Introduction to Neural Networks U. Minn. Psy 5038

Self-organization Decorrelation, and Principal Components Analysis with Neural **Networks**

Initialization

In[11]:=

Off[SetDelayed::write]
Off[General::spell1]
<<Statistics`ContinuousDistributions`</pre>

Introduction

Unsupervised learning--what does it mean to learn without a teacher?

Statistical view:

Learning as probability density estimation. From a relatively small number of samples (human faces), what can we conclude about the probabilistic structure of the whole ensemble (of human faces)?

Straightforward with a single random variable: mean, standard deviation, histogram

Less straightforward with vector random variable: vector means, autocovariance, higher-order statistics, histogram

Less straightforward because of the problem of getting enough samples to fill all the bins.

But for natural patterns, it is typically the case that even tho' the data maybe n-dimensional vectors, the ensemble lives in a much smaller space. How can we find that space?

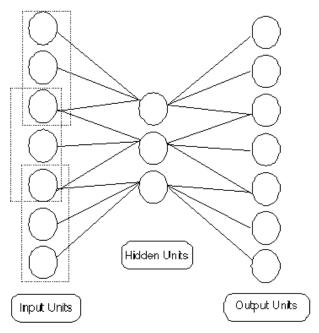
Once found, what is it good for?

Unsupervised learning, self-organization, and data compression

In an earlier lecture, we saw an example of the increased computational power of a multi-layer network. The reason for the increased power is that the hidden units discover effective ways of representing contingencies in the training data set. For example, a solution to the XOR problem in effect discovers how to do AND as well as OR relations, and piece these together.

One of the problems with multi-layer nets is understanding exactly what they have discovered and are representing in the hidden layers. It is perhaps easiest to begin tackling this problem by setting up a network to do autoassociation.

Let's turn the supervised 3-layer backprop network into an unsupervised learning algorithm simply by setting the output equal to the input. Then we are seeking weights that achieve the goal that the outputs come as close as possible to matching the inputs, in a least squares sense. If we have a smaller number of hidden units than input or output units, we can ask: What has the network discovered about the input ensemble that is captured with the smaller dimensionality of the hidden unit layer?



A theoretical result (Baldi and Hornik, 1988) showed that for the linear case this kind of network is closely related to a standard statistical technique called "Principal Components Analysis", (PCA) that dates back to 1933 (Hotelling, H. (1933). Analysis of a complex of statistical variables into principal components. J. Educ. Psych., 24, 417-441,498-520). The idea is that the variability in a data set consisting of n-dimensional vectors may concentrate along certain axes or subspaces of dimension m<n. Principal components analysis is one standard technique for finding the dimensions that capture the most variation. Suppose there are n input units, and m hidden units. Baldi and Hornik showed that the hidden units were finding the m-dimensional sub-space that capture the most variance. This is not exactly principal components analysis, but it is closely related.

In this notebook you will learn about PCA, and then see how it can be done by neural-like systems that use local hebbian learning, and avoid error back-propagation.

In order to understand PCA, let's start with the following simple two neuron system. This is the simplest system for which

correlational structure can be analyzed. The rationale is that the two neuron system will give us insight into the problem of finding structure in data sets with really high dimensionality, such as images or speech.

Modeling the input: Statistical model of the correlations of a 2D input ensemble

■ The generative model

Recall that the idea behind generative modeling is to understand the structure of the data coming into the network. This gives us a better idea of what the network is ideal for, and where it should have problems. Our goal is first create data that has a particular correlational structure, and then to see how a neural network can discover the structure.

Consider a "two-neuron" system whose inputs are correlated. The random variable, \mathbf{rv} , is a 2D vector representing the input. The scatter plot for this vector has a slope of Tan[theta] = 0.41. The variances along the axes are:

```
bigstd^2 = 4^2 = 16 and smallstd^2 = .25^2 = .0625.
```

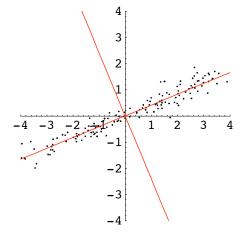
gprincipalaxes is a graph of the principal axes which we will use for later comparison with simulations. **ContinuousDistributions.m** is a *Mathematica* package that you have seen before and that provides routines for sampling from a Gaussian (or Normal) distribution, rather than the standard uniform distribution that **Random**[] provides.

We define ndist so that Random[ndist] returns numbers whose average is zero, and whose standard deviation is 1. Variance is equal to standard deviation squared. If we multiple Random[ndist] by bigstd, we get random numbers with variance bigstd^2. And similarly for smallstd. rv is the projection of these numbers onto the x and y axes.

```
In[14]:= ndist = NormalDistribution[0,1]; theta = Pi/8;
bigstd = 4.0; smallstd = 0.25;
alpha = N[Cos[theta]]; beta = N[Sin[theta]];
rv :=
    {bigstd x1 alpha + smallstd y1 beta, bigstd x1 beta -
    smallstd y1 alpha} /.
        {x1-> Random[ndist],y1-> Random[ndist]};

gprincipalaxes = Plot[{x (beta/alpha),
        x (-1/(beta/alpha))}, {x,-4,4},
        PlotRange->{{-4,4},{-4,4}},
        PlotStyle->{RGBColor[1,0,0]},
        AspectRatio->1,DisplayFunction->Identity];
```

x1 and y1 are said to be *correlated*. (Later we'll see how to use the package **<<Statistics`MultinormalDistribution`** to simplify synthesis of n-dimensional random numbers.) Let's view a scatterplot of samples from these two correlated Gaussian random variables.



Principal Components Analysis (PCA) using standard statistical methods

In the previous section, we developed a model for synthetic data--so we know the statistical structure. Usually, we don't have a good model of the statistical structure of an ensemble, but want to discover something about it. It is usually too hard to find a complete model of the underlying distribution, but we can still analyze the data to find means, variances and so forth. When dealing with a high-dimensional ensemble, sometimes most of the variation is occurring in some subspace. In the example above, most of the variation is occurring in the 1D subspace defined by a line of slope **theta**. How could we have discovered that only from the data--i.e. without having the model before us? We could graph it and look. But what if the dimensionality of the space is really big?

PCA provides a method. PCA seeks out a new coordinate system that is just a rotation of the original that does two very interesting things: 1) The data when projected onto the new rotated coordinates are no longer correlated—in fact the autocovariance matrix (see below) is diagonal; 2) The new coordinates can be ordered so that the main or "principal component" has the most variance, the next has the second most, and so forth. How is this done? It turns out that the eigenvectors of the autocovariance matrix are the principal components, and the eigenvalues are the variances of the data when projected onto the new axes.

What good is PCA for a data set? If the variance of some of the projections is near zero, one can in fact dispense with these components and achieve a good approximate coding of the data with just the remaining coordinates. We are going to see that in the 2D example, we can get an economical coding of the data with just one number, rather than two.

■ Calculate the autocovariance matrix

Let $E[\bullet]$ stand for the expected or average of a random variable, \bullet . Suppose we want a measure of the covariation of two random variables, x and y. One way is to first subtract off the mean from both giving: x1=x-E[x], and y1=y-E[y]. Then we find the average of the product $E[x1\ y1]$. This is called covariance. If x1 and y1 tend to go up together (a high value of x1 predicts a high value of y1, etc..), then the product will tend to be big on average—they are correlated. (If x=y, then this is just the standard definition of variance.)

Suppose we have a vector (like \mathbf{rv} , of dimension 2 or perhaps higher) whose elements are random variables. We can define a cross-covariance analogous to covariance. But all we need now is a measure of how the various elements of covary with each other. The autocovariance matrix of a of vector random variable, \mathbf{x} , can be defined by first subtracting off the mean vector, and then averaging over all the outer-products with itself: $\mathbf{E}[\mathbf{x}-\mathbf{E}[\mathbf{x}]][\mathbf{x}-\mathbf{E}[\mathbf{x}]]^T$]. (Note this could be estimated using the auto-associative memory rule--i.e. just add up all the outer products, and then normalize by the number of learning pairs.) The diagonal values of the autocovariance matrix correspond to the variances of each element. The off-diagonals are the covariances for each pair of elements. Because of the symmetry of the outer-product (multiplication commutes), the autocovariance matrix is symmetric.

Let's compute the autocovariance matrix for **rv**. The calculations are simpler because the average value of **rv** is zero. As we would expect, the matrix is symmetric:

Out[24]//MatrixForm=

```
\begin{pmatrix} 14.3324 & 6.00546 \\ 6.00546 & 2.5816 \end{pmatrix}
```

The variances of the two inputs (the diagonal elements) are due to the projections onto the horizontal and vertical axis of the generating random variable.

(Sidenote: The autocorrelation matrix is defined to be the expected or average value of the outer product without subtracting off the means.)

■ Calculate the principal components (eigenvectors of the autocovariance matrix)

Now we will calculate the eigenvectors of the autocovariance matrix

```
In[26]:= MatrixForm[eigauto = Eigenvectors[auto]]
```

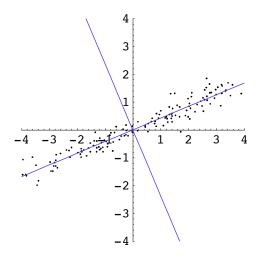
Out[26]//MatrixForm=

```
\begin{pmatrix} 0.921771 & 0.387734 \\ -0.387734 & 0.921771 \end{pmatrix}
```

Remember that the eigenvectors of a symmetric matrix are orthogonal. You can check that these are.

Let's graph the principal axes corresponding to the eigenvectors of the autocovariance matrix together with the scatterplot we plotted earlier. One axis is defined by: y=eigauto[[1,2]]/eigauto[[1,1]] x, and the other axis by: y=eigauto[[2,2]]/eigauto[[2,2]]/eigauto[[2,1]] x.

In[28]:= Show[g1,gPCA,DisplayFunction->\$DisplayFunction];



You can see that PCA has discovered important structure in the input ensemble as shown by the blue lines.

Try changing npoints=5. Then plot the true principal axes with gPCA, using show[g1,g-PCA,gprincipalaxes,DisplayFunction→\$DisplayFunction]. Do gPCA and gprincipalaxes match? Why not?

■ Calculating the variances (eigenvalues)

The eigenvalues give the ratio of the variances of the projections of the random variables $\mathbf{rv}[[1]]$, and $\mathbf{rv}[[2]]$ along the principal axes:

```
In[29]:= eigvalues = Eigenvalues[auto]

Out[29]= {16.8585, 0.0554654}
```

Let's project the data onto the principal axes and calculate the autocovariance matrix in the new coordinate system. The projected values are given by: **eigauto.rvsamples.**

We'll see that the new coordinates for this data set have zero correlation.

```
In[30]:= autolist = Table[
    Outer[Times,eigauto.rvsamples[[i]],
    eigauto.rvsamples[[i]]],{i,Length[rvsamples]}];

MatrixForm[Chop[
    Sum[autolist[[i]],
        {i,Length[autolist]}]/Length[autolist]]]

Clear[autolist];
```

Out[31]//MatrixForm=

```
\begin{pmatrix} 16.8585 & 0 \\ 0 & 0.0554654 \end{pmatrix}
```

Note that the off-diagonal elements (the terms that measure the covariation of the transformed random variables) are zero. Further, the diagonal elements are estimates of the population variances along the principal axes. The should be approximately equal to the population variances specified by the generative model: i.e. the **bigstd^2**, and **smallstd^2** from our synthetic data process. We've demonstrated a fundamental property of PCA: 1) PCA decorrelates previously correlated input data; 2) PCA discovers principal axes that capture the dimensions with the dominant variance.

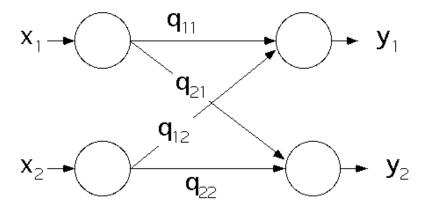
How can we do PCA using brain-style computation?

Principal Components Analysis (PCA) with neural networks

Neural network model using Hebb together with Oja's rule for extracting the dominant principal component

■ Introduction to Oja's network: weight normalization

Consider the following linear neural network. The input and output values are represented by vectors \mathbf{x} , and \mathbf{y} respectively. The connection weights are represented by matrix \mathbf{Q} .



We will combine the outer product form of Hebb's rule, together with Oja's modification. Without Oja's rule, the Hebb rule does not place a limit on the size of the weights.

$$\Delta q_{ij} = \alpha \left(x_j y_i - q_{ij} y_i^2 \right)$$

Oja's rule automatically tends to normalize the weights so that their squared sum is finite. In fact:

Show, when the weights are no longer changing, that:

$$\sum_{i,j} q_{ij}^2 = 1$$

■ Implementing Oja's network

Oja's rule constrains the sum of the squares of the weights to approach 1. We will set the intial values of the weight matrix to random values between 0 and 1.

Note that a space or * in *Mathematica* between two expressions does an element by element multiplication. We use this notation as economical way of writing Oja's rule. An example is:

```
In[37]:= MatrixForm[{{a,b},{c,d}} {x,y}]
```

Out[37]//MatrixForm=

```
\begin{pmatrix} ax & bx \\ cy & dy \end{pmatrix}
```

Note that this different from standard matrix/vector multiplication.

For each random input rv, we compute the output $y = Q \cdot x$, and the weights Q get adjusted on-line by Oja's rule. Unlike computing eigenvectors, we don't have to store all npoints of the random vectors to compute an autocovariance matrix.

The slopes of the rotated coordinates are given by the elements of p1. The last computed values are:

```
In[66]:= \begin{array}{c} Q\\ Q[[1, 2]]/Q[[1, 1]]\\ Q[[2, 2]]/Q[[2, 1]] \end{array}
Out[66]= \begin{array}{c} \left(0.923498 \ 0.383904\\ 0.923498 \ 0.383904 \right) \end{array}
Out[67]= \begin{array}{c} 0.415707\\ 0.415707 \end{array}
Out[68]= \begin{array}{c} 0.415707 \end{array}
```

■ Graph the evolution of the network: slopes of the projection axes

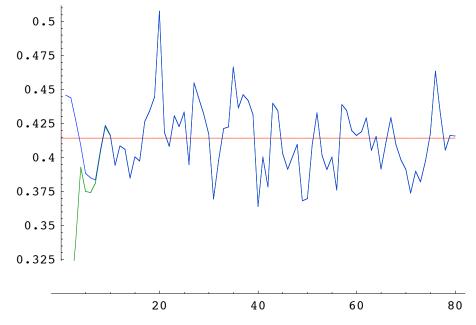
Let's plot the slopes of projection axes as a function of iterations. We've sampled every 5th value, using **Mod[i,5**], and stored it in **p1**. These values should approach the slope of the scatter plot, **Tan[theta].**

```
In[55]:= gg1=Plot[ Tan[theta], {x,0,Length[p1]}, AxesOrigin->{0,.3},
    DisplayFunction->Identity,
    PlotStyle->{RGBColor[1,0,0]}];

gg2=ListPlot[Map[#[[2]]&,p1], AxesOrigin->{0,0},
    PlotJoined->True, DisplayFunction->Identity,
    PlotStyle->{RGBColor[0,.5,0]}];

gg3=ListPlot[Map[#[[1]]&,p1], AxesOrigin->{0,0},
    PlotJoined->True, DisplayFunction->Identity,
    PlotStyle->{RGBColor[0,0,1]}];

Show[gg1,gg2,gg3,DisplayFunction->$DisplayFunction];
```

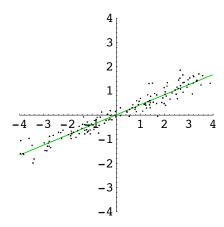


There is some random fluctuation in the weights. We can obtain more stability by having a time constant over which the Hebbian term and the variance of y are averaged.

■ Graph the slope of the slope of the projection axes (ratio of network weights) together with the data

We can see how well the coordinate transformation fits the principal axes of a sample scatter plot:

In[63]:= Show[gnetwork,g1,DisplayFunction->\$DisplayFunction];



You can verify that the network does a good job of extracting the principal component. Recall that the slope for the population distribution is **Tan[theta**]:

In[69]:= N[Tan[theta]]
Out[69]= 0.414214

It doesn't take long for the green and blue lines to converge to identical values.

The only problem with this network is that having two output neurons is redundant--they both pull out the same principal component--the dominant axis. The slopes for both are:

In[70]:= p1[[Length[p1]]]

Out[70]= {0.415707, 0.415707}

This isn't surprising because the network was symmetrical--both output neurons saw the same inputs and updated their weights using the same rule. How can this be fixed to pick out the other principal components? Some kind of asymmetry has to be introduced.

A generalization of Oja's rule for extracting all of the principal components (Sanger, 1989)

■ Introduction to Sanger's network for PCA

The problem with Oja's network is that it extracts just the main principal component. Our example had two outputs, but the network is symmetric, and both outputs were the same--the projection of the input onto the main principal axes. Sanger proposed a modification to the Oja network that can extract *all* of the principal components.

We will use the same network as in the above example. However, the normalization part of learning rule will be asymmetric. The generalization of Oja's term to update weights \mathbf{q} , is given by:

$$\Delta q_{ij} = \alpha \left(x_j y_i - y_i \sum_{k=1}^i q_{kj} y_k \right)$$

■ Implementing the Sanger network

The above learning rule can be evaluated in *Mathematica* as: LT Outer[Times,y,y]).Q, where LT is a lower triangular matrix. The entries above the diagonal are all zero, and the entries below and including the diagonal are one. You can verify the Sanger weight update formula with the following expressions:

```
In[71]:= Clear[Q,q,y,yy];
    n = 2;
    LT = Table[If[i>=j,1,0],{i,n},{j,n}];
    Q = Array[q,{n,n}];
    yy = Array[y,{n}];
    (LT Outer[Times,yy,yy]).Q//MatrixForm
```

Out[76]//MatrixForm=

```
\begin{pmatrix} q(1, 1) y(1)^2 & q(1, 2) y(1)^2 \\ q(2, 1) y(2)^2 + q(1, 1) y(1) y(2) & q(2, 2) y(2)^2 + q(1, 2) y(1) y(2) \end{pmatrix}
```

OK, let's try Sanger's network out on our synthetic data.

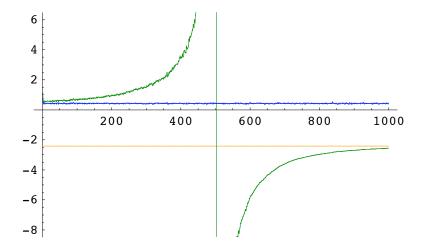
You may have to adjust the learning constant. It can take 1000's of iterations to converge, so don't give up easily. So run the above cell, graph the result using the input cell below. Then go back up and evaluate the cell above again. Check graphically below, and so forth until you see convergence.

■ Graph the evolution of the network weights in terms of the slope

From the model of our synthetic data, the two slopes should be:

Tan[theta] and -1/Tan[theta]. Let's take a look at the slopes of the transformed coordinates in the list p1:

```
In[111]:=
```



```
In[117]:= p1[[Length[p1]]]

Out[117]= {0.442973, -2.56778}
```

Compare your results with the slopes of gprincipalaxes:

```
In[121]:= slope = (beta/alpha) (-1/slope)

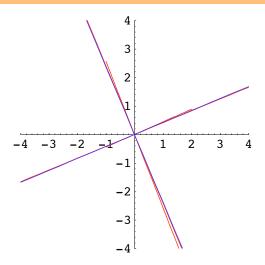
Out[121]= 0.414214

Out[122]= -2.41421
```

Note that the number of iterations is plotted in multiples determined by the Mod[] function above.

■ Graph the transformed axes of the Sanger network and compare them to those from the underlying distribution

Let's plot up the transformation axes of the Sanger network (**gnetwork2**), and compare them with the axes from the population distribution (**gprincipalaxes**), and the calculated principal component axes (**gPCA**):



Contingent Adaptation: McCollough effect

Celeste McCollough (1965).

Make stimulus

```
In[125]:= width = 128; freq=8;
    grating[x_,y_,xfreq_,yfreq_] := Sign[Cos[(2. Pi)*(xfreq*x + yfreq*y)]];
```

■ Vertical red adapting grating

■ Horizontal green adapting grating

■ Horizontal gray test grating

■ Vertical gray test grating

Test: Try it

- 1. First look at the two black and white gratings on the right. They should look black and white, and the white should have relatively little if any tinges of color.
- 2. Now look at the left vertical red grating, then the right horizontal green, then back at the left and so forth for 2-4 minutes. (You can use **Pause**[] for timing in seconds

and print "done" or Play[Sin[2Pi 440 t],{t,0,1}]; to play a sound.).

3. Then when adapted, look at the black and white test gratings again. The white bars of horizontal B&W should look pinkish, and the vertical bars greenish.

```
Show[GraphicsArray[{{gvertred, ghorizgreen, ghorizgray, gvertgray}},
DisplayFunction → $DisplayFunction, GraphicsSpacing → {.01, .01}]];
```

Pause[120]
"done"

done

■ Or display to a new notebook:

Is there a functional explanation for what is going on? Is there a neural network explanation?

Barlow suggested that the adaptation is the result of the visual system adjusting to new statistical dependencies between features. It isn't just that neurons are "getting tired". Specifically, he suggested that perceptual systems adjust their representations of features to be independent or uncorrelated with each other (technically, independence is a stronger condition). This is a problem of neural self-organization, perceptual learning based on experience. Next we'll look at a neural network that re-organize to decrease the correlations between their firing. This network may provide an explanation for McCulloch's color-contingent affter-effect.

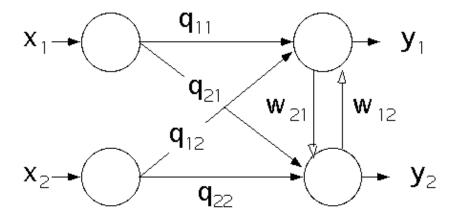
Non-orthogonal decorrelation

■ Foldiak's scheme combining Hebbian and anti-Hebbian learning

Rigid rotations aren't the only possible transformations that decorrelate the inputs. Further, one might want a new coordinate system that shares the variance equally--after all, we do not have strong evidence that neurons vary greatly in their ability to code the range of variation. This section looks at a network due to Peter Foldiak.

Foldiak and Barlow devised a neural network that combined a Hebbian learning rule on the forward connections with anti-Hebbian learning on the inhibitory connections between the output units. Oja's rule was used to normalize the weights. It can be shown that decorrelated output values are steady-state solutions for the weight changes.

One of the reasons for interest in this kind of model are the potential relations with the physiology. Inhibitory links are well-known, and evidence for anti-Hebbian learning is something to be looked for empirically.



Independence and decorrelation

Two random variables, x, y are uncorrelated if E(xy)=E(x)E(y) (i.e. the covariance is zero). They are independent if p(x,y)=p(x)p(y). For a multivariate Gaussian density, these two are equivalent. But in general, independence is the stronger condition, in that independence implies no correlation (but the converse is not true). Suppose a neural network recodes the input (x,y) into outputs (x',y'). The above networks "decorrelated" the inputs-E(x'y')=E(x')E(y')=0. If the inputs are not Gaussian random variables, is there a way to find an independent representation? There has been recent discussion of the utility of both decorrelated and statistically independent representations. We don't have time to go into the details, but the interested student should take a look at Barlow (1990), Bell and Sejnowski (1995), and Olshausen and Field (1996). As an application, Olshausen and Field (1996) showed that the pattern of simple cell receptive field weights in visual cortex can be obtained by seeking a coordinate transformation of image space that decorrelates the output values using two simple constraints: 1) keep the discrepancy between the image data and its linear reconstruction (as a weighted sum of receptive fields) small, and, 2) keep the overall activity level (e.g. total variance) small. The result is a sparse code for images.

Correlational or covariance structure is sometimes called 2nd order. Is there evidence that neural circuits discover and reduce other kinds of dependencies that go beyond correlations, to remove third or higher-order statistics? Schwartz, O., & Simoncelli, E. P. (2001) suggest a possible role for normalization as a mechanism that reduces higher order dependencies, producing neural codes where there is less information in one neuron's activity in predicting those in other nearby ones.

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