Advanced Machine Learning
Lecture 9

Mixture Models

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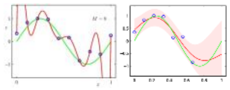
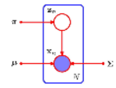
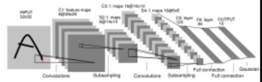
This Lecture: *Advanced Machine Learning*

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

- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Gaussian Processes
- Learning with Latent Variables
  - Probability Distributions
  - Approximate Inference
  - Mixture Models
  - EM and Generalizations
- Deep Learning
  - Neural Networks
  - CNNs, RNNs, RBMs, etc.





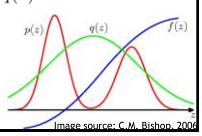


Recap: Importance Sampling

- Approach
  - Approximate expectations directly (but does not enable to draw samples from $p(\mathbf{z})$ directly).
  - Goal: $\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z}$
- Idea
  - Use a proposal distribution $q(\mathbf{z})$ from which it is easy to sample.
  - Express expectations in the form of a finite sum over samples $\{\mathbf{z}^{(l)}\}$ drawn from $q(\mathbf{z})$.

$$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z} = \int f(\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}q(\mathbf{z})d\mathbf{z}$$

$$\simeq \frac{1}{L}\sum_{l=1}^{L}\underbrace{\frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}}_{\text{Importance weights}}f(\mathbf{z}^{(l)})$$

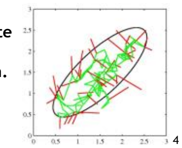


Slide adapted from Bernt Schiele

Image source: C.M. Bishop, 2006

Recap: MCMC - Markov Chain Monte Carlo

- Overview
  - Allows to sample from a large class of distributions.
  - Scales well with the dimensionality of the sample space.
- Idea
  - We maintain a record of the current state $\mathbf{z}^{(\tau)}$
  - The proposal distribution depends on the current state: $q(\mathbf{z} | \mathbf{z}^{(\tau)})$
  - The sequence of samples forms a Markov chain $\mathbf{z}^{(1)}$, $\mathbf{z}^{(2)}$,…
- Approach
  - At each time step, we generate a candidate sample from the proposal distribution and accept the sample according to a criterion.
  - Different variants of MCMC for different criteria.



Slide adapted from Bernt Schiele

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Recap: Markov Chains - Properties

- Invariant distribution
  - A distribution is said to be invariant (or stationary) w.r.t. a Markov chain if each step in the chain leaves that distribution invariant.
  - Transition probabilities:
    $$T\left(\mathbf{z}^{(m)}, \mathbf{z}^{(m+1)}\right) = p\left(\mathbf{z}^{(m+1)} | \mathbf{z}^{(m)}\right)$$
  - For homogeneous Markov chain, distribution $p^{*}(\mathbf{z})$ is invariant if:
    $$p^{\star}(\mathbf{z}) = \sum_{\mathbf{z}'} T(\mathbf{z}', \mathbf{z})\, p^{\star}(\mathbf{z}')$$
- Detailed balance
  - Sufficient (but not necessary) condition to ensure that a distribution is invariant:
    $$p^{\star}(\mathbf{z})T(\mathbf{z}, \mathbf{z}') = p^{\star}(\mathbf{z}')T(\mathbf{z}', \mathbf{z})$$
  - A Markov chain which respects *detailed balance* is reversible.

Slide credit: Bernt Schiele

Recap: MCMC - Metropolis Algorithm

- Metropolis algorithm **[Metropolis et al., 1953]**
  - Proposal distribution is symmetric: $q(\mathbf{z}_A | \mathbf{z}_B) = q(\mathbf{z}_B | \mathbf{z}_A)$
  - The new candidate sample $\mathbf{z}^{*}$ is accepted with probability
    $$A(\mathbf{z}^{\star}, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{p}(\mathbf{z}^{\star})}{\tilde{p}(\mathbf{z}^{(\tau)})}\right)$$

$\Rightarrow$ New candidate samples always accepted if $\tilde{p}(\mathbf{z}^{\star}) \geq \tilde{p}(\mathbf{z}^{(\tau)})$.
  - The algorithm sometimes accepts a state with lower probability.

Slide adapted from Bernt Schiele

MCMC – Metropolis-Hastings Algorithm

- Metropolis-Hastings Algorithm
  - Generalization: Proposal distribution not required to be symmetric.
  - The new candidate sample $\mathbf{z}^*$ is accepted with probability

$$A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{p}(\mathbf{z}^\star) q_k(\mathbf{z}^{(\tau)}|\mathbf{z}^\star)}{\tilde{p}(\mathbf{z}^{(\tau)}) q_k(\mathbf{z}^\star|\mathbf{z}^{(\tau)})}\right)$$

  - where k labels the members of the set of possible transitions considered.
- Note
  - Evaluation of acceptance criterion does not require normalizing constant Z_p.
  - When the proposal distributions are symmetric, Metropolis-Hastings reduces to the standard Metropolis algorithm.

Random Walks

- Example: Random Walk behavior
  - Consider a state space consisting of the integers $z \in \mathbb{Z}$ with initial state $z(1) = 0$ and transition probabilities

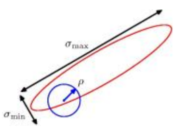
$$\begin{aligned} p(z^{(\tau+1)} = z^{(\tau)}) &= 0.5 \\ p(z^{(\tau+1)} = z^{(\tau)} + 1) &= 0.25 \\ p(z^{(\tau+1)} = z^{(\tau)} - 1) &= 0.25 \end{aligned}$$

- Analysis
  - Expected state at time τ: $\mathbb{E}[z^{(\tau)}] = 0$
  - Variance: $\mathbb{E}[(z^{(\tau)})^2] = \tau/2$
  - After τ steps, the random walk has only traversed a distance that is on average proportional to $\sqrt{\tau}$.

⇒ Central goal in MCMC is to avoid random walk behavior!

MCMC – Metropolis-Hastings Algorithm

- Schematic illustration
  - For continuous state spaces, a common choice of proposal distribution is a Gaussian centered on the current state.



⇒ What should be the variance of the proposal distribution?
  - Large variance: rejection rate will be high for complex problems.
  - The scale ρ of the proposal distribution should be as large as possible without incurring high rejection rates.

  ⇒ ρ should be of the same order as the smallest length scale σ_{min}.
  - This causes the system to explore the distribution by means of a random walk.
    - Undesired behavior: number of steps to arrive at state that is independent of original state is of order $(\sigma_{\text{max}}/\sigma_{\text{min}})^2$.
    - Strong correlations can slow down the Metropolis(-Hastings) algorithm!

Gibbs Sampling

- Approach
  - MCMC-algorithm that is simple and widely applicable.
  - May be seen as a special case of Metropolis-Hastings.
- Idea
  - Sample variable-wise: replace $\mathbf{z}_i$ by a value drawn from the distribution $p(z_i|\mathbf{z}_{\setminus i})$.
    - This means we update one coordinate at a time.
  - Repeat procedure either by cycling through all variables or by choosing the next variable.

Gibbs Sampling

- Example
  - Assume distribution $p(z_1, z_2, z_3)$.
  - Replace $z_1^{(\tau)}$ with new value drawn from $z_1^{(\tau+1)} \sim p(z_1|z_2^{(\tau)}, z_3^{(\tau)})$
  - Replace $z_2^{(\tau)}$ with new value drawn from $z_2^{(\tau+1)} \sim p(z_2|z_1^{(\tau+1)}, z_3^{(\tau)})$
  - Replace $z_3^{(\tau)}$ with new value drawn from $z_3^{(\tau+1)} \sim p(z_3|z_1^{(\tau+1)}, z_2^{(\tau+1)})$
  - And so on…

Gibbs Sampling

- Properties
  - Since the components are unchanged by sampling: $\mathbf{z}^*_{\setminus k} = \mathbf{z}_{\setminus k}$.
  - The factor that determines the acceptance probability in the Metropolis-Hastings is thus determined by

$$A(\mathbf{z}^\star, \mathbf{z}) = \frac{p(\mathbf{z}^\star) q_k(\mathbf{z}|\mathbf{z}^\star)}{p(\mathbf{z}) q_k(\mathbf{z}^\star|\mathbf{z})} = \frac{p(z_k^\star|\mathbf{z}_{\setminus k}^\star) p(\mathbf{z}_{\setminus k}^\star) p(z_k|\mathbf{z}_{\setminus k}^\star)}{p(z_k|\mathbf{z}_{\setminus k}) p(\mathbf{z}_{\setminus k}) p(z_k^\star|\mathbf{z}_{\setminus k})} = 1$$

  - (we have used $q_k(\mathbf{z}^*|\mathbf{z}) = p(z^*_k|\mathbf{z}_{\setminus k})$ and $p(\mathbf{z}) = p(z_k|\mathbf{z}_{\setminus k})\, p(\mathbf{z}_{\setminus k})$).
  - I.e. we get an algorithm which always accepts!

⇒ If you can compute (and sample from) the conditionals, you can apply Gibbs sampling.

⇒ The algorithm is completely parameter free.

⇒ Can also be applied to subsets of variables.

Discussion

- Gibbs sampling benefits from few free choices and convenient features of conditional distributions:
  - Conditionals with a few discrete settings can be explicitly normalized:

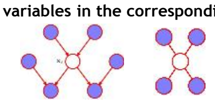
$$p(x_i|\mathbf{x}_{j\neq i}) = \frac{p(x_i, \mathbf{x}_{j\neq i})}{\sum_{x_i'} p(x_i', \mathbf{x}_{j\neq i})}$$

This sum is small and easy.

  - Continuous conditionals are often only univariate.

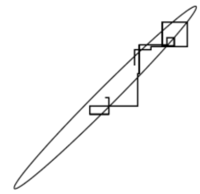
⇒ amenable to standard sampling methods.

  - In case of graphical models, the conditional distributions depend only on the variables in the corresponding Markov blankets.



Gibbs Sampling

- Example
  - 20 iterations of Gibbs sampling on a bivariate Gaussian.



  - Note: strong correlations can slow down Gibbs sampling.

How Should We Run MCMC?

- Arbitrary initialization means starting iterations are bad
  - Discard a "burn-in" period.
- How do we know if we have run for long enough?
  - You don't. That's the problem.
- The samples are not independent
  - Solution 1: Keep only every Mth sample ("thinning").
  - Solution 2: Keep all samples and use the simple Monte Carlo estimator on MCMC samples
    - It is consistent and unbiased if the chain has "burned in".

⇒ Use thinning only if computing $f(\mathbf{x}^{(s)})$ is expensive.

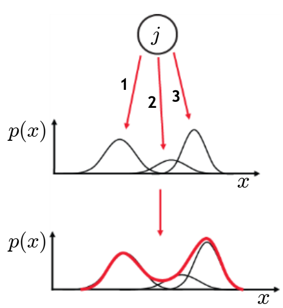
- For opinion on thinning, multiple runs, burn in, etc.
  - Charles J. Geyer, Practical Markov chain Monte Carlo, Statistical Science. 7(4):473{483, 1992. (http://www.jstor.org/stable/2246094)

Topics of This Lecture

- Recap: Mixtures of Gaussians
  - Mixtures of Gaussians
  - ML estimation
  - EM algorithm for MoGs
- An alternative view of EM
  - Latent variables
  - General EM
  - Mixtures of Gaussians revisited
  - Mixtures of Bernoulli distributions
- The EM algorithm in general
  - Generalized EM
  - Monte Carlo EM

Recap: Mixture of Gaussians (MoG)

- "Generative model"



$p(j) = \pi_j$ "Weight" of mixture component

$p(x|\theta_j)$ Mixture component

Mixture density $p(x|\theta) = \sum_{j=1}^{M} p(x|\theta_j)p(j)$

Recap: Mixture of Multivariate Gaussians

- Multivariate Gaussians

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

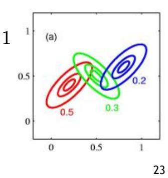
$$p(\mathbf{x}|\theta_j) = \frac{1}{(2\pi)^{D/2}|\mathbf{\Sigma}_j|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^{\mathrm{T}}\mathbf{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)\right\}$$

  - Mixture weights / mixture coefficients:

$p(j) = \pi_j$ with $0 \cdot \pi_j \cdot 1$ and $\sum_{j=1}^{M} \pi_j = 1$

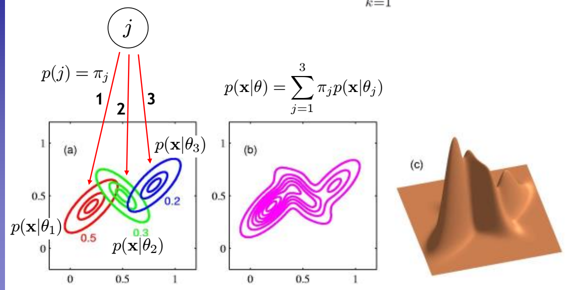
  - Parameters:

$$\theta = (\pi_1, \boldsymbol{\mu}_1, \mathbf{\Sigma}_1, \ldots, \pi_M, \boldsymbol{\mu}_M, \mathbf{\Sigma}_M)$$



Recap: Mixture of Multivariate Gaussians

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



Recap: ML for Mixtures of Gaussians

- Maximum Likelihood
  - Minimize $E = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(\mathbf{x}_n|\theta)$
  - We can already see that this will be difficult, since

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

This will cause problems!

Recap: ML for Mixture of Gaussians

- Minimization:

$$\boxed{\frac{\partial}{\partial \boldsymbol{\mu}_j} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_j)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}$$

$$\begin{aligned}
\frac{\partial E}{\partial \boldsymbol{\mu}_j} &= -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \boldsymbol{\mu}_j} p(\mathbf{x}_n|\theta_j)}{\sum_{k=1}^{K} p(\mathbf{x}_n|\theta_k)} \\
&= -\sum_{n=1}^{N} \left(\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_j) \frac{p(\mathbf{x}_n|\theta_j)}{\sum_{k=1}^{K} p(\mathbf{x}_n|\theta_k)} \right) \\
&= -\cancel{\boldsymbol{\Sigma}}^{-1} \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu}_j) \frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)} \stackrel{!}{=} 0
\end{aligned}$$

$= \gamma_j(\mathbf{x}_n)$

"responsibility" of component j for $\mathbf{x}_n$

- We thus obtain

$$\Rightarrow \boldsymbol{\mu}_j = \frac{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)\mathbf{x}_n}{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)}$$

Recap: ML for Mixtures of Gaussians

- But...

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

- I.e. there is no direct analytical solution!

$$\frac{\partial E}{\partial \boldsymbol{\mu}_j} = f(\pi_1, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \ldots, \pi_M, \boldsymbol{\mu}_M, \boldsymbol{\Sigma}_M)$$

  - Complex gradient function (non-linear mutual dependencies)
  - Optimization of one Gaussian depends on all other Gaussians!
  - It is possible to apply iterative numerical optimization here, but the EM algorithm provides a simpler alternative.

Recap: EM Algorithm

- Expectation-Maximization (EM) Algorithm
  - E-Step: softly assign samples to mixture components

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

  - M-Step: re-estimate the parameters (separately for each mixture component) based on the soft assignments

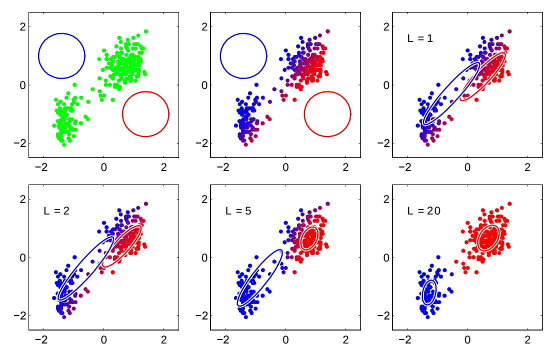
$$\hat{N}_j \leftarrow \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n) = \text{soft number of samples labeled } j$$

$$\hat{\pi}_j^{\text{new}} \leftarrow \frac{\hat{N}_j}{N}$$

$$\hat{\boldsymbol{\mu}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)\mathbf{x}_n$$

$$\hat{\boldsymbol{\Sigma}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})^{\mathrm{T}}$$

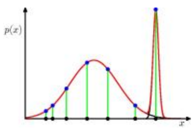
Recap: EM Algorithm - An Example



Recap: EM - Caveats

- When implementing EM, we need to take care to avoid singularities in the estimation!
  - Mixture components may collapse on single data points.
  - E.g. consider the case $\Sigma_k = \sigma_k^2 \mathbf{I}$ (this also holds in general)
  - Assume component j is exactly centered on data point $\mathbf{x}_n$. This data point will then contribute a term in the likelihood function

$$\mathcal{N}(\mathbf{x}_n|\mathbf{x}_n, \sigma_j^2 \mathbf{I}) = \frac{1}{\sqrt{2\pi}\sigma_j}$$



  - For $\sigma_j \rightarrow 0$, this term goes to infinity!

⇒ Need to introduce regularization
  - Enforce minimum width for the Gaussians

Image source: C.M. Bishop, 2006

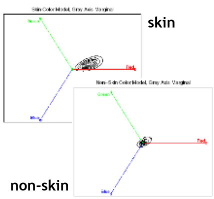
Application: Image Segmentation

(a) input image (b) user input (c) inferred segmentation

- User assisted image segmentation
  - User marks two regions for foreground and background.
  - Learn a MoG model for the color values in each region.
  - Use those models to classify all other pixels.
  - ⇒ Simple segmentation procedure (building block for more complex applications)

Application: Color-Based Skin Detection

- Collect training samples for skin/non-skin pixels.
- Estimate MoG to represent the skin/ non-skin densities



skin

non-skin

Classify skin color pixels in novel images

M. Jones and J. Rehg, Statistical Color Models with Application to Skin Detection, IJCV 2002.

Outlook for Today

- Criticism
  - This is all very nice, but in the ML lecture, the EM algorithm miraculously fell out of the air.
  - Why do we actually solve it this way?
- This lecture
  - We will take a more general view on EM
    - Different interpretation in terms of latent variables
    - Detailed derivation
  - This will allow us to derive EM algorithms also for other cases.
  - In particular, we will use it for estimating mixtures of Bernoulli distributions in the next lecture.

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Gaussian Mixtures as Latent Variable Model

- Mixture of Gaussians
  - Can be written as linear superposition of Gaussians in the form

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

- Let's write this in a different form…
  - Introduce a K-dimensional binary random variable $\mathbf{z}$ with a 1-of-K coding, i.e., $z_k = 1$ and all other elements are zero.
  - Define the joint distribution over $\mathbf{x}$ and $\mathbf{z}$ as

$$p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z})$$

  - This corresponds to the following graphical model:

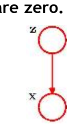


Image source: C.M. Bishop, 2006

Gaussian Mixtures as Latent Variable Models

- Marginal distribution over $\mathbf{z}$
  - Specified in terms of the mixing coefficients π_k, such that

$$p(z_k = 1) = \pi_k$$

where $0 \cdot \pi_j \cdot 1$ and $\sum_{j=1}^{K} \pi_j = 1.$

  - Since $\mathbf{z}$ uses a 1-of-K representation, we can also write this as

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

  - Similarly, we can write for the conditional distribution

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

Gaussian Mixtures as Latent Variable Models

- Marginal distribution of $\mathbf{x}$
  - Summing the joint distribution over all possible states of $\mathbf{z}$

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

- What have we gained by this?
  - The resulting formula looks still the same after all...
  - ⇒ 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...

Gaussian Mixtures as Latent Variable Models

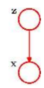
- Conditional probability of $\mathbf{z}$ given $\mathbf{x}$:
  - Use again the "responsibility" notation $\gamma_k(z_k)$

$$\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1) p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1) p(\mathbf{x}|z_j = 1)} = \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

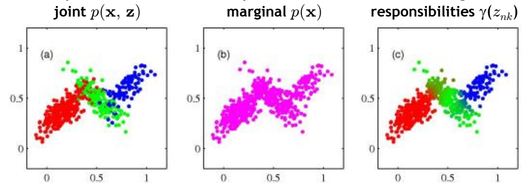
  - We can view π_k as the prior probability of $z_k = 1$ and $\gamma(z_k)$ as the corresponding posterior once we have observed $\mathbf{x}$.

Sidenote: 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 $\gamma(z_{nk})$



Alternative View of EM

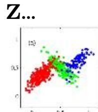
- Complementary view of the EM algorithm
  - The goal of EM is to find ML solutions for models having latent variables.
  - Notation
    - Set of all data $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_N]^T$
    - Set of all latent variables $\mathbf{Z} = [\mathbf{z}_1, \ldots, \mathbf{z}_N]^T$
    - Set of all model parameters $\boldsymbol{\theta}$
  - Log-likelihood function

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

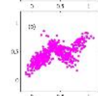
  - Key observation: summation inside logarithm ⇒ difficult.

Alternative View of EM

- Now, suppose we were told for each observation in $\mathbf{X}$ the corresponding value of the latent variable $\mathbf{Z}$...
  - Call $\{\mathbf{X}, \mathbf{Z}\}$ the complete data set and



refer to the actual observed data $\mathbf{X}$ as incomplete.



  - The likelihood for the complete data set now takes the form

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

  - ⇒ Straightforward to marginalize...

Alternative View of EM

- In practice, however,…
  - We are not given the complete data set $\{\mathbf{X}, \mathbf{Z}\}$, but only the incomplete data $\mathbf{X}$.
  - Our knowledge of the latent variable values in $\mathbf{Z}$ is given only by 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 θ^{new}.

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

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.

Remark: 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

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

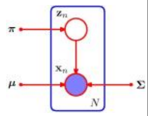
⇒ Suitable choices for the prior will remove the ML singularities!

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:

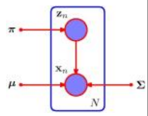


Image source: C.M. Bishop, 2006

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

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

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

  ⇒ 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):

$$\pi_k = \frac{1}{N} \sum_{n=1}^{N} z_{nk}$$

⇒ 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.

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

Gaussian Mixtures Revisited

- Continuing the estimation
  - The complete-data log-likelihood is therefore

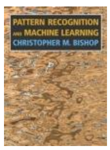
$$\mathbb{E}_{\mathbf{Z}}[\log p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi})] = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma z_{nk}\left\{\log \pi_k + \log \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}$$

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

References and Further Reading

- More information about EM and MoG 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