ANLY-601
Advanced Pattern Recognition

Spring 2018

L12 – Mixture Density Models, EM Algorithm

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Mixture Density Models

- Flexible models – able to fit lots of densities
- Fit parameters by maximum likelihood. Nonlinear equations require iterative fitting procedure. Standard is Expectation – Maximization (EM).
- “Soft” version of clustering.

General form is $p(x\,|\,\Theta) = \sum_{j=1}^{k} \alpha_j \; p(x\,|\,j)$

$p(x\,|\,j) \equiv p(x\,|\,\theta_j)$ are component densities with parameter (vectors) θ_j

$\Theta \equiv \left(\alpha_1,\ldots,\alpha_k,\ \theta_1,\ \theta_k\ \right)$

$\alpha_j \geq 0, \qquad \sum_{j=1}^{k} \alpha_j \; = 1 \qquad\qquad \alpha_j$ is prior probability for mixture component j

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Generative Model

Mixture model form $p(x \mid \Theta) = \sum_{j=1}^{k} \alpha_j \; p(x \mid j)$

$p(x \mid j) \equiv p(x \mid \theta_j)$ are component densities with parameter (vectors) θ_j

$\Theta \equiv (\alpha_1, \ldots, \alpha_k, \theta_1, \ldots, \theta_k)$

$\alpha_j \geq 0, \quad \sum_{j=1}^{k} \alpha_j = 1 \quad \alpha_j$ is prior probability for mixture component j

Generating *x* is a two-fold sampling procedure:

1. Pick a component density with probability α_j
2. Generate a sample *x* from *p(x | j)*

Mixture Models

Most common example is mixture of Gaussians

$$p(x \mid \Theta) = \sum_{j=1}^{k} \alpha_j \; p(x \mid j)$$

with

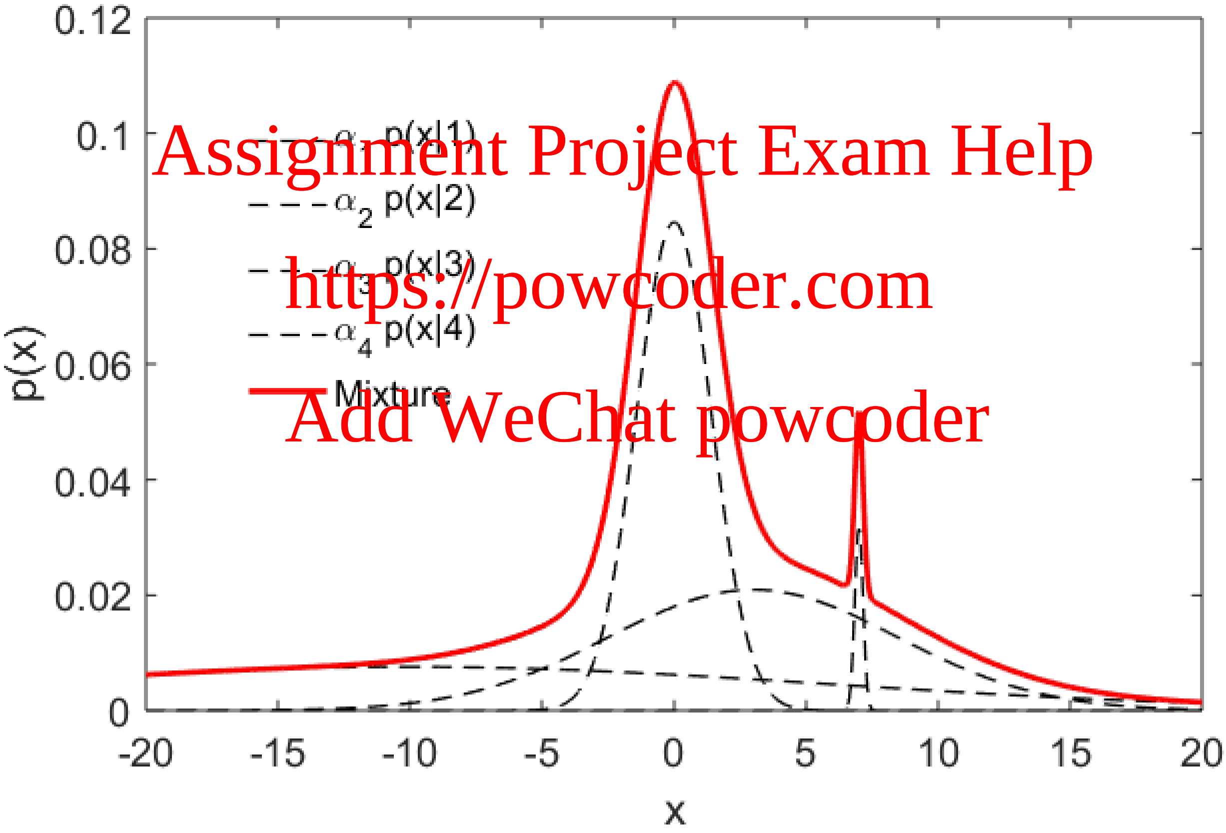
$$p(x \mid j) = \frac{1}{\sqrt{(2\pi)^n \left|\Sigma_j\right|}} \exp\left(\tfrac{-1}{2} \; (x - \mu_j)^T \; \Sigma_j^{-1} \; (x - \mu_j) \right)$$

There's a universal approximation theorem[1] for such mixtures that states that with enough components, a mixture of Gaussians fit by maximum likelihood can arbitrarily closely match any density on a compact subset of R^n.

1. Jonathan Li and Andrew Barron. Mixture Density Estimation, in Solla, Leen, and Mueller (eds.) *Advances in Neural Information Processing Systems 12*, The MIT Press, 2000.

Gaussian Mixture Model

Flexible --- can make lots of shapes!



Fitting Mixture Models

Suppose we have a data set

$$D = \{ x_a \ , \ a = 1, \ldots, N \} \quad \text{with each } x_a \text{ a vector in } R^n$$

we'd like to adjust the parameters

$$\Theta \equiv (\alpha_1, \ldots, \alpha_k, \theta_1, \ldots, \theta_k)$$

so as to maximize the data log likelihood

$$L(\Theta) = \ln P(D \mid \Theta) = \sum_{a=1}^{N} \ln \left(\sum_{j=1}^{k} \alpha_j \ p(x_a \mid \theta_j) \right)$$

Fitting Mixture Models

The data log likelihood

$$L(\Theta) = \ln P(D \mid \Theta) = \sum_{a=1}^{N} \ln\left(\sum_{j=1}^{k} \alpha_j \; p(x_a \mid \theta_j) \right)$$

cannot be maximized in one step --- the maximization equations don't have a closed form solution.

Instead, use an iterative approach --- the *EM* algorithm

For the moment, rewrite the log-likelihood as (suppressing the mixture form of $p(x|\Theta)$)

$$L(\Theta) = \ln P(D \mid \Theta) = \sum_{a=1}^{N} \ln p(x_a \mid \Theta) = \sum_{a=1}^{N} \ln\left(\sum_{i_a=1}^{k} p(i_a, x_a \mid \Theta) \right)$$

where i_a is the <u>unknown</u> index of the component responsible for generating x_a.

Fitting Mixture Models

Next, we write a lower bound for *L*. Introduce an average over <u>any</u> probability distribution on the unknown indices i_a , $Q(i_a)$

$$L = \sum_{a=1}^{N} \ln p\left(x_a \mid \Theta\right) = \sum_{a=1}^{N} \ln \left\{ \sum_{i_a=1}^{k} p(i_a, x_a \mid \Theta) \right\} = \sum_{a=1}^{N} \ln \left\{ \sum_{i_a=1}^{k} Q(i_a) \frac{p(i_a, x_a \mid \Theta)}{Q(i_a)} \right\}$$

Jensen's inequality gives:

$$L = \sum_{a=1}^{N} \ln \left\{ \sum_{i_a=1}^{k} Q(i_a) \frac{p(i_a, x_a)}{Q(i_a)} \right\} \geq \sum_{a=1}^{N} \sum_{i_a=1}^{k} \left(Q(i_a) \ln \frac{p(i_a, x_a)}{Q(i_a)} \right)$$

$$= \sum_{a=1}^{N} \sum_{i_a=1}^{k} Q(i_a) \ln p(i_a, x_a) - \sum_{a=1}^{N} \sum_{i_a=1}^{k} Q(i_a) \ln Q(i_a) \equiv \Gamma(\Theta)$$

The equality holds when $Q(i_a)$ is the posterior distribution on the unknown indices

$$Q(i_a) = p(i_a \mid x_a , \Theta)$$

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EM Algorithm

Iterative optimization algorithm: Expectation Maximization (EM) maximizes Γ (which maximizes *L).* There are multiple optima, EM only finds a local optimum.

Initialize the algorithm to some choice of the parameters. At the n+1th iteration :

E Step: With Θ fixed at $\Theta(n)$, estimate the index distribution as

$$Q_{n+1}(i_a) = h_{i,a}(n+1) \equiv p(i|x_a, \Theta(n)) = \frac{\alpha_i(n)\ p\left(x_a|\theta_i(n)\right)}{\sum_{j=1}^{k} \alpha_j(n)\ p\left(x_a|\theta_j(n)\right)}$$

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EM

M Step: With $Q = h_{i,a}(n+1)$ fixed, maximize Γ with respect to Θ

$$\Theta(n+1) = \arg\max_{\Theta} \Gamma\big(\Theta, h_{i,a}(n+1)\big) = \arg\max_{\Theta} \sum_{a=1}^{N}\sum_{i=1}^{k} h_{i,a}(n+1)\ \ln\ \big(\alpha_i\ \ p\big(x_a\,|\,\theta_i\big)\big)$$

subject to the condition $\sum_{i=1}^{k} \alpha_i = 1$

This gives

$$\boxed{\alpha_i(n+1) = \frac{1}{N}\sum_{a=1}^{N} h_{ia} = \frac{1}{N}\sum_{a=1}^{N} p(i\ |\ x_a\,,\,\Theta(n))}$$

for the α_i $i=1,\ldots k$

EM

<u>M Step </u> (continued) With $Q = h_{ia}(n+1)$ fixed,
maximize $\Gamma(\Theta,h)$ with respect to the θ_j

$$\Theta(n+1) = \arg\max_{\Theta} \Gamma\left(\Theta, h_{i,a}(n+1)\right) = \arg\max_{\Theta} \sum_{a=1}^{N} \sum_{i=1}^{k} h_{i,a}(n+1) \ln \left(\alpha_i \; p\left(x_a \,|\, \theta_i\right)\right)$$

Maximize Γ with respect to each θ_j (e.g. set $\nabla_{\theta_j}\Gamma = 0$)
separately, so the above reduces to

$$\boxed{\theta_j(n+1) = \arg\max_{\theta_j} \sum_{a=1}^{N} h_{j,a}(n+1) \ln \left(\alpha_j \, p(x_a \,|\, \theta_j)\right)}$$

Example – Mixture of Gaussians

Component densities $$p(x\,|\,\theta_j) = \frac{1}{\sqrt{(2\pi)^n \,|\Sigma_i|}} \exp -\tfrac{1}{2}(x-\mu_i)^T \Sigma_i^{-1} (x-\mu_i)$$

E-Step $$h_{a,i}(n+1) \equiv p(i_a \,|\, x_a, \Theta(n)) = \frac{\alpha_i(n)\; p(x_a\,|\,\theta_i(n))}{\sum_{j=1}^{k} \alpha_j(n)\; p(x_a\,|\,\theta_j(n))}$$

M-Step

$$\alpha_i(n+1) = \frac{1}{N}\sum_{a=1}^{N} h_{i,a}(n+1) \qquad \mu_i(n+1) = \frac{\sum_{a=1}^{N} h_{i,a}(n+1)\; x_a}{\sum_{a} h_{i,a}(n+1)}$$

$$\Sigma_i(n+1) = \frac{\sum_{a=1}^{N} h_{i,a}(n+1)\,\big(x_a - \mu_i(n+1)\big)\big(x_a - \mu_i(n+1)\big)^T}{\sum_{a} h_{i,a}(n+1)}$$

Gaussian Mixtures

Let's interpret equations for the M-Step

$$\alpha_i(n+1) = \frac{1}{N}\sum_{a=1}^{N} h_{i,a}(n+1)$$

New estimate of prior for ith component is the average over the data points of the posteriors for ith component.

$$\mu_i(n+1) = \frac{\sum_{a=1}^{N} h_{i,a}(n+1)\; x_a}{\sum_a h_{i,a}(n+1)}$$

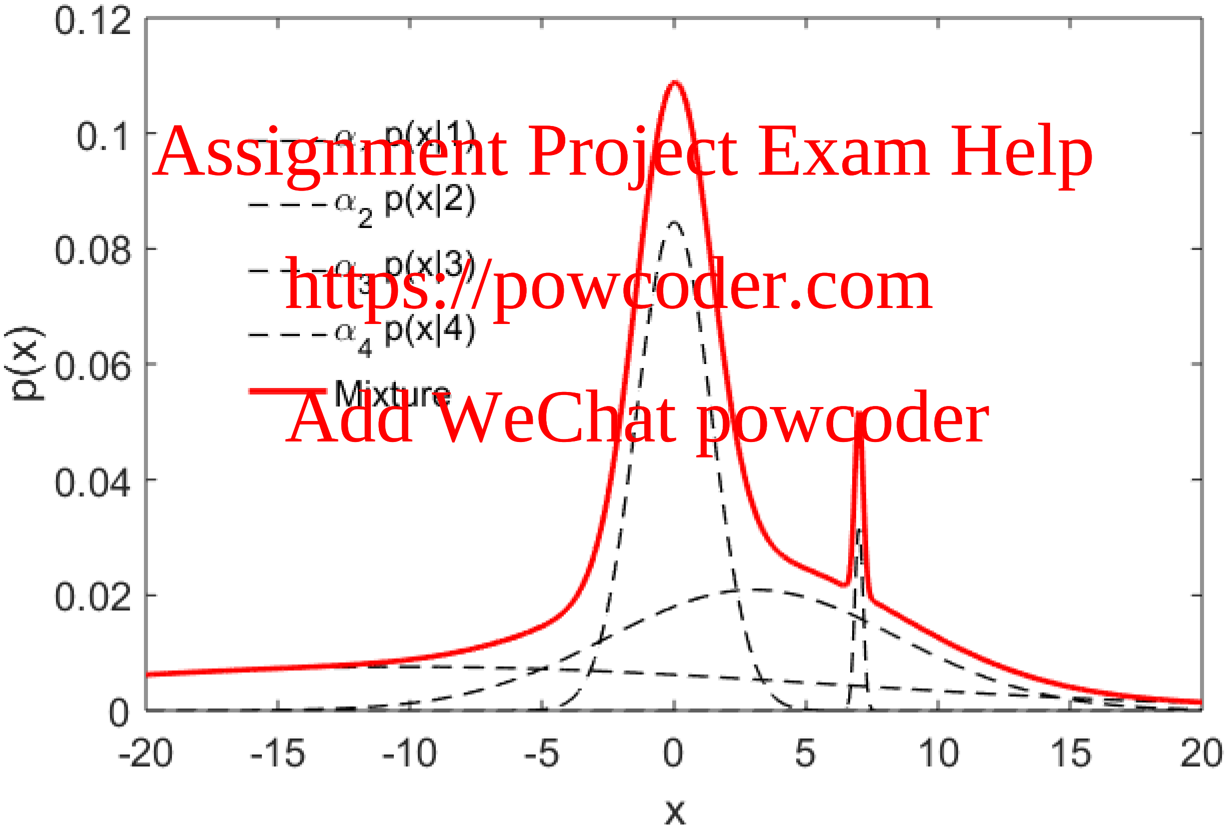
New mean for ith component is weighted average of data points. Weighting is fraction of the data point x_a attributed to component *i*,

$$\Sigma_i(n+1) = \frac{\sum_{a=1}^{N} h_{i,a}(n+1)\,\left(x_a - \mu_i(n+1)\right)\left(x_a - \mu_i(n+1)\right)^T}{\sum_a h_{i,a}(n+1)}$$

New covariance is constructed from weighted outer product.

Gaussian Mixture Model

Flexible --- can make lots of shapes!



EM Summary --- Gaussian Mixtures

Initialize parameters

$\alpha_i(0) = 1/k$ all components equally likely

$\mu_i(0) = x_i$ k randomly chosen points from training data

$\Sigma_{\mathrm{i}}(0)$ a positive symmetric, positive definite matrix e.g. $\sigma^2 I$

EM Summary --- Gaussian Mixtures

Iterate

E-Step (estimate posteriors) $h_{a,i}(n+1) \equiv p(i_a \mid x_a, \Theta(n)) = \dfrac{\alpha_i(n)\ p(x_a \mid \theta_i(n))}{\sum_{j=1}^{k} \alpha_j(n)\ p(x_a \mid \theta_j(n))}$

M-Step

Re-estimate priors $\alpha_i(n+1) = \dfrac{1}{N} \sum_{a=1}^{N} h_{i,a}(n+1)$

Re-estimate means $\mu_i(n+1) = \dfrac{\sum_{a=1}^{N} h_{i,a}(n+1)\ x_a}{\sum_a h_{i,a}(n+1)}$

Re-estimate covariances

$$\Sigma_i(n+1) = \frac{\sum_{a=1}^{N} h_{i,a}(n+1) \left(x_a - \mu_i(n+1)\right) \left(x_a - \mu_i(n+1)\right)^T}{\sum_a h_{i,a}(n+1)}$$

Caveats

In high dimensions *n*, there are loads of covariance matrix elements. Likely to overfit.

Fixes – constrain covariance matrices to have fewer components

Diagonal
$$\Sigma_i = \begin{pmatrix} \lambda_{i1} & & 0 \\ & \lambda_{i2} & \\ 0 & & \ddots \end{pmatrix}$$

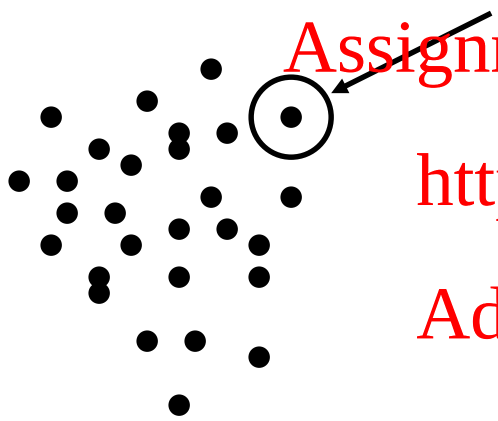
Spherically symmetric $\Sigma_i = \sigma_i^2 I$, with I the identity matrix

Some other clever form (???)

Note that any constraints modify the M-step equations for the covariance --- can you derive the forms?

Caveats

There are regions of the parameter space where the likelihood goes through the roof but the resulting model is bad



One Gaussian wrapped around this one point x'. Let $\mu_i = x'$, and take σ_i^2 to 0.

Then $p(x' \mid \mu_i, \sigma_i^2) \rightarrow \infty$

and the likelihood grows without bound. This is particularly likely in high-dimensions where the average distance between datapoints becomes large.

Regularization (has a grounding in Bayesian priors and MAP estimation). After re-estimation, add a small diagonal matrix to the covariance

$$\Sigma_i(n+1) \rightarrow \Sigma_i(n+1) + \varepsilon I$$

References

- Dempster, Laird, and Rubin. Maximum likelihood from incomplete data via the EM algorithm, *J. Royal Statistical Soc. B,* 39, 1-39, 1977.
- Rener and Walker. Mixture densities, maximum likelihood and the EM algorithm, SIAM Review, 26, 195-239, 1984.
- Ormoneit and Tresp. In *Advances in Neural Information Processing Systems 8,* The MIT Press, 1996.
- Jonathan Li and Andrew Barron. Mixture Density Estimation, in Solla, Leen, and Mueller (eds.) *Advances in Neural Information Processing Systems 12*, The MIT Press, 2000.

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