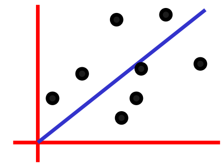
This part of the lecture is derived from: Regression and Classification with Neural Networks

Andrew W. Moore

 Sep 25th, 2001

Linear Regression



DATASET

inputs	outputs
$x_1 = 1$	$y_1 = 1$
$x_2 = 3$	$y_2 = 2.2$
$x_3 = 2$	$y_3 = 2$
$x_4 = 1.5$	$y_4 = 1.9$
$x_5 = 4$	$y_5 = 3.1$

Empirical view: Hmm, looks like the data can be fit by a line going through the origin: y = wx. (w is a "weight")

Score = $\Sigma \text{error}^2 = \Sigma(y-wx)^2$

(Why square the error? Minimizing score, want to penalize positive and negative errors)

Getting the best score

- For functions that are linear in the unknown parameters, we can simply compute the globally best parameters to fit a training set. Formulating our example problem in matrix notation:

$X = (x_1, x_2, x_3, \ldots, x_n)^T$

$y = Xw$

so estimate of $w = (X^TX)^{-1}X^Ty = \Sigma xy/\Sigma x^2$

(Where did this formula come from? Take the derivative of the score and set it to zero)

Getting the best score

- However, many functions we might like to use aren't linear in the unknown parameters.
- In this case, the score is a function of the training set and the parameters:
- Score = $\Sigma(y-f(x,w))^2$
- We can use gradient descent to minimize the score.

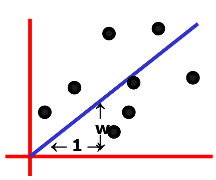
$$\Delta w = -\varepsilon(\partial score / \partial w)$$

$$\partial score / \partial w = -2\Sigma(y - f(x,w))\partial f / \partial w$$

"Numerical Recipes in X" is a good reference,

Matlab provides software

Linear Regression: Probabilistic Version



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Linear regression assumes that the expected value of the output given an input, $E[y|x]$, is linear.

Simplest case: $Out(x) = wx$ for some unknown w.

Given the data, we can estimate w.

1-parameter linear regression

Assume that the data is formed by

$$y_i = wx_i + \text{noise}_i$$

where…

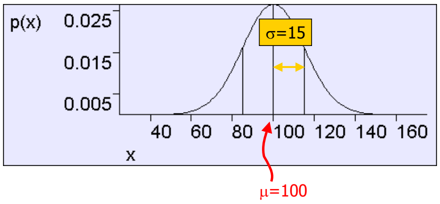
- the noise signals are independent
- the noise has a normal distribution with mean 0 and unknown variance σ^2

$P(y|w,x)$ has a normal distribution with

- mean wx
- variance σ^2

General Gaussian

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2} \right)$$



$$E[X] = \mu$$

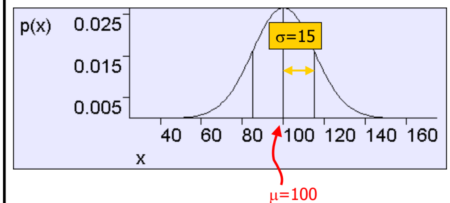
$$\text{Var}[X] = \sigma^2$$

What is a normal distribution?

General Gaussian

Also known as the normal distribution or Bell-shaped curve

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2} \right)$$



$$E[X] = \mu$$

$$\text{Var}[X] = \sigma^2$$

Shorthand: We say X ~ N(μ,σ^2) to mean "X is distributed as a Gaussian with parameters μ and σ^2".

In the above figure, X ~ N(100,15^2)

Maximum likelihood estimation of *w*

Asks the question:

"For which value of *w* is this data most likely to have happened?"

<=>

For what *w* is

P($y_1, y_2 \ldots y_n \mid x_1, x_2, x_3, \ldots x_n, w$) maximized?

<=>

For what *w* is

$$\prod_{i=1}^{n} P(y_i \mid w, x_i) \text{ maximized?}$$

For what *w* is

$$\prod_{i=1}^{n} P(y_i \mid w, x_i) \quad \text{maximized?}$$

For what *w* is

$$\prod_{i=1}^{n} \exp\left(-\frac{1}{2}\left(\frac{y_i - wx_i}{\sigma}\right)^2\right) \text{ maximized?}$$

For what *w* is

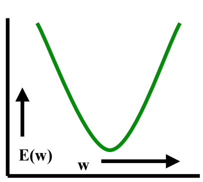
$$\sum_{i=1}^{n} -\frac{1}{2}\left(\frac{y_i - wx_i}{\sigma}\right)^2 \quad \text{maximized?}$$

For what *w* is

$$\sum_{i=1}^{n} (y_i - wx_i)^2 \quad \text{minimized?}$$

Linear Regression

The maximum likelihood *w* is the one that minimizes sum-of-squares of residuals



$$\text{E} = \sum_i (y_i - wx_i)^2$$

$$= \sum_i y_i^2 - \left(2\sum x_i y_i\right)w + \left(\sum x_i^2\right)w^2$$

We want to minimize a quadratic function of *w*.

Linear Regression

Easy to show the sum of squares is minimized when

$$w = \frac{\sum x_i y_i}{\sum x_i^2}$$

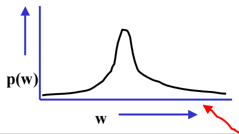
The maximum likelihood model is $\text{Out}(x) = wx$

We can use it for prediction

Linear Regression

Easy to show the sum of squares is minimized when

$$w = \frac{\sum x_i y_i}{\sum x_i^2}$$



The maximum likelihood model is $\mathrm{Out}(x) = wx$

We can use it for prediction

Note: In Bayesian stats you'd have ended up with a prob dist of *w*

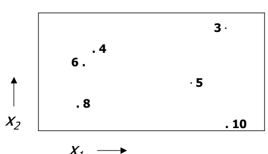
And predictions would have given a prob dist of expected output

Often useful to know your confidence. Max likelihood can give some kinds of confidence too.

Multivariate Linear Regression

Multivariate Regression

What if the inputs are vectors?



2-d input example

Dataset has form

$\mathbf{x}_1$	y_1
$\mathbf{x}_2$	y_2
$\mathbf{x}_3$	y_3
.:	:
.	
$\mathbf{x}_R$	y_R

Multivariate Regression

Write matrix X and Y thus:

$$\mathrm{X} = \begin{bmatrix} \ldots..\mathbf{x}_1\ldots.. \\ \ldots..\mathbf{x}_2\ldots.. \\ \vdots \\ \ldots..\mathbf{x}_R\ldots.. \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \ldots & x_{1m} \\ x_{21} & x_{22} & \ldots & x_{2m} \\ & & \vdots & \\ x_{R1} & x_{R2} & \ldots & x_{Rm} \end{bmatrix} \quad \mathrm{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_R \end{bmatrix}$$

(there are *R* datapoints. Each input has m components)

The linear regression model assumes a vector **w** such that

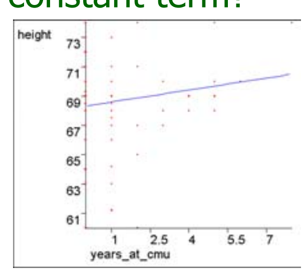
Out(**x**) = $\mathbf{x}^T\mathbf{w} = w_1 x[1] + w_2 x[2] + \ldots . w_m x[D]$

The max. likelihood estimate of **w** is **w** = $(X^TX)^{-1}(X^TY)$

Constant Term in Linear Regression

What about a constant term?

We may expect linear data that does not go through the origin.



Statisticians and Neural Net Folks all agree on a simple obvious hack.

Can you guess??

The constant term

- The trick is to create a fake input "X_0" that always takes the value 1

X_1	X_2	Y
2	4	16
3	4	17
5	5	20

Before:

$Y=w_1X_1+ w_2X_2$

…has to be a poor model

X_0	X_1	X_2	Y
1	2	4	16
1	3	4	17
1	5	5	20

After:

$Y= w_0X_0+w_1X_1+ w_2X_2$

$= w_0+w_1X_1+ w_2X_2$

…has a fine constant term

In this example, You should be able to see the MLE w_0 , w_1 and w_2 by inspection

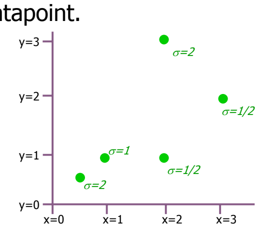
Heteroscedasticity…

Linear Regression with varying noise

Regression with varying noise

- Suppose you know the variance of the noise that was added to each datapoint.

x_i	y_i	σ_i^2
½	½	4
1	1	1
2	1	1/4
2	3	4
3	2	1/4



Assume $y_i \sim N(wx_i, \sigma_i^2)$

What's the MLE estimate of w?

MLE estimation with varying noise

$$\underset{w}{\operatorname{argmax}} \log p(y_1, y_2, \ldots, y_R \mid x_1, x_2, \ldots, x_R, \sigma_1^2, \sigma_2^2, \ldots, \sigma_R^2, w) =$$

$$\underset{w}{\operatorname{argmin}} \sum_{i=1}^{R} \frac{(y_i - wx_i)^2}{\sigma_i^2} =$$

Assuming i.i.d. and then plugging in equation for Gaussian and simplifying.

$$\left(w \text{ such that } \sum_{i=1}^{R} \frac{x_i(y_i - wx_i)}{\sigma_i^2} = 0 \right) =$$

Setting dLL/dw equal to zero

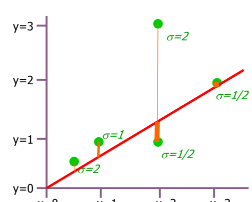
$$\frac{\left(\sum_{i=1}^{R} \frac{x_i y_i}{\sigma_i^2} \right)}{\left(\sum_{i=1}^{R} \frac{x_i^2}{\sigma_i^2} \right)}$$

Trivial algebra

This is Weighted Regression

- We are asking to minimize the weighted sum of squares

$$\underset{w}{\operatorname{argmin}} \sum_{i=1}^{R} \frac{(y_i - wx_i)^2}{\sigma_i^2}$$



where weight for i'th datapoint is $\frac{1}{\sigma_i^2}$

Weighted Multivariate Regression

The max. likelihood **w** is **w** = $(WX^TWX)^{-1}(WX^TWY)$

(WX^TWX) is an m x m matrix: i,j'th elt is $\sum_{k=1}^{R} \frac{x_{ki}x_{kj}}{\sigma_i^2}$

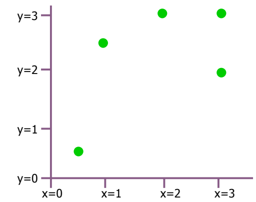
(WX^TWY) is an m-element vector: i'th elt $\sum_{k=1}^{R} \frac{x_{ki}y_k}{\sigma_i^2}$

Non-linear Regression

Non-linear Regression

- Suppose you know that y is related to a function of x in such a way that the predicted values have a non-linear dependence on w, e.g:

x_i	y_i
½	½
1	2.5
2	3
3	2
3	3



Assume $y_i \sim N(\sqrt{w + x_i}, \sigma^2)$

What's the MLE estimate of w?

Non-linear MLE estimation

$$\underset{w}{\operatorname{argmax}} \log p(y_1, y_2, \ldots, y_R \mid x_1, x_2, \ldots, x_R, \sigma, w) =$$

$$\underset{w}{\operatorname{argmin}} \sum_{i=1}^{R} \left(y_i - \sqrt{w + x_i}\right)^2 =$$

Assuming i.i.d. and then plugging in equation for Gaussian and simplifying.

$$\left(w \text{ such that } \sum_{i=1}^{R} \frac{y_i - \sqrt{w + x_i}}{\sqrt{w + x_i}} = 0 \right) =$$

Setting dLL/dw equal to zero

Non-linear MLE estimation

$$\underset{w}{\operatorname{argmax}} \log p(y_1, y_2, \ldots, y_R \mid x_1, x_2, \ldots, x_R, \sigma, w) =$$

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Setting dLL/dw equal to zero

We're down the algebraic toilet

So guess what we do?

Non-linear MLE estimation

$$\underset{w}{\operatorname{argmax}} \log p(y_1, y_2, \ldots, y_R \mid x_1, x_2, \ldots, x_R, \sigma, w) =$$

Common (but not only) approach:
Numerical Solutions:

- Line Search
- Simulated Annealing
- Gradient Descent
- Conjugate Gradient
- Levenberg Marquardt
- Newton's Method

Also, special purpose statistical-optimization-specific tricks such as E.M. (See Gaussian Mixtures lecture for introduction)

Assuming i.i.d. and then plugging in equation for Gaussian and simplifying.

Setting dLL/dw equal to zero

We're down the algebraic toilet

So guess what we do?

GRADIENT DESCENT

Suppose we have a scalar function $f(w): \Re \rightarrow \Re$

We want to find a local minimum.
Assume our current weight is *w*

GRADIENT DESCENT RULE: $w \leftarrow w - \eta \frac{\partial}{\partial w} f(w)$

η is called the LEARNING RATE. A small positive number, e.g. η = 0.05

GRADIENT DESCENT

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Recall Andrew's favorite default value for anything

η is called the LEARNING RATE. A small positive number, e.g. η = 0.05

QUESTION: Justify the Gradient Descent Rule

Gradient Descent in "m" Dimensions

Given $f(\mathbf{w}) : \Re^m \rightarrow \Re$

$$\nabla f(\mathrm{w}) = \begin{pmatrix} \frac{\partial}{\partial w_1} f(\mathrm{w}) \\ \vdots \\ \frac{\partial}{\partial w_m} f(\mathrm{w}) \end{pmatrix}$$ points in direction of steepest ascent.

$|\nabla f(\mathrm{w})|$ is the gradient in that direction

GRADIENT DESCENT RULE: $\mathrm{w} \leftarrow \mathrm{w} - \eta \nabla f(\mathrm{w})$

Equivalently

$w_j \leftarrow w_j - \eta \frac{\partial}{\partial w_j} f(\mathrm{w})$ ….where w_j is the *j*th weight

"just like a linear feedback system"

What's all this got to do with Neural Nets, then, eh??

For supervised learning, neural nets are also models with vectors of **w** parameters in them. They are now called weights.

As before, we want to compute the weights to minimize sum-of-squared residuals.

Which turns out, under "Gaussian i.i.d noise" assumption to be max. likelihood.

Instead of explicitly solving for max. likelihood weights, we use **GRADIENT DESCENT** to **SEARCH** for them.

"Why?" you ask, a querulous expression in your eyes.
"Aha!!" I reply: "We'll see later."

Linear Perceptrons

They are multivariate linear models:

$$\text{Out}(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x}$$

And "training" consists of minimizing sum-of-squared residuals by gradient descent.

$$E = \sum_k \left(\text{Out}(\mathrm{x}_k) - y_k\right)^2$$
$$= \sum_k \left(\mathrm{w}^T \mathrm{x}_k - y_k\right)^2$$

QUESTION: Derive the perceptron training rule.

Linear Perceptron Training Rule

$$E = \sum_{k=1}^{R} (y_k - \mathbf{w}^T \mathbf{x}_k)^2$$

Gradient descent tells us we should update **w** thusly if we wish to minimize *E:*

$$w_j \leftarrow w_j - \eta \frac{\partial E}{\partial w_j}$$

So what's $\frac{\partial E}{\partial w_j}$?

Linear Perceptron Training Rule

$$E = \sum_{k=1}^{R} (y_k - \mathbf{w}^T \mathbf{x}_k)^2$$

Gradient descent tells us we should update **w** thusly if we wish to minimize *E:*

$$w_j \leftarrow w_j - \eta \frac{\partial E}{\partial w_j}$$

So what's $\frac{\partial E}{\partial w_j}$?

$$\frac{\partial E}{\partial w_j} = \sum_{k=1}^{R} \frac{\partial}{\partial w_j} (y_k - \mathbf{w}^T \mathbf{x}_k)^2$$
$$= \sum_{k=1}^{R} 2(y_k - \mathbf{w}^T \mathbf{x}_k) \frac{\partial}{\partial w_j} (y_k - \mathbf{w}^T \mathbf{x}_k)$$
$$= -2 \sum_{k=1}^{R} \delta_k \frac{\partial}{\partial w_j} \mathbf{w}^T \mathbf{x}_k$$

…where…
$\delta_k = y_k - \mathbf{w}^T \mathbf{x}_k$

$$= -2 \sum_{k=1}^{R} \delta_k \frac{\partial}{\partial w_j} \sum_{i=1}^{m} w_i x_{ki}$$
$$= -2 \sum_{k=1}^{R} \delta_k x_{kj}$$

Linear Perceptron Training Rule

$$E = \sum_{k=1}^{R} (y_k - \mathbf{w}^T \mathbf{x}_k)^2$$

Gradient descent tells us we should update **w** thusly if we wish to minimize *E*:

$$w_j \leftarrow w_j - \eta \frac{\partial E}{\partial w_j}$$

...where...

$$\frac{\partial E}{\partial w_j} = -2 \sum_{k=1}^{R} \delta_k x_{kj}$$

$$\boxed{w_j \leftarrow w_j + 2\eta \sum_{k=1}^{R} \delta_k x_{kj}}$$

We frequently neglect the 2 (meaning we halve the learning rate)

The "Batch" perceptron algorithm

1) Randomly initialize weights w_1 w_2 … w_m

2) Get your dataset (append 1's to the inputs if you don't want to go through the origin).

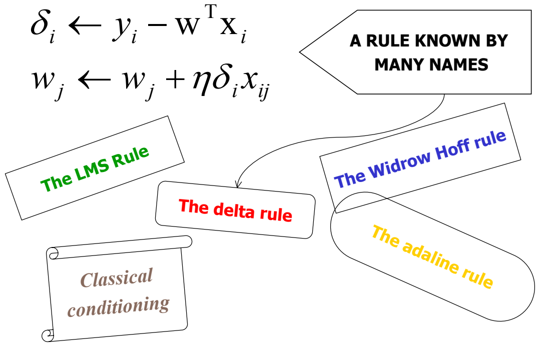
3) for i = 1 to R $\quad \delta_i := y_i - \mathbf{w}^T \mathbf{x}_i$

4) for j = 1 to m $\quad w_j \leftarrow w_j + \eta \sum_{i=1}^{R} \delta_i x_{ij}$

5) if $\sum \delta_i^2$ stops improving then stop. Else loop back to 3.

$$\delta_i \leftarrow y_i - \mathrm{w}^T \mathrm{x}_i$$

$$w_j \leftarrow w_j + \eta \delta_i x_{ij}$$



If data is voluminous and arrives fast

Input-output pairs (***x***,*y*) come streaming in very quickly. THEN

Don't bother remembering old ones.
Just keep using new ones.

observe (**x**,*y*)

$$\delta \leftarrow y - \mathrm{w}^T \mathrm{x}$$

$$\forall j \;\; w_j \leftarrow w_j + \eta \, \delta \, x_j$$

Gradient Descent vs Matrix Inversion for Linear Perceptrons

GD Advantages (MI disadvantages):

-
-
-

GD Disadvantages (MI advantages):

-
-
-
-
-

Gradient Descent vs Matrix Inversion for Linear Perceptrons

GD Advantages (MI disadvantages):

- Biologically plausible
- With very very many attributes each iteration costs only O(mR). If fewer than m iterations needed we've beaten Matrix Inversion
- More easily parallelizable (or implementable in wetware)?

GD Disadvantages (MI advantages):

- It's moronic
- It's essentially a slow implementation of a way to build the XTX matrix and then solve a set of linear equations
- If m is small it's especially outageous. If m is large then the direct matrix inversion method gets fiddly but not impossible if you want to be efficient.
- Hard to choose a good learning rate
- Matrix inversion takes predictable time. You can't be sure when gradient descent will stop.

Gradient Descent vs Matrix Inversion for Linear Perceptrons

GD Advantages (MI disadvantag…):

- Biologically plausible
- With very very many attrib… each i… on… (mR). If fewer than m iterations nee… …rsion
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GD Disadvantag…

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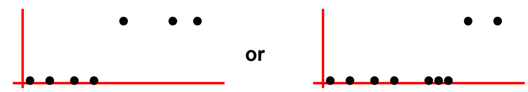
- If m is small it's espec… …hen the direct matrix inversion me… …possible if you want to be efficient.
- Hard to choose a good lear… …g rate
- Matrix inversion takes pred…table time. You can't be sure when gradient descent will stop.

But we'll soon see that GD has an important extra trick up its sleeve

Perceptrons for Classification

What if all outputs are 0's or 1's ?



We can do a linear fit.

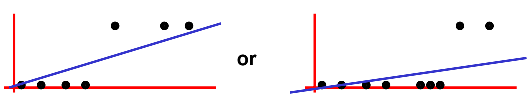
Our prediction is 0 if out($\boldsymbol{x}$)≤1/2

1 if out($\boldsymbol{x}$)>1/2

WHAT'S THE BIG PROBLEM WITH THIS???

Perceptrons for Classification

What if all outputs are 0's or 1's ?



Blue = Out(x)

We can do a linear fit.

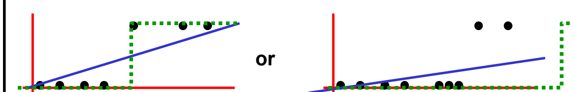
Our prediction is 0 if out($\boldsymbol{x}$)≤½

1 if out($\boldsymbol{x}$)>½

WHAT'S THE BIG PROBLEM WITH THIS???

Perceptrons for Classification

What if all outputs are 0's or 1's ?



Blue = Out(x)

Green = Classification

We can do a linear fit.

Our prediction is 0 if out($\boldsymbol{x}$)≤½

1 if out($\boldsymbol{x}$)>½

Fix #1

- Only pay attention to points at border.
- This leads to SVM approach.

Fix #2: Change definition of error

Don't minimize $\sum \left(y_i - \mathrm{w}^{\mathrm{T}}\mathrm{x}_i\right)^2$.

Minimize number of misclassifications instead. [Assume outputs are +1 & -1, not +1 & 0]

$$\sum \left(y_i - \mathrm{Round}\left(\mathrm{w}^{\mathrm{T}}\mathrm{x}_i\right)\right)$$

where $\mathrm{Round}(x) = \begin{cases} -1 & \text{if } x<0 \\ 1 & \text{if } x \geq 0 \end{cases}$

NOTE: CUTE & NON OBVIOUS WHY THIS WORKS!!

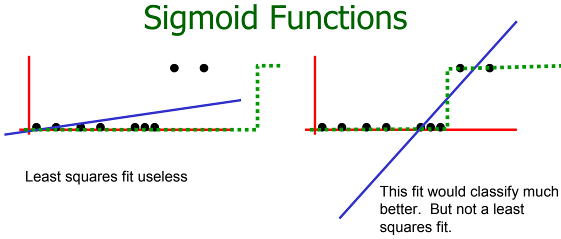
The gradient descent rule can be changed to:

if $(\boldsymbol{x}_i, y_i)$ correctly classed, don't change

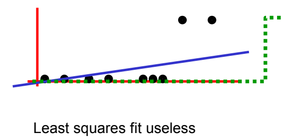
if wrongly predicted as 1 $\quad \boldsymbol{w} \leftarrow \boldsymbol{w} - \boldsymbol{x}_i$

if wrongly predicted as -1 $\quad \boldsymbol{w} \leftarrow \boldsymbol{w} + \boldsymbol{x}_i$

Classification with Perceptrons II: Sigmoid Functions



Fix #3: Use a different function

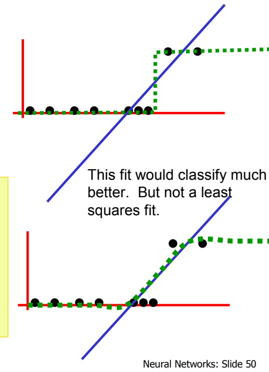


SOLUTION:

Instead of Out($\boldsymbol{x}$) = $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$

We'll use Out($\boldsymbol{x}$) = $g(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$

where $g(x): \Re \rightarrow (0,1)$ is a squashing function



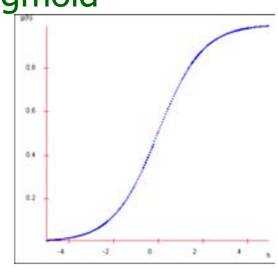
The Sigmoid

$$g(h) = \frac{1}{1+\exp(-h)}$$

Note that if you rotate this curve through 180° centered on *(0,1/2)* you get the same curve.

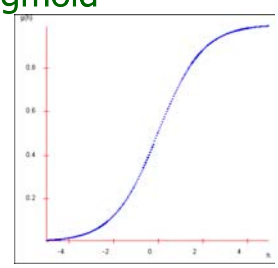
i.e. *g(h)=1-g(-h)*

Can you prove this?



The Sigmoid

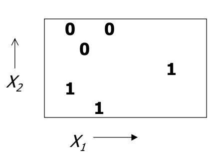
$$g(h) = \frac{1}{1+\exp(-h)}$$



Now we choose $\boldsymbol{w}$ to minimize

$$\sum_{i=1}^{R}[y_i - \mathrm{Out}(\mathrm{x}_i)]^2 = \sum_{i=1}^{R}[y_i - g(\mathrm{w}^{\mathrm{T}}\mathrm{x}_i)]^2$$

Linear Perceptron Classification Regions



We'll use the model Out($\boldsymbol{x}$) = $g(\boldsymbol{w}^{\mathrm{T}}(\boldsymbol{x},1))$

$= g(w_1x_1 + w_2x_2 + w_0)$

Which region of above diagram classified with +1, and which with 0 ??

Gradient descent with sigmoid on a perceptron

First, notice $g'(x) = g(x)(1-g(x))$

Because: $g(x) = \frac{1}{1+e^{-x}}$ so $g'(x) = \frac{-e^{-x}}{\left(1+e^{-x}\right)^2}$

$$= \frac{1-1-e^{-x}}{\left(1+e^{-x}\right)^2} = \frac{1}{\left(1+e^{-x}\right)^2} - \frac{1}{1+e^{-x}} = \frac{-1}{1+e^{-x}}\left(1-\frac{1}{1+e^{-x}}\right) = -g(x)(1-g(x))$$

$$\mathrm{Out(x)} = g\left(\sum_k w_k x_k\right)$$

$$\mathrm{E} = \sum_i \left(y_i - g\left(\sum_k w_k x_{ik}\right)\right)^2$$

$$\frac{\partial \mathrm{E}}{\partial w_j} = \sum_i 2\left(y_i - g\left(\sum_k w_k x_{ik}\right)\right)\left(-\frac{\partial}{\partial w_j} g\left(\sum_k w_k x_{ik}\right)\right)$$

$$= \sum_i -2\left(y_i - g\left(\sum_k w_k x_{ik}\right)\right) g'\left(\sum_k w_k x_{ik}\right)\frac{\partial}{\partial w_j}\sum_k w_k x_{ik}$$

$$= \sum_i -2\delta_i g(\mathrm{net}_i)(1-g(\mathrm{net}_i))x_{ij}$$

where $\delta_i = y_i - \mathrm{Out}(\mathrm{x}_i)$ $\quad \mathrm{net}_i = \sum_k w_k x_k$

The sigmoid perceptron update rule:

$$w_j \leftarrow w_j + \eta \sum_{i=1}^{R} \delta_i g_i (1-g_i) x_{ij}$$

where $g_i = g\left(\sum_{j=1}^{m} w_j x_{ij}\right)$

$$\delta_i = y_i - g_i$$

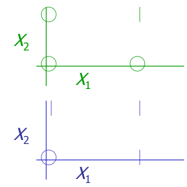
Other Things about Perceptrons

- Invented and popularized by Rosenblatt (1962)
- Even with sigmoid nonlinearity, correct convergence is guaranteed
- Stable behavior for overconstrained and underconstrained problems

Perceptrons and Boolean Functions

If inputs are all 0's and 1's and outputs are all 0's and 1's…

- Can learn the function $x_1 \wedge x_2$
- Can learn the function $x_1 \vee x_2$.
- Can learn <u>any</u> conjunction of literals, e.g. $x_1 \wedge \sim x_2 \wedge \sim x_3 \wedge x_4 \wedge x_5$



QUESTION: WHY?

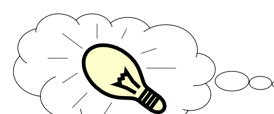
Perceptrons and Boolean Functions

- Can learn any disjunction of literals
  e.g. $x_1 \wedge \sim x_2 \wedge \sim x_3 \wedge x_4 \wedge x_5$
- Can learn majority function
  $$f(x_1, x_2 \dots x_n) = \begin{cases} 1 \text{ if } n/2 \; x_i\text{'s or more are} = 1 \\ 0 \text{ if less than } n/2 \; x_i\text{'s are} = 1 \end{cases}$$
- What about the exclusive or function?
  $f(x_1, x_2) = x_1 \forall x_2 =$
  $(x_1 \wedge \sim x_2) \vee (\sim x_1 \wedge x_2)$

Multilayer Networks

The class of functions representable by perceptrons is limited

$$\text{Out}(\mathbf{x}) = g(\mathbf{w}^T\mathbf{x}) = g\left(\sum_j w_j x_j\right)$$



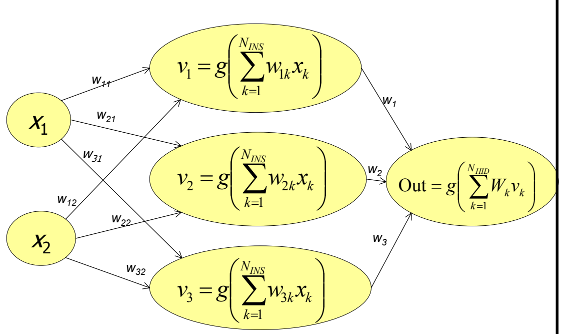
Use a wider representation !

$$\text{Out}(\mathbf{x}) = g\left(\sum_j W_j g\left(\sum_k w_{jk} x_{jk}\right)\right)$$

This is a nonlinear function
Of a linear combination
Of non linear functions
Of linear combinations of inputs

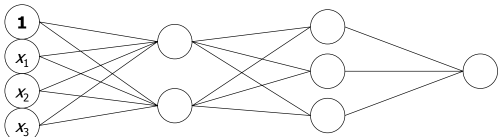
A 1-HIDDEN LAYER NET

$N_{INPUTS} = 2$ $N_{HIDDEN} = 3$



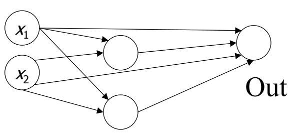
Why not use multiple layers of linear networks?

OTHER NEURAL NETS



2-Hidden layers + Constant Term

"JUMP" CONNECTIONS



$$\text{Out} = g\left(\sum_{k=1}^{N_{INS}} w_{0k} x_k + \sum_{k=1}^{N_{HID}} W_k v_k\right)$$

Backpropagation (Chain Rule)

$$\text{Out}(\text{x}) = g\left(\sum_j W_j g\left(\sum_k w_{jk} x_k\right)\right)$$

Find a set of weights $\{W_j\}, \{w_{jk}\}$

to minimize

$$\sum_i (y_i - \text{Out}(\text{x}_i))^2$$

by gradient descent.

That's it!
That's the backpropagation algorithm.

Backpropagation Convergence

Convergence to a global minimum is <u>not</u> guaranteed.

•In practice, this is not a problem, apparently.

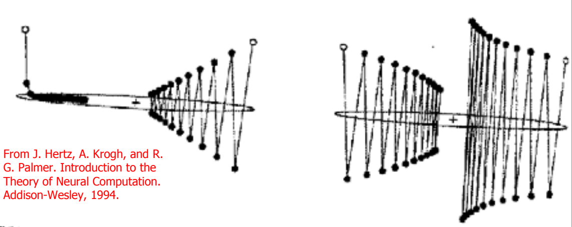
Tweaking to find the right number of hidden units, or a useful learning rate η, is more hassle, apparently.

IMPLEMENTING BACKPROP: Differentiate Monster sum-square residual Write down the Gradient Descent Rule It turns out to be easier & computationally efficient to use lots of local variables with names like h_j o_k v_j net_i etc…

Choosing the learning rate

- This is a subtle art.
- Too small: can take days instead of minutes to converge
- Too large: diverges (MSE gets larger and larger while the weights increase and usually oscillate)
- Sometimes the "just right" value is hard to find.

Learning-rate problems



From J. Hertz, A. Krogh, and R. G. Palmer. Introduction to the Theory of Neural Computation. Addison-Wesley, 1994.

FIGURE 5.10 Gradient descent on a simple quadratic surface (the left and right parts are copies of the same surface). Four trajectories are shown, each for 20 steps from the open circle. The minimum is at the + and the ellipse shows a constant error contour. The only significant difference between the trajectories is the value of η, which was 0.02, 0.0476, 0.049, and 0.0505 from left to right.

Improving Simple Gradient Descent

Momentum

Don't just change weights according to the current datapoint.
Re-use changes from earlier iterations.

Let $\Delta\mathbf{w}(t)$ = weight changes at time t.

Let $-\eta \frac{\partial \text{E}}{\partial \text{w}}$ be the change we would make with regular gradient descent.

Instead we use

$$\Delta\mathbf{w}(t+1) = -\eta \frac{\partial \text{E}}{\partial \mathbf{w}} + \alpha \Delta\mathbf{w}(t)$$

$$\mathbf{w}(t+1) = \mathbf{w}(t) + \Delta\mathbf{w}(t)$$

momentum parameter

Momentum damps oscillations.

A hack? Well, maybe.

Momentum illustration

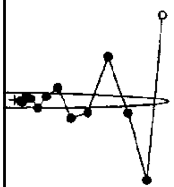


FIGURE 6.3 Gradient descent on the simple quadratic surface of Fig. 5.10. Both trajectories are for 12 steps with $\eta = 0.0476$, the best value in the absence of momentum. On the left there is no momentum ($\alpha = 0$), while $\alpha = 0.5$ on the right.

Improving Simple Gradient Descent

Newton's method

$$E(\mathbf{w}+\mathbf{h}) = E(\mathbf{w}) + \mathbf{h}^T \frac{\partial E}{\partial \mathbf{w}} + \frac{1}{2}\mathbf{h}^T \frac{\partial^2 E}{\partial \mathbf{w}^2}\mathbf{h} + O(|\mathbf{h}|^3)$$

If we neglect the $O(h^3)$ terms, this is a ***quadratic form***

Quadratic form fun facts:

If $y = c + \boldsymbol{b}^T \boldsymbol{x} - 1/2\, \boldsymbol{x}^T \boldsymbol{A}\, \boldsymbol{x}$

And if $\boldsymbol{A}$ is SPD

Then

$\boldsymbol{x}^{opt} = \boldsymbol{A}^{-1}\boldsymbol{b}$ is the value of $\boldsymbol{x}$ that maximizes y

Improving Simple Gradient Descent

Newton's method

$$E(\mathbf{w}+\mathbf{h}) = E(\mathbf{w}) + \mathbf{h}^T \frac{\partial E}{\partial \mathbf{w}} + \frac{1}{2}\mathbf{h}^T \frac{\partial^2 E}{\partial \mathbf{w}^2}\mathbf{h} + O(|\mathbf{h}|^3)$$

If we neglect the $O(h^3)$ terms, this is a ***quadratic form***

$$\mathbf{w} \leftarrow \mathbf{w} - \left[\frac{\partial^2 E}{\partial \mathbf{w}^2}\right]^{-1} \frac{\partial E}{\partial \mathbf{w}}$$

This should send us directly to the global minimum if the function is truly quadratic.

And it might get us close if it's locally quadraticish

Improving Simple Gradient Descent

Newton's method

$$E(\mathbf{w}+\mathbf{h}) = E(\mathbf{w}) + \mathbf{h}^T \frac{\partial E}{\partial \mathbf{w}} + \frac{1}{2}\mathbf{h}^T \frac{\partial^2 E}{\partial \mathbf{w}^2}\mathbf{h} + O(|\mathbf{h}|^3)$$

If ... neglect the $O(h^3)$ terms, this is a ***quadratic form***

BUT (and it's a big but)…

That second derivative matrix can be expensive and fiddly to compute.

If we're not already in the quadratic bowl, we'll go nuts.

...mum if the function...

And it might get us close ... aticish

Improving Simple Gradient Descent

Conjugate Gradient

Another method which attempts to exploit the "local quadratic bowl" assumption

But does so while only needing to use $\dfrac{\partial E}{\partial \mathbf{w}}$

and not $\dfrac{\partial^2 E}{\partial \mathbf{w}^2}$

It is also more stable than Newton's method if the local quadratic bowl assumption is violated.

It's complicated, outside our scope, but it often works well. More details in Numerical Recipes in C.

BEST GENERALIZATION

Intuitively, you want to use the smallest, simplest net that seems to fit the data.

HOW TO FORMALIZE THIS INTUITION?

1. Don't. Just use intuition
2. Bayesian Methods Get it Right
3. Statistical Analysis explains what's going on
4. Cross-validation

Other "Neural Networks"

- Polynomials (linear in weights)
- Projection Pursuit $\Sigma g_i(w_i^T x)$, $g_i()$ arbitrary, say splines.
- Additive Regression $\Sigma g_i(x_i)$, align units with coordinate axes, $g_i()$ arbitrary
- Radial Basis Functions $\Sigma g_i(|x-c_i|^2)$

Non-parametric Neural Networks

- Add parameters (neurons/units) as you go along.
- GMDH (do it with polynomials)
- Cascade Correlation

GMDH (c.f. BACON, AIM)

- Group Method Data Handling
- A very simple but very good idea:

1. Do linear regression
2. Use cross-validation to discover whether any quadratic term is good. If so, add it as a basis function and loop.
3. Use cross-validation to discover whether any of a set of familiar functions (log, exp, sin etc) applied to any previous basis function helps. If so, add it as a basis function and loop.
4. Else stop

GMDH (c.f. BACON, AIM)

- Group Method Data Handling
- A very simple but very good idea:

1. D
2. U

Typical learned function:

age^{est} = height - 3.1 sqrt(weight) +

4.3 income / (cos (NumCars))

y

qu … sis

function and loop.

3. Use cross-validation to discover whether any of a set of familiar functions (log, exp, sin etc) applied to any previous basis function helps. If so, add it as a basis function and loop.
4. Else stop

When will GMDH fail?

When will GMDH fail?

- Will not learn XYZ if X, Y, and Z are zero mean and independent such that E(XY), E(XZ), and E(YZ) are all zero.

What You Should Know

- How to use matlab to do multivariate Least-squares linear regression.
- Derivation of least squares as max. likelihood estimator of linear coefficients
- The general gradient descent rule, relationship to chain rule
- How to use matlab to fit data with nonlinear functions

Which approach is better?

