Introduction to Neural Networks
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Expectation-Maximization (EM)

Initialize

■ Read in Statistical and Graphics Add-in packages:

```
Off[General::spell1];
```

```
<< Statistics`NormalDistribution`
<< Statistics`ContinuousDistributions`
<< Statistics`MultinormalDistribution`
<< Statistics`DiscreteDistributions`
```

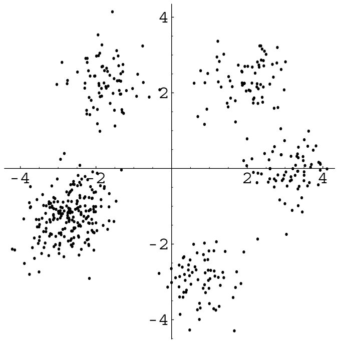
```
<< Graphics`MultipleListPlot`
<< Graphics`Graphics`
```

Introduction

The Expectation Maximization algorithm can be viewed as an example of *unsupervised learning* and crops up in a wide range of applications, including probability density estimation, clustering, and discovering prototypes from data. In principle, it is very general and is guaranteed to converge to a local likelihood maximum. The EM algorithm is a common procedure for integrating out "hidden variables"--i.e. for marginalizing.

Integrating out secondary variables

Suppose we have 5 (hidden) processes each of which can contribute to our data.



For mixture distributions, we are often not directly interested in the mixing probabilities--we are mainly interested in the parameters of the distributions, e.g. the 5 means. These means, in an N-dimensional space for example, could represent prototypes in memory.

■ Simple case & intuition

(Example from draft chapter by: Yuille, Coughlan, Kerten & Schrater)

Suppose there is some agent that randomly chooses whether to flash a bright (a=1) or the dim (a=2) light, and for each flash we make a measurement x . To keep things simple, we'll assume that the probability of the bright and dim switch settings are both equal, p(a=1) = p(a=2) = 1/2 . Further suppose that the light measurements x are Gaussian distributed, and the standard deviations are known (we will drop these assumptions later).

Rather than making decisions about whether a given flash is bright or dim, we want to estimate the two means from a series of measurements (e.g. photon counts), {x_i: i =1,...,N } , without knowing which measurement came from which light setting. Of course, if we knew which measurement came from which switch setting, our job would be easy. Let V_{ia}=1 if data x_i is generated by model P(x| mu _a, sigma ^2) and V_{ia}=0 otherwise, for a=1,2 . Then,

$$\mu_a \approx \frac{\sum_{i=1}^{N} V_{ia} x_i}{\sum_{i=1}^{N} V_{ia}}$$

The problem is that the values of V_{ia} are unknown secondary (hidden) variables which influence the observations. However, if we could somehow estimate the probability of which switch generated each measurement x_i , then the means could be approximated as:

$$\mu_a \approx \frac{\sum_{i=1}^{M} \bar{V}_{ia} x_i}{\sum_{i=1}^{M} \bar{V}_{ia}}, \ \forall \ a$$

where $\overline{V}$ {ia} is the average value of V{ia} and is given by $\overline{V}$ {ia} = p(V{ia}=1 | x_i) = p(a |x_i) . This brings us a step closer to a solution, but raises another problem--to calculate $\overline{V}$ {ia} we will need to know the means--the very parameters we were trying to estimate in the first place!

Let's see how to justify our intuitive estimate of the means, and in the process solve the dilemma of how to determine the probability of which switch generated each measurement. Our goal will be to find the maximum likelihood estimates of the means (and eventually other state variables) conditional on the observations. We will derive the EM rules for a mixture of multi-variate gaussians.Then we will derive a more general rule for arbitrary discrete distributions.

Mixtures of multivariate gaussians

Let x represent a d-dimensional vector generated from a mixture of M Gaussian densities, with s= {mu_a,C_a } and h= {a} , where mu_a , C_a , and p(a) are the vector means, covariance matrices, and mixture probs, respectively.

(The notation s, and h is used later for an unknown parameter s (or a set s), that we want to estimate, and another parameter h (or set h) that is hidden.)

$$p(x) = p(x|\mu_a, C_a) = \sum_a p(x|a)p(a)$$

where a = 1,...,M , and $\sum_a$ p(a) = 1 . The p(x |a) are the class-conditional probability densities:

$$p(x|a) = \frac{1}{\sqrt{(2\pi)^d|C_a|}} exp\{-(x-\mu_a)^T \cdot C_a^{-1} \cdot (x-\mu_a)/2\}$$

We are given a sequence of vector measurements {x_i: i =1,...,N } and wish to estimate the means, the covariances and mixing parameters. Let the probability that x_i came from mixture component a be p(x_i|a) .

$$p(x_1, x_2, \ldots, x_N|\mu_a, C_m) = \prod_i \sum_a p(x_i|a)p(a)$$

The log-likelihood of the data is given by:

$$E(\mu_a, C_a) = \log(p(x_1, x_2, \ldots, x_N)) = \sum_i \log\{\sum_a p(x_i|a)$$

For the moment, suppose the mixing parameters and covariance matrices are known, and we want to estimate the means. The values of mu_a which maximize E can be found analytically by solving:

$$\partial E/\partial\mu_j = \sum_i \frac{p(x_i|j)p(j)}{\sum_a p(x_i|a)p(a)} \frac{(\mu_j - x_i)}{\sigma_j^2} = \sum_i p(j|x_i) \frac{(\mu_j -}{\sigma_j^2}$$

where we've used:

$$p(a|x_i) = \frac{p(x_i, a)}{p(x_i)} = \frac{p(x_i|a)p(a)}{\sum_a p(x_i|a)p(a)}$$

Solving for the μ_j ' s (= μ_a ' s), we have

$$\mu_a = \frac{\sum_i x_i p(a|x_i)}{\sum_i p(a|x_i)}.$$

The rub, of course, is that p(a|x_i) depends on mu_a..., so

E&M iteration steps

- **Estimate conditional mixing probabilities: E-step**

Let mu_{a,t} be an initial guess. Then in the E-step we let:

$$p(a|x_i, \mu_{a,t}) = \frac{p(x_i|a, \mu_{a,t})p(a)}{\sum_a p(x_i|a, \mu_{a,t})p(a)}$$

- **And then find the mean that maximizes the likelihood of the data: M-step**

The M-step,

$$\mu_{a,t+1} = \frac{\sum_i x_i p(a|x_i, \mu_{a,t})}{\sum_i p(a|x_i, \mu_{a,t})}.$$

■ **How about the covariance?**

Suppose we don't know the covariance matrix or the mixing probabilities? We can use the updated values of p_t(a|x_i) ,

$$p_{t+1}(a|x_i,) = p_t(a|x_i, \mu_a(t), C_a(t), p_t(a))$$

to progressively estimate the state parameters C_a and p(a) , as well as mu_a . The M-step for the covariance is:

■ **M-step for covariance & p(a)**

$$C_a(t+1) = \frac{\sum_i (x_i - \mu_a)(x_i - \mu_a)^T p_t(a|x_i)}{\sum_i p_t(a|x_i)}$$

(where ab^T is the outer product between vectors a and b). The mixing probabilities are estimated by:

$$p_{t+1}(a) = \frac{1}{N} \sum_i p_t(a|x_i)$$

Demo: Two gaussians, unknown μ's σ's , and mixing probabilities (revised)

Generating samples from a Gaussian Mixture Distribution

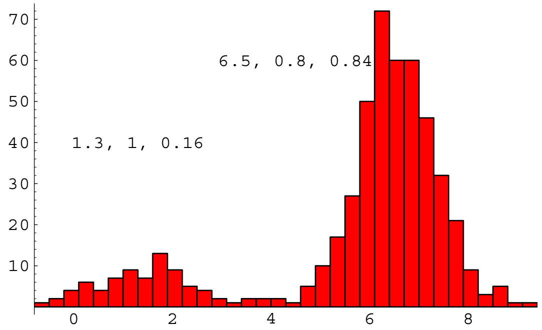
■ **Generative model**

```
μ1=1.3;σ1=1;
μ2=6.5;σ2=.8;
a1=.16; a2 = 1-a1;
p1dist=NormalDistribution[μ1,σ1];
p2dist=NormalDistribution[μ2,σ2];
p1[x_]:=PDF[p1dist,x];
p2[x_]:=PDF[p2dist,x];

(*mix[x_]:=a1*p1[x]+a2*p2[x];*)

samplemix:=If[Random[]<a1,Random[p1dist],Random[p2dist]];
```

```
data = Table[samplemix, {i, 1, 500}];
Histogram[data, HistogramCategories → Range[-20, 20, .3],
  Epilog → {Text[ToString[μ1] <> ", " <> ToString[σ1] <> ", " <> ToString[a1],
     {μ1, 40}], Text[ToString[μ2] <> ", " <>
      ToString[σ2] <> ", " <> ToString[a2], {μ2 - 2, 60}]}];
```



EM algorithm--Now learn the parameters--means, standard deviations, and mixing probabilities

```
pxdm[x_, mu_, σ_] := PDF[NormalDistribution[mu, σ], x];
```

E-step: The prob of mixing labels conditional on the data x is:

$$p(a|x_i, \mu_{a,t}) = \frac{p(x_i|a, \mu_{a,t})p(a)}{\sum_a p(x_i|a, \mu_{a,t})p(a)}$$

In *Mathematica* code,

```
pmcx[a_, x_] := pxdm[x, μ[[a]], σ[[a]]] * pa[[a]] /
    (pxdm[x, μ[[1]], σ[[1]]] * pa[[1]] + pxdm[x, μ[[2]], σ[[2]]] * pa[[2]]);
```

M-step: The maximum liklihood estimates of the means is:

$$\mu_a = \frac{\sum_i x_i p(a|x_i)}{\sum_i p(a|x_i)}.$$

or in *Mathematica*:

μ[[1]]=pmcx[1,data].data/Plus@@(pmcx[1,#]&/@data)

μ[[2]]=pmcx[2,data].data/Plus@@(pmcx[2,#]&/@data)

Similarly, the variances and mixing probabilities are also weighted averages:

σ[[1]]=Sqrt[pmcx[1,data].(data-μ[[1]])^2/Plus@@(pmcx[1,#]&/@data)]

σ[[2]]=Sqrt[pmcx[2,data].(data-μ[[2]])^2/Plus@@(pmcx[2,#]&/@data)]

pa[[1]]=Plus@@(pmcx[1,#]&/@data)/Length[data]

pa[[2]]=Plus@@(pmcx[2,#]&/@data)/Length[data]

To estimate the unknown parameters from the data, we first initialize to random values:

```
μ = {Random[Real, {-10, 10}], Random[Real, {-10, 10}]};
σ = {Random[Real, {0, 10}], Random[Real, {0, 10}]};
pa = {temp = Random[], 1 - temp};
```

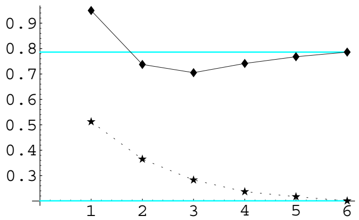
The interate for i=1 to iter. Note that the E-step occurs on the right-hand side, where pmcx[] is a function of the most recent value of the mean, std, and mixing parameters.

```
iter = 6;
μparameterList = Table[0, {a, 1, 2}, {k, 1, iter}];
σparameterList = μparameterList; paparameterList = μparameterList;
For[k = 1, k ≤ iter, k++,
  For[a = 1, a ≤ 2, a++,
    μ[[a]] = pmcx[a, data].data / Plus @@ (pmcx[a, #] & /@ data);
    σ[[a]] =
     Sqrt[pmcx[a, data].(data - μ[[a]]) ^2 / Plus @@ (pmcx[a, #] & /@ data)];
    pa[[a]] = Plus @@ (pmcx[a, #] & /@ data) / Length[data];
    μparameterList[[a, k]] = μ[[a]];
    σparameterList[[a, k]] = σ[[a]];
    paparameterList[[a, k]] = pa[[a]];
   ];
 ];
```

■ Plot the evolution of the mixing parameters

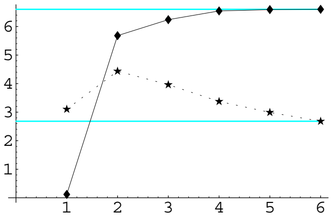
Blue line shows true values from the generative model.

```
Show[{Plot[{pa[[1]], pa[[2]]}, {x, 0, iter},
    PlotStyle → Hue[.5], DisplayFunction → Identity],
   MultipleListPlot[paparameterList[[1]], paparameterList[[2]],
    PlotJoined → True, DisplayFunction → Identity]},
  DisplayFunction → $DisplayFunction];
```



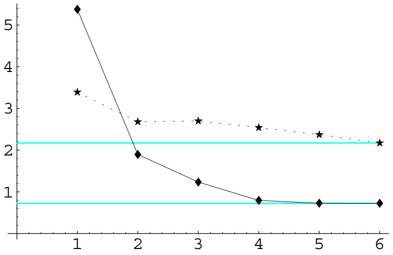
Plot the evolution of the means

```
Show[{Plot[{μ[[1]], μ[[2]]}, {x, 0, iter},
    PlotStyle → Hue[.5], DisplayFunction → Identity],
   MultipleListPlot[μparameterList[[1]], μparameterList[[2]],
    PlotJoined → True, DisplayFunction → Identity]},
  DisplayFunction → $DisplayFunction];
```



Plot the evolution of the standard deviations

```
Show[{Plot[{σ[[1]], σ[[2]]}, {x, 0, iter},
    PlotStyle → Hue[.5], DisplayFunction → Identity],
   MultipleListPlot[σparameterList[[1]], σparameterList[[2]],
    PlotJoined → True, DisplayFunction → Identity]},
  DisplayFunction → $DisplayFunction];
```



EM: Theory for arbitrary discrete probability distributions

We'd like to generalize the theory, and also make clearer the function of EM in integrating out hidden or secondary variables. The notation s, and h is used for an unknown parameter s (or a set s), that we want to estimate, and another parameter h (or set {hi}) that is hidden.)

We'd like to find the value of s that maximizes the likelihood of the data {xi}, given other intervening variables hi.

The log-likelihood of the observations is given by:

$$\log p(x_1, \ldots, x_N|s) = \log \prod_{i=1}^{N+1} p(x_i|s) = \sum_i \log p(x_i|s) = \sum_i \log \sum_{h_i} p(x_i, h$$

To find the maximum of the likelihood, we calculate the derivative of the log-likelihood with respect to s , and then set the derivative equal to zero:

$$\frac{\partial \log p(x_1, \ldots, x_N|s)}{\partial s} = \sum_i \frac{1}{\sum_{h_i} p(x_i, h_i|s)} \frac{\partial}{\partial s}\{\sum_{h_i} p(x_i, h_i$$

Where we have used the relation,

$$\frac{\partial \log \phi(s)}{\partial s} = \frac{1}{\phi(s)} \frac{\partial \phi(s)}{\partial s}$$

Bringing the summation over h_i in front, we have:

$$\sum_i \sum_{h_i} \frac{1}{\sum_{h_i} p(x_i, h_i|s)} \frac{\partial}{\partial s} p(x_i, h_i|s)$$

Again using the above derivative of a log relation, we have

$$\sum_i \sum_{h_i} \frac{p(x_i, h_i|s)}{\sum_{h_i} p(x_i, h_i|s)} \frac{\partial}{\partial s} \log p(x_i, h_i|s)$$

and by Bayes,

$$\sum_i \sum_{h_i} p(h_i|x_i, s) \frac{\partial}{\partial s} \log p(x_i, h_i|s) = 0$$

■ Summary of EM strategy

The EM strategy for solving equation for s involves two steps:

1) Given a guess, s=s_t , calculate

$$p(h_i|x_i, s_t) \qquad (E - step)$$

2) Solve

$$\sum_i \sum_{h_i} p(h_i|x_i, s_t) \frac{\partial}{\partial s} \log p(x_i, h_i|s) = 0 \qquad (M - step)$$

to find the next s_{t+1} . Then iterate back to the E-step until convergence. Although the EM algorithm does converge, it doesn't necessarily converge to the maximum likelihood estimate.

Expectation Maximization -- Segmentation simulation

We've studied the problem of interpolation given missing data. We motivated the problem by the visual phenomenon of surface completion. Another aspect of surface perception is our ability to take noisy data (e.g. depth cues), and not only interpolate the data, but also decide which of several surfaces the data belong using stereo data (Madarasmi et al., 1993; Kersten & Madarasmi, 1995) or optic flow. A number of ways have been proposed to deal with this problem, but the technique of most general application is expectation-maximization--a general statistical technique developed in the 1970's that appears in various forms in many algorithms, including belief propagation. The algorithm has been applied to the surface estimation problem, e.g. from optic flow (Jepson, 1993; Weiss, 1997). We go to Weiss again for a nice simple demo.

Consider **Generative Model 1.**

Generative models

Two lines with slopes and intercepts (a1,b1) and (a2,b2).

```
ndist = NormalDistribution[0, 1];
```

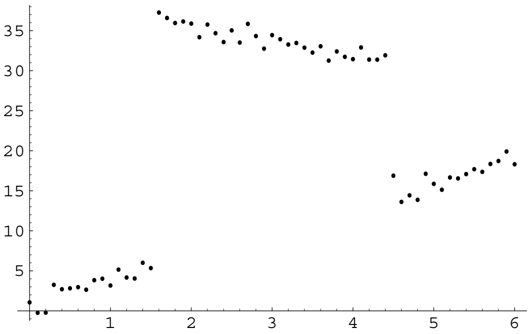
■ Generative model 1

```
y1[x_] := -2 * x + 40 + Random[ndist];
y2[x_] := 3 * x + 1 + Random[ndist];
data = Table[{x, If[Abs[x - 3] < 1.5, y1[x], y2[x]]}, {x, 0, 6, .1}];
{x, y} = Transpose[data];
```

■ Generative model 2

```
y1[x_] := -2 * x + 15;
y2[x_] := 3 * x + 1;
data = Table[{x, If[Random[] < .5, y1[x], y2[x]]}, {x, 0, 6, .1}];
{x, y} = Transpose[data];
```

```
gdata = ListPlot[data];
```



Which data belong together? We'll assume that we know there are two linear models, but we don't know their parameters--i.e. we don't know their slopes and intercepts.

EM algorithm

■ Initialize parameters to random values

```
σ = .1;
{a1, b1, a2, b2} = Table[10 * Random[], {4}];
```

■ E-step

Compute residuals r1, r2, the error in the predicted and actual y values under each of the two models.

```
r1 = a1 * x + b1 - y;
r2 = a2 * x + b2 - y;
```

Using the residuals, compute weights. We'll assign these weights to data in the M-step later.

```
w1 = Exp[-r1^2 / σ] / (Exp[-r1^2 / σ] + Exp[-r2^2 / σ]);
w2 = Exp[-r2^2 / σ] / (Exp[-r1^2 / σ] + Exp[-r2^2 / σ]);
```

■ M-step

Standard linear regression doesn't assume that the data may have come from different sources. The least-squares solution (derivable from i.i.d. gaussian model for the data) is equivalent to solving:

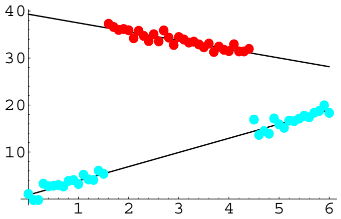
$$\begin{pmatrix} \sum_i x_i^2 & \sum_i x_i \\ \sum_i x_i & \sum_i 1 \end{pmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum_i x_i y_i \\ \sum_i y_i \end{bmatrix}$$

But if the data come from different sources, with above weights we can compute weighted linear regression to estimate the slope and intercept parameters:

$$\begin{pmatrix} \sum_i w_i x_i^2 & \sum_i w_i x_i \\ \sum_i w_i x_i & \sum_i w_i 1 \end{pmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum_i w_i x_i y_i \\ \sum_i w_i y_i \end{bmatrix}$$

```
{a1, b1} =
  Inverse[{{w1.(x x), w1.x}, {w1.x, Apply[Plus, w1]}}].{w1.(x y), w1.y};
{a2, b2} = Inverse[{{w2.(x x), w2.x}, {w2.x, Apply[Plus, w2]}}].
   {w2.(x y), w2.y};
```

```
gfit = Plot[{a1 * x + b1, a2 * x + b2}, {x, 0, 6}, DisplayFunction → Identity];
Show[{gfit, Graphics[
    {PointSize[0.03], Transpose[{Hue[#1] & /@ (w1 / 2), Point /@ data}]}]},
  PlotRange → All, DisplayFunction → $DisplayFunction];
```



Exercises

Run EM with Generative Model 2. Increase the additive noise. How does attribution accuracy change? ("attribution" means assigning a point to its correct line)

N=5 Multivariate gaussians, only data known: Implement EM to estimate means, variance, and mixing probabilities

---

■ Generating samples from a Gaussian Mixture Distribution

```
Clear[ndist];
ndist[μ_, Σ_] := MultinormalDistribution[μ, Σ];
```

```
r = .05;
σ = .3;
μ = Table[3 * N[{Cos[2 Pi i], Sin[2 Pi i]}], {i, 0, 2 Pi, Pi / 4}];
Σ = Table[{{σ, r}, {r, σ}}, {i, 0, 2 Pi, Pi / 4}];

Det[{{σ, r}, {r, σ}}]
```

```
0.0875
```

The generator: randomindex := Random[Integer,{1,5}]; would give uniformly distributed mix labels.

The following gives mixing mix probabilities of 1/7, 1/7, 3/7, 1/7 and 1/7 for subdistributions 1,2,3,4,5 respectively.

```
randomindex := {1, 2, 3, 3, 3, 4, 5}[[Random[Integer, {1, 7}]]]
```

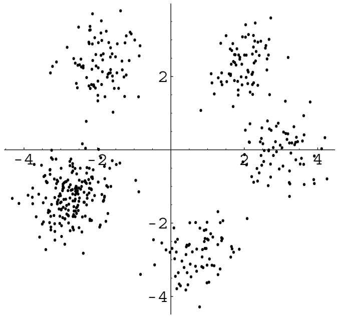
Thus our stochastic generative process can be written:

```
Random[ndist[μ[[t = randomindex]], Σ[[t]]]]
```

```
{0.432208, -3.03454}
```

```
scatterdata = Table[Random[ndist[μ[[t = randomindex ]], Σ[[t]]]], {i, 1, 500}];
```

```
ListPlot[scatterdata, AspectRatio → Automatic];
```



■ Implement EM to estimate means, variance, and mixing probabilities

$$p(a|x_i, \mu_{a,t}) = \frac{p(x_i|a, \mu_{a,t})p(a)}{\sum_a p(x_i|a, \mu_{a,t})p(a)}$$

$$\mu_{a,t+1} = \frac{\sum_i x_i p(a|x_i, \mu_{a,t})}{\sum_i p(a|x_i, \mu_{a,t})}.$$

$$C_a(t+1) = \frac{\sum_i (x_i - \mu_a)(x_i - \mu_a)^T p_t(a|x_i)}{\sum_i p_t(a|x_i)}$$

$$p_{t+1}(a|x_i,) = p_t(a|x_i, \mu_a(t), C_a(t), p_t(a))$$

References

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