Mixture models and the EM algorithm

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Outline

Latent variable models

K-meansClustering

Mixture models

The EM algorithm

Latent variable models (LVMs)

- **Graphial model:** model dependence between two variables by adding an edge between them.
- **Latent variable:** assume that the observed variables are correlated because they arise from a hidden common "cause".
- **Pros 1**: LVMs have fewer parameters than models that directly represent correlation in the visible space.
- **Pros 2**: good for compression of x.
- **Cons**: Harder to fit than models with no latent variables.

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K-Means Objective: Compression

- Observed feature vectors: $\boldsymbol{x}_i \in \mathbb{R}^d, \quad i = 1, \ldots, N$.
- Hidden cluster labels: $z_i \in \{1, 2, \ldots, K\}, \quad i = 1, \ldots, N$.
- Hidden cluster centers: $\boldsymbol{\mu}_k \in \mathbb{R}^d, \quad k = 1, \ldots, K$.

$$J(\boldsymbol{z}, \boldsymbol{\mu} | \boldsymbol{x}, K) = \sum_{k=1}^{K} \sum_{i | z_i = k} \|\boldsymbol{x}_i - \boldsymbol{\mu}_k\|^2 = \sum_{i=1}^{N} \|\boldsymbol{x}_i - \boldsymbol{\mu}_{z_i}\|^2$$

$$J(\boldsymbol{z}, \boldsymbol{\mu} | \boldsymbol{x}, K) = \sum_{k=1}^{K} \sum_{i=1}^{N} z_{ik} \|\boldsymbol{x}_i - \boldsymbol{\mu}_k\|^2, \quad z_{ik} = \mathbb{I}(z_i = k)$$

- K-Means alternates between:
  - $\boldsymbol{z}^t = \operatorname{argmin}_{\boldsymbol{z}} J(\boldsymbol{z}, \boldsymbol{\mu}^{t-1} | \boldsymbol{x}, K)$
  - $\boldsymbol{\mu}^t = \operatorname{argmin}_{\boldsymbol{\mu}} J(\boldsymbol{z}^t, \boldsymbol{\mu} | \boldsymbol{x}, K)$

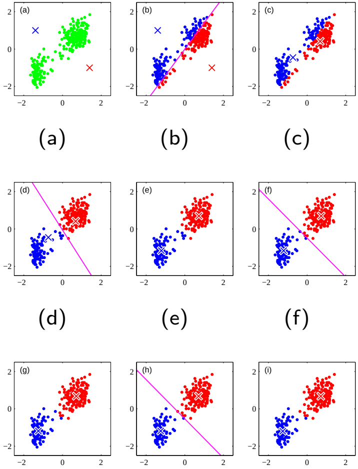
K-Means Algorithm

Objective function: $J(\boldsymbol{z}, \boldsymbol{\mu} | \boldsymbol{x}, K) = \sum_{k=1}^{K} \sum_{i=1}^{N} z_{ik} \|\boldsymbol{x}_i - \boldsymbol{\mu}_k\|^2$.

```
given Choose random cluster centers. $\boldsymbol{\mu}^{(0)}$.
repeat
    1. Assignment Step: $\boldsymbol{z}^t = \operatorname{argmin}_{\boldsymbol{z}} J(\boldsymbol{z}, \boldsymbol{\mu}^{t-1} | \boldsymbol{x}, K)$,    $z_i^{(t)} = \operatorname{argmin}_k \|\boldsymbol{x}_i - \boldsymbol{\mu}_k^{(t-1)}\|^2$.
    2. Mean Update Step: $\boldsymbol{\mu}^t = \operatorname{argmin}_{\boldsymbol{\mu}} J(\boldsymbol{z}^t, \boldsymbol{\mu} | \boldsymbol{x}, K)$,    $\boldsymbol{\mu}_k^{(t)} = \frac{1}{N_k^{(t)}} \sum_{i=1}^{N} z_{ik} \boldsymbol{x}_i$.
return $z_{ik}$.
```

Step 1: assign data to closest cluster centers, breaking ties arbitrarily.
Step 2: means of data assigned to each cluster center (least squares).

Illustration of K-Means



(a) (b) (c)

(d) (e) (f)

(g) (h) (i)

Figure: Illustration of the K-means algorithm using the re-scaled Old Faithful data set. Figure generated by `KmeansDemoFaithful`.

K-Means Implementation & Properties

Initialization: Choose random cluster centers $\boldsymbol{\mu}_{(0)}$

- Should be distinct (breaking symmetry) and in "region" of data.
- Common heuristic: Randomly pick K data points.
- K-Means++: Randomly pick K widely separated data points.

Theoretical Guarantees:

- Converges after finitely many iterations $z^{(t+1)} = z^{(t)}$.
- Worst-case convergence time poor (super-polynomial in N).
- Different initializations may produce very different solutions.
- Converged objective may be arbitrarily worse than optimum, but smart initializations (K-Means++) do allow some guarantees.
- In practice, can usually still find "useful" local optima.
- Optimal reconstruction error always decreases with $K, 0$ if $K = N$.

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Gaussian Mixture Models

- Observed feature vectors: $\boldsymbol{x}_i \in \mathbb{R}^d, \quad i = 1, \dots, N$.
- Hidden cluster labels: $z_i \in \{1, 2, \dots, K\}, \quad i = 1, \dots, N$.
- Hidden cluster centers: $\boldsymbol{\mu}_k \in \mathbb{R}^d, \quad k = 1, \dots, K$.
- Hidden mixture covariances: $\boldsymbol{\Sigma}_k \in \mathbb{R}^{d \times d}, \quad k = 1, \dots, K$.
- Hidden mixture probabilities: $\pi_k, \quad \sum_{i=1}^{K} \pi_k = 1$
- Gaussian mixture generative model:

$$
\begin{aligned}
p(z_i) &= \mathsf{Cat}(z_i | \boldsymbol{\pi}) \\
p(\boldsymbol{x}_i | z_i) &= N(\boldsymbol{x}_i | \boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}) \\
p(\boldsymbol{x}_i | \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) &= \sum_{z_i=1}^{K} \pi_{z_i} N(\boldsymbol{x}_i | \boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i})
\end{aligned}
$$

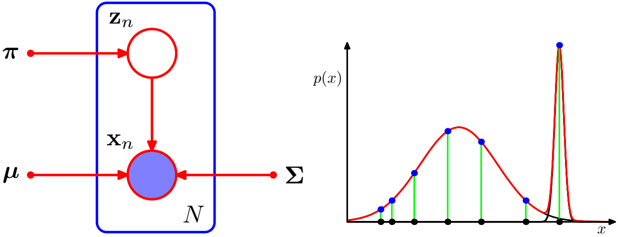
Unsupervised Learning

- Learning:

$$\operatorname*{argmax}_{\boldsymbol{\pi},\boldsymbol{\theta}} \log p(\boldsymbol{\pi}) + \log p(\boldsymbol{\theta}) + \sum_{i=1}^{N} \left[\sum_{z_i} p(z_i|\boldsymbol{\pi}) p(\boldsymbol{x}_i|z_i, \boldsymbol{\theta}) \right]$$

- No notion of training and test data: labels are never observed.
- As before, maximize posterior probability of model parameters.
- For hidden variables associated with each observation, we marginalize over possible values rather than estimating.
  - Fully accounts for uncertainty in these variables.
  - There is one hidden variable per observation, so cannot perfectly estimate even with infinite data.
- Must use generative model (discriminative degenerates).

Singularities: ML for Gaussian Mixtures



(a)

(b)

Figure: (a) Graphical representation of a Gaussian mixture model. (b) Illustration of how singularities in the likelihood function arise with mixtures of Gaussians.

Unsupervised Learning Algorithms

- Initialization: Randomly select starting parameters.
- Estimation: Given parameters, infer likely hidden data.
  - Similar to testing phase of supervised learning.
- Learning: Given hidden & observed data, find likely parameters.
  - Similar to training phase of supervised learning.
- Iteration: Alternate estimation & learning until convergence.

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Expectation Maximization (EM)

Goal: maximize the likelihood function $p(\boldsymbol{X}|\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$.

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

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

  where $Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\boldsymbol{Z}} p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})$
- Check for convergence of either the log likelihood or the parameter values. If the convergence criterion is not satisfied, then let

  $$\boldsymbol{\theta}^{\text{old}} \leftarrow \boldsymbol{\theta}^{\text{new}}$$

  and return to step 2.

Example: EM for Gaussian Mixtures

- Initialize the means $\boldsymbol{\mu}_k$, covariances $\boldsymbol{\Sigma}_k$ and mixing coefficients π_k, and evaluate the initial value of the log likelihood.
- **E step.** Evaluate the responsibilities using the current parameter values

$$\gamma(z_{ik}) = p(z_i = k|\boldsymbol{x}_i, \boldsymbol{\pi}, \boldsymbol{\theta}) = \frac{\pi_k N(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j N(\boldsymbol{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

- **M step.** Re-estimate the parameters using the current responsibilities

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{ik}) \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{ik}) (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^T$$

$$\pi_k^{\text{new}} = \frac{N_k}{N}$$

where $N_k = \sum_{n=1}^{N} \gamma(z_{ik})$.

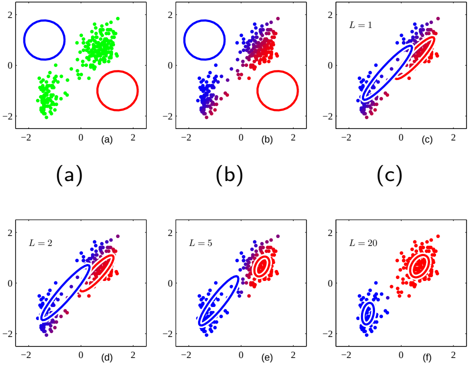
Example: EM for Gaussian Mixtures(cont'd)

- Evaluate the log likelihood

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

  and check for convergence of the parameters or the log likelihood. If the convergence criterion is not satisfied return to step 2.

Illustration of EM Algorithm for GGM



(a) (b) (c)

(d) (e) (f)

Figure: Illustration of the EM algorithm using the Old Faithful set. Figure generated by `MixGaussDemoFaithful`.

EM as Lower Bound Maximization

$$\ln p(\boldsymbol{x}|\boldsymbol{\theta}) = \ln(\sum_{\boldsymbol{z}} p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta}))$$

$$\ln p(\boldsymbol{x}|\boldsymbol{\theta}) \geq \sum_{\boldsymbol{z}} q(\boldsymbol{z}) \ln(\frac{p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta})}{q(\boldsymbol{z})}) \quad \text{(Jensen's Inequality)}$$

$$\ln p(\boldsymbol{x}|\boldsymbol{\theta}) \geq \sum_{\boldsymbol{z}} q(\boldsymbol{z}) \ln p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta}) - \sum_{\boldsymbol{z}} q(\boldsymbol{z}) \ln q(\boldsymbol{z}) = L(q, \boldsymbol{\theta})$$

- Initialization: Randomly select starting parameters $\boldsymbol{\theta}_{(0)}$.
- Estimation: Given parameters, infer likely hidden data.

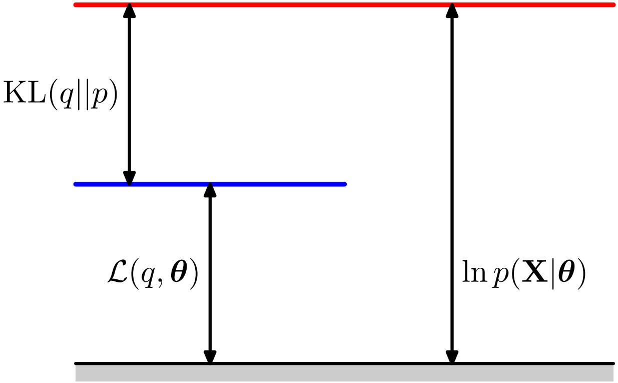
$$q^{(t)} = \underset{q}{\operatorname{argmax}}\, L(q, \boldsymbol{\theta}^{(t-1)})$$

- Learning: Given hidden & observed data, find likely parameters.

$$\boldsymbol{\theta}^{(t)} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, L(q^{(t)}, \boldsymbol{\theta})$$

- Iteration: Alternate estimation & learning until convergence.

Lower Bounds on Marginal Likelihood



$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$

EM: Expectation Step

$$\ln p(\boldsymbol{x}|\boldsymbol{\theta}) \geq \sum_{z} q(z) \ln p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta}) - \sum_{\boldsymbol{z}} q(\boldsymbol{z}) \ln q(\boldsymbol{z}) = L(q, \boldsymbol{\theta})$$

$$q^{(t)} = \operatorname*{argmax}_{q} L(q, \boldsymbol{\theta}^{(t-1)})$$

- General solution, for any probabilistic model

$$q^{(t)} = \operatorname*{argmax}_{q} L(q, \boldsymbol{\theta}^{(t-1)})$$

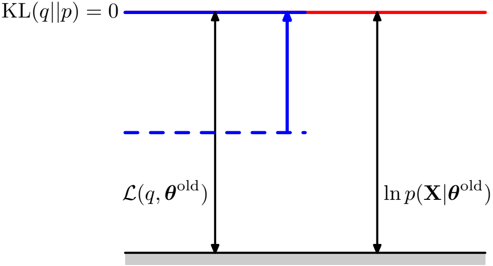
- For mixture models, data independent given parameters

$$p(z_i|\boldsymbol{\pi}) = \mathsf{Cat}(z_i|\boldsymbol{\pi})$$

$$p(\boldsymbol{x}_i|z_i, \boldsymbol{\theta}) = p(\boldsymbol{x}_i|\boldsymbol{\theta}_{z_i})$$

$$\gamma(z_{ik}) = p(z_i = k|\boldsymbol{x}_i, \boldsymbol{\pi}, \boldsymbol{\theta}) = \frac{\pi_k N(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j N(\boldsymbol{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

Illustration of the E step



$\mathrm{KL}(q||p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}})$

Figure: Illustration of the E step of the EM algorithm. The q distribution is set equal to the posterior distribution for the current parameter values $\boldsymbol{\theta}^{\text{old}}$, causing the lower bound to move up to the same value as the log likelihood function, with the KL divergence vanishing.

EM: Maximization Step

$$\ln p(\boldsymbol{x}|\boldsymbol{\theta}) \geq \sum_{\boldsymbol{z}} q(\boldsymbol{z}) \ln p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta}) - \sum_{\boldsymbol{z}} q(\boldsymbol{z}) \ln q(\boldsymbol{z}) = L(q, \boldsymbol{\theta})$$

$$\boldsymbol{\theta}^{(t)} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, L(q^{(t)}, \boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} = \sum_{\boldsymbol{z}} q(\boldsymbol{z}) \ln p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta})$$

- Unlike E-step, no simplified general solution.
- Applying to GMM

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{ik}) \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{ik}) (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^T$$

$$\pi_k^{\text{new}} = \frac{N_k}{N}$$

Illustration of the M step

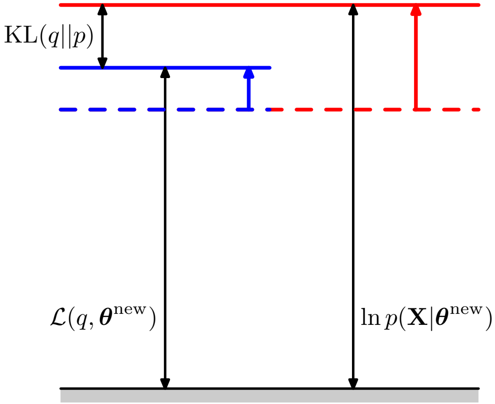

$\mathrm{KL}(q||p)$
$\mathcal{L}(q,\boldsymbol{\theta}^{\mathrm{new}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{new}})$

Figure: Illustration of the M step of the EM algorithm. The distribution $q(\boldsymbol{Z})$ is held fixed and the lower bound $L(q,\boldsymbol{\theta})$ is maximized with respect to the parameter vector $\boldsymbol{\theta}$ to give a revised value $\boldsymbol{\theta}^{\text{new}}$. Because the KL divergence is nonnegative, this causes the log likelihood $\ln p(\boldsymbol{X}|\boldsymbol{\theta})$ to increase by at least as much as the lower bound does.

EM: A Sequence of Lower Bounds

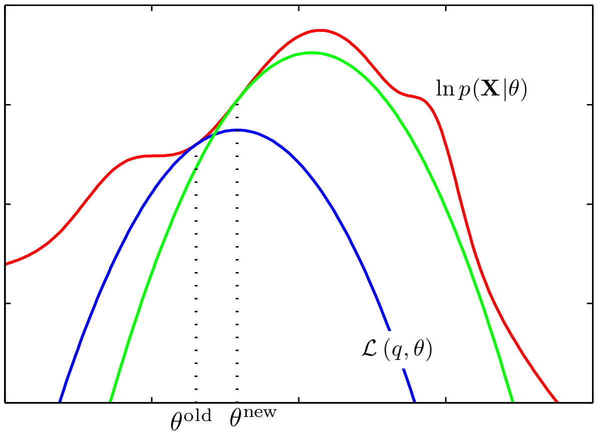


Figure: The EM algorithm involves alternately computing a lower bound on the log likelihood for the current parameter values and then maximizing this bound to obtain the new parameter values.