# Introduction to Machine Learning Logistic Regression 

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## Outline

(1) Logistic Regression

- Introduction
- Constraints
- The Initial Model
- The Two Case Class
- Graphic Interpretation
- Fitting The Model
- The Two Class Case
- The Final Log-Likelihood
- The Newton-Raphson Algorithm
- Matrix Notation
(2) More on Optimization Methods
- Can we do better?
- Using Cholesky Decomposition
- Cholesky Decomposition
- The Proposed Method
- Quasi-Newton Method
- The Second Order Approximation
- The BFGS Algorithm
- A Neat Trick: Coordinate Ascent
- Coordinate Ascent Algorithm
- Conclusion


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## Assume the following

## Let $Y_{1}, Y_{2}, \ldots, Y_{N}$ independent random variables

Taking values in the set $\{0,1\}$

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## Now, you have a set of fixed vectors

$$
\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{N}
$$

Mapped to a series of numbers by a weight vector $\boldsymbol{w}$

$$
\boldsymbol{w}^{T} \boldsymbol{x}_{1}, \boldsymbol{w}^{T} \boldsymbol{x}_{2}, \ldots, \boldsymbol{w}^{T} \boldsymbol{x}_{N}
$$

## In our simplest from $[1,2]$

## There is a suspected relation

Between $\theta_{i}=P\left(Y_{i}=1\right)$ and $\boldsymbol{w}^{T} \boldsymbol{x}_{i}$

- Here $Y$ is the random variable and $y$ is the value that the random variable can take.


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- Here $Y$ is the random variable and $y$ is the value that the random variable can take.

Thus we have

$$
y= \begin{cases}1 & \boldsymbol{w}^{T} \boldsymbol{x}+e>0 \\ 0 & \text { else }\end{cases}
$$

Note: Where $e$ is an error with a certain distribution!!!

For Example, Graphically

We have


## It is better to user a logit version

We have


## Logit Distribution

PDF with support $z \in(-\infty, \infty), \mu$ location and $s$ scale

$$
p(x \mid \mu, s)=\frac{\exp \left\{-\frac{z-\mu}{s}\right\}}{s\left(1+\exp \left\{-\frac{z-\mu}{s}\right\}\right)^{2}}
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$$

## With a CDF

$$
P(Y<z)=\int_{-\infty}^{z} p(y \mid \mu, s) d y=\frac{1}{1+\exp \left\{-\frac{z-\mu}{s}\right\}}
$$

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## In Bayesian Classification

## Assignment of a pattern

It is performed by using the posterior probabilities, $P\left(\omega_{i} \mid \boldsymbol{x}\right)$

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$$

## Such that each

$$
0 \leq P\left(\omega_{i} \mid \boldsymbol{x}\right) \leq 1
$$

## Observation

This is a typical example of the discriminative approach

- Where the distribution of data is of no interest.
- In the Logistic Regression the Distribution is imposed over the output!!!


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## The Model

We have the following under the extended features

$$
\log \frac{P\left(\omega_{1} \mid \boldsymbol{x}\right)}{P\left(\omega_{K} \mid \boldsymbol{x}\right)}=\boldsymbol{w}_{1}^{T} \boldsymbol{x}
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\log \frac{P\left(\omega_{2} \mid \boldsymbol{x}\right)}{P\left(\omega_{K} \mid \boldsymbol{x}\right)} & =\boldsymbol{w}_{2}^{T} \boldsymbol{x} \\
\vdots & \\
\log \frac{P\left(\omega_{K-1} \mid \boldsymbol{x}\right)}{P\left(\omega_{K} \mid \boldsymbol{x}\right)} & =\boldsymbol{w}_{K-1}^{T} \boldsymbol{x}
\end{aligned}
$$

## Further

## We have

The model is specified in terms of $K-1$ log-odds or logit transformations.

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## And

Although the model uses the last class as the denominator in the odds-ratios.

The choice of denominator is arbitrary

- However, because the estimates are equivariant under this choice.
- The action taken in a decision problem should not depend on transformation on the measurement used

Now

How do we find the terms?

$$
P\left(\omega_{1} \mid \boldsymbol{x}\right), P\left(\omega_{2} \mid \boldsymbol{x}\right), \ldots, P\left(\omega_{K} \mid \boldsymbol{x}\right)
$$

## It is possible to show that

We have that, for $l=1,2, \ldots, K-1$

$$
\frac{P\left(\omega_{l} \mid \boldsymbol{x}\right)}{P\left(\omega_{K} \mid \boldsymbol{x}\right)}=\exp \left\{\boldsymbol{w}_{l}^{T} \boldsymbol{x}\right\}
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Therefore

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\sum_{l=1}^{K-1} \frac{P\left(\omega_{l} \mid \boldsymbol{x}\right)}{P\left(\omega_{K} \mid \boldsymbol{x}\right)}=\sum_{l=1}^{K-1} \exp \left\{\boldsymbol{w}_{l}^{T} \boldsymbol{x}\right\}
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$$

## Thus

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\frac{1-P\left(\omega_{K} \mid \boldsymbol{x}\right)}{P\left(\omega_{K} \mid \boldsymbol{x}\right)}=\sum_{l=1}^{K-1} \exp \left\{\boldsymbol{w}_{l}^{T} \boldsymbol{x}\right\}
$$

## Basically

We have, (Take a look a the board)

$$
P\left(\omega_{K} \mid \boldsymbol{x}\right)=\frac{1}{1+\sum_{l=1}^{K-1} \exp \left\{\boldsymbol{w}_{l}^{T} \boldsymbol{x}\right\}}
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Then

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\frac{P\left(\omega_{i} \mid \boldsymbol{x}\right)}{\frac{1+\sum_{l=1}^{K-1} \exp \left\{\boldsymbol{w}_{l}^{T} x\right\}}{1}}=\exp \left\{\boldsymbol{w}_{l}^{T} \boldsymbol{x}\right\}
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## For $i=1,2, \ldots, k-1$

$$
P\left(\omega_{i} \mid \boldsymbol{x}\right)=\frac{\exp \left\{\boldsymbol{w}_{i}^{T} \boldsymbol{x}\right\}}{1+\sum_{l=1}^{K-1} \exp \left\{\boldsymbol{w}_{l}^{T} \boldsymbol{x}\right\}}
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## Additionally

## For K

$$
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## Additionally

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$$
P\left(\omega_{K} \mid \boldsymbol{x}\right)=\frac{1}{1+\sum_{l=1}^{K-1} \exp \left\{\boldsymbol{w}_{l}^{T} \boldsymbol{x}\right\}}
$$

## Easy to see

They sum to one.

## A Note in Notation

Given all these parameters, we summarized them

$$
\Theta=\left\{\boldsymbol{w}_{1}, \boldsymbol{w}_{2}, \ldots, \boldsymbol{w}_{K-1}\right\}
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$$
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Therefore

$$
P\left(\omega_{l} \mid \boldsymbol{X}=\boldsymbol{x}\right)=p_{l}(\boldsymbol{x} \mid \Theta)
$$

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## In the two class case

We have

$$
\begin{aligned}
P_{1}\left(\omega_{1} \mid \boldsymbol{x}\right) & =\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}\right\}} \\
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\end{aligned}
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## A similar model

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\begin{aligned}
& P_{1}\left(\omega_{1} \mid \boldsymbol{x}\right)=\frac{\exp \left\{-\boldsymbol{w}^{T} \boldsymbol{x}\right\}}{1+\exp \left\{-\boldsymbol{w}^{T} \boldsymbol{x}\right\}} \\
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We have the following split

Using $f(\boldsymbol{x})=\boldsymbol{w}^{T} \boldsymbol{x}$


## Then, we have the mapping to

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## A Classic application of Maximum Likelihood

Given a sequence of smaples iid

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We have the following pdf

$$
p\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{N} \mid \Theta\right)=\prod_{i=1}^{N} p\left(x_{i} \mid \Theta\right)
$$

## $P(g=v \mid X)$ Distribution

## Where $P(g=v \mid X)$ completely specify the conditional distribution

 We have a multinomial distribution which under the log-likelihood of $N$ observations:$\mathcal{L}(\Theta)=$

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$$

## Where

$g_{i}$ represent the class that $\boldsymbol{x}_{i}$ belongs.

$$
g_{i}= \begin{cases}1 & \text { if } \boldsymbol{x}_{i} \in \text { Class } 1 \\ 2 & \text { if } \boldsymbol{x}_{i} \in \text { Class } 2\end{cases}
$$

## How do we integrate this into a Cost Function?

Clearly, we have two distributions
We need to represent the distributions into the functions $p_{g_{i}}\left(\boldsymbol{x}_{i} \mid \theta\right)$.

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Why not to have all the distributions into this function

$$
p_{g_{i}}\left(\boldsymbol{x}_{i} \mid \theta\right)=\prod_{l=1}^{K-1} p\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}_{l}\right)^{I\left\{\boldsymbol{x}_{i} \in \omega_{l}\right\}}
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## It is easy with the two classes

Given that we have a binary situation!!!

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## Given the two case

## We have then a Bernoulli distribution

$$
\begin{aligned}
& p_{1}\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)=\left[\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}\right\}}\right]^{y_{i}} \\
& p_{2}\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)=\left[\frac{1}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}\right\}}\right]^{1-y_{i}}
\end{aligned}
$$

## Given the two case

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\end{aligned}
$$

## With

$$
\begin{aligned}
& y_{i}=1 \text { if } \boldsymbol{x}_{i} \in \text { Class } 1 \\
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\end{aligned}
$$

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## We have the following

## Cost Function

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{w})= & \sum_{i=1}^{N}\left\{y_{i} \log p_{1}\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)+\right. \\
& \left.\left(1-y_{i}\right) \log \left(1-p_{1}\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)\right)\right\}
\end{aligned}
$$

We have the following

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& \left.\left(1-y_{i}\right) \log \left(1-p_{1}\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)\right)\right\}
\end{aligned}
$$

## After some reductions

$$
\mathcal{L}(\boldsymbol{w})=\sum_{i=1}^{N}\left\{y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}-\log \left(1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}\right)\right\}
$$

Now, we derive and set it to zero
We have

$$
\frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w}}=\sum_{i=1}^{N} \boldsymbol{x}_{i}\left(y_{i}-\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right)=0
$$

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## We have

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\frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w}}=\sum_{i=1}^{N} \boldsymbol{x}_{i}\left(y_{i}-\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right)=0
$$

## Which are $d+1$ equations nonlinear

$$
\sum_{i=1}^{N} \boldsymbol{x}_{i}\left(y_{i}-p\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)\right)=\left(\begin{array}{c}
\sum_{i=1}^{N} 1 \times\left(y_{i}-\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right) \\
\sum_{i=1}^{N} x_{1}^{i}\left(y_{i}-\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right) \\
\sum_{i=1}^{N} x_{2}^{i}\left(y_{i}-\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right) \\
\vdots \\
\sum_{i=1}^{N} x_{d}^{i}\left(y_{i}-\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right)
\end{array}\right)=\mathbf{0}
$$

It is know as a scoring function.

## Finally

## In other words you

(1) $d+1$ nonlinear equations in $\boldsymbol{w}$.

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(3) For example, from the first equation:

$$
\sum_{i=1}^{N} y_{i}=\sum_{i=1}^{N} p\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)
$$

- The expected number of class ones matches the observed number.


## Finally

## In other words you

(1) $d+1$ nonlinear equations in $\boldsymbol{w}$.
(c) For example, from the first equation:

$$
\sum_{i=1}^{N} y_{i}=\sum_{i=1}^{N} p\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}\right)
$$

- The expected number of class ones matches the observed number.
- And hence also class twos.


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(3) $\operatorname{Or} h=r-x_{0}$

## We have then

From Taylor

$$
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## Thus

$$
r=x_{0}+h \approx x_{0}-\frac{f\left(x_{0}\right)}{f^{\prime}\left(x_{0}\right)}
$$

## We have our final improving

We have

$$
x_{1} \approx x_{0}-\frac{f\left(x_{0}\right)}{f^{\prime}\left(x_{0}\right)}
$$

Then, on the scoring function

For this, we need the Hessian of the function

$$
\frac{\partial^{2} \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w} \partial \boldsymbol{w}^{T}}=-\sum_{i=1}^{N} \boldsymbol{x}_{i} \boldsymbol{x}_{i}^{T}\left[\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right]\left[1-\frac{\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}{1+\exp \left\{\boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right]
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$$

Thus, we have at a starting point $w^{\text {old }}$

$$
\boldsymbol{w}^{\text {new }}=\boldsymbol{w}^{\text {old }}-\left(\frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w} \partial \boldsymbol{w}^{T}}\right)^{-1} \frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w}}
$$

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## We can rewrite all as matrix notations

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(9) $W$ a $N \times N$ diagonal matrix of weights with the $i^{t h}$ diagonal element

$$
p\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}^{o l d}\right)\left[1-p\left(\boldsymbol{x}_{i} \mid \boldsymbol{w}^{o l d}\right)\right]
$$

Then, we have

For each updating term

$$
\begin{aligned}
\frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w}} & =X^{T}(\boldsymbol{y}-\boldsymbol{p}) \\
\frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w} \partial \boldsymbol{w}^{T}} & =-X^{T} W X
\end{aligned}
$$

Then, we have

Then, the Newton Step
$\boldsymbol{w}^{\text {new }}=\boldsymbol{w}^{\text {old }}+\left(X^{T} W X\right)^{-1} X^{T}(\boldsymbol{y}-\boldsymbol{p})$

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\boldsymbol{w}^{\text {new }} & =\boldsymbol{w}^{\text {old }}+\left(X^{T} W X\right)^{-1} X^{T}(\boldsymbol{y}-\boldsymbol{p}) \\
& =I \boldsymbol{w}^{\text {old }}+\left(X^{T} W X\right)^{-1} X^{T} I(\boldsymbol{y}-\boldsymbol{p})
\end{aligned}
$$

Then, we have

## Then, the Newton Step

$$
\begin{aligned}
\boldsymbol{w}^{n e w} & =\boldsymbol{w}^{\text {old }}+\left(X^{T} W X\right)^{-1} X^{T}(\boldsymbol{y}-\boldsymbol{p}) \\
& =I \boldsymbol{w}^{\text {old }}+\left(X^{T} W X\right)^{-1} X^{T} I(\boldsymbol{y}-\boldsymbol{p}) \\
& =\left(X^{T} W X\right)^{-1} X^{T} W X \boldsymbol{w}^{\text {old }}+\left(X^{T} W X\right)^{-1} X^{T} W W^{-1}(\boldsymbol{y}-\boldsymbol{p})
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$$

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\boldsymbol{w}^{\text {new }} & =\boldsymbol{w}^{o l d}+\left(X^{T} W X\right)^{-1} X^{T}(\boldsymbol{y}-\boldsymbol{p}) \\
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& =\left(X^{T} W X\right)^{-1} X^{T} W\left[X \boldsymbol{w}^{o l d}+W^{-1}(\boldsymbol{y}-\boldsymbol{p})\right]
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& =\left(X^{T} W X\right)^{-1} X^{T} W\left[X \boldsymbol{w}^{\text {old }}+W^{-1}(\boldsymbol{y}-\boldsymbol{p})\right] \\
& =\left(X^{T} W X\right)^{-1} X^{T} W \boldsymbol{z}
\end{aligned}
$$

## Then


#### Abstract

We have Re-expressed the Newton step as a weighted least squares step.


## Then

## We have

Re-expressed the Newton step as a weighted least squares step.
With a the adjusted response as

$$
\boldsymbol{z}=X \boldsymbol{w}^{\text {old }}+W^{-1}(\boldsymbol{y}-\boldsymbol{p})
$$

## This New Algorithm

It is know as
Iteratively Re-weighted Least Squares or IRLS

## This New Algorithm

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Iteratively Re-weighted Least Squares or IRLS

After all at each iteration, it solves

A weighted Least Square Problem

$$
\boldsymbol{w}^{n e w} \leftarrow \arg \min _{\boldsymbol{w}}(\boldsymbol{z}-X \boldsymbol{w})^{T} W(\boldsymbol{z}-X \boldsymbol{w})
$$

## Observations

## Good Starting Point $w=0$

However, convergence is never guaranteed!!!

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## However

- Typically the algorithm does converge, since the log-likelihood is concave.
- But overshooting can occur.


## Observations

## $L\left(\boldsymbol{\theta}_{j}\right)=\log \prod_{j=1}^{n} p\left(\boldsymbol{x}_{j} \mid \boldsymbol{\theta}_{j}\right)$



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$L\left(\boldsymbol{\theta}_{j}\right)=\log \prod_{j=1}^{n} p\left(\boldsymbol{x}_{j} \mid \boldsymbol{\theta}_{j}\right)$


## Halving Solve the Problem

## Perfect!!!

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## The final question

## After all, we always want to have a better solution

- We know that $\left(\frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w} \partial \boldsymbol{w}^{T}}\right)^{-1}$ takes $O\left(d^{3}\right) \ldots$ and we want something better!!!


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We have the following methods

- Colesky Decomposition


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## We can decompose the matrix

Given $A=X^{T} W X$ and $Y=X^{T} W \boldsymbol{z}$, you have

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A x=Y
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Given $A=X^{T} W X$ and $Y=X^{T} W \boldsymbol{z}$, you have

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We want to obtain

$$
x=A^{-1} Y
$$

## This can be seen as a system of linear equations

## As you can see

- We start with a set of linear equations with $d+1$ unknowns:


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$$
x_{1}, x_{2}, \ldots, x_{d+1} \begin{cases}a_{11} x_{1}+a_{12} x_{2}+\ldots+a_{1 d+1} x_{d+1} & =y_{1} \\ a_{21} x_{1}+a_{22} x_{2}+\ldots+a_{2 d+1} x_{d+1} & =y_{2} \\ \vdots & \vdots \\ a_{d+11} x_{1}+a_{d+12} x_{2}+\ldots+a_{d+1 d+1} x_{n} & =y_{d+1}\end{cases}
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$$

## Thus

- A set of values for $x_{1}, x_{2}, \ldots, x_{n}$ that satisfy all of the equations simultaneously is said to be a solution to these equations.


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## What is the Cholesky Decomposition? [4]

## It is a method that factorize a matrix

- $A \in \mathbb{R}^{d+1 \times d+1}$ is a positive definite Hermitian matrix


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Positive definite matrix

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Hermitian matrix in the Real Domain (Symmetric Matrix)

$$
A=A^{T}
$$

## Therefore

Cholesky decomposes $A$ into lower or upper triangular matrix and their conjugate transpose

$$
\begin{aligned}
A & =L L^{T} \\
A & =R^{T} R
\end{aligned}
$$

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$$

Thus, we can use the Cholensky decomposition

- The Cholensky decomposition is of order $O\left(d^{3}\right)$ and requires $\frac{1}{6} d^{3}$ FLOP operations.


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## We have

The matrices $A \in \mathbb{R}^{d+1 \times d+1}$ and $X=A^{-1}$

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If we define $R X=B$

$$
R^{T} B=I
$$

## Now

If $B=\left(R^{T}\right)^{-1}=L^{-1}$ for $L=R^{T}$
(1) We note that the inverse of the lower triangular matrix $L$ is lower triangular.
(2) The diagonal entries of $L^{-1}$ are the reciprocal of diagonal entries of $L$

$$
\begin{gathered}
\left(\begin{array}{cccc}
a_{1,1} & 0 & \cdots & 0 \\
a_{2,1} & a_{2,2} & 0 & \vdots \\
\vdots & \vdots & \ddots & 0 \\
a_{d+1,1} & a_{d+1,2} & \cdots & a_{d+1, d+1}
\end{array}\right)\left(\begin{array}{cccc}
b_{1,1} & 0 & \cdots & 0 \\
b_{2,1} & b_{2,2} & 0 & \vdots \\
\vdots & \vdots & \ddots & 0 \\
b_{d+1,1} & b_{d+1,2} & \cdots & b_{d+1, d+1}
\end{array}\right) \\
\left(\begin{array}{cccc}
1 & 0 & \cdots & 0 \\
0 & 1 & 0 & \vdots \\
\vdots & 0 & \ddots & 0 \\
0 & \cdots & 0 & 1
\end{array}\right)
\end{gathered}
$$

Now

Now, we construct the following matrix $S$ with entries

$$
s_{i, j}= \begin{cases}\frac{1}{l_{i, i}} & \text { if } i=j \\ 0 & \text { otherwise }\end{cases}
$$

Now, we have

The matrix $S$ is the correct solution to upper diagonal element of the matrix $B$
i.e. $s_{i j}=b_{i j}$ for $i \leq j \leq d+1$

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i.e. $s_{i j}=b_{i j}$ for $i \leq j \leq d+1$

Then, we use backward substitution to solve $x_{i, j}$ at equation $R x_{i}=s_{i}$
Assuming:

$$
\begin{aligned}
X & =\left[\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{d+1}\right] \\
S & =\left[\boldsymbol{s}_{1}, \boldsymbol{s}_{2}, \ldots, \boldsymbol{s}_{d+1}\right]
\end{aligned}
$$

## Back Substitution

## Back substitution

Since $R$ is upper-triangular, we can rewrite the system $R x_{i}=s_{i}$ as

$$
\begin{aligned}
r_{1,1} x_{1, i}+r_{1,2} x_{2, i}+\ldots+r_{1, d-1} x_{d-1, i}+r_{1, d} x_{d, i}+r_{1, d+1} x_{d+1, i} & =s_{1, i} \\
r_{2,2} x_{2}+\ldots+r_{2, d-1} x_{d-1, i}+r_{2, d} x_{d, i}+r_{2, d+1} x_{d+1, i} & =s_{2, i} \\
& \vdots \\
r_{d-1, d-1} x_{d-1, i}+r_{d-1, d} x_{d, i}+r_{d-1, d+1} x_{d+1, i} & =s_{d-1, i} \\
r_{d, d} x_{d, i}+r_{d, d+1} x_{d, i} & =s_{d, i} \\
r_{d+1, d+1} x_{d+1, i} & =s_{d+1, i}
\end{aligned}
$$

## Then

We solve only for $x_{i j}$ such that

- We have $i<j \leq N$ (Upper triangle elements).


## Then

## We solve only for $x_{i j}$ such that

- We have $i<j \leq N$ (Upper triangle elements).

$$
x_{j i}=\overline{x_{i j}}
$$

- In our case the same value given that we live on the reals.


## Complexity

## Equation solving requires

- $\frac{1}{3}(d+1)^{3}$ multiply operations.


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The total number of multiply operations for matrix inverse

- Including Cholesky decomposition is $\frac{1}{2}(d+1)^{3}$


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The total number of multiply operations for matrix inverse

- Including Cholesky decomposition is $\frac{1}{2}(d+1)^{3}$


## Therefore

- We have complexity $O\left(d^{3}\right)$ !!! Per iteration!!! But actually $\frac{1}{2}(d+1)^{3}$ multiply operations


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## However

## As Good Computer Scientists

We want to obtain a better complexity as $O\left(n^{2}\right)!!!$

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## We can obtain such improvements

Using Quasi Newton Methods

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Let's us to develop the solution

- For the most popular one
- Broyden-Fletcher-Goldfarb-Shanno (BFGS) method


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## The Second Order Approximation

## We have

$$
f(\boldsymbol{x}) \approx f\left(\boldsymbol{x}_{k}\right)+\nabla f\left(\boldsymbol{x}_{k}\right)\left(\boldsymbol{x}-\boldsymbol{x}_{k}\right)+\frac{1}{2}\left(\boldsymbol{x}-\boldsymbol{x}_{k}\right)^{T} \boldsymbol{H} f\left(\boldsymbol{x}_{k}\right)\left(\boldsymbol{x}-\boldsymbol{x}_{k}\right)
$$

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$$

We develop a new equation based in the previous idea by using $\boldsymbol{x}=\boldsymbol{x}_{k}+\boldsymbol{p}$

$$
f(\boldsymbol{x}) \approx f\left(\boldsymbol{x}_{k}\right)+\nabla f\left(\boldsymbol{x}_{k}\right) \boldsymbol{p}+\frac{1}{2} \boldsymbol{p}^{T} H_{k} \boldsymbol{p}
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We develop a new equation based in the previous idea by using $\boldsymbol{x}=\boldsymbol{x}_{k}+\boldsymbol{p}$

$$
f(\boldsymbol{x}) \approx f\left(\boldsymbol{x}_{k}\right)+\nabla f\left(\boldsymbol{x}_{k}\right) \boldsymbol{p}+\frac{1}{2} \boldsymbol{p}^{T} H_{k} \boldsymbol{p}
$$

## Here

- $H_{k}$ is an $d+1 \times d+1$ symmetric positive definite matrix that will be updated through the entire process


## For the BFGS

Then, the inverse update of it $H_{k}=B_{k}^{-1}$
In BFGS we go directly for the inverse by setting up:

$$
\begin{gathered}
\min _{H}\left\|H-H_{k}\right\| \\
\text { s.t. } H=H^{T} \\
H y_{k}=s_{k}
\end{gathered}
$$

with

$$
\begin{aligned}
& s_{k}=\boldsymbol{x}_{k+1}-\boldsymbol{x}_{k} \\
& y_{k}=\nabla f\left(\boldsymbol{x}_{k+1}\right)-\nabla f\left(\boldsymbol{x}_{k}\right)
\end{aligned}
$$

## Then, we have

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## A unique solution will be

$$
\begin{equation*}
H_{k+1}=\left(I-\rho_{k} s_{k} y_{k}^{T}\right) H_{k}\left(I-\rho_{k} y_{k} s_{k}^{T}\right)+\rho s_{k} s_{k}^{T} \tag{1}
\end{equation*}
$$

where $\rho_{k}=\frac{1}{y_{k}^{T} s_{k}}$

## Complexity of Generating $H_{k+1}$

## We notice that the complexity of calculating

$$
s_{k} s_{k}^{T}, s_{k} s_{k}^{T}, s_{k} y_{k}^{T}
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- It is $O\left(d^{2}\right)$


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## Why? For Example

$$
\left(\begin{array}{c}
s_{1} \\
s_{2} \\
\vdots \\
s_{d}
\end{array}\right)\left(\begin{array}{llll}
s_{1} & s_{2} & \cdots & s_{d}
\end{array}\right)=\left(\begin{array}{cccc}
s_{1}^{2} & s_{1} s_{2} & \cdots & s_{1} s_{d} \\
s_{2} s_{1} & s_{2}^{2} & \cdots & s_{2} s_{d} \\
\vdots & \vdots & \ddots & \vdots \\
s_{d} s_{1} & s_{d} s_{2} & \cdots & s_{d}^{2}
\end{array}\right) \text {-Equal to } d^{2}
$$

Finally

## Finally

## Thus

- The sum on the term $H_{k+1}$ has a complexity of $O\left(d^{2}\right)$

The total complexity

$$
O\left(d^{2}\right)
$$

## Problem

## There is no magic formula to find an initial $H_{0}$

We can use specific information about the problem:

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- For instance by setting it to the inverse of an approximate Hessian calculated by finite differences at $\boldsymbol{x}_{0}$


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We can use specific information about the problem:

- For instance by setting it to the inverse of an approximate Hessian calculated by finite differences at $\boldsymbol{x}_{0}$
- In our case, we have $\frac{\partial \mathcal{L}(\boldsymbol{w})}{\partial \boldsymbol{w} \partial \boldsymbol{w}^{T}}$, or in matrix format $X^{T} W X$, we could get initial setup


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The

- Cost of update or inverse update is $O\left(d^{2}\right)$ operations per iteration.


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## For More

- Nocedal, Jorge \& Wright, Stephen J. (1999). Numerical Optimization. Springer-Verlag.


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## Given the following [5]

## Because the likelihood is concave



## Caution

Here, we change the labeling to $y_{i}= \pm 1$ with

$$
p\left(y_{i}= \pm 1 \mid \boldsymbol{x}, \boldsymbol{w}\right)=\sigma\left(y \boldsymbol{w}^{T} \boldsymbol{x}\right)=\frac{1}{1+\exp \left\{-y \boldsymbol{w}^{T} \boldsymbol{x}\right\}}
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Thus, we have the following log likelihood under regularization $\lambda>0$

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\mathcal{L}(\boldsymbol{w})=-\sum_{i=1}^{N} \log \left\{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}\right\}-\frac{\lambda}{2} \boldsymbol{w}^{T} \boldsymbol{w}
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$$

It is possible to get a Gradient Descent

$$
\nabla_{\boldsymbol{w}} l(\boldsymbol{w})=\sum_{i=1}^{N}\left\{1-\frac{1}{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right\} y_{i} \boldsymbol{x}_{i}-\lambda \boldsymbol{w}
$$

## Danger Will Robinson!!!

Gradient descent using resembles the Perceptron learning algorithm Problem!!! It will always converge for a suitable step size, regardless of whether the classes are separable!!!

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## Here

We will simplify our work
By stating the algorithm for coordinate ascent

## Here

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By stating the algorithm for coordinate ascent
Then
A more precise version will be given

## Coordinate Ascent

## Algorithm

- Input Max, an initial $\boldsymbol{w}_{0}$
(1) counter $\leftarrow 0$
(2) while counter $<$ Max
(3) for $i \leftarrow 1, \ldots, d$
©
Randomly pick $i$
Compute a step size $\delta^{*}$ by approximately maximize $\arg \min _{\delta} f\left(\boldsymbol{x}+\delta \boldsymbol{e}_{i}\right)$
©

$$
x_{i} \leftarrow x_{i}+\delta^{*}
$$

## Coordinate Ascent

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6

$$
x_{i} \leftarrow x_{i}+\delta^{*}
$$

## Where

$$
\boldsymbol{e}_{i}=\left(\begin{array}{lllllll}
0 & \cdots & 0 & 1 \leftarrow i & 0 & \cdots & 0
\end{array}\right)^{T}
$$

## In the case of Logistic Regression

Thus, we can optimize each $w_{k}$ alternatively by a coordinate-wise Newton update

$$
w_{k}^{\text {new }}=w_{k}^{o l d}+\frac{-\lambda w_{k}^{o l d}+\sum_{i=1}^{N}\left\{1-\frac{1}{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right\} y_{i} x_{i k}}{\lambda+\sum_{i=1}^{N} x_{i k}^{2}\left(\frac{1}{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right)\left(1-\frac{1}{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right)}
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$$

## Complexity of this update

| Item | Complexity |
| :---: | :---: |
| $\sum_{i=1}^{N}\left\{1-\frac{1}{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right\} y_{i} x_{i k}$ | $O(N)$ |
| $\sum_{i=1}^{N} x_{i k}^{2}\left(\frac{1}{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right)\left(1-\frac{1}{1+\exp \left\{-y_{i} \boldsymbol{w}^{T} \boldsymbol{x}_{i}\right\}}\right)$ | $O(N)$ |
| Total Complexity | $O(N)$ |
| For all the dimensions | $O(N d)$ |

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We have the following Complexities per iteration

## Complexities

| Method | Per Iteration | Convergence Rate |
| :---: | :---: | :---: |
| Cholesky Decomposition | $\frac{d^{3}}{2}=O\left(d^{3}\right)$ | Quadratic |
| Quasi-Newton BFGS | $O\left(d^{2}\right)$ | Super-linearly |
| Coordinate Ascent | $O(N d)$ | Not established |

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