Neural Networks and Deep Learning 3

-Statistical Learning and Data Mining-

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Overview

Representation learning is the idea that performance of ML methods is highly dependent on the choice of data representation

For this reason, much of ML is geared towards transforming the data into the relevant features and then using these as inputs

This idea is as old as statistics itself, really,

(E.g. Pearson (1901), where PCA was first introduced)

However, the idea is constantly revisited in a variety of fields and contexts

Overview

Commonly, these learned representations capture ‘low level’ information like overall shape types

Other sharp features, such as images, aren’t captured

It is possible to quantify this intuition for PCA at least

PCA

PCA

Principal components analysis (PCA) is an (unsupervised) dimension reduction technique

It solves various equivalent optimization problems

(Maximize variance, minimize L_2 distortions, find closest subspace of a given rank,...)

At its core, we are finding linear combinations of the original (centered) covariates

$$Z_{ij} = \alpha_j^\top X_i$$

This is expressed via the SVD $\mathbb{X} - \overline{\mathbb{X}} = UDV^\top$ as

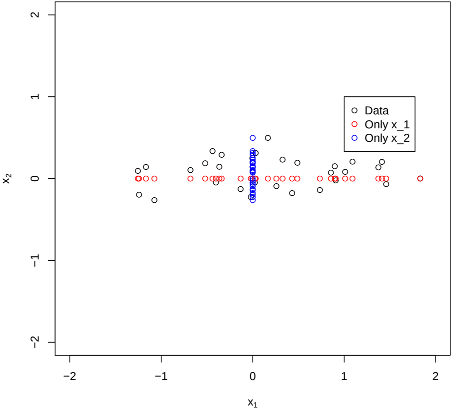
$$Z = \mathbb{X}V = UD$$

PCA

Lower dimensional embeddings

Suppose we have predictors x_1 and x_2

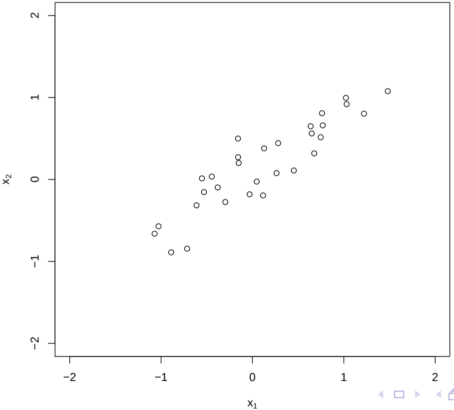
- We more faithfully preserve the structure of the data by keeping x_1 and setting x_2 to zero than the opposite



Lower dimensional embeddings

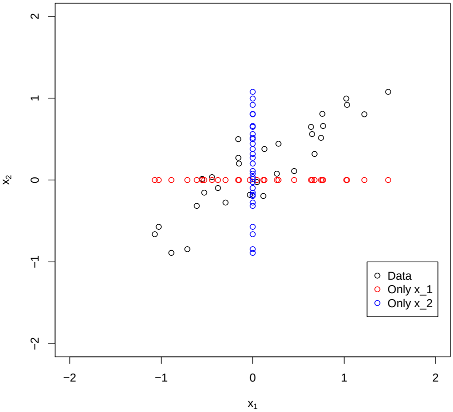
An important feature of the previous example that x_1 and x_2 aren't correlated

What if they are?



Lower dimensional embeddings

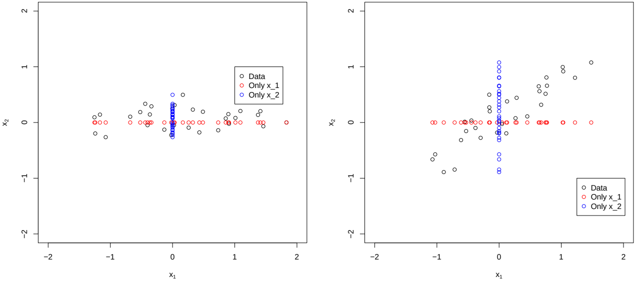
We do lose a lot of structure by setting either x_1 or x_2 to zero



Lower dimensional embeddings

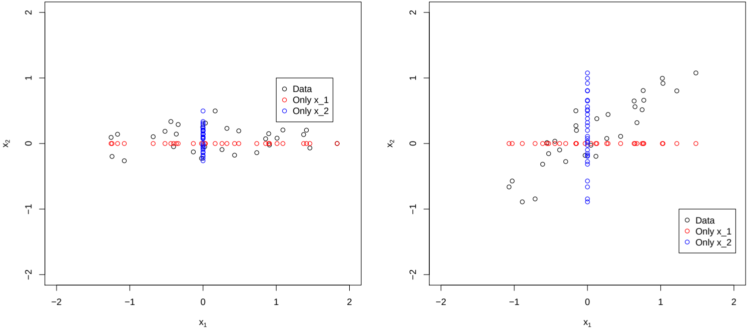
There isn't that much structurally different between the examples

One is just a rotation of the other



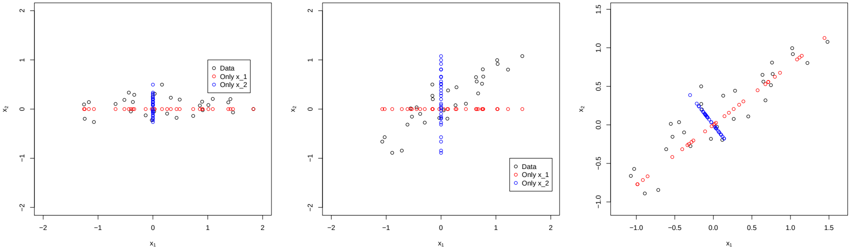
Lower dimensional embeddings

If we knew how to rotate our data, then we would be able to preserve more structure



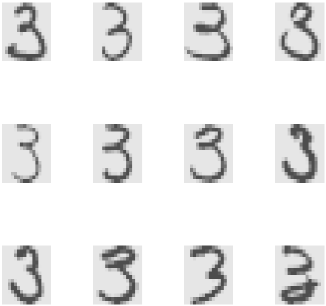
Lower dimensional embeddings

It turns out that PCA gives us exactly this rotation.



Digits example

PCA



Source: http://www-stat.stanford.edu/∼tibs/ElemStatLearn/

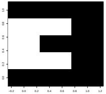
The data: 658 handwritten 3s each drawn by a different person

Each image is 16x16 pixels, each taking grayscale values between -1 and 1.

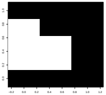
PCA

Think about each pixel location as a measurement

Consider these simple drawings of 3's. We convert this to an observation in a matrix by unraveling it along rows

$X_1 =$ 

$$X_1 = [1, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 1, 1, 1, 1]^\top$$

$X_2 =$ 

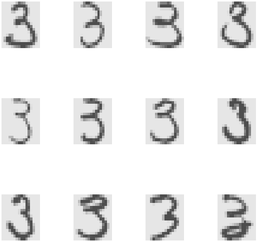
$$X_2 = [1, 1, 1, 0, 1, 1, 0, 0, 1, 0, 0, 1, 1, 1, 1]^\top$$

(Here, let black be 1 and white be 0)

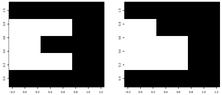
PCA

We will consider digits with...

- more pixels ($p = 256$)
- a continuum of intensities



Vs.



PCA

```
threesCenter = scale(threes,scale=FALSE)

svd.out = svd(threesCenter)

pcs    = svd.out$v
scores = svd.out$u%*%diag(svd.out$d)
```

Or, using prcomp:

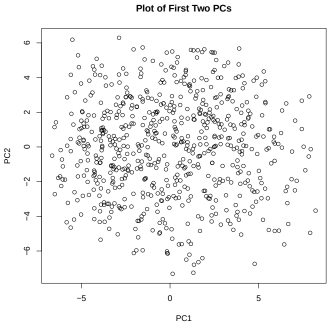
```
out = prcomp(threes,scale=F)
pcs = out$rot
scores = out$x
```

(Note that here we aren't scaling: the measurements are already on a consistent scale)

PCA

We can plot the scores of the first two principal components versus each other:

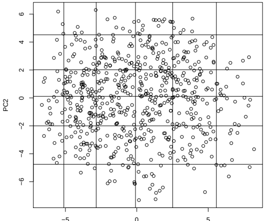
```
plot(scores[,1],scores[,2],xlab = 'PC1',ylab='PC2',
    main='Plot of First Two PCs')
```



Note: Each circle in this plot represents a hand written ‘3’.

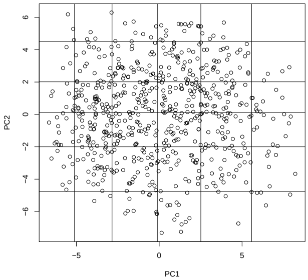
PCA

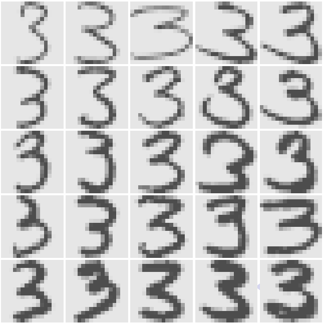
```
quantile.vec = c(0.05,0.25,0.5,0.75,0.95)
quant.score1 = quantile(scores[,1],quantile.vec)
quant.score2 = quantile(scores[,2],quantile.vec)
plot(scores[,1],scores[,2],xlab = 'PC1',ylab='PC2')
for(i in 1:5){
  abline(h = quant.score2[i])
  abline(v = quant.score1[i])
}
identify(scores[,1],scores[,2],n=25) #to find points
```



PCA

```
pcs.order = c(73,238,550,82,640,284,84,133,4,322,392,241,
    554,220,500,247,344,142,405,649,184,149,234,375,176)
par(mfrow=c(5,5))
par(mar=c(.2,.2,.2,.2))
for(i in pcs.order){
  plot.digit(threes[i,])
}
```

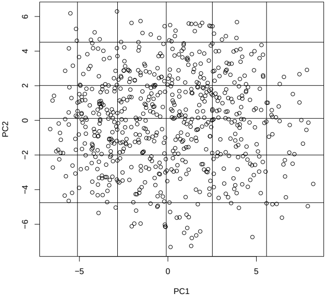


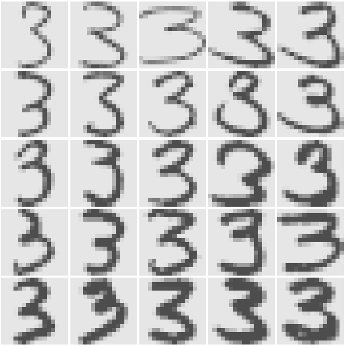


PCA

The 3's get lighter as the location on PC2 increases.

The 3's get more elongated as the location along PC1 increases





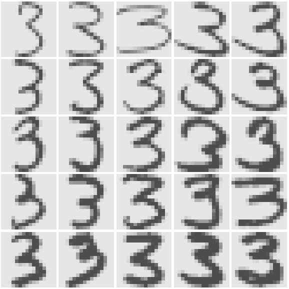
PCA

Each number represents a vector in $\mathbb{R}^{256}$

(as each square is 16x16 pixels)

However, hopefully we can reduce this number by re-expressing the digits in PC-land

(For instance, the top-right pixel is always 0 and hence that covariate is uninteresting)



PCA

Lastly, we can also look at the loadings as well:

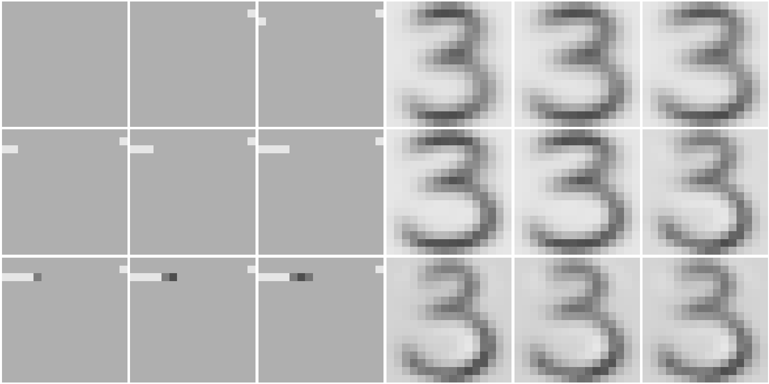
1st PC: Takes a compact 3 and smears it out

2nd PC: Deletes a portion of the inner part of a 3 and augments the outer (right) part

3rd PC: Moves a 3 down and tips it to the right

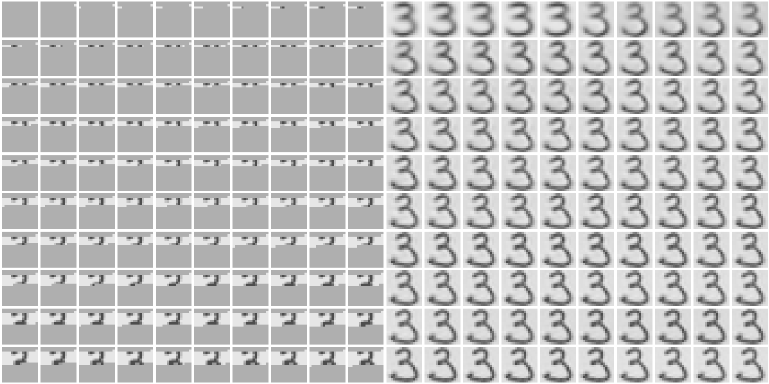
Reconstruction

Using 9 axis dimensions



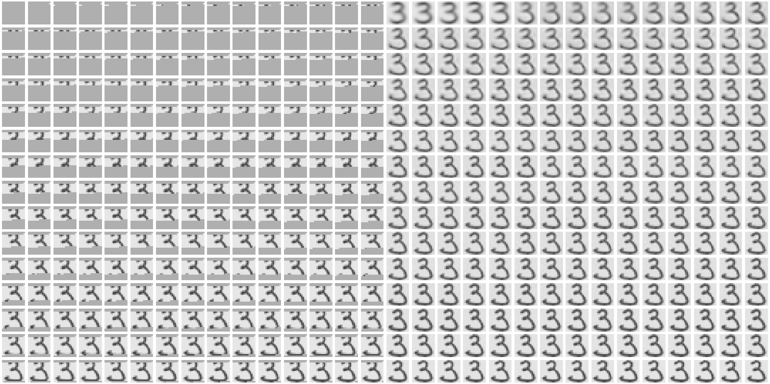
Reconstruction

Using 100 axis dimensions

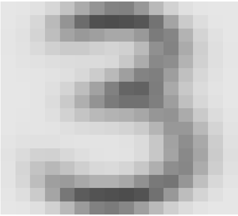


Reconstruction

Using 225 axis dimensions



Reconstruction



This is the mean (From centering $\mathbb{X}$: $(\mathbb{X} - \overline{\mathbb{X}}) = UDV^\top$)
(that is, the origin of the PCA axis, or $\overline{\mathbb{X}}$)[1]

```
plot.digit(attributes(digitsCenter)$'scaled:center')
```

[1]Technically, $\overline{X}_i$ for any i

Back to deep learning

PCA

If we want to find the first K principal components, the relevant optimization program is:

$$\min_{\mu,(\lambda_i),V_K} \sum_{i=1}^{n} ||X_i - \mu - V_K \lambda_i||^2$$

This representation is important

It shows that we are trying to reconstruct lower dimensional representations of the covariates

PCA

$$\min_{\mu,(\lambda_i),V_K} \sum_{i=1}^{n} ||X_i - \mu - V_K \lambda_i||^2$$

We can partially optimize for μ and (λ_i) to find

- $\hat{\mu} = \overline{X}$
- $\hat{\lambda}_i = V_K^\top (X_i - \hat{\mu})$

We can find

$$\min_{V} \sum_{i=1}^{n} \left|\left|(X_i - \hat{\mu}) - VV^\top (X_i - \hat{\mu})\right|\right|^2$$

where V is constrained to be orthogonal

(This is the so called Steifel manifold of rank-K orthogonal matrices)

The solution is given by the singular vectors V

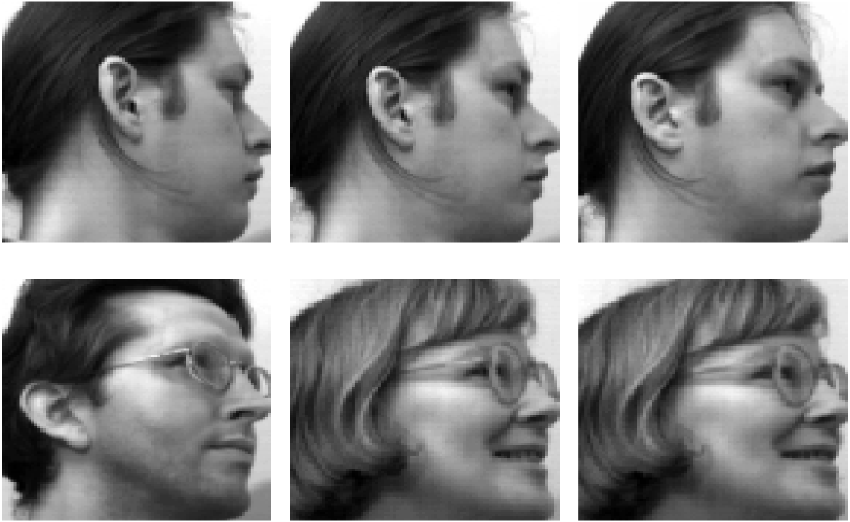
Example: Facial recognition

Images

- There are 575 total images
- Each image is 92×112 pixels and grey scale
- These images come from the Sheffield face database

  (See `http://www.face-rec.org/databases/` for this and other databases. See my rcode for how to read the images into R)

FACES



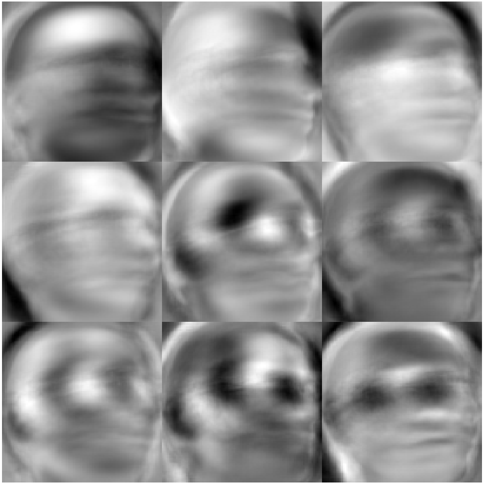
Faces

Regardless of how you formulate the optimization problem for PCA, it can be done in R by:

```
svd.out    = svd(scale(X,scale=F))
pc.basis   = svd.out$v
pc.scores = X %*% pc.basis
```

Let's apply this to the faces

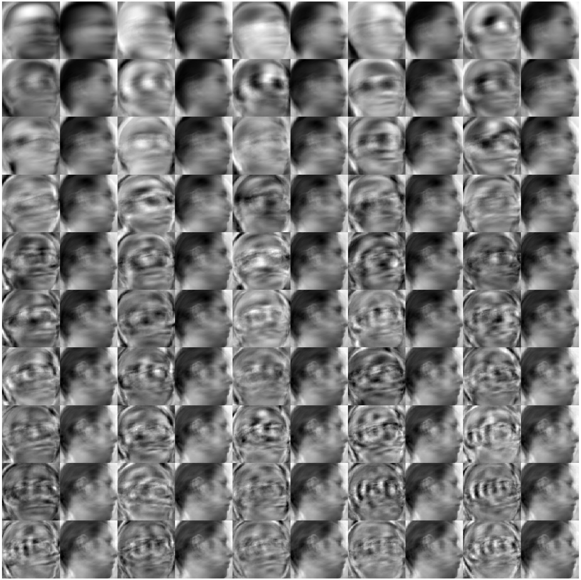
Faces: PC basis



Faces: PC projections

Varying levels of K: $\tilde{\mathbb{X}} = \sum_{k=1}^{K} d_k u_k v_k^\top + \overline{\mathbb{X}}$

Faces: PC projections and basis



Deep learning

Deep learning: Overview

Neural networks are models for supervised learning

Linear combinations of features are fed through nonlinear functions repeatedly

At the top layer, the resulting latent factor is fed into a linear/logistic regression

Deep learning: Overview

Deep learning is a new idea that has generated renewed interest in neural networks

Here, we wish to learn a hierarchy of features one level at a time, using

1. unsupervised feature learning to learn a new transformation at each level
2. which gets composed with the previously learned transformations

The top layer (which would be the output) is used to initialize a (supervised) neural network

Deep learning: Overview

Traditionally, a neural net is fit to all labelled data in one operation, with weights randomly chosen near zero

Due to the nonconvexity of the objective function, the final solution can get 'caught' in poor local minima

Deep learning seeks to find a good starting value, while allowing for:

- ...modeling the joint distribution of the covariates separately
- ...use of unlabeled data (including the test covariates)

Examples of unlabeled data

- Emails: For labelling spam or not spam, we might have a large number of emails where the label is known that we'd like to use somehow for classification
- Images: For labelling face or not face, we could have a huge number of images which we don't know the content

  (For instance, all the frames of all the videos on youtube)

If we are trying to estimate the Bayes' rule, it tends to rely on a conditional distribution

$$\mathbb{P}(Y|X) = \frac{\mathbb{P}(X, Y)}{\mathbb{P}(X)}$$

We can use unlabeled data to get a better estimate of $\mathbb{P}(X)$

(And hence the Bayes' rule)

Auto-encoders

Auto-encoders

An auto-encoder generalizes PCA by specifying

- Feature-extracting function: This function $h : \mathbb{R}^p \to \mathbb{R}^K$ maps the covariates to a new representation and is also known as the encoder
- Reconstruction function: This function[2] $h^{-1} : \mathbb{R}^K \to \mathbb{R}^p$ is also known as the decoder and it maps the representation back into the original space

Goal: Optimize any free parameters in the encoder/decoder pair that minimizes reconstruction error

[2] I've labeled this function h^{-1} to be suggestive, but I don't mean that $h^{-1}(h(x)) = x$

Auto-encoder

Let $W \in \mathbb{R}^{p \times K}$ (with $K < p$) be a matrix of weights

Linear combinations of X are fed through a function σ

$$h(X) = \sigma(W^\top X) \in \mathbb{R}^K$$

The output layer is then modeled as a linear combination of these inputs[3]

$$h^{-1}(h(X)) = Wh(X) = W\sigma(W^\top X) \in \mathbb{R}^p$$

[3] There is no restriction that the same matrix to be used in h and h^{-1}. Keeping them the same is known as weight-tying

Deep learning

Reminder Given inputs $X_1, \ldots, X_n$, the PCA problem

$$\min_{(\lambda_i), V_K} \sum_{i=1}^{n} ||X_i - V_K \lambda_i||^2$$

(Note I've implictly subtracted of the mean)

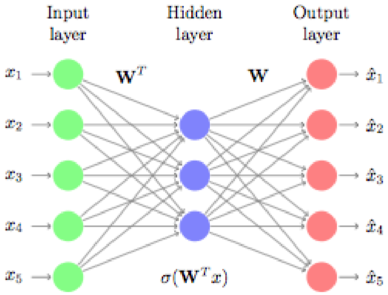
More general autoencoder: weight matrix W is estimated by solving the (non convex) optimization problem:

$$\min_{W \in \mathbb{R}^{p \times K}} \sum_{i=1}^{n} ||X_i - Wh(X_i)||^2 = \min_{W \in \mathbb{R}^{p \times K}} \sum_{i=1}^{n} \left|\left|X_i - W\sigma(W^\top X_i)\right|\right|^2$$

(If $\sigma(X) \equiv X$, then we've recovered the PCA program)

Deep learning schematic

An autoencoder might look like:



Neural networks: Representations

Important: Neural networks themselves create (supervised) representations

Compare:

$$\alpha^\top X \Leftrightarrow W^\top X$$

Neural networks: Representations

Return to the US crime data

Run a single layer, two hidden unit neural network

(with sigmoid activation function)

```
Y = subset(UScrime,select=y,drop=T)
X = scale(subset(UScrime,select=-y))
X = as.data.frame(X)
names(X) = names(subset(UScrime,select=-y))
model.out = as.formula(paste("Y ~ ",paste(names(X),
                      collapse='+')))
nn.out = neuralnet(model.out,data=UScrime, hidden=2,
                  threshold=0.01,rep=1)

W = nn.out$weights[[1]][[1]]
plot(W[-1,],type='n',xlab='W_1',ylab='W_2')
text(W[-1,],names(X),cex=.75)
```

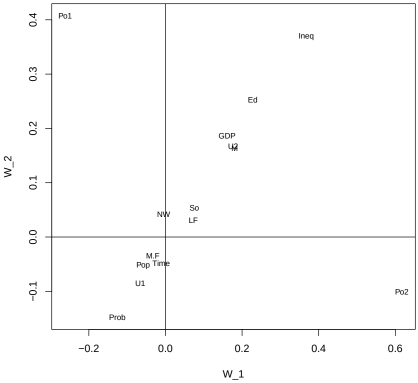
Neural networks: Representations

The interpretation is that each latent variable $Z_k = \sigma(\alpha_k^\top X)$ is a neuron that is tuned to detect a particular type of structure

Covariates that "positive" signs in the representations indicate the neuron is "tuned" to that signal-type

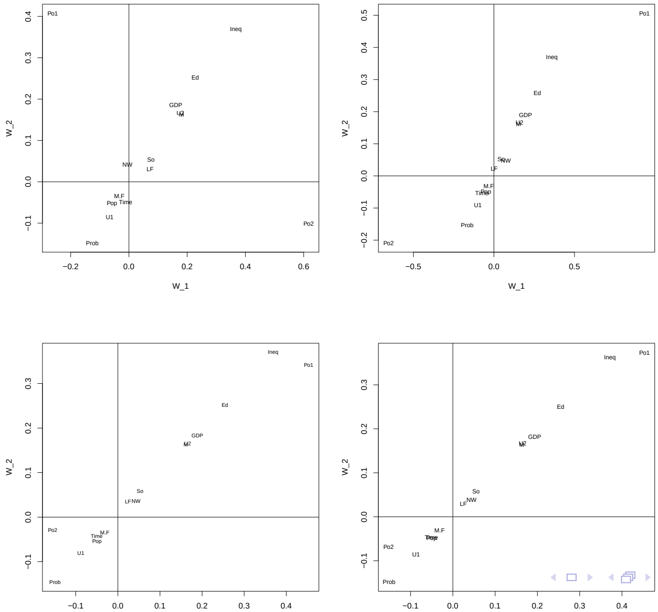
Note that this isn't a derivative or importance-based interpretation

Neural networks: Representations



M: % males aged 14-24.
So: indicator for a Southern stat
Ed: mean years of schooling.
Po1: police 1960.
Po2: police 1959.
LF: labor force participation ra
M.F: # of males per 1000 females.
Pop: state population.
NW: # of non-whites per 1000 peop
U1: unemployment rate of urban ma
U2: unemployment rate of urban ma
GDP: gross domestic product per h
Ineq: income inequality.
Prob: probability of imprisonment
Time: average time served in stat

Neural networks: Representations



DEEP LEARNING

The following is a brief overview of NNs from some researchers at Google

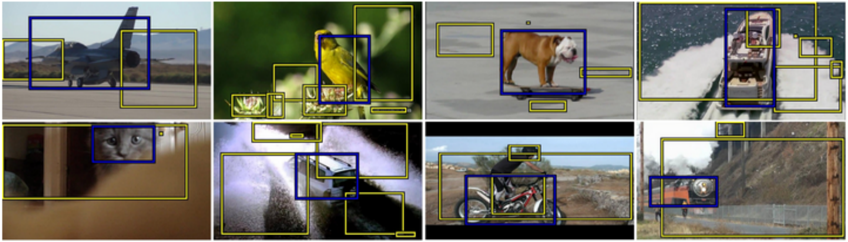
(Le, Ranzato, Monga, Devin, Chen, Dean, Ng (2012))

It has about 1 billion trainable parameters and uses advanced parallelism to make computation feasible

It also uses a decoupled encoder-decoder pair, plus regularization and a linear activation

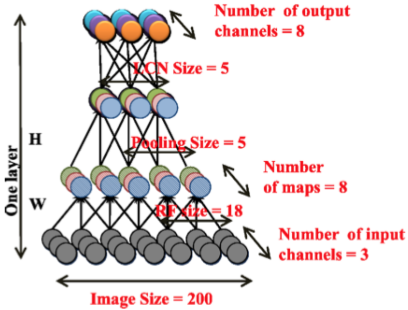
(This means that we write the representation as $W_O W_I^\top X$, where $W_O \neq W_I$)

Deep learning: Data



Deep learning schematic

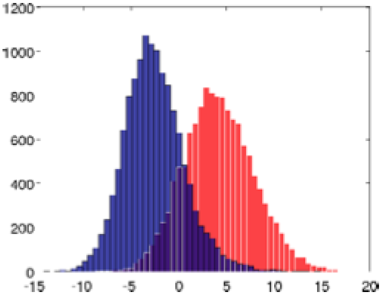
A representation of their implementation



Deep learning results

If we look at every neuron (that is, hidden unit) in the network and take the output for a given body of test images

Maximize the classification rate of taking the $\mathrm{sign}(\cdot)$, they find:



Deep learning results

The test images with maximum activation of that optimal neuron

Deep learning results

Finding the pixel wise maximizing input: