## Introduction to Neural Networks Daniel Kersten

Clustering, K-Means, Expectation-Maximization (EM) Note on probabilistic population codes

## Review: neural architecture of vision

Hierarchical view of visual neural architecture consisting of lateral, feedforward and feedback computations.


## Lateral organization/computation

Assumption is that lateral organization represents features or "concepts" at a given level of abstraction. E.g. an "edge" is a concept, but so is "elbow", "face", "body" and "scene".

Self-organization of maps based on bringing similar features at the same level of abstraction close together on the cortical gray matter. E.g. edge orientation, spatial frequency, location in V1. Poses of the human head in the columnar structure of temporal areas.

Self-organization of receptive fields based on efficient coding. With connections to classical dimensionality reduction methods such as principal components analysis, sparse coding/dictionary methods (including ICA), and contingent adaptation to maximize representational capacity. The idea is that statistical regularities in visual sensory patterns can be exploited to recode information into forms that are less redundant.

Examples of lateral computations involving active linking and suppression of features that are likely or unlikely to be grouped.


Left panel: patches from fox emerging behind tree. Middle panel: MRFs. Third panel: Das A, Gilbert CD (1999) Topography of contextual modulations mediated by short-range interactions in primary visual cortex.
Nature 399:655-661.
One of the problems of early local linking is that one may suffer from premature commitment--i.e. passing along the wrong assignments to a higher level.


This is an argument for a "probabilistic principle of least commitment", and for probabilistic representations of information, discussed in the last section of this notebook.

## Motivation for today

Today we are going to continue the general topic of methods lateral organization or grouping as unsuper-
vised learning. We'll first discuss a simple clustering algorithm called K-Means, and then proceed to study EM, the "expectation maximization" algorithm, where we will be estimating the parameters of probability distributions.

We'll revisit linear regression but in the more general case where the data come from one of two lines, but we aren't told which line. This problem is also encountered in vision where the visual system decides which of several surfaces the visual features come from.



Given a distribution of patterns, for example below where each point represents a pattern with 2 features, can one discover an underlying organization that assigns each pattern to one of $n$ clusters, either exclusively or with a probability of membership:

## Clustering

The larger goal is: given a set of unlabeled data $\mathrm{x}, 1$ ) decompose them into M classes ( $w_{1}, \ldots, w_{M}$ ), where M may or may not be known. 2) Learn $p(x \mid w)$; 3) Discover new classes.

We will look at the case of discovering classes when $M$ is known, first with a deterministic model ( K means), and then with a probabilistic model where the underlying generative processes has hidden or latent variables (EM).

## K-means

Assume that data x in D is clustered around unknown mean values, $m_{a}$. Assume the $\#$ of clusters is known -- fixed at $k$.

Simultaneously associate data to the means and estimate the means by minimizing:

$$
\sum_{a=1}^{k} \sum_{x \in D_{a}}\left(x-m_{a}\right)^{2}
$$

There are various algorithms. Deterministic K-means works by

1) randomly choosing data points $x$ and put them in $k$ sets $D_{a}, a=1$ to $k$.
2) calculate the mean of each cluster;
3) for each data point calculate how far it is from each of these provisional means and assign it to the nearest one;
4) repeat 2 and 3 until convergence.
```
ln[12]:= data = RandomReal[{-1, 1},{10^4, 2}];
ln[13]:=
    cc = ClusteringComponents[data, 3, 1,
        Method -> "KMeans", "DistanceFunction" }->\mathrm{ SquaredEuclideanDistance];
ln[14]:=
    means = Mean /@ {Pick[data, cc, 1], Pick[data, cc, 2], Pick[data, cc, 3]}
Out[14]= {{0.0262886, 0.609233}, {-0.561074, -0.329898}, {0.524062, -0.371086}}
ln[t5]:= Graphics[{LightBrown, Point@Pick[data, cc, 1], LightPurple, Point@Pick[data, cc, 2],
        LightCyan, Point@Pick[data, cc, 3], {Brown, PointSize[Medium], Point@means[[1]]},
    {Purple, PointSize[Medium], Point@means[[2]]},
    {Cyan, PointSize[Medium], Point@means[[3]]}}]
```

Here's a second example:

Generative model:
$\ln [31]$ := $\mathrm{x} 1=$ RandomVariate[MultinormalDistribution[\{0, 0\}, \{\{1, 0\}, \{0, 2\}\}], 500]; $x 2=\operatorname{RandomVariate[MultinormalDistribution[\{ 3,~0\} ,~}\{\{1,0\},\{0,2\}\}], 500]$;
$x 3$ = RandomVariate[MultinormalDistribution[\{3, 3\}, \{\{1, 0\}, \{0, 2\}\}], 500]; ggenerativem = Graphics@\{Red, Point@x1, Green, Point@x2, Blue, Point@x3\}


Given unlabeled data:

In[25]:= data2 = Join[x1, x2, x3];
ListPlot[data2, AspectRatio $\rightarrow 1$, Axes $\rightarrow$ False]

Out[26]=
$\ln [28]:=$ cc2 $=$ ClusteringComponents[data2, 3, 1, Method $\rightarrow$ "KMeans", "DistanceFunction" $\rightarrow$ SquaredEuclideanDistance];

In[29]:= means = Mean /@ \{Pick[data2, cc2, 1], Pick[data2, cc2, 2], Pick[data2, cc2, 3] \}
Out [29] $=\{\{2.58404,0.348759\},\{-0.273624,-0.633823\},\{3.03263,3.59689\}\}$
$\ln [41]:=$ gkmeans =
Graphics[\{Green, Point@Pick[data2, cc2, 1], Red, Point@Pick[data2, cc2, 2], Blue,
Point@Pick[data2, cc2, 3] , \{Yellow, PointSize[Large], Point@means[[1]]\},
\{Yellow, PointSize[Large], Point@means[ [2]]\},
\{Yellow, PointSize[Large], Point@means [ [3]]\}\}];
GraphicsRow[ \{ggenerativem, gkmeans\}, ImageSize $\rightarrow$ Medium]

Out[42]=



## Expectation Maximization (EM)

The Expectation Maximization algorithm 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

## Generating samples from a Gaussian Mixture Distribution

Similar to the generative model used above, suppose we have several (hidden) processes each of which can contribute to our data. In particular, let's assume a mixture distribution consisting of five different bivariate gaussian distributions.
$\ln [55]:=$ Clear[ndist];
ndist[ $\left.\mu_{-}, \Sigma_{-}\right]:=$MultinormalDistribution $[\mu, \Sigma$ ];
$\ln [57]:=r=.05 ;$
$\sigma=1.0 ;$
$\mu=$ Table[3 * $\mathrm{N}[\{\operatorname{Cos}[2 \mathrm{Pi} \mathrm{i}], \operatorname{Sin}[2 \mathrm{Pi} i]\}],\{i, 0,2 \mathrm{Pi}, \mathrm{Pi} / 4\}]$;
$\Sigma=\operatorname{Table}[\{\{\sigma, r\},\{r, \sigma\}\},\{i, 0,2 \operatorname{Pi}, \operatorname{Pi} / 4\}] ;$
$\operatorname{Det}[\{\{\sigma, r\},\{r, \sigma\}\}]$
Out[61]= 0.9975

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

The following gives mixing probabilities of $1 / 7,1 / 7,3 / 7,1 / 7$ and $1 / 7$ for distributions $1,2,3,4,5$ respectively.
$\ln [63]:=$
randomindex $:=\{1,2,3,3,3,4,5\} \llbracket R a n d o m I n t e g e r[\{1,7\}] \rrbracket$
Thus our stochastic generative process can be written:
$\ln [64]:=$
RandomReal[ndist[ $\mu[$ [t = randomindex]], $\Sigma[[t]]]$
Out[64]=
$\{-0.521357,-1.08368\}$
$\ln [65]:=$
scatterdata $=$ Table[RandomReal[ndist[ $\mu[$ [t = randomindex ] ], $\Sigma[[t]]]],\{i, 1,1500\}] ;$
ListPlot[scatterdata, AspectRatio $\rightarrow$ Automatic, ImageSize $\rightarrow$ Small]


The means, in an N-dimensional space for example, could represent prototypes in memory, and standard deviations the range of variability in the exemplars.

Given the kind of unlabeled data in the above example, how could one go about estimating not only the mixing probabilities, but also the means and covariances of the underlying generative processes?

## Simple case \& intuition

Let's see how to estimate means in the simplest case of two unknown distributions.

Suppose there is some agent that randomly chooses whether to flash a bright (a=1) or a dim (a=2) light, and for each flash we make a measurement $x$ of the light intensity.

We want to estimate the two means ( $\mu_{a}$, where $\mathrm{a}=1$ or 2 ) from a series of measurements (e.g. photon counts corresponding to light intensity), $\left\{x_{i}: i=1, \ldots, N\right\}$, 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 $V_{\mathrm{ia}}$ be an indicator variable, where $V_{\mathrm{ia}}=1$ if data point $x_{i}$ is generated by model $\mathrm{P}\left(\mathrm{x} \mid \mu_{\mathrm{a}}\right.$, sigma $\left.{ }^{\wedge} 2\right)$ and $V_{\mathrm{ia}}=0$ otherwise, for $\mathrm{a}=1,2$.
(Recall that we've used indicator functions before, as in the example of interpolation with missing data.)

Then using the usual formula for the estimate of the mean:

$$
\mu_{a} \approx \frac{\sum_{i=1}^{N} V_{i a} x_{i}}{\sum_{i=1}^{N} V_{i a}}
$$

The problem is that the values of $V_{\mathrm{i}}$ are unknown hidden variables that 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:

$$
\mu_{a} \approx \frac{\sum_{i=1}^{M} \bar{V}_{i a} x_{i}}{\sum_{i=1}^{M} \bar{V}_{i a}}, \forall a
$$

where $\overline{V_{\mathrm{ia}}}$ is the average value of $V_{\mathrm{ia}}$ and is given by $\overline{V_{\mathrm{ia}}}=\mathrm{p}\left(V_{\mathrm{ia}}=1 \mid x_{i}\right)=\mathrm{p}\left(\mathrm{a} \mid x_{i}\right)$. This brings us a step closer to a solution, but raises another problem--to calculate $\overline{V_{i a}}$ we will need to know the means-the very parameters we were trying to estimate in the first place! This is because $\mathrm{p}\left(\mathrm{a} \mid x_{i}\right)$ depends on the means for switch setting $\mathrm{a}=1$ or $\mathrm{a}=2$. In other words, we need the formula for $\mathrm{p}\left(\mathrm{a} \mid x_{i}, \mu_{\mathrm{a}}\right)\left(=\mathrm{p}\left(\mathrm{a} \mid x_{i}\right)\right.$ ). But the K-means example provides a clue.

We could: 1) guess the two means, then assign each data point to one of them based on which is closer. Then,
2) estimate the means again based on this provisional assignment. And then repeat these two steps until convergence

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

It is almost as easy to understand the derivation for a random vector (i.e. multivariate) as a random scalar, so we'll derive the results for the general vector case.

Let x represent a d-dimensional vector generated from a mixture of M Gaussian densities, with $\mathrm{s}=$ $\left\{\mu_{a}, C_{a}\right\}$ and $\mathrm{h}=\{\mathrm{a}\}$, where $\mu_{a}, C_{a}$, and $\mathrm{p}(\mathrm{a})$ are the vector means, covariance matrices, and mixture probabilities, respectively.
(The notation s , and h is used later for an unknown parameter s (or a set s )-- a "primary variable", that
we want to estimate, and another parameter $h$ (or set $h$ ) that is hidden--a "secondary" or "latent" variable. But we'll also see how to estimate $p(a))$.

So the mixture probability distribution of $x$ is:

$$
p(x)=p\left(x \mid \mu_{a}, C_{a}\right)=\sum_{a} p(x \mid a) p(a)
$$

where $a=1, \ldots, M$, and $\sum_{a} p(a)=1$. The $p(x \mid a)$ are the "class-conditional" probability densities, given by the standard expression for a multivariate gaussian distribution:

$$
p(x \mid a)=\frac{1}{\sqrt{(2 \pi)^{d}\left|C_{a}\right|}} \exp \left\{-\left(x-\mu_{a}\right)^{T} \cdot C_{a}^{-1} \cdot\left(x-\mu_{a}\right) / 2\right\}
$$

We are given a sequence of vector measurements $\left\{x_{i}: i=1, \ldots, N\right\}$, where $x_{i}$ now represents the ith sample vector (not the ith element of a vector $x$ ), and wish to estimate the means, the covariances and mixing parameters.

Let the probability that $x_{i}$ came from mixture component a be $\mathrm{p}\left(x_{i} \mid \mathrm{a}\right)$. We assume independence, so the likelihood is given by the product:

$$
p\left(x_{1}, x_{2}, \ldots, x_{N} \mid \mu_{a}, C_{a}\right)=\prod_{i} \sum_{a} p\left(x_{i} \mid a\right) p(a)
$$

Again taking the logs will help by turning products into sums. The log-likelihood is:

$$
E\left(\mu_{a}, C_{a}\right)=\log \left(p\left(x_{1}, x_{2}, \ldots, x_{N}\right)\right)=\sum_{i} \log \left\{\sum_{a} p\left(x_{i} \mid a\right) p(a)\right\}
$$

To maximize the likelihood, we can find the distribution parameters ( $\mu_{a}, C_{a}$ ) that minimize E . For the moment to keep things simple, 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 finding values of the means where the gradient values of $E$ are zero:

$$
\partial E / \partial \mu_{j}=\sum_{i} \frac{p\left(x_{i} \mid j\right) p(j)}{\sum_{a} p\left(x_{i} \mid a\right) p(a)} \frac{\left(\mu_{j}-x_{i}\right)}{\sigma_{j}^{2}}=\sum_{i} p\left(j \mid x_{i}\right) \frac{\left(\mu_{j}-x_{i}\right)}{\sigma_{j}^{2}}=0
$$

where we've used Bayes rule:

$$
p\left(a \mid x_{i}\right)=\frac{p\left(x_{i}, a\right)}{p\left(x_{i}\right)}=\frac{p\left(x_{i} \mid a\right) p(a)}{\sum_{a} p\left(x_{i} \mid a\right) p(a)}
$$

Solving for the $\mu_{j}{ }^{\prime} s\left(=\mu_{a}{ }^{\prime} s\right)$, we have

$$
\mu_{a}=\frac{\sum_{i} x_{i} p\left(a \mid x_{i}\right)}{\sum_{i} p\left(a \mid x_{i}\right)}
$$

This corresponds to the intuition we had above for the bright/dim example.
Recall, the problem, of course, is that we don't know $p\left(a \mid x_{i}\right)$. It depends on $\mu_{a}$ which we want to estimate..., so to get started we will just guess values for the means, $\mu_{a}$, and proceed with fingers crossed....

## E\&M iteration steps

## Estimate conditional mixing probabilities: E-step

Let $\mu_{a, t}$ be an initial guess of the mean for class a at time step t. Then in the E-step (E for "expectation") we let:

$$
p\left(a \mid x_{i}, \mu_{a, t}\right)=\frac{p\left(x_{i} \mid a, \mu_{a, t}\right) p(a)}{\sum_{a} p\left(x_{i} \mid a, \mu_{a, t}\right) p(a)}
$$

We can think of this as estimating the probability of which process the data, $x_{i}$, belongs to (e.g. a = the bright vs. dim switch setting) based on our current guess of the mean.

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

Now that we have an estimate of the current conditional mixing probability, we proceed to update our estimates of the mean.
This is the M-step ("maximization" step).

$$
\mu_{a, t+1}=\frac{\sum_{i} x_{i} p\left(a \mid x_{i}, \mu_{a, t}\right)}{\sum_{i} p\left(a \mid x_{i}, \mu_{a, t}\right)}
$$

The EM algorithm then proceeds by going back to the E-step to recompute $p\left(a \mid x_{i}, \mu_{a}\right)$ using the updated $\mu_{\mathrm{a}}$, followed by another M-step, and so on, until convergence.
(It has been shown that in the general case of non-Gaussian distributions discussed below that EM will converge to a local minimum of the likelihood function.)

How about the covariance?
Suppose we don't know the covariance matrix or the mixing probabilities? We can use the updated values of $p_{t}\left(\mathrm{a} \mid x_{i}\right)$,

$$
p_{t+1}\left(a \mid x_{i},\right)=p_{t}\left(a \mid x_{i}, \mu_{a}(t), C_{a}(t), p_{t}(a)\right)
$$

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 \& $p(a)$

$$
C_{a}(t+1)=\frac{\sum_{i}\left(x_{i}-\mu_{a}\right)\left(x_{i}-\mu_{a}\right)^{T} p_{t}\left(a \mid x_{i}\right)}{\sum_{i} p_{t}\left(a \mid x_{i}\right)}
$$

(where $\mathbf{a b}^{\wedge} \mathbf{T}$ is the outer product between vectors $\mathbf{a}$ and $\mathbf{b}$ ).
The mixing probabilities are estimated by:

$$
p_{t+1}(a)=\frac{1}{N} \sum_{i} p_{t}\left(a \mid x_{i}\right)
$$

## Demo: Two gaussians, unknown $\mu$ 's, $\sigma$ 's , and mixing probabilities

## Generating samples from a Gaussian Mixture Distribution

## Generative model

```
\operatorname{ln[6]]:= }\mu1=1.3; \sigma1 = 1; \mu2 = 6.5; \sigma2 = 0.8; a1 = 0.16; a2 = 1 - a1;
    p1dist = NormalDistribution[ }\mu1,\sigma1]
    p2dist = NormalDistribution[ }\mu2,\sigma2]
    p1[x_] := PDF[p1dist, x];
    p2[x_] := PDF[p2dist, x];
    samplemix := If[RandomReal[] < a1, RandomReal[p1dist], RandomReal[p2dist]];
```


data $=$ Table[samplemix, \{i, 1, 500\}];
Histogram[data, Epilog $\rightarrow$
\{Text[" $\mu 1="<>\operatorname{ToString}[\mu 1]<>", \sigma 1="<>\operatorname{ToString}[\sigma 1]<>", p a 1="<>$ ToString[a1],
$\{\mu 1,40\}]$, Text [" $\mu 2="<>\operatorname{ToString}[\mu 2]<>", \sigma 2="<>$
ToString[o2] <> ", pa2=" <> ToString[a2], \{ $\mu 2-2,150\}]\}]$

EM algorithm--Now learn all the parameters--means, standard deviations, and mixing probabilities from the data
$\ln [72]:=\operatorname{pxdm}\left[x_{-}, m u_{-}, \sigma_{-}\right]:=\operatorname{PDF}[$ NormalDistribution[mu, $\sigma$ ], $x$ ];
E-step: The prob of mixing labels conditional on the data x is:

$$
p\left(a \mid x_{i}, \mu_{a, t}\right)=\frac{p\left(x_{i} \mid a, \mu_{a, t}\right) p(a)}{\sum_{a} p\left(x_{i} \mid a, \mu_{a, t}\right) p(a)}
$$

In Mathematica code,
$\ln [73]:=\operatorname{pmcx}\left[a_{-}, x_{-}\right]:=\operatorname{pxdm}[x, \mu[[a]], \sigma[[a]]] *$
pa[[a]] / (pxdm[x, $\mu[$ [1] ], $\sigma[[1]]] * \operatorname{pa[[1]]+pxdm[x,~} \mu[[2]], \sigma[[2]]] * p a[[2]])$;
SetAttributes[pmcx, Listable]; (*pmcx is made listable so that
that it will automatically map over the data below*)
M-step: The maximum likelihood estimate of the means is:

$$
\mu_{a}=\frac{\sum_{i} x_{i} p\left(a \mid x_{i}\right)}{\sum_{i} p\left(a \mid x_{i}\right)} .
$$

or in Mathematica:
$\mu[[1]]=\mathrm{pmcx}[1$, data $]$. data/Plus@@(pmcx[1,\#]\&/@data)
$\mu[[2]]=p m c x[2$, data $]$.data/Plus@@(pmcx[2,\#]\&/@data)
Similarly, the variances and mixing probabilities are also weighted averages:
$\sigma[[1]]=$ Sqrt[pmcx[1,data].(data- $\mu[[1]])^{\wedge} 2 /$ Plus@@(pmcx[1,\#]\&/@data)]

```
\sigma[[2]]=Sqrt[pmcx[2,data].(data- }\mu[[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：
$\ln [75]:=\mu=\operatorname{RandomReal}[\{-10,10\}, 2]$ ；
$\sigma=$ RandomReal［\｛0，10\}, 2];
pa＝\｛temp＝RandomReal［］， 1 －temp $\}$
Then iterate for $\mathrm{i}=1$ 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．
$\ln [76]:=$

```
iter = 6;
\muparameterList = Table[0, {a, 1, 2}, {k, 1, iter}];
\sigmaparameterList = \muparameterList; paparameterList = \muparameterList;
For [k = 1, k s iter, k++,
    For[a=1, a < 2,a++,
        \mu[[a]] = pmcx[a, data].data / Plus @@ (pmcx[a, #] & /@ data);
        \sigma[[a]] = Sqrt[pmcx[a, data].(data - \mu[[a]])^2 / Plus @@ (pmcx[a,#] & /@ data)];
        pa[[a]] = Plus @@ (pmcx[a,#] & /@ data) / Length[data];
        \muparameterList[[a, k]] = \mu[[a]];
        \sigmaparameterList[[a, k]] = \sigma[[a]];
        paparameterList[[a,k]] = pa[[a]];
        ];
    ];
```


## Graph of the evolution of the mixing parameters

Blue line shows true values from the generative model．
In［80］：$=$ ga＝Show［\｛Plot［\｛pa【1］，pa【2】\}, \{x, 0, iter\}, PlotStyle $\rightarrow$ Hue［0．5］］， ListPlot［\｛paparameterList【1］，paparameterList【2』\}, Joined $\rightarrow$ True］\}, PlotRange $\rightarrow$ \｛0，1\}, AxesOrigin $\rightarrow$ \｛0，0\}, AxesLabel $\rightarrow$ \｛＂iteration＂，＂pa＂\}];

## Graph of the evolution of the means

$\ln [81]:=$ gmeans $=$ Show［\｛Plot［\｛ $\mu \llbracket 1 \rrbracket, \mu \llbracket 2 \rrbracket\},\{x, 0$, iter $\}, ~ P l o t S t y l e ~ \rightarrow ~ H u e[0.5]], ~$ ListPlot［\｛ $\mu$ parameterList【1】，$\mu$ parameterList【2】\}, Joined $\rightarrow$ True］\}, PlotRange $\rightarrow\{0,8\}$ ，AxesOrigin $\rightarrow\{0,0\}$ ，AxesLabel $\rightarrow$ \｛＂iteration＂，＂$\mu$＂$\}$ ］；

## Graph of the evolution of the standard deviations

```
ln[82]:= gsds = Show[{Plot[{\sigma\llbracket1\rrbracket, \sigma\llbracket2\rrbracket}, {x, 0, iter}, PlotStyle }->\mathrm{ Hue[0.5]],
        ListPlot[{\sigmaparameterList\llbracket1\rrbracket, oparameterList\llbracket2\rrbracket}, Joined }->\mathrm{ True]},
    PlotRange }->\mathrm{ {0, 5}, AxesOrigin }->\mathrm{ {0, 0}, AxesLabel }->\mathrm{ {"iteration", "б"}];
```

In[83]:= GraphicsRow[\{ga, gmeans, gsds\}, ImageSize $\rightarrow$ Large]




## EM: Theory for arbitrary 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 is used for an unknown parameter s (or a set s), that we want to estimate (e.g. the means and covariances), and another parameter h (or set $\left\{h_{i}\right\}$ ) that is hidden (e.g. an indicator variable representing the probability of mixing, $\mathrm{p}(\mathrm{a})$ ).)

We'd like to find the value of $s$ that maximizes the likelihood of the data $\left\{x_{i}\right\}$, given other intervening variables hi.
The log-likelihood of the observations is given by:

$$
\log p\left(x_{1}, \ldots, x_{N} \mid s\right)=\log \prod_{i=1}^{N+1} p\left(x_{i} \mid s\right)=\sum_{i} \log p\left(x_{i} \mid s\right)=\sum_{i} \log \sum_{h_{i}} p\left(x_{i}, h_{i} \mid s\right)
$$

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:

$$
\frac{\partial \log p\left(x_{1}, \ldots, x_{N} \mid s\right)}{\partial s}=\sum_{i} \frac{1}{\sum_{h_{i}} p\left(x_{i}, h_{i} \mid s\right)} \frac{\partial}{\partial s}\left\{\sum_{h_{i}} p\left(x_{i}, h_{i} \mid s\right)\right\}
$$

Where we have used the relation (that you can prove from basic calculus):

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

Bringing the summation over $h_{i}$ towards the front, we have:

$$
\sum_{i} \sum_{h_{i}} \frac{1}{\sum_{h_{i}} p\left(x_{i}, h_{i} \mid s\right)} \frac{\partial}{\partial s} p\left(x_{i}, h_{i} \mid s\right)
$$

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

$$
\sum_{i} \sum_{h_{i}} \frac{p\left(x_{i}, h_{i} \mid s\right)}{\sum_{h_{i}} p\left(x_{i}, h_{i} \mid s\right)} \frac{\partial}{\partial s} \log p\left(x_{i}, h_{i} \mid s\right)
$$

Using Bayes rule and setting the expression to zero, we want to find s that satisfy:

$$
\sum_{i} \sum_{h_{i}} p\left(h_{i} \mid x_{i}, s\right) \frac{\partial}{\partial s} \log p\left(x_{i}, h_{i} \mid s\right)=0
$$

## Summary of EM strategy in the general case

So following the above reasoning for the Gaussian case, the EM strategy for solving equation for s involves two steps:

1) Given a guess, $s=s_{t}$ at step $t$, calculate

$$
p\left(h_{i} \mid x_{i}, s_{t}\right) \quad(E-\text { step })
$$

2) Use this to solve

$$
\sum_{i} \sum_{h_{i}} p\left(h_{i} \mid x_{i}, s_{t}\right) \frac{\partial}{\partial s} \log p\left(x_{i}, h_{i} \mid s\right)=0 \quad(M-s t e p)
$$

to find the next $s=s_{t+1}$. 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. In a previous example, we used a local smoothness constraint. Another way is to do a parametric fit, which imposes global, rather than local, constraints. For example, a global constraint might look for surface fits among planes or quadratic surfaces, or splines.

Or even more complex shape models could be invoked. In the earlier ape-human figure, one could use a higher-level, global shape model (homo sapiens vs. Pan troglodyte) to disambiguate local edge groupings where the noses meet.



Another aspect of surface perception is our ability to take noisy data (e.g. depth cues), and not only interpolate the data as we saw with the Markov Random Field example, but also decide which of several surfaces the data belong. This problem appears with stereo and motion data (Madarasmi et al., 1993; Kersten \& Madarasmi, 1995) or optic flow (Jepson, 1993; Weiss, 1997).


Free-fusing the above sparse stereogram pair produces a perception of two surfaces in depth, as illustrated by the depth vs. horizontal distance plot on the right.

A number of ways have been proposed to deal with this problem. EM (described above) is 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 Yair Weiss for a simple tutorial and demo.

Consider first Generative Model 1.

## Generative models

Two lines with (slopes, intercepts) $=(a t 1, b t 1)$ and (at2, bt2).
$\ln [84]:=$ ndist $=$ NormalDistribution [0, 2];

## Generative model I

```
ln[85]:= {at1, bt1} = {-2, 40};
    {at2, bt2} = {3, 1};
    y1[x_] := at1 * x + bt1 + Random[ndist];
    y2[x_] := at2 * x + bt2 + 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 (you will need to make the cell property "evaluatable" to work)


## EM algorithm

We now pretend we don't know the values of the slopes and intercepts, and want to estimate them from the data.

The simplified logic of the EM algorithm is as follows. Start with random parameter values (slopes and intercepts, or a's and b's) for the two models. Iterate the E and M steps until convergence:

1. E-step: assign points to the line that are the best fit
2. M-step: update the line parameters using only the points assigned to it
...but with EM we will do "soft" assignment where probabilities are given to each data point as to whether it might have been caused by line 1 vs. line 2 . And in the M-step, we will uses these weights to do weighted linear regression.

Initialize parameters to random values

```
ln[92]:= \sigma= 0.1;
    {a1, b1, a2, b2} = Table[10 RandomReal[], {4}];
```


## E-step

Compute residuals $\mathrm{r} 1, \mathrm{r} 2$, the error in the predicted and actual y values under each of the two models.
$\ln [111]:=r 1=a 1$ * $x+b 1-y ;$
r2 = a2 * $x$ + b2 - y;
Now we could just assign points based on which line parameters give the smallest residual. But we'd like to take into account our model of the conditional mixing probabilities, which also depend on the noisiness in the data. So we'll compute weights that correspond to the conditional mixing probabilities. Using the residuals, compute weights. We'll assign these weights to data in the M-step later.
$\ln [113]:=\mathrm{w} 1=\operatorname{Exp}\left[-r 1^{\wedge} 2 / \sigma\right] /\left(\operatorname{Exp}\left[-r 1^{\wedge} 2 / \sigma\right]+\operatorname{Exp}\left[-r 2^{\wedge} 2 / \sigma\right]\right) ;$
$w 2=\operatorname{Exp}\left[-r 2^{\wedge} 2 / \sigma\right] /\left(\operatorname{Exp}\left[-r 1^{\wedge} 2 / \sigma\right]+\operatorname{Exp}\left[-r 2^{\wedge} 2 / \sigma\right]\right) ;$

## 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:

$$
\left(\begin{array}{cc}
\sum_{i} x_{i}^{2} & \sum_{i} x_{i} \\
\sum_{i} x_{i} & \sum_{i} 1
\end{array}\right)\left[\begin{array}{c}
a \\
b
\end{array}\right]=\left[\begin{array}{c}
\sum_{i} x_{i} y_{i} \\
\sum_{i} y_{i}
\end{array}\right]
$$

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

$$
\left(\begin{array}{cc}
\sum_{i} w_{i} x_{i}^{2} & \sum_{i} w_{i} x_{i} \\
\sum_{i} w_{i} x_{i} & \sum_{i} w_{i} 1
\end{array}\right)\left[\begin{array}{l}
a \\
b
\end{array}\right]=\left[\begin{array}{c}
\sum_{i} w_{i} x_{i} y_{i} \\
\sum_{i} w_{i} y_{i}
\end{array}\right]
$$

(For simplicity, we've dropped the subscript on the weights that indicates whether it is line 1 or line 2 , and just keep the subscript indicating the weight for point i).
$\ln [115]:=\{a 1, b 1\}=\operatorname{Inverse}[\{\{w 1 \cdot(x x), w 1 \cdot x\},\{w 1 \cdot x, A p p l y[P l u s, w 1]\}\}] \cdot\{w 1 \cdot(x y), w 1 \cdot y\} ;$
$\{a 2, b 2\}=\operatorname{Inverse[\{ \{ w2.(xx),w2.x\} ,\{ w2.x,Apply[Plus,w2]\} \} ]\cdot \{ w2.(xy),w2.y\} ;~}$
$\ln [177]:=$ gfit $=P \operatorname{lot}[\{a 1 x+b 1, a 2 x+b 2\},\{x, 0,6\}] ;$
Show
$\left\{\right.$ gfit, Graphics $\left[\left\{\operatorname{PointSize}[0.03], \operatorname{Transpose}\left[\left\{(H u e[\# 1] \&) / @ \frac{w 1}{2}\right.\right.\right.\right.$, Point /@data $\left.\left.\left.\left.\}\right]\right\}\right]\right\}$,
PlotRange $\rightarrow$ All]
Out[118]= 20
Now manually run through the E and M steps again...and again, until convergence.
$\ln [102]:=\{\{a t 1, b t 1\},\{a 1, b 1\},\{a t 2, b t 2\},\{a 2, b 2\}\} / /$ TableForm
Out[102]/TableForm=
-2 4
10.09135 .21563
$3 \quad 1$
$3.39444 \quad 3.61352$

- 1. Run EM with Generative Model 2. Increase the additive noise. How does attribution accuracy change? ("attribution" means assigning a point to its correct line)
- 2. N=5 Multivariate gaussians, only data known: Implement EM to estimate means, variance, and mixing probabilities

Implement EM to estimate means, variance, and mixing probabilities

$$
\begin{aligned}
& p\left(a \mid x_{i}, \mu_{a, t}\right)=\frac{p\left(x_{i} \mid a, \mu_{a, t}\right) p(a)}{\sum_{a} p\left(x_{i} \mid a, \mu_{a, t}\right) p(a)} \\
& \mu_{a, t+1}=\frac{\sum_{i} x_{i} p\left(a \mid x_{i}, \mu_{a, t}\right)}{\sum_{i} p\left(a \mid x_{i}, \mu_{a, t}\right)} \\
& C_{a}(t+1)=\frac{\sum_{i}\left(x_{i}-\mu_{a}\right)\left(x_{i}-\mu_{a}\right)^{T} p_{t}\left(a \mid x_{i}\right)}{\sum_{i} p_{t}\left(a \mid x_{i}\right)} \\
& \quad p_{t+1}\left(a \mid x_{i},\right)=p_{t}\left(a \mid x_{i}, \mu_{a}(t), C_{a}(t), p_{t}(a)\right)
\end{aligned}
$$

Neural representation of probability distributions?

## Population codes

Lecture 24 supplementary material described an influential model of population coding for orientation that has been around for many decades.


Receptive fields of visual neurons typically overlap in space (e.g. a bright spot at one location creates a neural point spread function, the "projective field"). E.g. a bar at one orientation will more or less activate cells within a certain feature range ( $+/-15$ deg in V1). Cell S firing at a rate of g spikes per second may not tell us the orientation of the stimulus (because the rate per second also depends on other dimensions of the stimulus, such as contrast). But suppose we have access to the responses of a bunch (i.e. population) of neurons all "seeing" the same stimulus bar. How can information (e.g. about orientation) be extracted from this pattern of activity?

One can combine information across a population in terms of a "population vector". Let $\boldsymbol{x}_{\boldsymbol{k}}$ be a vector representing a stimulus feature (e.g. the kth 2-D position, or kth motion direction, or kth orientation, etc.). Let the firing rate of the ith cell be $R_{i}\left(\boldsymbol{x}_{\boldsymbol{k}}\right)$ in response to input $\boldsymbol{x}_{\boldsymbol{k}}$. Let the feature that produces the peak response of the ith cell be $x_{i}^{p}-$ i.e. $\boldsymbol{x}_{i}^{p}$ is the ith cell's preferred feature, the one that fires the cell the most (the center of the tuning function, so $R_{i}\left(x_{i}^{p}\right)$ is the maximum firing rate).

Given an input feature $\boldsymbol{x}_{\boldsymbol{k}}$, the firing rate of the ith cell can be interpreted as the strength of its "vote" for its preferred feature. So for the example of positional coding, position could be represented by the weighted average over the population of cells, each responding with various firing rates to $x_{k}$ :

$$
x=\sum_{i} R_{i}\left(x_{k}\right) x_{i}^{p}
$$

This can be interpreted as a weighted average. (With a grandmother cell code, $\mathrm{R}_{\mathrm{i}}\left(\mathrm{x}_{\mathrm{k}}\right)=\delta_{\mathrm{ik}}$.)
Analogous to computing the center of mass, or an average, we can normalize the estimate by the total activity:

$$
x=\sum_{i} R_{i}\left(x_{k}\right) x_{i}^{p} / \sum_{i} R_{i}\left(x_{k}\right)
$$

This measure has been applied to modeling sensory coding, and in the motor system, and cognitive processes involving direction of movement (Georgopoulos et al., 1993). In certain tasks the population vector can be measured in real neuronal ensembles and be seen to evolve in time consistent with behavioral measures (mental rotation, reach planning).

## Population codes as probability distributions

How to avoid (or correct) problems with ealry, local commitment.


The Lecture 24 web page includes material on a probabilistic interpretation of population codes.

There are several ideas relevant to this lecture 26, and earlier course material on integrating information based on reliability.

First, a probabilistic representation can be viewed as a specific example of the principle of least commit-ment--i.e. represent the probabilities of ambiguous early features such as information for edge orientation, rather than make a decision. So if you have a local measurement say of an orientation at one location, and of another orientation at another location, decide whether to link them based on a weighted average. (Recall homework assignment on combining information from two different estimates of means.)

But the weights needs to be represented somehow in the brain. This is where probabilistic coding becomes important. The work by Pouget, Zemel, Ma, Knill, Latham and others provides the theoretical framework for how neural populations could not only represent probability distributions, but also compute with them, including information integration, and do marginalization.

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