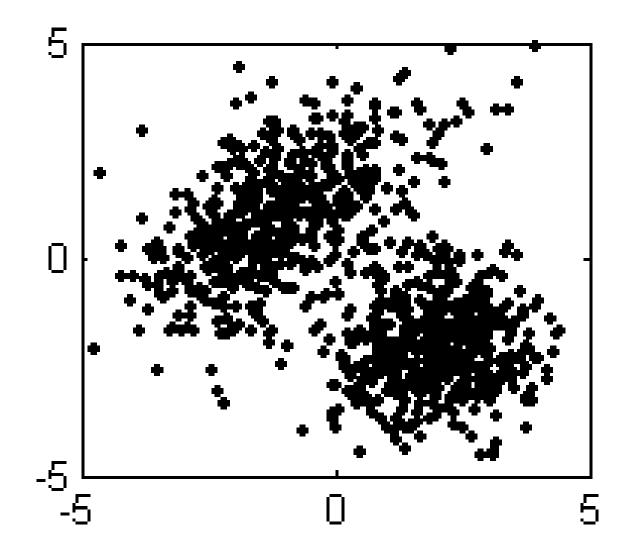
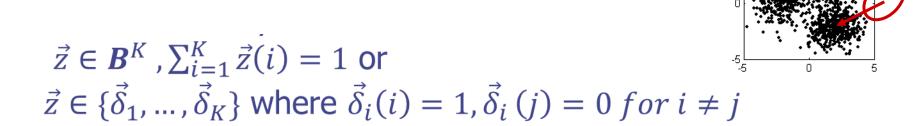
Machine Learning 4771

Instructor: Itsik Pe'er

Reminder: Mixture of Gaussians

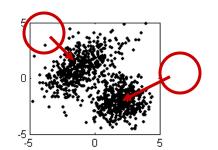


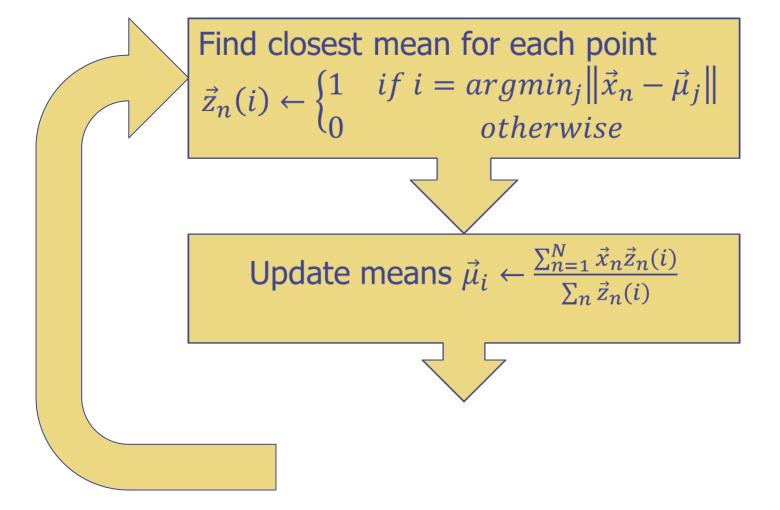
Kmeans: Notation Reminder

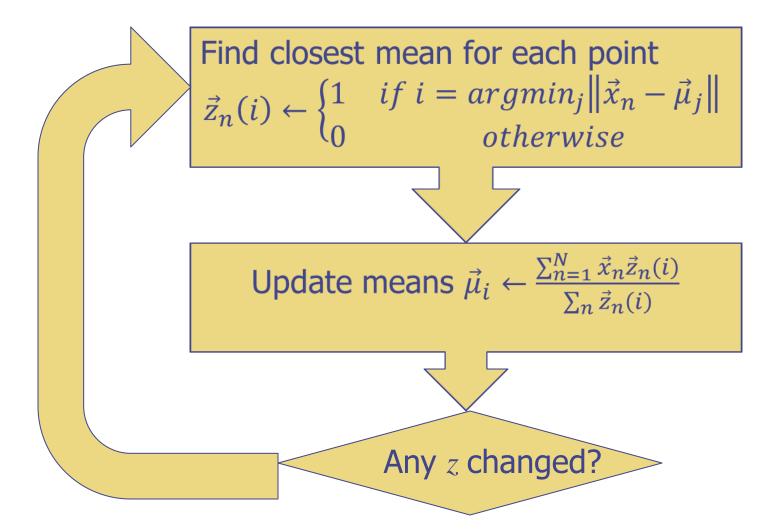


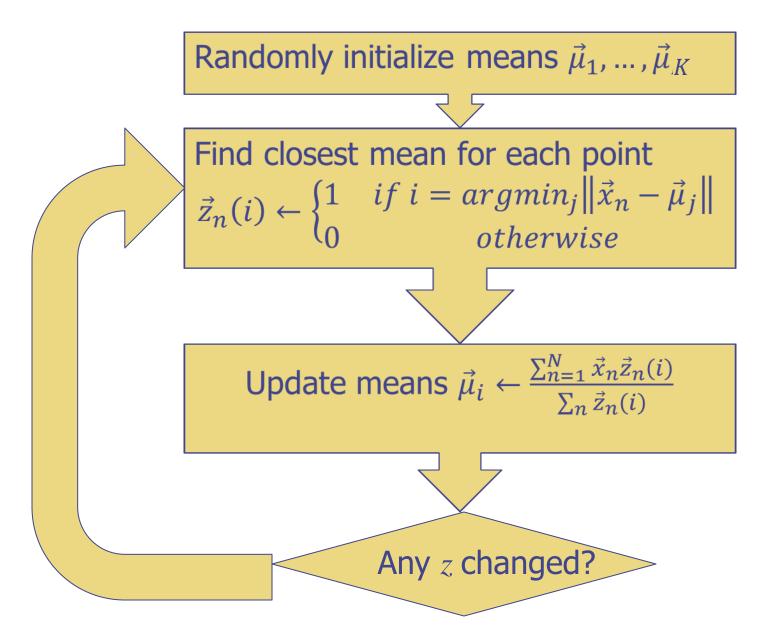
```
mixing proportions (prior) =\pi = p(\vec{z} = \vec{\delta}_i | \pi)
mixture components =p(\vec{x} | \vec{z} = \vec{\delta}_i, \theta)
posteriors (responsibilities) =\tau_{n,i} = p(\vec{z} = \vec{\delta}_i | \vec{x}_n, \theta) = \frac{p(\vec{x}_n | \vec{z} = \vec{\delta}_i, \theta)p(\vec{z} = \vec{\delta}_i | \theta)}{p(\vec{x}_n | \theta)}
```

- An old "heuristic" clustering algorithm
- Gobble up data with a divide & conquer scheme
- •Assume each point *x* has an discrete multinomial vector *z*
- •Chicken and Egg problem:
- If know classes, we can get model (max likelihood!)
- If know the model, we can predict the classes (classifier!)









- •Geometric, each point goes to closest Gaussian
- Recompute the means by their assigned points
- •Minimizing $\min_{n} J(\vec{\mu}_1, ..., \vec{\mu}_K, \vec{z}_1, ..., \vec{z}_N)$ cost function:

$$J(\vec{\mu}_1, \dots, \vec{\mu}_K, \vec{z}_1, \dots, \vec{z}_N) = \sum_{n=1}^{N} \sum_{i=1}^{K} \vec{z}_n(i) ||\vec{x}_n - \vec{\mu}_i||^2$$

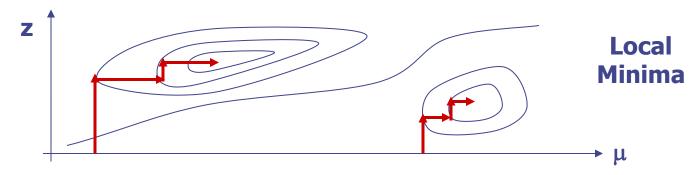
$$\vec{z}_n(i) = \begin{cases} 1 & \text{if } i = argmin_j ||\vec{x}_n - \vec{\mu}_j|| \\ 0 & \text{otherwise} \end{cases} \text{ and } \vec{\mu}_i = \frac{\sum_{n=1}^{N} \vec{x}_n \vec{z}_n(i)}{\sum_n \vec{z}_n(i)}$$

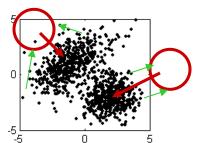
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- Guaranteed to improve per iteration and converge
- •Like Coordinate Descent (lock one var, maximize the other)
- A.k.a. Axis-Parallel Optimization or Alternating Minimization



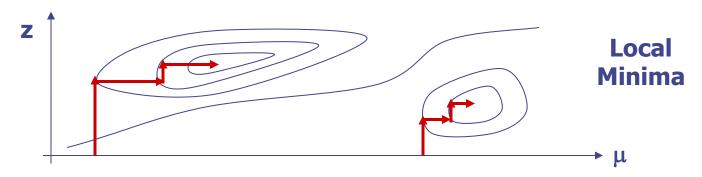


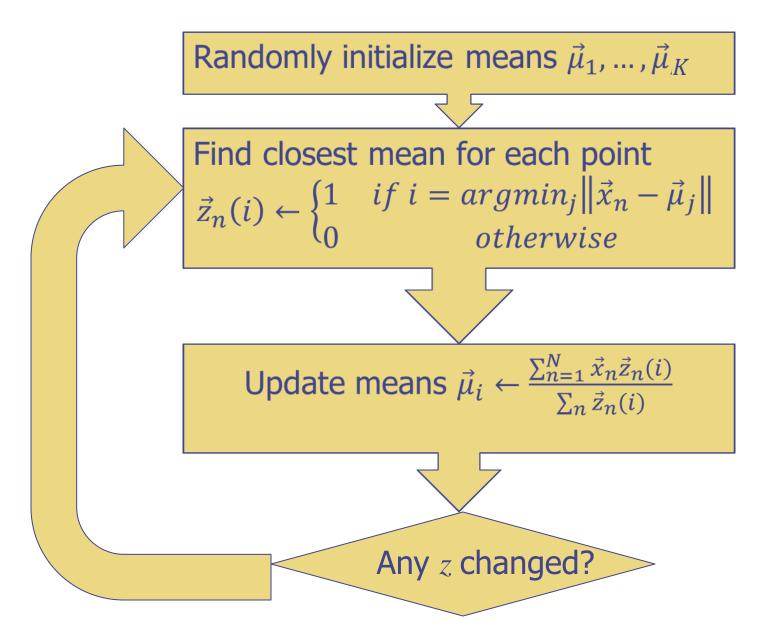
- •Geometric, each point goes to closest Gaussian
- Recompute the means by their assigned points
- •Minimizing $\min_{\mu,\Sigma} \min_{z} J(\vec{\mu}_1, ..., \vec{\mu}_K, \Sigma_1, ..., \Sigma_K, \vec{z}_1, ..., \vec{z}_N)$ cost:

$$J(\vec{\mu}_{1},...,\vec{\mu}_{K},\vec{z}_{1},...,\vec{z}_{N}) = \sum_{n=1}^{N} \sum_{i=1}^{K} \vec{z}_{n}(i) (\vec{x}_{n} - \vec{\mu}_{i})^{T} \Sigma^{-1} (\vec{x}_{n} - \vec{\mu}_{i})$$

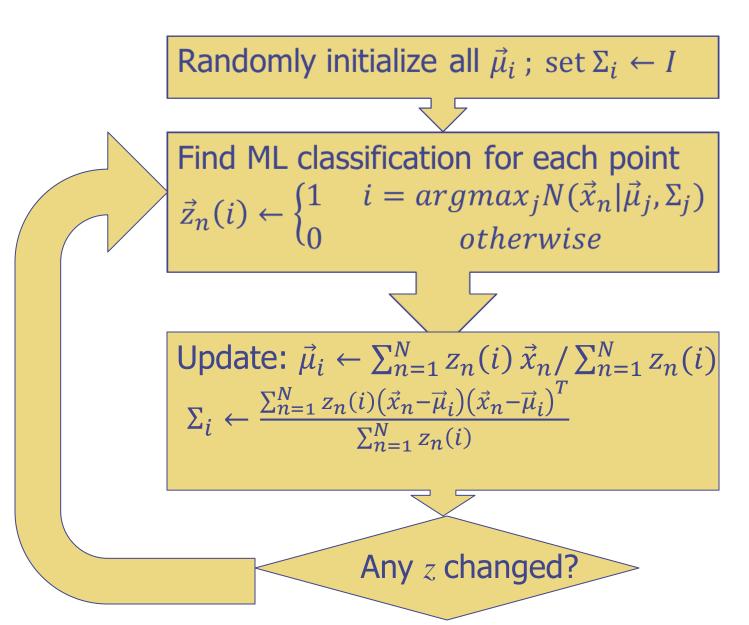
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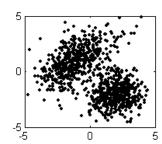


The Gaussian K-Means Algorithm



Kmeans—Expectation Maximization

At each stage of K-means, an element chooses the most likely (responsible) cluster



Hedging allows smoother optimization surface

Take expectation over responsible cluster

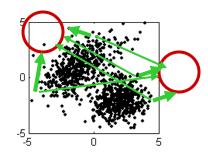
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•EM is a soft/fuzzy version of K-Means (which does winner-takes-all, closest Gaussian Mean completely wins datapoint)

$$\vec{z}_n(i) = \begin{cases} 1 & i = argmax_j N(\vec{x}_n | \vec{\mu}_j, \Sigma_j) \\ 0 & otherwise \end{cases}$$

 Instead, consider soft percentage assignment of datapoint (responsibility)



$$\tau_{n,i} = p(\vec{z}_n = \vec{\delta}(j) | \vec{x}_n, \theta) \propto \pi_j \frac{\exp\left(-\frac{1}{2}(\vec{x}_n - \vec{\mu}_j)^T \Sigma^{-1}(\vec{x}_n - \vec{\mu}_j)\right)}{(2\pi)^{\frac{D}{2}}\sqrt{|\Sigma|}}$$

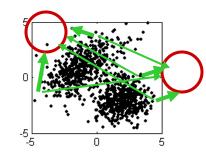
$$\tau_{n,1}, \dots, \tau_{n,K} = \begin{bmatrix} 0.8 & 0.8 & 0.6 & 0.4 & 0.2 \\ 0.2 & 0.4 & 0.2 & 0 \end{bmatrix}$$

Update for the means are then

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Update for the means are then

'weighted' by responsibilities:
$$\vec{\mu}_i = \frac{\sum_{n=1}^N \tau_{n,i} \vec{x}_n}{\sum_n \tau_{n,i}}$$

Same for other parameters

•EM uses expected value of $\vec{z}_n(i)$ rather than max

$$\tau_{n,i} = E\{\vec{z}_n(i)|\vec{x}_n\} = p(\vec{z}_n = \vec{\delta}(j)|\vec{x}_n, \theta)$$

- •EM updates covariances, mixing proportions AND means...
- •The algorithm for Gaussian mixtures:

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$$\tau_{n,i}^{(t)} \leftarrow$$

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$$\rightarrow \text{EXPECTATION: } \tau_{n,i}^{(t)} \leftarrow \frac{\pi_i^{(t)} N\left(\vec{x}_n \middle| \vec{\mu}_i^{(t)}, \Sigma_i^{(t)}\right)}{\sum_j \pi_j^{(t)} N\left(\vec{x}_n \middle| \vec{\mu}_j^{(t)}, \Sigma_j^{(t)}\right)}$$

MAXIMIZATION:
$$\vec{\mu}_i^{(t+1)} \leftarrow \frac{\sum_{n=1}^N \tau_{n,i}^{(t)} \vec{x}_n}{\sum_n \tau_{n,i}^{(t)}}$$

$$\Sigma_i^{(t+1)} \leftarrow$$

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$$\tau_{n,i} = E\{\vec{z}_n(i)|\vec{x}_n\} = p(\vec{z}_n = \vec{\delta}(j)|\vec{x}_n, \theta)$$

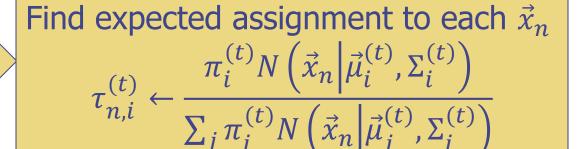
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$$\begin{array}{c}
\text{MAXIMIZATION: } \vec{\mu}_{i}^{(t+1)} \leftarrow \frac{\sum_{n=1}^{N} \tau_{n,i}^{(t)} \vec{x}_{n}}{\sum_{n} \tau_{n,i}^{(t)}} \quad \pi_{i}^{(t+1)} \leftarrow \frac{\sum_{n} \tau_{n,i}^{(t)}}{N} \\
\sum_{i} \tau_{n,i}^{(t+1)} \leftarrow \frac{\sum_{n=1}^{N} \tau_{n,i}^{(t)} (\vec{x}_{n} - \vec{\mu}_{i}^{(t+1)})^{T} (\vec{x}_{n} - \vec{\mu}_{i}^{(t+1)})}{\sum_{n} \tau_{n,i}^{(t)}}
\end{array}$$

The EM Clustering Algorithm

Initialize: random
$$\vec{\mu}_i^{(1)}$$
, $\Sigma_i^{(1)} = I$, $\pi_i^{(1)} = \frac{1}{K}$



Expectation

Update
$$\vec{\mu}_{i}^{(t+1)} \leftarrow \sum_{n=1}^{N} \tau_{n,i}^{(t)} \vec{x}_{n} / \sum_{n=1}^{N} \tau_{n,i}^{(t)}$$

$$\sum_{i}^{(t+1)} \leftarrow \frac{\sum_{n=1}^{N} \tau_{n,i}^{(t)} (\vec{x}_{n} - \vec{\mu}_{i}^{(t+1)}) (\vec{x}_{n} - \vec{\mu}_{i}^{(t+1)})^{T}}{\sum_{n=1}^{N} \tau_{n,i}^{(t)}}$$

$$\pi_{i}^{(t+1)} \leftarrow \sum_{n=1}^{N} \tau_{n,i}^{(t)} / N$$

Little changed?

Maximization

The EM Clustering Algorithm

Initialize: random
$$\vec{\mu}_i^{(1)}$$
, $\Sigma_i^{(1)} = I$, $\pi_i^{(1)} = \frac{1}{K}$

Find expected assignment to each \vec{x}_n $\tau_{n,i}^{(t)} \leftarrow E\{\vec{z}_n(i)\}$

Expectation

Update

$$\vec{\mu}_{i}^{(t+1)} \leftarrow argmax_{\mu^{*}} E_{\vec{z}} \{ l(\theta, z s.t. \vec{\mu}_{i} = \mu^{*}) \}$$

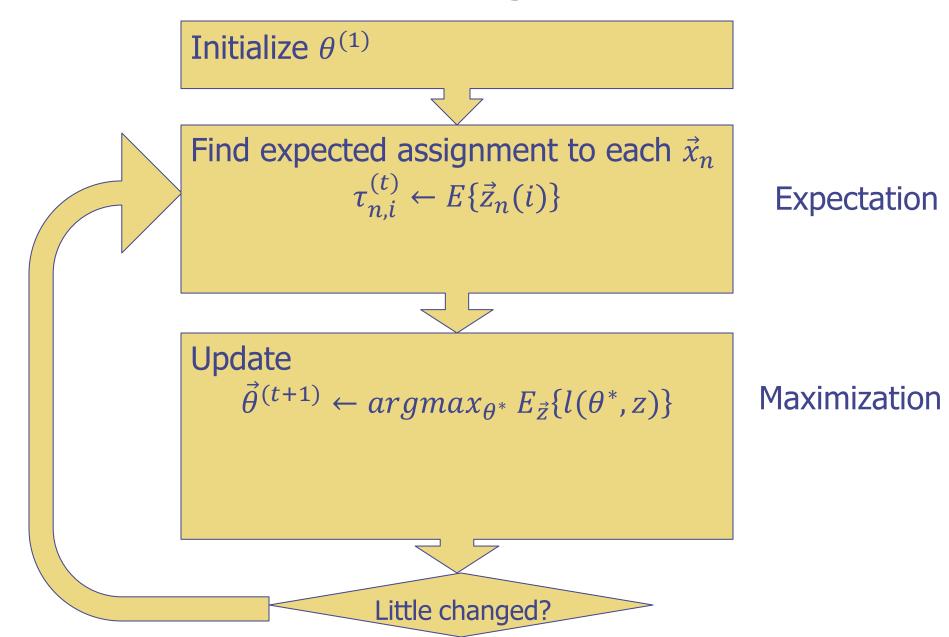
$$\Sigma_{i}^{(t+1)} \leftarrow argmax_{\Sigma^{*}} E_{\vec{z}} \{ l(\theta, z s.t. \Sigma_{i} = \Sigma^{*}) \}$$

$$\pi_{i}^{(t+1)} \leftarrow argmax_{\pi^{*}} E_{\vec{z}} \{ l(\theta, z s.t. \pi_{i} = \pi^{*}) \}$$

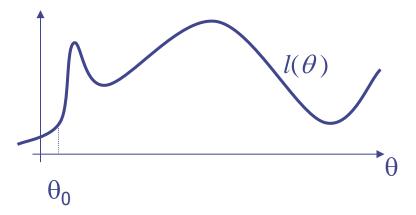
Maximization

Little changed?

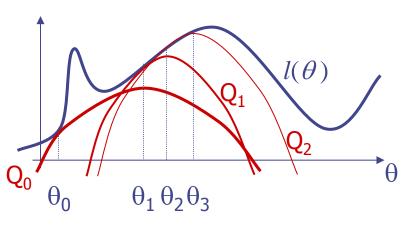
The General EM Algorithm



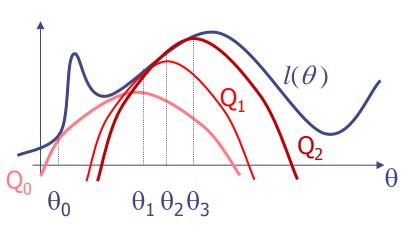
- Let's now show that EM indeed maximizes likelihood
- •Bound Maximization: optimize a lower bound on $l(\theta)$
- •Since log-likelihood $l(\theta)$ not concave, can't max it directly
- •Consider an auxiliary function $Q(\theta)$ which is concave
- $Q(\theta)$ kisses $l(\theta)$ at a point and is less than it elsewhere



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$$\forall \theta \forall t: \ l(\theta) \geq Q_t(\theta)$$

$$l(\theta_t) = Q_t(\theta_t)$$

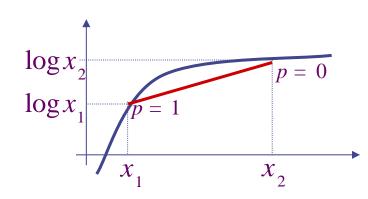
$$Q_t(\theta_{t+1}) > Q_t(\theta_t)$$
 because $\theta_{t+1} = \arg\max_{\theta} Q_t(\theta)$
$$l(\theta_{t+1}) \geq Q_t(\theta_{t+1}) > Q_t(\theta_t) = l(\theta_t)$$

- Monotonically increases log-likelihood
- •But how to find a bound and guarantee we max it?

Jensen's Inequality



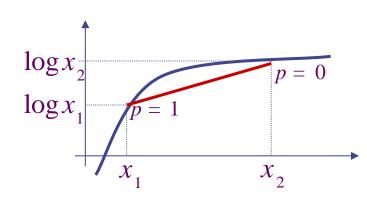
- •Example: f(x) = log(x) =concave and M = 2 $log(px_1 + (1 - p)x_2) \ge p log x_1 + (1 - p) log x_2$
- Bound log(sum) with sum(log)



Jensen's Inequality



- Expectation in discrete case is sum weight by probability
- •For convex f: $f\left(\sum_{i=1}^{M} p_i x_i\right) \leq \sum_{i=1}^{M} p_i f(x_i)$ when $\sum_{i=1}^{M} p_i = 1$, $p_i \geq 0$
- •For concave $f: f\left(\sum_{i=1}^{M} p_i x_i\right) \ge \sum_{i=1}^{M} p_i f(x_i)$ when $\sum_{i=1}^{M} p_i = 1$, $p_i \ge 0$
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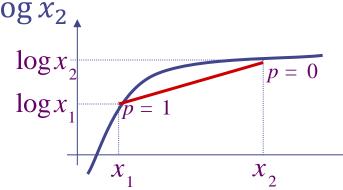


Jensen's Inequality

- •An important general bound from Jensen (1906)
- •For convex f: $f(E\{x\}) \le E\{f(x)\}$
- •For concave f: $f(E\{x\}) \ge E\{f(x)\}$
- Expectation in discrete case is sum weight by probability
- •For convex f: $f\left(\sum_{i=1}^{M} p_i x_i\right) \leq \sum_{i=1}^{M} p_i f(x_i)$ when $\sum_{i=1}^{M} p_i = 1$, $p_i \geq 0$
- •For concave $f: f\left(\sum_{i=1}^{M} p_i x_i\right) \ge \sum_{i=1}^{M} p_i f(x_i)$ when $\sum_{i=1}^{M} p_i = 1$, $p_i \ge 0$
- •Example: f(x) = log(x) =concave and M=2

$$\log(px_1 + (1-p)x_2) \ge p\log x_1 + (1-p)\log x_2$$

- Bound log(sum) with sum(log)
- •How to apply this to mixture models?



$$l(\theta) =$$

$$l(\theta) = \sum_{n=1}^{N} \log p(x_n | \theta)$$
 Original Log-Likelihood
$$= \sum_{n=1}^{N} \log \sum_{z} p(x_n, z | \theta)$$
 Has Hidden Variables (messy)
$$= \sum_{n=1}^{N} \log \sum_{z} p(x_n, z | \theta) \frac{p(z | x_n, \theta_t)}{p(z | x_n, \theta_t)}$$
 Posterior density
$$= \sum_{n=1}^{N} \log \sum_{z} p(z | x_n, \theta_t) \frac{p(x_n, z | \theta)}{p(z | x_n, \theta_t)}$$
 Rearrange

called Q (not messy)

Expectation-Maximization

•Now have the following bound and maximize it: $l(\theta) \ge$

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$$l(\theta) \ge Q(\theta|\theta_t) - \sum_{n=1}^N \sum_z p(z|x_n, \theta_t) \log p(z|x_n, \theta_t)$$

$$\theta_{t+1} = \arg \max Q(\theta|\theta_t) = \arg \max \sum_{n=1}^N \sum_z p(z|x_n, \theta_t) \log p(x_n, z|\theta_t)$$

- = $\arg \max \sum_{n=1}^{N} \sum_{z} \tau_{n,z} \log p(x_n, z | \theta_t)$
- • $Q(\theta | \theta_t)$ is called Auxiliary Function... take derivatives of it
- •This is easy for many functions... just weighted max likelihood!
- •For example, Gaussian mixture:

$$\frac{\partial Q(\theta)}{\partial \overrightarrow{\mu}_k} =$$

•Now have the following bound and maximize it:

$$l(\theta) \geq Q(\theta|\theta_t) - \sum_{n=1}^N \sum_z p(z|x_n,\theta_t) \log p(z|x_n,\theta_t)$$

$$\theta_{t+1} = \arg\max Q(\theta|\theta_t) = \arg\max \sum_{n=1}^{\infty} \sum_{z} p(z|x_n, \theta_t) \log p(x_n, z|\theta_t)$$

- = $\arg \max \sum_{n=1}^{N} \sum_{z} \tau_{n,z} \log p(x_n, z | \theta_t)$
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$$\frac{\partial Q(\theta)}{\partial \vec{\mu}_k} = \frac{\partial}{\partial \vec{\mu}_k} \sum_{n=1}^{N} \sum_{j=1}^{K} \tau_{n,k} \log \pi_k N(\vec{x}_n | \vec{\mu}_k, \Sigma_k)$$

$$0 = \sum_{n=1}^{N} \tau_{n,k} \frac{\partial}{\partial \vec{\mu}_{k}} \left(-\frac{1}{2} (\vec{x}_{n} - \vec{\mu}_{k})^{T} \Sigma^{-1} (\vec{x}_{n} - \vec{\mu}_{k}) \right)$$

$$\vec{\mu}_k = \frac{\sum_{n=1}^N \tau_{n,k} \vec{x}_n}{\sum_{n=1}^N \tau_{n,k}}$$
 ... similarly get π_k and Σ_k

•Incomplete Log-Likelihood

Complete Log-Likelihood

Incomplete Log-Likelihood

$$l(\theta) = \log p(observed|\theta) = \sum_{n=1}^{N} \log \sum_{z} p(x_n, z_n|\theta)$$

Complete Log-Likelihood

$$l(\theta) = \log p(observed, hidden|\theta) = \sum_{n=1}^{N} \log p(x_n, z_n|\theta)$$

- •We don't know the hidden variables z
- •EM computes expected values of hidden z under current θ_t
- •EM chooses Q to be the Expected Complete Log-Likelihood

Incomplete Log-Likelihood

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- Incomplete Log-Likelihood
- $l(\theta) = \log p(observed|\theta) = \sum_{n=1}^{N} \log \sum_{z} p(x_n, z_n|\theta)$
- Complete Log-Likelihood
- $l(\theta) = \log p(observed, hidden|\theta) = \sum_{n=1}^{N} \log p(x_n, z_n|\theta)$
- We don't know the hidden variables z
- •EM computes expected values of hidden z under current θ_t
- •EM chooses Q to be the Expected Complete Log-Likelihood

$$E\{l^{c}(\theta)\} = \sum_{hidden} p(hidden|observed, \theta_{t})l^{c}(\theta)$$

$$= \sum_{z_1} \sum_{z_2} ... \sum_{z_N} p(z_1, ..., z_N | x_1, ..., x_N, \theta_t) l^c(\theta)$$

$$= \sum_{z_1} \sum_{z_2} \dots \sum_{z_N} \prod_n p(z_n | x_n, \theta_t) l^c(\theta)$$

$$= \sum_{z_1} \sum_{z_2} \dots \sum_{z_N} \prod_n p(z_n | x_n, \theta_t) \sum_n \log p(x_n, z_n | \theta)$$

$$= \sum_n \sum_{z_n} p(z_n|x_n,\theta_t) \log p(x_n,z_n|\theta) \sum_{z_1} \dots \sum_{z_{i\neq n}} \dots \sum_{z_N} \prod_{i\neq n} p(z_i|x_i,\theta_t)$$

$$= \sum_{n} \sum_{n} p(z_n | x_n, \theta_t) \log p(x_n, z_n | \theta) = Q(\theta | \theta_t)$$

Summary

- Mixture Models and Hidden Variables
- Clustering
- K-Means
- Expectation Maximization

Happy Spring Break!