Mixture Models and the EM Algorithm

15-496/782: Artificial Neural Networks
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1

Mixture Models

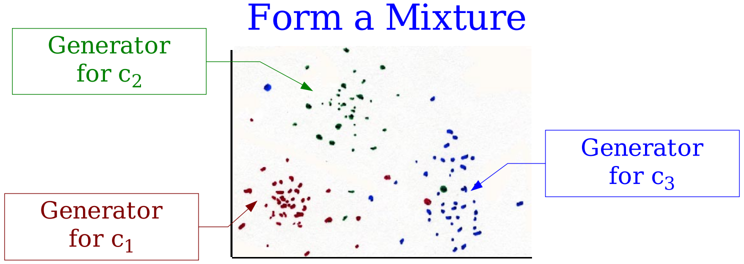
We can model a dataset as a collection of points generated by a mixture of Gaussians.

μ_j mean
σ_j standard deviation
α_j weight/prevalence/prior probability

$$\left(\sum_j \alpha_j\right) = 1, \qquad \text{so } \alpha_j = P(c_j)$$

2

Gaussian Generators Form a Mixture



Class priors $P_j = P(c_j)$ (mixture coefficients)

$$\sum_j P_j = 1$$

$$\text{Density distribution} = \sum_j P_j \cdot \exp\left[\frac{-(\mathbf{x}-\mu_j)^2}{\sigma_j^2}\right]$$

3

Probability Densities

$P(j)$ = prior probability of class c_j

so $\sum_j P(j) = 1$

Probability density of the mixture:

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

Posterior probability:

$$P(j|\mathbf{x}) = \frac{p(\mathbf{x}|j)P(j)}{p(\mathbf{x})}$$

so $\sum_j P(j|\mathbf{x}) = 1$

4

Conditional Density

Assume covariance matrix is diagonal with equal elements. Then:

$$p(\mathbf{x}|j) = \underbrace{\frac{1}{(2\pi\sigma^2)^{d/2}}}_{\text{normalization term}} \cdot \exp\left\{\frac{-\|\mathbf{x}-\mu_{\mathbf{j}}\|^2}{2\sigma^2}\right\}$$

How can we determine the "most probable" values of μ_j and σ_j and P(j), given the dataset $\{\mathbf{x}_i\}$?

Likelihood of a Dataset

What is the likelihood L that a dataset $\{\mathbf{x}i\}$ was generated by a given mixture model?

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

$$p(\{\mathbf{x}_{\mathbf{i}}\}) = \prod_{i=1}^{n} p(\mathbf{x}_{\mathbf{i}}) = L$$

Log Likelihood

For gradient descent, we want a sum, not a product, because the derivative of a product is messy. So take the negative log.

$$\begin{aligned} E &= -\log L = -\sum_{i=1}^{n} \log p(\mathbf{x}_{\mathbf{i}}) \\ &= -\sum_{i=1}^{n} \log\left\{\sum_{j=1}^{M} p(\mathbf{x}_{\mathbf{i}}|j)P(j)\right\} \end{aligned}$$

Gradient Descent on E

$$E = -\sum_{i=1}^{n} \log p(\mathbf{x}_{\mathbf{i}}) = -\sum_{i=1}^{n} \log\left(\sum_{j=1}^{M} p(\mathbf{x}_{\mathbf{i}}|j)P(j)\right)$$

$$\begin{aligned} \frac{\partial E}{\partial \mu_j} &= -\sum_{i=1}^{n}\left(\frac{1}{p(\mathbf{x}_{\mathbf{i}})} \cdot \sum_{k=1}^{M} P(k) \frac{\partial}{\partial \mu_{\mathbf{j}}} p(\mathbf{x}_{\mathbf{i}}|k)\right) \\ &= -\sum_{i=1}^{n}\left(\frac{1}{p(\mathbf{x}_{\mathbf{i}})} \cdot p(\mathbf{x}_{\mathbf{i}}|j)P(j) \cdot \frac{\|\mathbf{x}_{\mathbf{i}}-\mu_{\mathbf{j}}\|}{\sigma}\right) \\ &= -\sum_{i=1}^{n} P(j|\mathbf{x}_{\mathbf{i}}) \cdot \frac{\|\mathbf{x}_{\mathbf{i}}-\mu_{\mathbf{j}}\|}{\sigma} \end{aligned}$$

Gradient Descent (cont.)

$E = -\log L$ is our error function.

Do gradient descent on E:

$$\frac{\partial E}{\partial \mu_j} = \sum_{i=1}^{n} P(j|\mathbf{x_i}) \cdot \frac{\|\mathbf{x_i} - \mu_j\|}{\sigma_j^2}$$

$$\frac{\partial E}{\partial \sigma_j} = \sum_{i=1}^{n} \left(P(j|\mathbf{x_i}) \cdot \left(\frac{d}{\sigma_j} - \frac{\|\mathbf{x_i} - \mu_j\|^2}{\sigma_j^3} \right) \right)$$

Constrained Gradient Descent

There's a problem:

We can't just nudge μ_i and σ_j around by small amounts, since their values affect P(j).

Must satisfy these constraints:

$$\sum_{j=1}^{M} P(j) = 1$$

$$0 \leqslant P(j) \leqslant 1$$

The EM Algorithm (Expectation-Maximization)

Iterative algorithm for optimizing μ_j and σ_j, and P_j to minimize E.

Definitions:

$$P_{ji} = P(j|\mathbf{x_i}) = \frac{P(\mathbf{x_i}|j) \cdot P(j)}{p(\mathbf{x_i})}$$

Class priors:

$$P(j) = P_j = \frac{1}{N} \sum_{i=1}^{N} P_{ji}$$

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

Expectation (E) Step

Calculate P_{ji} for all points i and gaussians j,

using current parameter values $\mu_\mathbf{j}$, σ_j^2, and P_j.

Maximization (M) Step

$$P_j \leftarrow \frac{1}{N}\sum_{i=1}^{N} P_{ji}$$

$$\boldsymbol{\mu}_{\mathbf{j}} \leftarrow \frac{\sum_i P_{ji}\cdot \mathbf{x_i}}{\sum_i P_{ji}} = \frac{\sum_i P_{ji}\cdot \mathbf{x_i}}{P_j}$$

$$\sigma_j^2 \leftarrow \frac{\frac{1}{d}\sum_i P_{ji}\cdot\|\mathbf{x_i}-\boldsymbol{\mu}_{\mathbf{j}}\|^2}{P_j}$$

Repeat E and M steps until convergence.

13

EM Finds a Local Minimum in E (or Local Maximum in *L*)

$$\frac{\partial E}{\partial \boldsymbol{\mu}_{\mathbf{j}}} = 0 = -\sum_{i=1}^{n} P(j|\mathbf{x_i})\cdot\frac{\|\mathbf{x_i}-\mu_j\|}{\sigma_j^2}$$

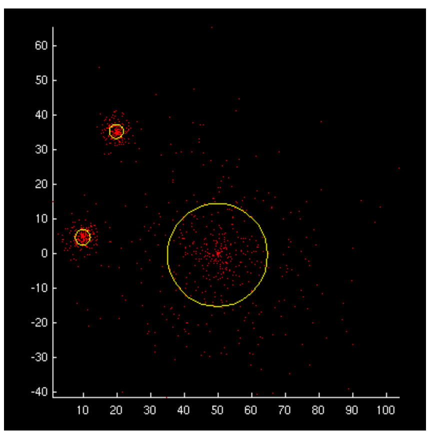
$$\boldsymbol{\mu}_{\mathbf{j}}\sum_{i=1}^{n}\frac{P(j|\mathbf{x_i})}{\sigma_j^2} = \frac{\sum_{i=1}^{n} P(j|\mathbf{x_i})\,\mathbf{x_i}}{\sigma_j^2}$$

$$\boldsymbol{\mu}_{\mathbf{j}} = \frac{\sum_{i=1}^{n} P(j|\mathbf{x_i})\,\mathbf{x_i}}{\sum_{i=1}^{n} P(j|\mathbf{x_i})}$$

μ_j is the weighted mean of the $\mathbf{x_i}$'s credited to the jth mixture component.

14

EM Demo

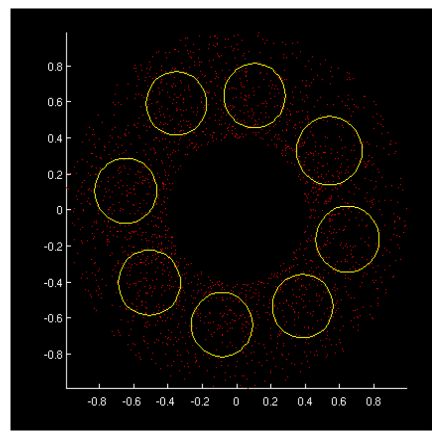


EmDataSet =4

emdemo

15

EM Demo



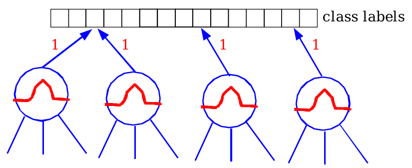
EmDataSet = 3

emdemo

16

Williamson: Gaussian ARTMAP

1. Use an RBF network to do pattern classification:



Each unit votes for one class. Tally votes from all active units. The class with the most votes wins. No LMS training.

2. Use a variant of EM to train the gaussians.

17

Characteristics of EM

- Learns in a small number of iterations.
- Can get stuck in local minima.
  - But you can add heuristics to help unstick the algorithm.
- Must decide in advance how many Gaussians.

18

"Match Tracking" in ARTMAP

Establish a match threshold ρ.

Units count as "active" only if $P(\mathbf{x}_i|j) > \rho$.

All other units are reset to zero; they do not vote.

If the network guesses the wrong class, increase ρ slightly and try again.

If ρ gets too high and all units are reset, then add a new unit to handle this data point.

19

Performance of Gaussian ARTMAP

Note: EM is a batch (offline) learning algorithm. Guassian ARTMAP uses an online variant.

Did well on several tasks:

- Letter image classification
- Landsat satellite image segmentation
- Speaker-independent vowel recognition

Match tracking helps Gaussian ARTMAP outperform EM by "backpropagating" the effects of erroneous classifications.

20

Offline Calculation of μ and σ²

$$\mu = \langle x \rangle$$

$$\begin{aligned}
\sigma^2 &= \langle (x-\mu)^2 \rangle \\
&= \langle x^2 - 2x\mu + \mu^2 \rangle \\
&= \langle x^2 \rangle - 2\langle x \rangle \mu + \langle \mu^2 \rangle \\
&= \langle x^2 \rangle - 2\mu^2 + \mu^2 \\
&= \langle x^2 \rangle - \langle x \rangle^2
\end{aligned}$$

On-line Calculation of μ

$$\begin{aligned}
\mu_n &= \frac{1}{n}\sum_{i=1}^{n} x_i \\
\mu_{n+1} &= \frac{n\cdot\mu_n + x_{n+1}}{n+1} \\
&= \frac{n}{n+1}\mu_n + \frac{x_n}{n+1} \\
&= \left(1-\frac{1}{n+1}\right)\mu_n + \frac{1}{n+1}x_{n+1}
\end{aligned}$$

On-line Calculation of σ²

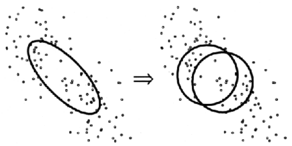
$$\sigma_n^2 = \frac{1}{n}\sum_{i=1}^{n}\left(x_i-\mu_n\right)^2$$

$$\sigma_{n+1}^2 = \left(1-\frac{1}{n+1}\right)\sigma_n^2 + \frac{1}{n+1}\left(x_{n+1}-\mu_{n+1}\right)^2$$

σ_n^2 is slightly biased because μ_n changes, but the effect is not significant.

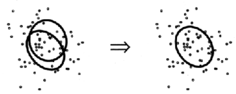
Split and Merge EM
(Ueda, Nakano, Gharamani, and Hinton)

- Split a component if it does a poor job estimating the local density.
- Example: a component stuck between two clusters will have low density near its mean and high density near the true cluster centers.
- To split, make two copies, and perturb each one away from the mean by a small amount.



Split and Merge EM (cont.)

• Merge two components if their paramaters are close. Set the merged component's parameters to the weighted average.



• Combine one merge step with one split step, so the number of mixture components M stays the same.

Combined Split and Merge Steps

Old components: i j k ...

merge split

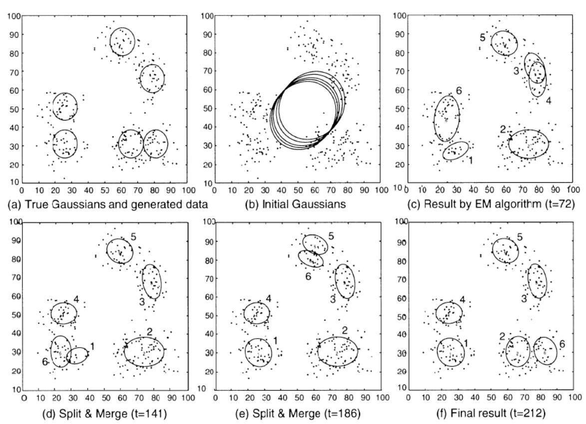
New components: i' j' k' ...

Run a mini-EM step to adapt elements i', j', and k'. Then run full EM to asymptote.

If overall likelihood is not improved, undo the split/merge and try a different set of candidates.

Candidates are ranked heuristically; only need to look at about 5.

Performance of SMEM



Mixture of Factor Analyzers

Project high-D space down to lower-D space. Compute a mixture of low-D functions.

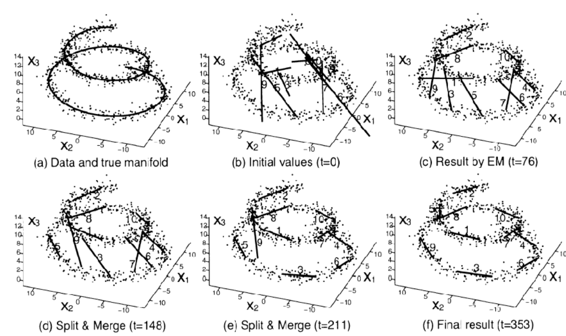
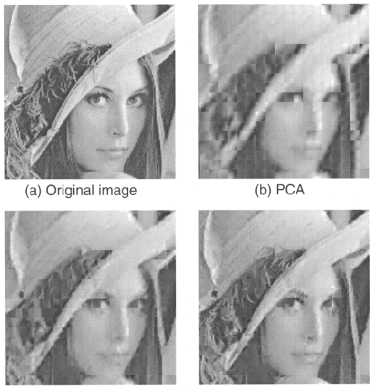


Image Reconstruction



(a) Original image (b) PCA (c) MFA with EM (d) MFA with SMEM

29

Cheapo Heuristic

Not as good as SMEM, but easy to program:

If a component captures fewer than 1/(2M) points, reset its μ to a random $\mathbf{x}_i$ and recalculate its σ^2.

Assumes the P(j) values are roughly equal.

EmHeuristic = 1
emdemo

30