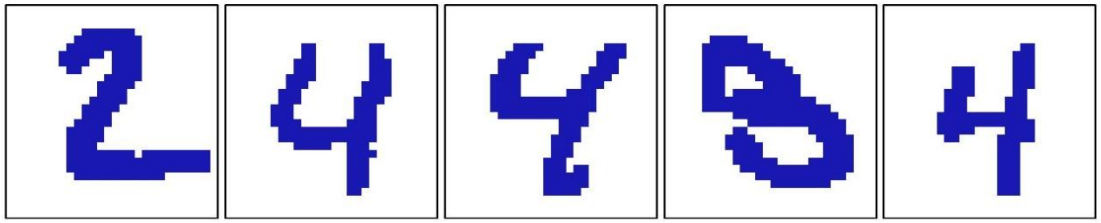
$$\mathbb{E}_{\mathbf{Z}}[\log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\pi})] = \ldots [x_{ni} \log \mu_{ki} + (1 - x_{ni}) \log(1 - \mu_{ki})]$$

  $\Rightarrow$ Need to enforce a range [MIN_VAL,1-MIN_VAL] for either μ_{ki} or γ.

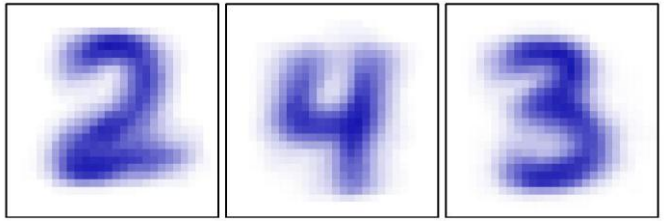
- General remarks
  - Bernoulli mixtures are used in practice in order to represent binary data.
  - The resulting model is also known as latent class analysis.

Example: Handwritten Digit Recognition

- Binarized digit data (examples from set of 600 digits)



- Means of a 3-component Bernoulli mixture (10 EM iter.)



- Comparison: ML result of single multivariate Bernoulli distribution

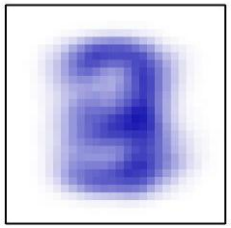


Image source: C.M. Bishop, 2006

Topics of This Lecture

- **The EM algorithm in general**
  - Recap: General EM
  - Example: Mixtures of Bernoulli distributions
  - Monte Carlo EM
- Bayesian Mixture Models
  - Towards a full Bayesian treatment
  - Dirichlet priors
  - Finite mixtures
  - Infinite mixtures
  - Approximate inference
- Outlook: Dirichlet Processes

Monte Carlo EM

- EM procedure
  - M-step: Maximize expectation of complete-data log-likelihood

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \int p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) \mathrm{d}\mathbf{Z}$$

  - For more complex models, we may not be able to compute this analytically anymore…
- Idea
  - Use sampling to approximate this integral by a finite sum over samples $\{\mathbf{Z}^{(l)}\}$ drawn from the current estimate of the posterior

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) \sim \frac{1}{L} \sum_{l=1}^{L} \log p(\mathbf{X}, \mathbf{Z}^{(l)}|\boldsymbol{\theta}^{\text{old}})$$

  - This procedure is called the Monte Carlo EM algorithm.

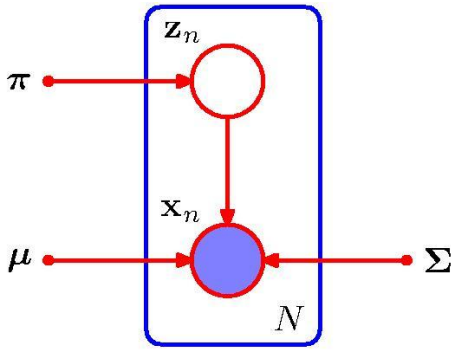
Topics of This Lecture

- The EM algorithm in general
  - Recap: General EM
  - Example: Mixtures of Bernoulli distributions
  - Monte Carlo EM
- **Bayesian Mixture Models**
  - **Towards a full Bayesian treatment**
  - **Dirichlet priors**
  - **Finite mixtures**
  - **Infinite mixtures**
  - **Approximate inference**
- Outlook: Dirichlet Processes

Towards a Full Bayesian Treatment…

- **Mixture models**
  - We have discussed mixture distributions with K components

$$p(\mathbf{X}|\boldsymbol{\theta}) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$$



  - So far, we have derived the ML estimates ⇒ EM
  - Introduced a prior $p(\theta)$ over parameters ⇒ MAP-EM

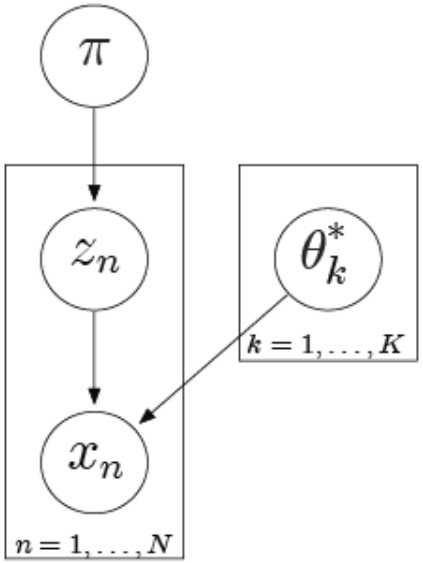
  - One question remains open: how to set K ?

⇒ Let's also set a prior on the number of components…

Bayesian Mixture Models

- Let's be Bayesian about mixture models
  - Place priors over our parameters
  - Again, introduce variable $\mathbf{z}_n$ as indicator which component data point $\mathbf{x}_n$ belongs to.

$$\begin{aligned} \mathbf{z}_n|\boldsymbol{\pi} &\sim \text{Multinomial}(\boldsymbol{\pi}) \\ \mathbf{x}_n|\mathbf{z}_n = k, \boldsymbol{\mu}, \boldsymbol{\Sigma} &\sim \mathcal{N}(\boldsymbol{\mu}_k, \Sigma_k) \end{aligned}$$



  - This is similar to the graphical model we've used before, but now the π and $\theta_k = (\mu_k, \Sigma_k)$ are also treated as random variables.
  - *What would be suitable priors for them?*

Bayesian Mixture Models

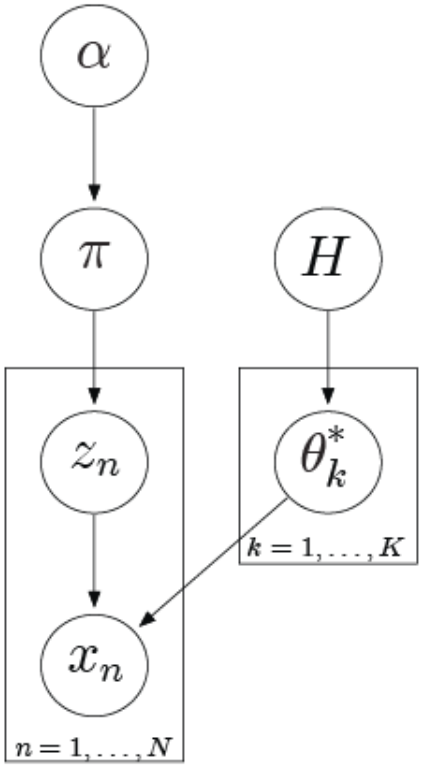
- Let's be Bayesian about mixture models
  - Place priors over our parameters
  - Again, introduce variable $\mathbf{z}_n$ as indicator which component data point $\mathbf{x}_n$ belongs to.

$$\begin{aligned} \mathbf{z}_n|\boldsymbol{\pi} &\sim \text{Multinomial}(\boldsymbol{\pi}) \\ \mathbf{x}_n|\mathbf{z}_n = k, \boldsymbol{\mu}, \boldsymbol{\Sigma} &\sim \mathcal{N}(\boldsymbol{\mu}_k, \Sigma_k) \end{aligned}$$

  - Introduce conjugate priors over parameters

$$\begin{aligned} \boldsymbol{\pi} &\sim \text{Dirichlet}(\frac{\alpha}{K}, \ldots, \frac{\alpha}{K}) \\ \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k &\sim H = \mathcal{N} - \mathcal{IW}(0, s, d, \phi) \end{aligned}$$

"Normal - Inverse Wishart"



Bayesian Mixture Models

- **Full Bayesian Treatment**
  - Given a dataset, we are interested in the cluster assignments

$$p(\mathbf{Z}|\mathbf{X}) = \frac{p(\mathbf{X}|\mathbf{Z})p(\mathbf{Z})}{\sum_{\mathbf{Z}} p(\mathbf{X}|\mathbf{Z})p(\mathbf{Z})}$$

  where the likelihood is obtained by marginalizing over the parameters θ

$$\begin{aligned} p(\mathbf{X}|\mathbf{Z}) &= \int p(\mathbf{X}|\mathbf{Z},\boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} \\ &= \int \prod_{n=1}^{N}\prod_{k=1}^{K} p(\mathbf{x}_n|z_{nk},\boldsymbol{\theta}_k)p(\boldsymbol{\theta}_k|H)\mathrm{d}\boldsymbol{\theta} \end{aligned}$$

- **The posterior over assignments is intractable!**
  - Denominator requires summing over all possible partitions of the data into K groups!

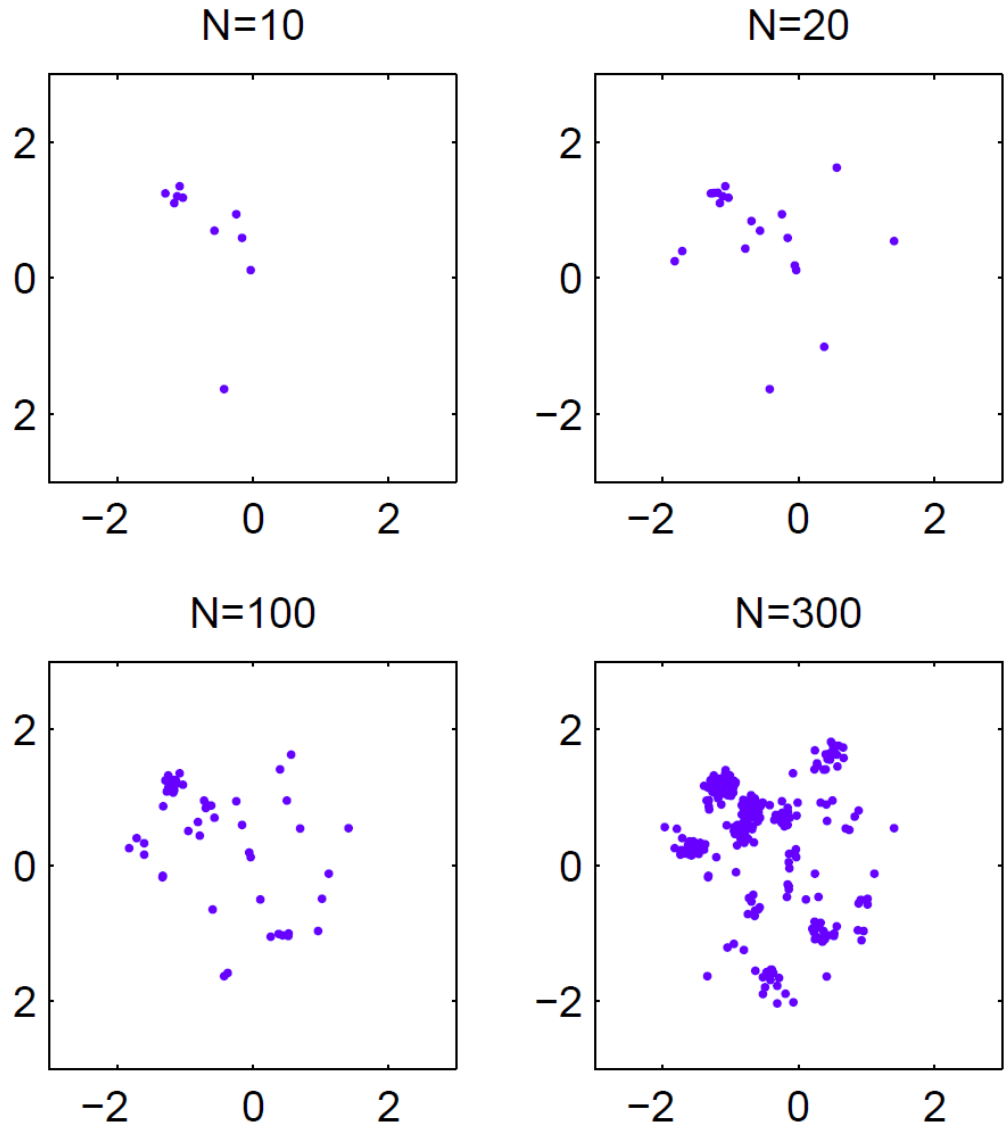
$\Rightarrow$ We will see efficient approximate inference methods later on...

Bayesian Mixture Models

- Let's examine this model more closely
  - Role of Dirichlet priors?
  - How can we perform efficient inference?
  - What happens when K goes to infinity?

- This will lead us to an interesting class of models…
  - Dirichlet Processes
  - Possible to express infinite mixture distributions with their help
  - Clustering that automatically adapts the number of clusters to the data and *dynamically creates new clusters on-the-fly*.

Sneak Preview: Dirichlet Process MoG



Samples drawn from DP mixture

⇒ More structure appears as more points are drawn

Slide credit: Zoubin Gharamani

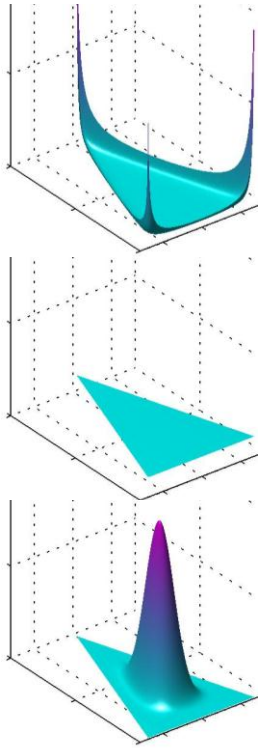
Recap: The Dirichlet Distribution

- **Dirichlet Distribution**
  - **Conjugate prior for the Categorical and the Multinomial distrib.**

$$\mathrm{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_K)}\prod_{k=1}^{K}\mu_k^{\alpha_k-1} \quad \text{with} \quad \alpha_0 = \sum_{k=1}^{K}\alpha_k$$

  - **Symmetric version (with concentration parameter α)**

$$\mathrm{Dir}(\boldsymbol{\mu}|\alpha) = \frac{\Gamma(\alpha)}{\Gamma(\alpha/K)^K}\prod_{k=1}^{K}\mu_k^{\alpha/K-1}$$



  - **Properties** **(symmetric version)**

$$\mathbb{E}[\mu_k] = \frac{\alpha_k}{\alpha_0} = \frac{1}{K}$$

$$\mathrm{var}[\mu_k] = \frac{\alpha_k(\alpha_0-\alpha_k)}{\alpha_0^2(\alpha_0+1)} = \frac{K-1}{K^2(\alpha+1)}$$

$$\mathrm{cov}[\mu_j\mu_k] = -\frac{\alpha_j\alpha_k}{\alpha_0^2(\alpha_0+1)} = -\frac{1}{K^2(\alpha+1)}$$

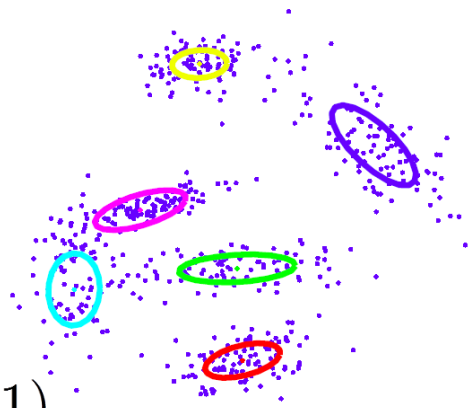
Image source: C. Bishop, 2006

Mixture Model with Dirichlet Priors

- **Finite mixture of K components**

$$p(\mathbf{x}_n|\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}_n|\theta_k)$$

$$= \sum_{k=1}^{K} p(z_{nk}=1|\pi_k) p(\mathbf{x}_n|\theta_k, z_{nk}=1)$$



  - **The distribution of latent variables $\mathbf{z}_n$ given π is multinomial**

$$p(\mathbf{z}|\boldsymbol{\pi}) = \prod_{k=1}^{K} \pi_k^{N_k}, \quad N_k \stackrel{\text{def}}{=} \sum_{n=1}^{N} z_{nk}$$

  - **Assume mixing proportions have a given symmetric conjugate Dirichlet prior**

$$p(\boldsymbol{\pi}|\alpha) = \frac{\Gamma(\alpha)}{\Gamma(\alpha/K)^K} \prod_{k=1}^{K} \pi_k^{\alpha/K-1}$$

Mixture Model with Dirichlet Priors

- **Integrating out the mixing proportions π:**

$$
\begin{aligned}
p(\mathbf{z}|\alpha) &= \int p(\mathbf{z}|\boldsymbol{\pi})p(\boldsymbol{\pi}|\alpha)\mathrm{d}\boldsymbol{\pi} \\
&= \int \prod_{k=1}^{K} \pi_k^{N_k} \cdot \frac{\Gamma(\alpha)}{\Gamma(\alpha/K)^K} \prod_{k=1}^{K} \pi_k^{\alpha/K-1} \mathrm{d}\boldsymbol{\pi} \\
&= \int \frac{\Gamma(\alpha)}{\Gamma(\alpha/K)^K} \prod_{k=1}^{K} \pi_k^{N_k+\alpha/K-1} \mathrm{d}\boldsymbol{\pi}
\end{aligned}
$$

  - **This is again a Dirichlet distribution (reason for conjugate priors)**

$$
= \frac{\Gamma(\alpha)}{\Gamma(\alpha/K)^K} \frac{\prod_{k=1}^{K}\Gamma(N_k+\alpha/K)}{\Gamma(N+\alpha)} \int \frac{\Gamma(N+\alpha)}{\prod_{k=1}^{K}\Gamma(N_k+\alpha/K)} \prod_{k=1}^{K} \pi_k^{N_k+\alpha/K-1} \mathrm{d}\boldsymbol{\pi}
$$

Completed Dirichlet form → integrates to 1

Mixture Models with Dirichlet Priors

- **Integrating out the mixing proportions π (cont'd)**

$$p(\mathbf{z}|\alpha) = \frac{\Gamma(\alpha)}{\Gamma(\alpha/K)^K} \frac{\prod_{k=1}^K \Gamma(N_k + \alpha/K)}{\Gamma(N+\alpha)}$$

$$= \frac{\Gamma(\alpha)}{\Gamma(N+\alpha)} \prod_{k=1}^K \frac{\Gamma(N_k + \alpha/K)}{\Gamma(\alpha/K)}$$

- **Conditional probabilities**
  - **Let's examine the conditional of $\mathbf{z}_n$ given all other variables**

$$p(z_{nk} = 1|\mathbf{z}_{-n}, \alpha) = \frac{p(z_{nk} = 1, \mathbf{z}_{-n}|\alpha)}{p(\mathbf{z}_{-n}|\alpha)}$$

where $\mathbf{z}_{-n}$ denotes all indizes except n.

Mixture Models with Dirichlet Priors

$$p(\mathbf{z}|\alpha) = \frac{\Gamma(\alpha)}{\Gamma(N+\alpha)} \prod_{k=1}^{K} \frac{\Gamma(N_k+\alpha/K)}{\Gamma(\alpha/K)}$$

- **Conditional probabilities**

$$p(z_{nk}=1|\mathbf{z}_{-n},\alpha) = \frac{p(z_{nk}=1,\mathbf{z}_{-n}|\alpha)}{p(\mathbf{z}_{-n}|\alpha)}$$

$$= \frac{\cancel{\frac{\Gamma(\alpha)}{\Gamma(N+\alpha)}} \frac{\Gamma(N_k+\alpha/K)}{\cancel{\Gamma(\alpha/K)}} \cancel{\prod_{j=1,j\neq k}^{K} \frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}}{\cancel{\frac{\Gamma(\alpha)}{\Gamma(N_{-n}+\alpha)}} \frac{\Gamma(N_{-n,k}+\alpha/K)}{\cancel{\Gamma(\alpha/K)}} \cancel{\prod_{j=1,j\neq k}^{K} \frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}}$$

$$= \frac{\Gamma(N_{-n}+\alpha)}{\Gamma(N+\alpha)} \frac{\Gamma(N_k+\alpha/K)}{\Gamma(N_{-n,k}+\alpha/K)}$$

Mixture Models with Dirichlet Priors

- **Conditional probabilities**

$$\Gamma(n+1) = n\Gamma(n)$$

$$p(z_{nk}=1|\mathbf{z}_{-n},\alpha) = \frac{p(z_{nk}=1,\mathbf{z}_{-n}|\alpha)}{p(\mathbf{z}_{-n}|\alpha)}$$

$$= \frac{\frac{\Gamma(\alpha)}{\Gamma(N+\alpha)} \frac{\Gamma(N_k+\alpha/K)}{\Gamma(\alpha/K)} \prod_{j=1,j\neq k}^{K} \frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}{\frac{\Gamma(\alpha)}{\Gamma(N_{-n}+\alpha)} \frac{\Gamma(N_{-n,k}+\alpha/K)}{\Gamma(\alpha/K)} \prod_{j=1,j\neq k}^{K} \frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}$$

$$= \frac{\Gamma(N_{-n}+\alpha)}{\Gamma(N+\alpha)} \frac{\Gamma(N_k+\alpha/K)}{\Gamma(N_{-n,k}+\alpha/K)}$$

$$= \frac{1}{N-1+\alpha} \frac{N_{-n,k}+\alpha/K}{1}$$

$$= \frac{N_{-n,k}+\alpha/K}{N-1+\alpha}$$

Finite Dirichlet Mixture Models

- **Conditional probabilities: Finite K**

$$p(z_{nk} = 1 | \mathbf{z}_{-n}, \alpha) = \frac{N_{-n,k} + \alpha/K}{N - 1 + \alpha}, \qquad N_{-n,k} \stackrel{\text{def}}{=} \sum_{i=1, i \neq n}^{N} z_{ik}$$

- **This is a very interesting result. *Why?***
  - **We directly get a numerical probability, no distribution.**
  - **The probability of joining a cluster mainly depends on the number of existing entries in a cluster.**

  $\Rightarrow$ The more populous a class is, the more likely it is to be joined!
  - **In addition, we have a base probability of also joining as-yet empty clusters.**
  - **This result can be directly used in Gibbs Sampling…**

Infinite Dirichlet Mixture Models

- **Conditional probabilities: Finite K**

$$p(z_{nk} = 1 | \mathbf{z}_{-n}, \alpha) = \frac{N_{-n,k} + \alpha/K}{N - 1 + \alpha}, \qquad N_{-n,k} \stackrel{\text{def}}{=} \sum_{i=1, i \neq n}^{N} z_{ik}$$

- **Conditional probabilities: Infinite K**
  - **Taking the limit as $K \to \infty$ yields the conditionals**

$$p(z_{nk} = 1 | \mathbf{z}_{-n}, \alpha) = \begin{cases} \frac{N_{-n,k}}{N-1+\alpha} & \text{if } k \text{ represented} \\ \frac{\alpha}{N-1+\alpha} & \text{if all } k \text{ not represented} \end{cases}$$

  - **Left-over mass $\alpha \Rightarrow$ countably infinite number of indicator settings**

Discussion

- Infinite Mixture Models
  - What we have just seen is a first example of a Dirichlet Process.
  - DPs will allow us to work with models that have an infinite number of components.
  - This will raise a number of issues
    - How to represent infinitely many parameters?
    - How to deal with permutations of the class labels?
    - How to control the effective size of the model?
    - How to perform efficient inference?

  $\Rightarrow$ More background needed here!
  - We will hear much more about DPs in the next lecture…

Topics of This Lecture

- The EM algorithm in general
  - Recap: General EM
  - Example: Mixtures of Bernoulli distributions
  - Monte Carlo EM
- **Bayesian Mixture Models**
  - **Towards a full Bayesian treatment**
  - **Dirichlet priors**
  - **Finite mixtures**
  - **Infinite mixtures**
  - **Approximate inference**
- Outlook: Dirichlet Processes

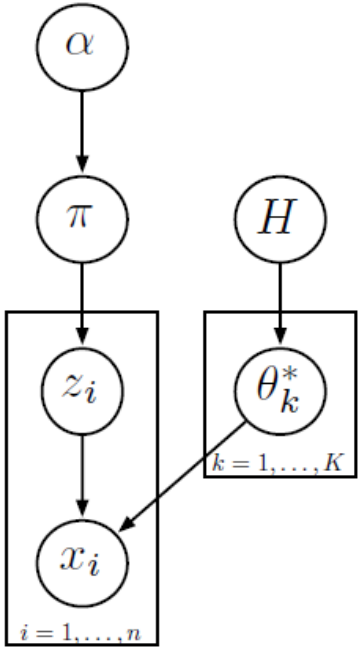
Gibbs Sampling for Finite Mixtures

- **We need approximate inference here**
  - **Gibbs Sampling: Conditionals are simple to compute**

$$p(\mathbf{z}_n = k|\text{others}) \propto \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$\boldsymbol{\pi} \mid \mathbf{z} \sim \text{Dir}(N_1 + \alpha/K, \ldots, N_K + \alpha/K)$$

$$\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k|\text{others} \sim \mathcal{N} - \mathcal{IW}(v', s', d', \phi')$$



Gibbs Sampling for Finite Mixtures

- **Standard finite mixture sampler**
  - Given mixture weights $\pi^{(t-1)}$ and cluster parameters $\left\{\theta_k^{(t=1)}\right\}_{k=1}^{K}$ from the previous iteration, sample new parameters as follows

1. Independently assign each point $\mathbf{x}_n$ to one of the K clusters by sampling the variables $\mathbf{z}_n$ from the multinomial distributions

$$\mathbf{z}_n^{(t)} \sim \frac{1}{Z_n} \sum_{k=1}^{K} z_{nk}^{(t-1)} \pi_k^{(t-1)} p(\mathbf{x}_n | \theta_k^{(t-1)}) \qquad Z_n = \sum_{k=1}^{K} \pi_k^{(t-1)} p(\mathbf{x}_n | \theta_k^{(t-1)})$$

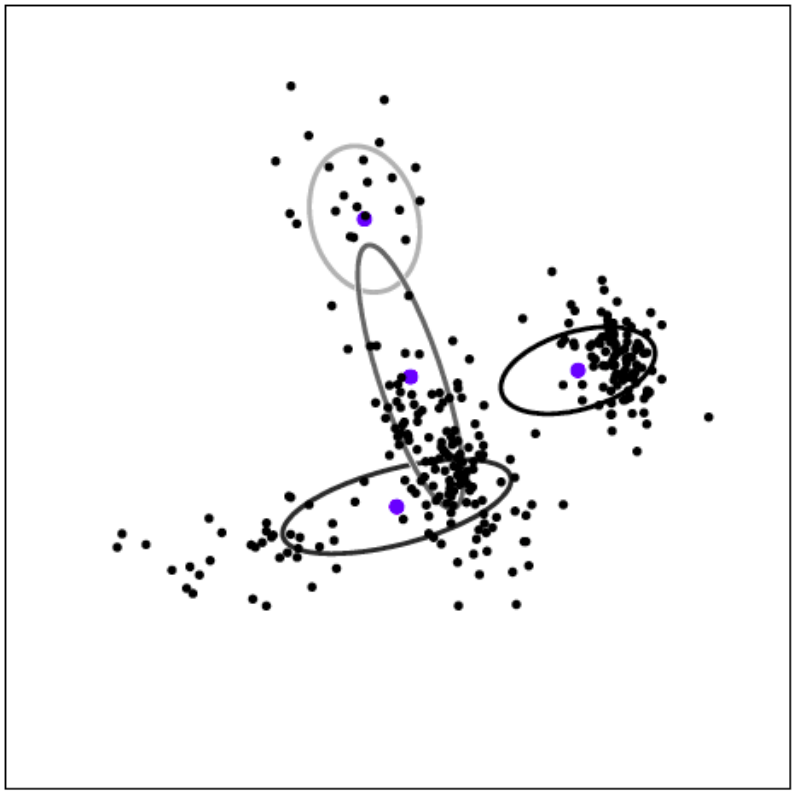
2. Sample new mixture weights from the Dirichlet distribution

$$\boldsymbol{\pi}^{(t)} \sim \mathrm{Dir}(N_1 + \alpha/K, \ldots, N_K + \alpha/K) \qquad N_k = \sum_{n=1}^{N} z_{nk}^{(t)}$$

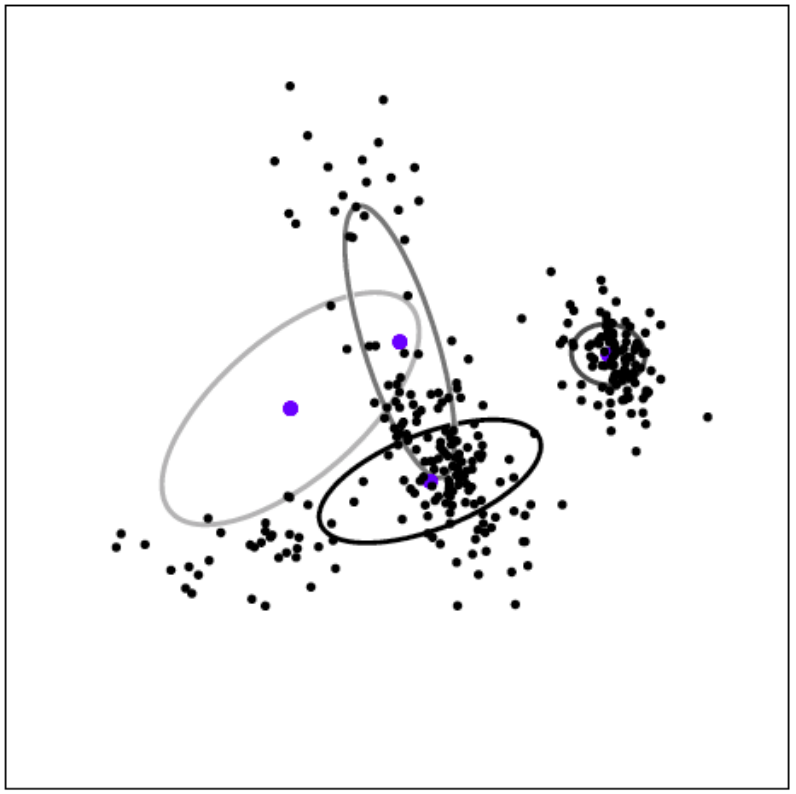
3. For each of the K clusters, independently sample new parameters from the conditional of the assigned observations

$$\boldsymbol{\theta}_k^{(t)} \sim p(\boldsymbol{\theta}_k | \{\mathbf{x}_n | z_{nk} = 1\}, H)$$

Standard Sampler: 2 Iterations



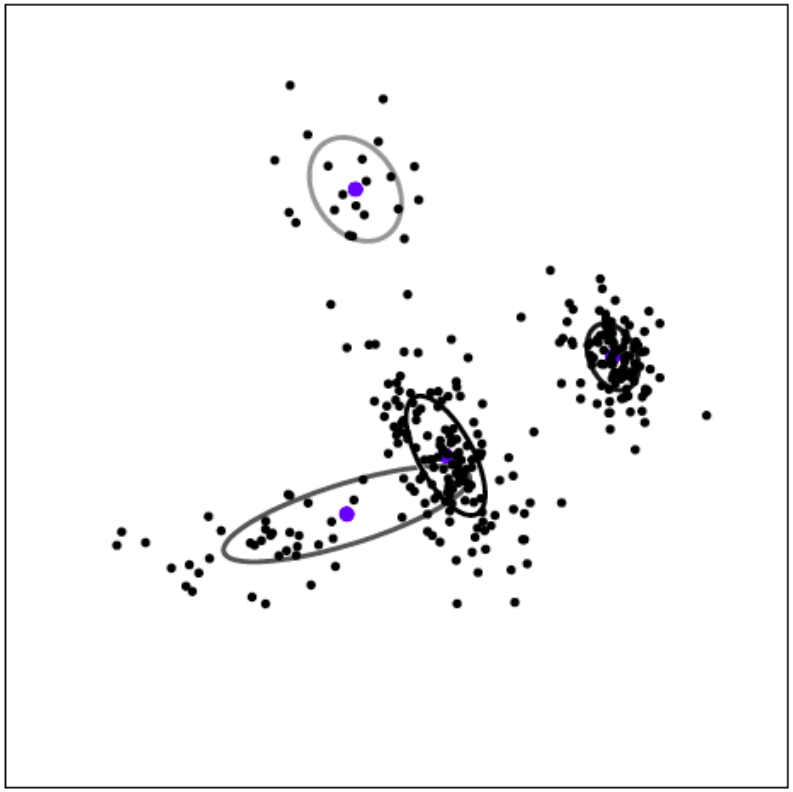
$\log p(x \mid \pi, \theta) = -539.17$



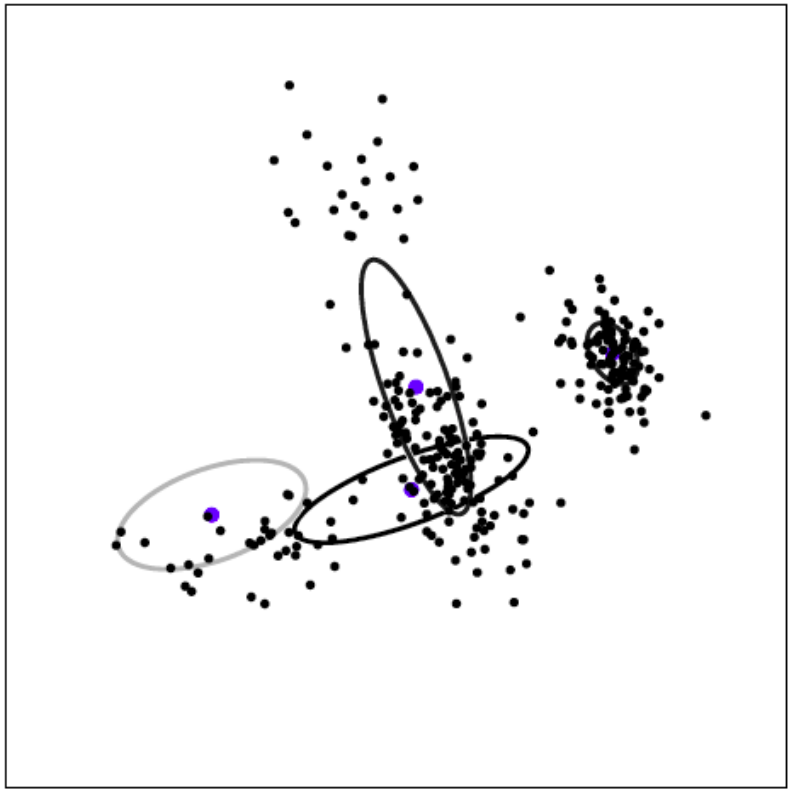
$\log p(x \mid \pi, \theta) = -497.77$

Slide credit: Erik Sudderth

Standard Sampler: 10 Iterations



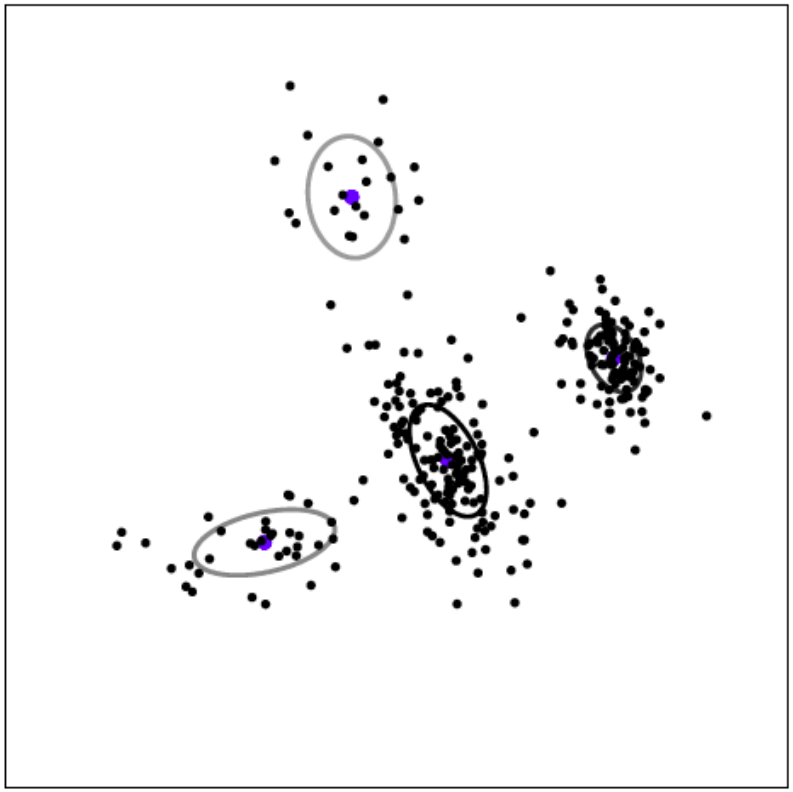
log p(x | π, θ) = –404.18



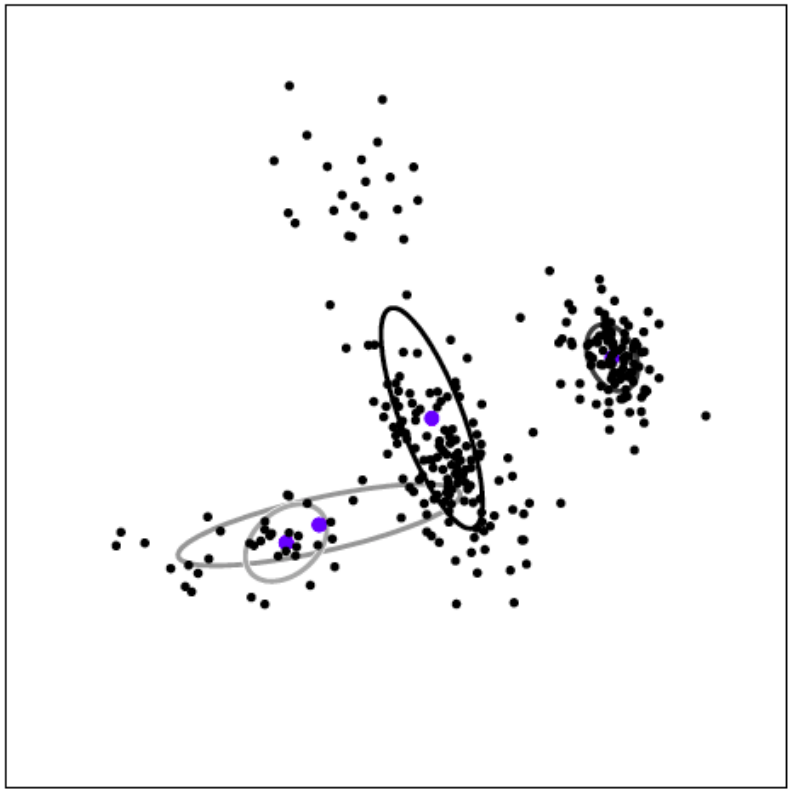
log p(x | π, θ) = –454.15

Slide credit: Erik Sudderth

Standard Sampler: 10 Iterations



log p(x | π, θ) = –397.40



log p(x | π, θ) = –442.89

Slide credit: Erik Sudderth

Gibbs Sampling for Finite Mixtures

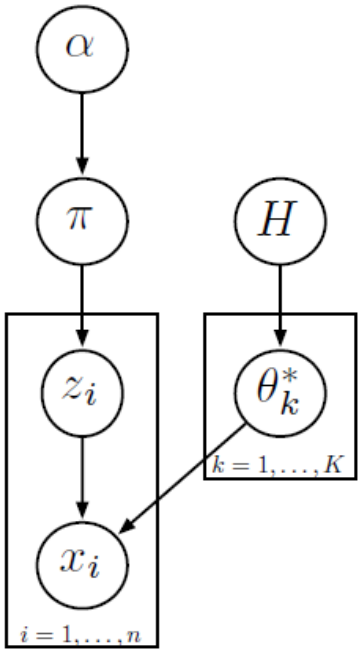
- We need approximate inference here
  - Gibbs Sampling: Conditionals are simple to compute

$$p(\mathbf{z}_n = k|\text{others}) \propto \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$\boldsymbol{\pi} \mid \mathbf{z} \sim \text{Dir}(N_1 + \alpha/K, \ldots, N_K + \alpha/K)$$

$$\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k|\text{others} \sim \mathcal{N} - \mathcal{IW}(v', s', d', \phi')$$

- However, this will be rather inefficient…
  - In each iteration, algorithm can only change the assignment for individual data points.
  - There are often groups of data points that are associated with high probability to the same component. ⇒ Unlikely that group is moved.
  - Better performance by collapsed Gibbs sampling which integrates out the parameters π, μ, Σ.



Collapsed Finite Bayesian Mixture

- More efficient algorithm
  - Conjugate priors allow analytic integration of some parameters
  - Resulting sampler operates on reduced space of cluster assignments (implicitly considers all possible cluster shapes)

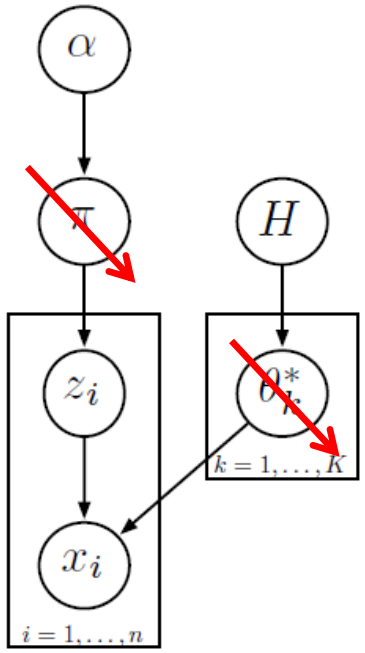
- Necessary steps
  - Derive

$$p(\mathbf{z}|\alpha) = \int p(\mathbf{z}|\boldsymbol{\pi})p(\boldsymbol{\pi}|\alpha)\mathrm{d}\boldsymbol{\pi}$$

  - Derive

$$p(\mathbf{x}_n|\mathbf{z}_n, H) = \int \sum_{k=1}^{K} z_{nk} p(\mathbf{x}_n|\boldsymbol{\theta}_k)p(\boldsymbol{\theta}_k|H)\mathrm{d}\boldsymbol{\theta}$$

  ⇒ Conjugate prior, Normal - Inverse Wishart



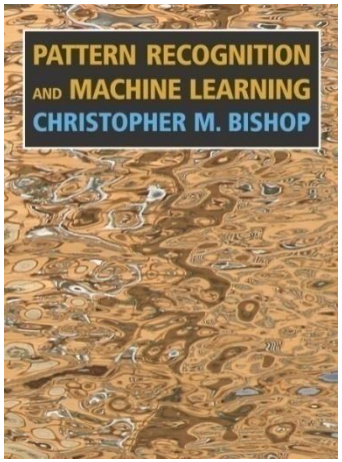
Collapsed Finite Mixture Sampler

- To be added…

References and Further Reading

- More information about EM estimation is available in Chapter 9 of Bishop's book (recommendable to read).

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006



- Additional information
  - Original EM paper:
    - A.P. Dempster, N.M. Laird, D.B. Rubin, „Maximum-Likelihood from incomplete data via EM algorithm", In Journal Royal Statistical Society, Series B. Vol 39, 1977
  - EM tutorial:
    - J.A. Bilmes, "A Gentle Tutorial of the EM Algorithm and its Application to Parameter Estimation for Gaussian Mixture and Hidden Markov Models", TR-97-021, ICSI, U.C. Berkeley, CA,USA