Advanced Machine Learning
Lecture 10

Mixture Models II

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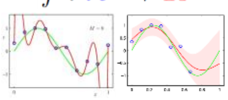
Announcement

- Exercise sheet 2 online
  - Sampling
  - Rejection Sampling
  - Importance Sampling
  - Metropolis-Hastings
  - EM
  - Mixtures of Bernoulli distributions [today's topic]
  - Exercise will be on Wednesday, 07.12.
  - ⇒ *Please submit your results until 06.12. midnight.*

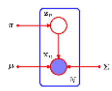
This Lecture: *Advanced Machine Learning*

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

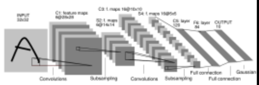
$$f : \mathcal{X} \to \mathbb{R}$$



- Learning with Latent Variables
  - Probability Distributions
  - Approximate Inference
  - Mixture Models
  - EM and Generalizations



- Deep Learning
  - Neural Networks
  - CNNs, RNNs, RBMs, etc.



Topics of This Lecture

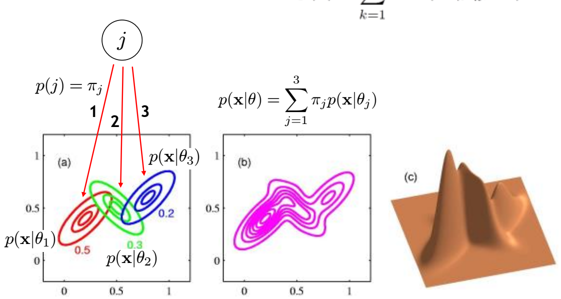
- The EM algorithm in general
  - Recap: General EM
  - Example: Mixtures of Bernoulli distributions
  - Monte Carlo EM
- Bayesian Mixture Models
  - Towards a full Bayesian treatment
  - Dirichlet priors
  - Finite mixtures
  - Infinite mixtures
  - Approximate inference (only as supplementary material)

Recap: Mixture of Gaussians

- "Generative model"

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

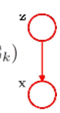
$$p(\mathbf{x}|\theta) = \sum_{j=1}^{3} \pi_j p(\mathbf{x}|\theta_j)$$



Recap: GMMs as Latent Variable Models

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

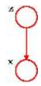
$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$



- 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 $p(\mathbf{x})$.
  - ⇒ 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 $\gamma(z_{nk})$

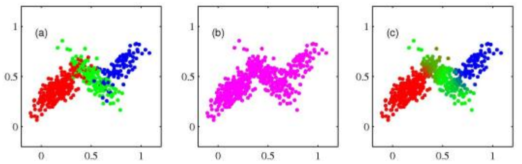


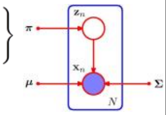
Image source: C.M. Bishop, 2006

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…

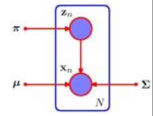


Image source: C.M. Bishop, 2006

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!

Gaussian Mixtures Revisited

- Maximize the likelihood
  - For the complete-data set $\{\mathbf{X},\mathbf{Z}\}$, the likelihood has the form

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

  - Taking the logarithm, we obtain

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

  - Compared to the incomplete-data case, the order of the sum and logarithm has been interchanged.

$\Rightarrow$ Much simpler solution to the ML problem.

  - Maximization w.r.t. a mean or covariance is exactly as for a single Gaussian, except that it involves only the subset of data points that are "assigned" to that component.

Gaussian Mixtures Revisited

- Maximization w.r.t. mixing coefficients
  - More complex, since the π_k are coupled by the summation constraint
$$\sum_{j=1}^{K} \pi_j = 1$$
  - Solve with a Lagrange multiplier
$$\log p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}) + \lambda\left(\sum_{k=1}^{K}\pi_k - 1\right)$$
  - Solution (after a longer derivation):
$$\pi_k = \frac{1}{N}\sum_{n=1}^{N} z_{nk}$$

$\Rightarrow$ The complete-data log-likelihood can be maximized trivially in closed form.

Gaussian Mixtures Revisited

- In practice, we don't have values for the latent variables
  - Consider the expectation w.r.t. the posterior distribution of the latent variables instead.
  - The posterior distribution takes the form
$$p(\mathbf{Z}|\mathbf{X},\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}) \propto \prod_{n=1}^{N}\prod_{k=1}^{K}\left[\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right]^{z_{nk}}$$
    and factorizes over n, so that the $\{\mathbf{z}_n\}$ are independent under the posterior.

    Expected value of indicator variable z_{nk} under the posterior.
$$\mathbb{E}[z_{nk}] = \frac{\sum_{z_{nk}} z_{nk}\left[\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right]^{z_{nk}}}{\sum_{z_{nj}}\left[\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)\right]^{z_{nj}}} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K}\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)} = \gamma(z_{nk})$$

Gaussian Mixtures Revisited

- Continuing the estimation
  - The complete-data log-likelihood is therefore
$$\mathbb{E}_{\mathbf{Z}}[\log p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi})] = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\left\{\log \pi_k + \log \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}$$

$\Rightarrow$ This is precisely the EM algorithm for Gaussian mixtures as derived before.

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 (only as supplementary material)

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

Diagonal covariance $\Rightarrow$ variables independently modeled

Mixtures of Bernoulli Distributions

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

$$\begin{aligned} p(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\pi}) &= \sum_{k=1}^{K} \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k) \\ &= \sum_{k=1}^{K} \pi_k \prod_{i=1}^{D} \mu_{ki}^{x_i}(1-\mu_{ki})^{(1-x_i)} \end{aligned}$$

  - Mean and covariance of the mixture are given by

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

Covariance not diagonal
⇒ Model can capture dependencies between variables

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

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

$$\begin{aligned} p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\pi}) &= \prod_{n=1}^{N}\prod_{k=1}^{K} \left[\pi_k p(\mathbf{x}_n|\boldsymbol{\mu}_k)\right]^{z_{nk}} \\ &= \prod_{n=1}^{N}\prod_{k=1}^{K} \left\{ \pi_k \prod_{i=1}^{D} \mu_{ki}^{x_{ni}}(1-\mu_{ki})^{(1-x_{ni})} \right\}^{z_{nk}} \end{aligned}$$

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

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

EM for Bernoulli Mixtures: E-Step

- E-Step
  - Evaluate the responsibilities

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

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

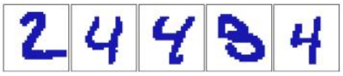
Discussion

- 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
$$0 \le p(\mathbf{x}_n|\boldsymbol{\mu}_k) \le 1$$
  - However, there are still problem cases when μ_{ki} becomes 0 or 1
$$\mathbb{E}_{\mathbf{Z}}[\log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\pi})] = \ldots [x_{ni} \log \mu_{ki} + (1 - x_{ni}) \log(1 - \mu_{ki})]$$

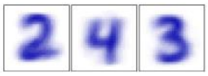
  ⇒ Need to enforce a range [MIN_VAL,1-MIN_VAL] for either μ_{ki} or γ.
- General remarks
  - Bernoulli mixtures are used in practice in order to represent binary data.
  - The resulting model is also known as latent class analysis.

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

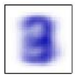


Image source: C.M. Bishop, 2006

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 (only as supplementary material)

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.

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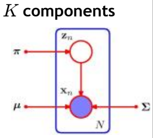
Towards a Full Bayesian Treatment…

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

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

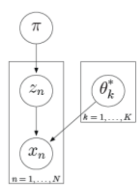


  - So far, we have derived the ML estimates ⇒ EM
  - Introduced a prior $p(\theta)$ over parameters ⇒ MAP-EM
  - One question remains open: how to set K ?
  - ⇒ Let's also set a prior on the number of components…

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.

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



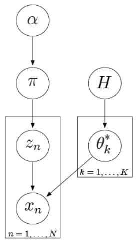
  - This is similar to the graphical model we've used before, but now the π and $\theta_k = (\mu_k, \boldsymbol{\Sigma}_k)$ are also treated as random variables.
  - *What would be suitable priors for them?*

Slide inspired by Yee Whye Teh

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.

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



  - Introduce conjugate priors over parameters

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

"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

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

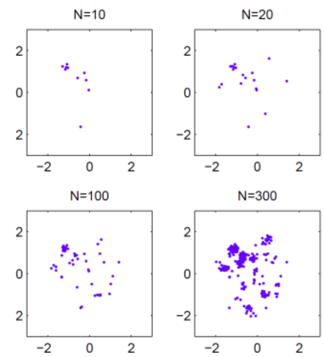
- The posterior over assignments is intractable!
  - Denominator requires summing over all possible partitions of the data into K groups!

$\Rightarrow$ Need efficient approximate inference methods to solve this...

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

$\Rightarrow$ More structure appears as more points are drawn

Recap: The Dirichlet Distribution

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

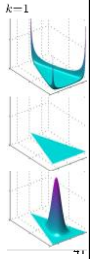
$$\mathrm{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_K)} \prod_{k=1}^{K} \mu_k^{\alpha_k - 1} \quad \text{with} \quad \alpha_0 = \sum_{k=1}^{K} \alpha_k$$

  - Symmetric version (with concentration parameter α)

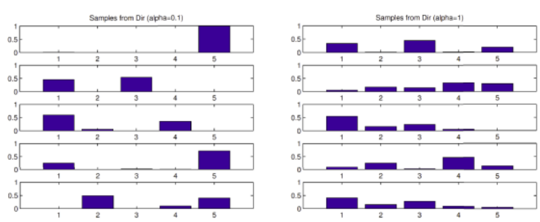
$$\mathrm{Dir}(\boldsymbol{\mu}|\alpha) = \frac{\Gamma(\alpha)}{\Gamma(\alpha/K)^K} \prod_{k=1}^{K} \mu_k^{\alpha/K - 1}$$

  - Properties (symmetric version)

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



Dirichlet Samples

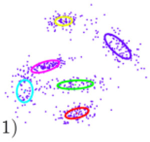


$\mathrm{Dir}(\theta \mid 0.1, 0.1, 0.1, 0.1, 0.1)$ $\mathrm{Dir}(\theta \mid 1.0, 1.0, 1.0, 1.0, 1.0)$

- Effect of concentration parameter α
  - Controls sparsity of the resulting samples

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:**

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

  - 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

- **Conditional probabilities**

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

$$p(z_{nk}=1|\mathbf{z}_{-n},\alpha) = \frac{p(z_{nk}=1,\mathbf{z}_{-n}|\alpha)}{p(\mathbf{z}_{-n}|\alpha)}$$
$$= \frac{\frac{\cancel{\Gamma(\alpha)}}{\Gamma(N+\alpha)}\frac{\Gamma(N_k+\alpha/K)}{\cancel{\Gamma(\alpha/K)}}\cancel{\prod_{j=1,j\neq k}^{K}\frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}}{\frac{\cancel{\Gamma(\alpha)}}{\Gamma(N_{-n}+\alpha)}\frac{\Gamma(N_{-n,k}+\alpha/K)}{\cancel{\Gamma(\alpha/K)}}\cancel{\prod_{j=1,j\neq k}^{K}\frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}}$$
$$= \frac{\Gamma(N_{-n}+\alpha)}{\Gamma(N+\alpha)}\frac{\Gamma(N_k+\alpha/K)}{\Gamma(N_{-n,k}+\alpha/K)}$$

Mixture Models with Dirichlet Priors

- **Conditional probabilities**

$$\boxed{\Gamma(n+1) = n\Gamma(n)}$$

$$p(z_{nk}=1|\mathbf{z}_{-n},\alpha) = \frac{p(z_{nk}=1,\mathbf{z}_{-n}|\alpha)}{p(\mathbf{z}_{-n}|\alpha)}$$
$$= \frac{\frac{\cancel{\Gamma(\alpha)}}{\Gamma(N+\alpha)}\frac{\Gamma(N_k+\alpha/K)}{\cancel{\Gamma(\alpha/K)}}\cancel{\prod_{j=1,j\neq k}^{K}\frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}}{\frac{\cancel{\Gamma(\alpha)}}{\Gamma(N_{-n}+\alpha)}\frac{\Gamma(N_{-n,k}+\alpha/K)}{\cancel{\Gamma(\alpha/K)}}\cancel{\prod_{j=1,j\neq k}^{K}\frac{\Gamma(N_j+\alpha/K)}{\Gamma(\alpha/K)}}}$$
$$= \frac{\Gamma(N_{-n}+\alpha)}{\Gamma(N+\alpha)}\frac{\Gamma(N_k+\alpha/K)}{\Gamma(N_{-n,k}+\alpha/K)}$$
$$= \frac{1}{N-1+\alpha}\frac{N_{-n,k}+\alpha/K}{1}$$
$$= \frac{N_{-n,k}+\alpha/K}{N-1+\alpha}$$

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.

  ⇒ 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 $K\rightarrow\infty$ 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

Slide adapted from Zoubin Gharamani

Discussion

- Infinite Mixture Models
  - What we have just seen is a first example of a Dirichlet Process.
  - DPs 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?

  ⇒ More background needed here!

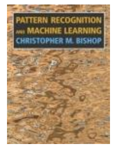
  - DPs are a very interesting class of models, but would take us too far here.
  - If you're interested in learning more about them, take a look at the Advanced ML slides from Winter 2012.

Next Lecture...

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