Lecture Notes for
Machine Learning in Python

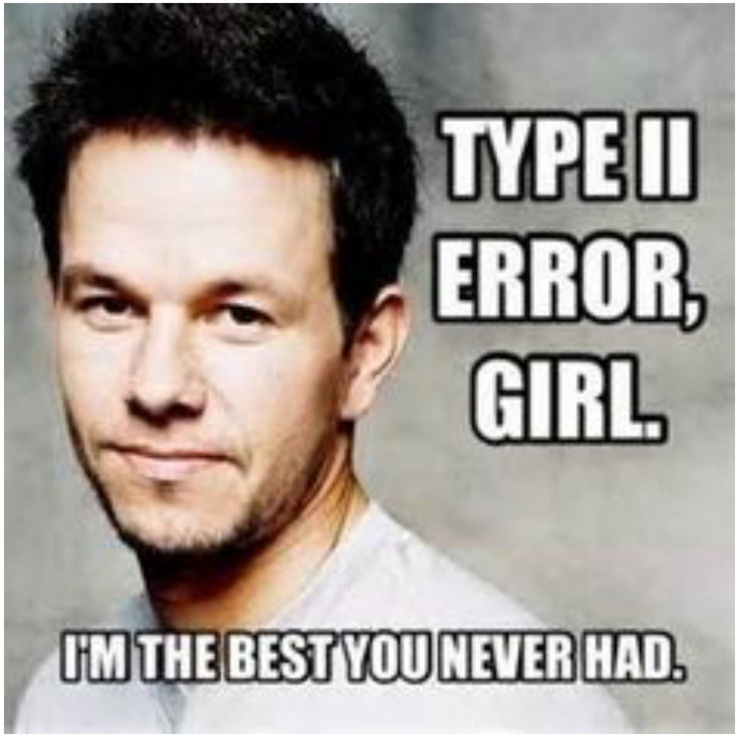
Professor Eric Larson

Logistic Regression

Class Logistics and Agenda

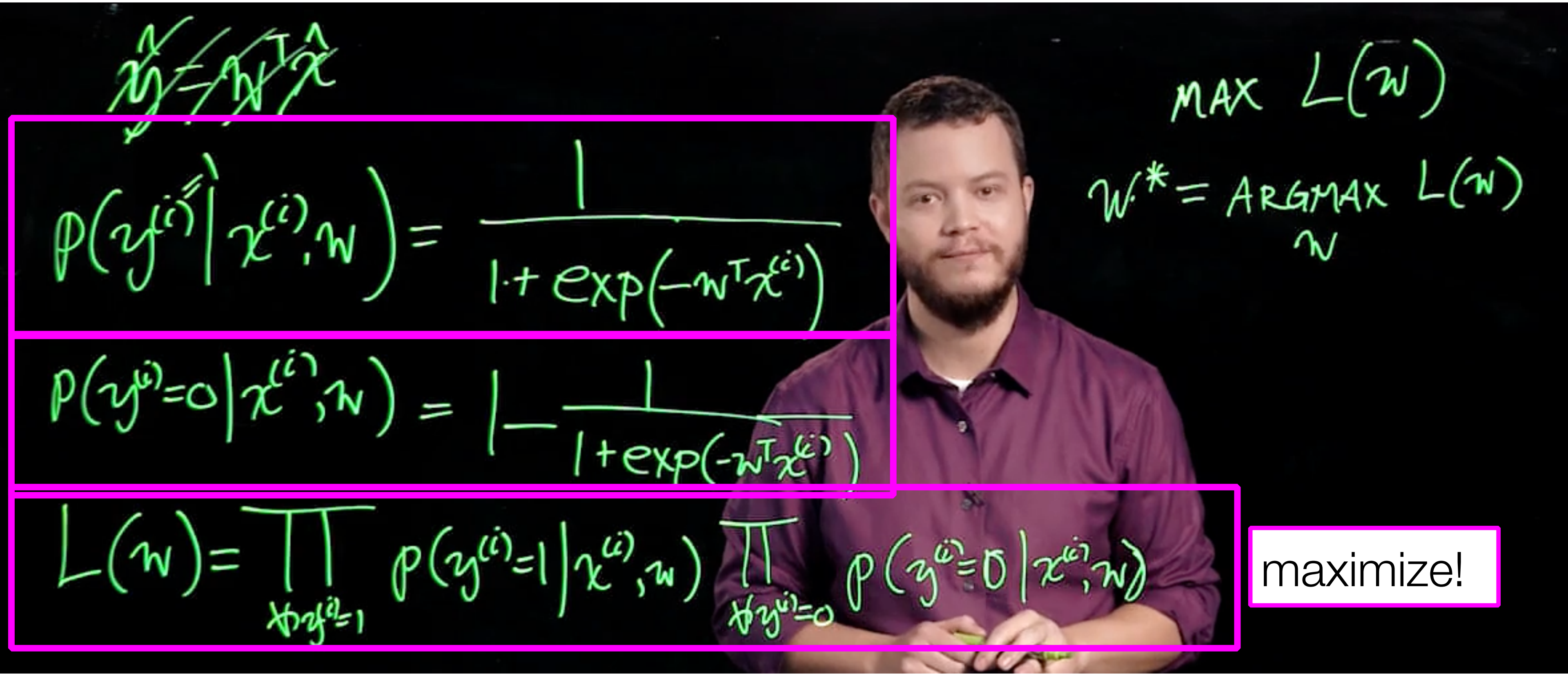
- Welcome back to lecture!
- Logistics
  - Nothing due this week
  - Next week: ICA2 and A4
- Agenda
  - Logistic Regression
    - Solving
    - Programming

Solving Logistic Regression



Setting Up Binary Logistic Regression

- From flipped lecture:



Binary Solution for Update Equation

- Video Supplement:
  - https://www.youtube.com/watch?v=FGnoHdjFrJ8

- General Procedure:
  - Simplify L(w) with logarithm, l(w)

$$l(w) = \sum_i y^{(i)} \ln\left(g(w^T x^{(i)})\right) + (1-y^{(i)}) \ln\left(1-g(w^T x^{(i)})\right)$$

  - Take Gradient

$$= -\sum_i \left(y^{(i)} - g(w^T x^{(i)})\right) x_j^{(i)}$$

  - Use gradient inside update equation for **w**

Binary Solution for Update Equation

- Use gradient inside update equation for **w**

$$\underbrace{w_j}_{\text{new value}} \leftarrow \underbrace{w_j}_{\text{old value}} + \eta \underbrace{\sum_{i=1}^{M} (y^{(i)} - g(x^{(i)}))x_j^{(i)}}_{\text{gradient}}$$

$$w \leftarrow w + \eta \sum_{i=1}^{M} (y^{(i)} - g(x^{(i)}))x^{(i)}$$

05. Logistic Regression.ipynb

Demo

Reinvent sklearn

Logistic Regression

- Programming
- Vectorization
- Regularization
- Multi-class extension

Other Tutorials:

http://blog.yhat.com/posts/logistic-regression-python-rodeo.html

http://scikit-learn.org/stable/auto_examples/linear_model/plot_iris_logistic.html

For Next Lecture

- **Next time**: Gradient based optimization for logistic regression
- **Next Next time**: SVMs in-class assignment

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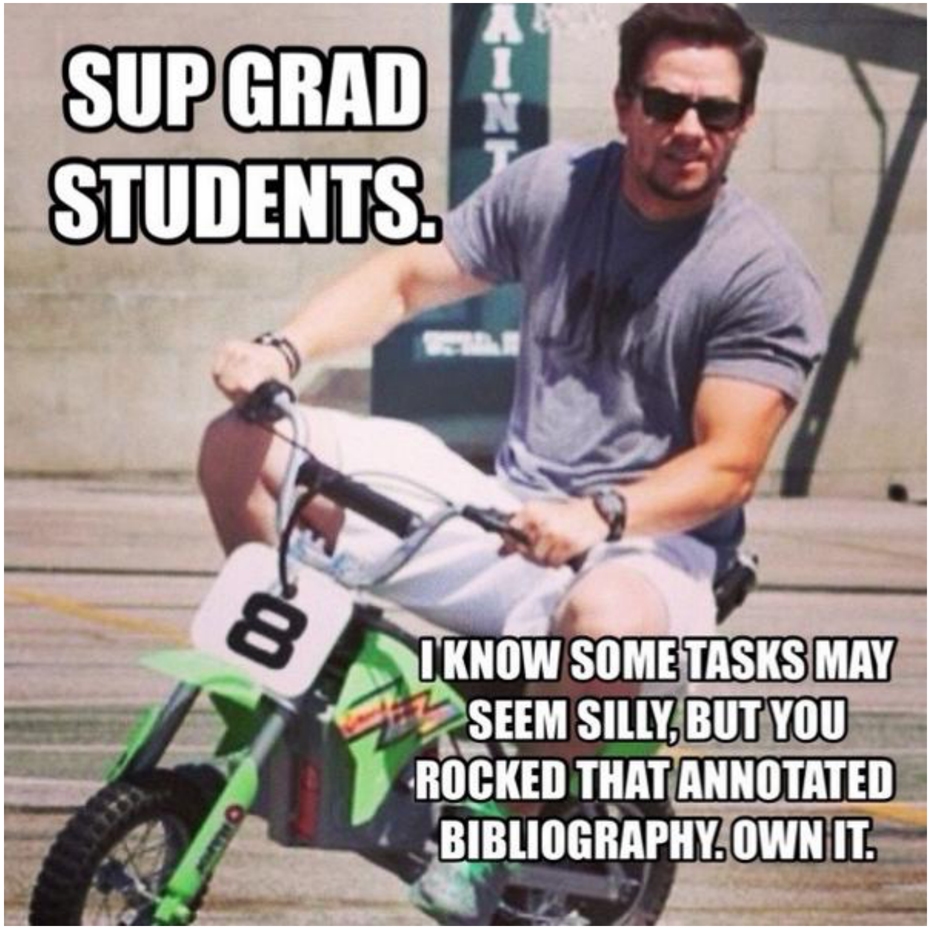
Optimization Techniques for Logistic Regression

Class Logistics and Agenda

- Agenda
  - Numerical Optimization Techniques
    - Types of Optimization
    - Programming the Optimization
- **Whirlwind Lecture Alert**: entire classes cover these concepts
  - We only want an intuition and implications for learning algorithms

Gradient Descent Techniques

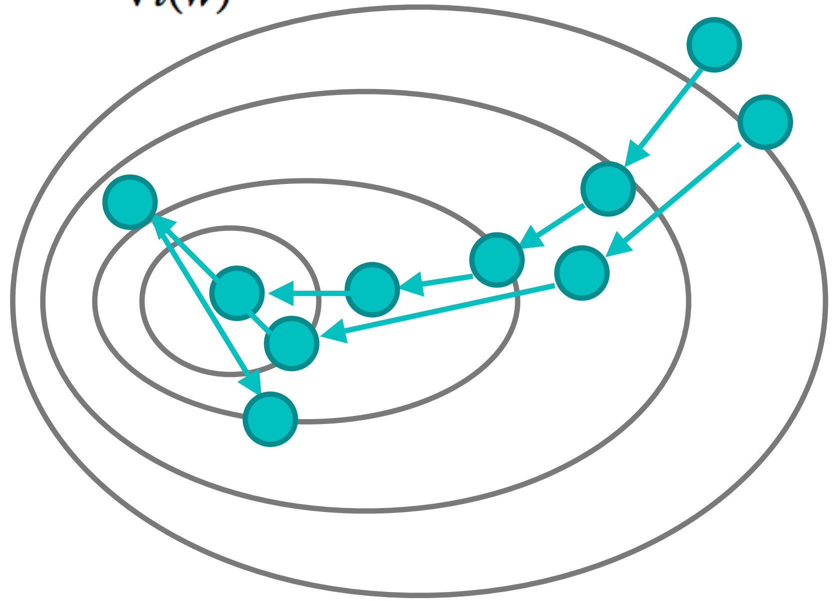


Optimization: gradient descent

- What we know thus far:

$$\underbrace{w_j}_{\text{new value}} \leftarrow \underbrace{w_j}_{\text{old value}} + \eta \underbrace{\left[\left(\sum_{i=1}^{M} (y^{(i)} - g(x^{(i)}))x_j^{(i)} \right) - C \cdot 2w_j \right]}_{\nabla l(w)}$$

$$w \leftarrow w + \eta \nabla l(w)$$



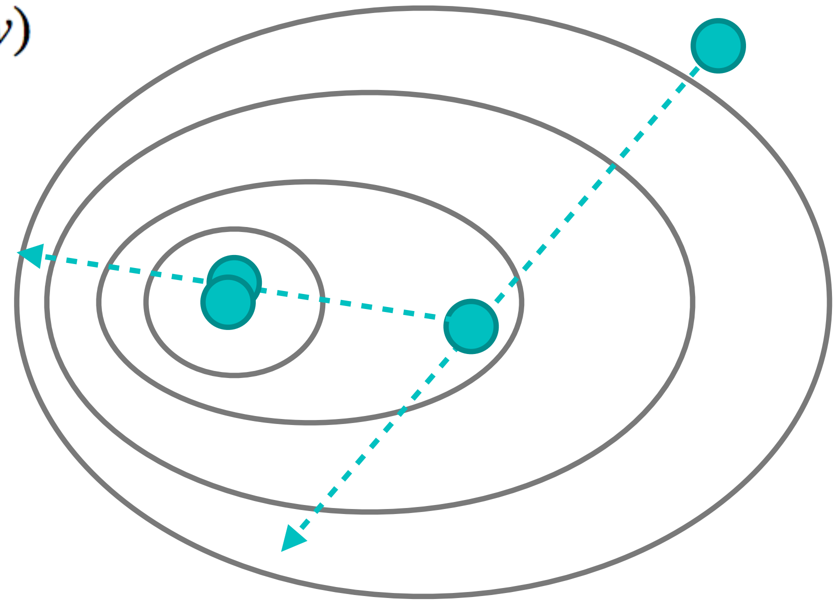
Line Search: a better method

- Line search in direction of gradient:

$$\eta \leftarrow \arg\max_{\eta} \underbrace{\sum_{i=1}^{M} (y^{(i)} - \hat{y}^{(i)})^2 - C \cdot \sum_{j} w_j^2}_{l(w)}$$

$$w \leftarrow w + \eta \nabla l(w)$$

$$w \leftarrow w + \underbrace{\eta}_{\text{best step?}} \nabla l(w)$$



Stochastic Methods

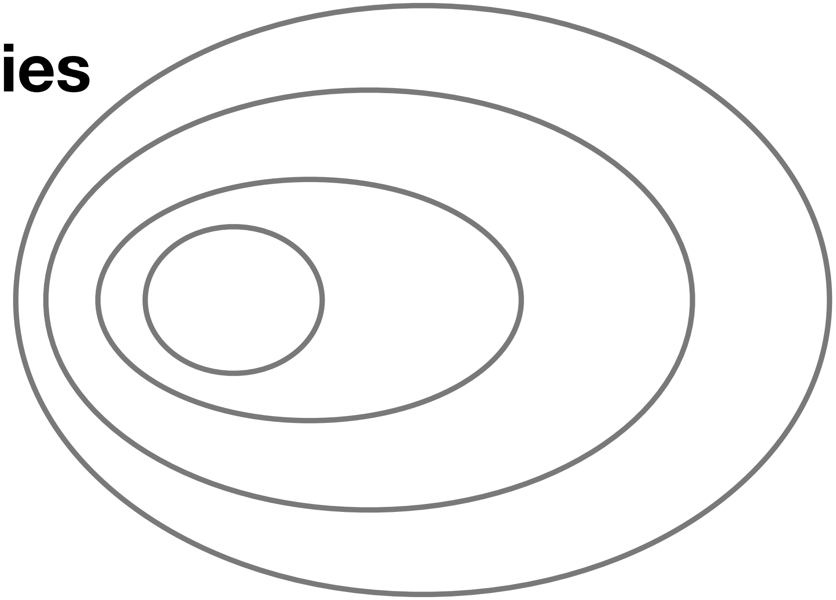
- How much computation is required (for gradient)?

$$\sum_{i=1}^{M}(y^{(i)} - \hat{y}^{(i)})x^{(i)} - 2C \cdot w$$

M = number of instances
N = number of features

Self Test: How many multiplies per gradient calculation?

A. M+N multiplications
B. M*N multiplications
C. 2N multiplications
D. 2N-M multiplications



Stochastic Methods

- How much computation is required (for gradient)?

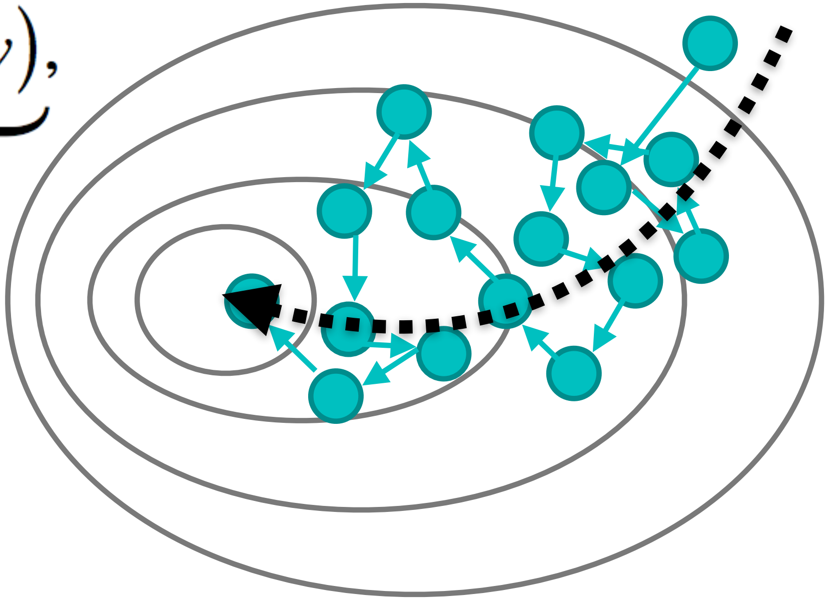
$$\sum_{i=1}^{M}(y^{(i)} - \hat{y}^{(i)})x^{(i)} - 2C \cdot w$$

Per iteration:

M*N multiplications

2M add/subtract

$$w \leftarrow w + \eta \underbrace{\left((y^{(i)} - \hat{y}^{(i)})x^{(i)} - 2C \cdot w\right)}_{\text{approx. gradient}},$$



i chosen at random

Per iteration:

N multiplications

1 add/subtract

`06. Optimization.ipynb` **Demo**

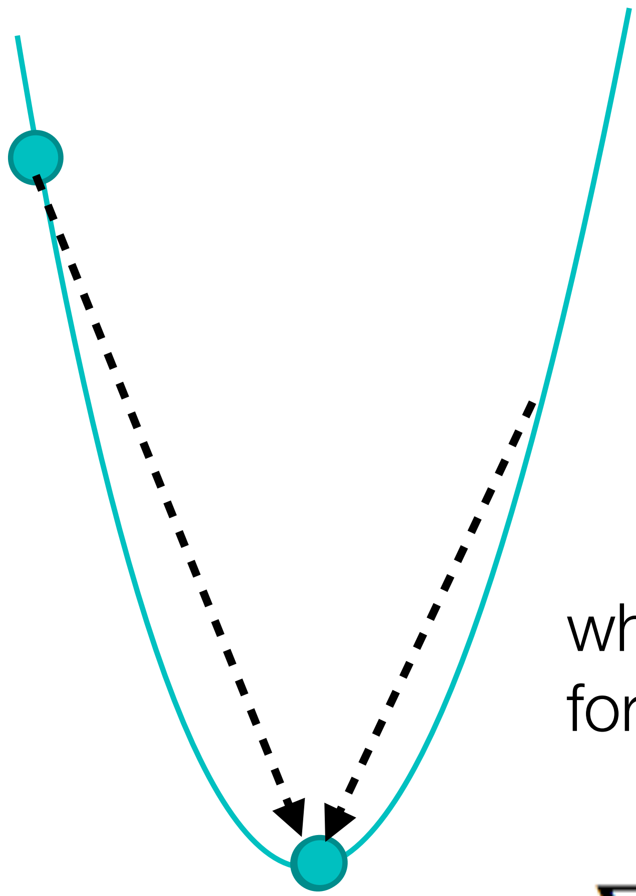
Numerical Optimization

- Gradient Descent (with line search)
- Stochastic Gradient Descent

Optimization Techniques with the Hessian

The Hessian

- Assume function is quadratic:



function of one variable:

$$w \leftarrow w - \underbrace{[\frac{\partial^2}{\partial w} l(w)]^{-1}}_{\text{inverse 2nd deriv}} \underbrace{\frac{\partial}{\partial w} l(w)}_{\text{derivative}}$$

will solve in one step!

what is the second order derivative for a multivariate function?

$$\nabla^2 l(w) = \mathbf{H}[l(w)]$$

The Hessian

- Assume function is quadratic:

function of one variable:

$$\mathbf{H}[l(w)] = \begin{bmatrix} \frac{\partial^2}{\partial w_1} l(w) & \frac{\partial}{\partial w_1}\frac{\partial}{\partial w_2} l(w) & \dots & \frac{\partial}{\partial w_1}\frac{\partial}{\partial w_N} l(w) \\ \frac{\partial}{\partial w_2}\frac{\partial}{\partial w_1} l(w) & \frac{\partial^2}{\partial w_2} l(w) & \dots & \frac{\partial}{\partial w_2}\frac{\partial}{\partial w_N} l(w) \\ & \vdots & & \\ \frac{\partial}{\partial w_N}\frac{\partial}{\partial w_1} l(w) & \frac{\partial}{\partial w_N}\frac{\partial}{\partial w_2} l(w) & \dots & \frac{\partial^2}{\partial w_N} l(w) \end{bmatrix}$$

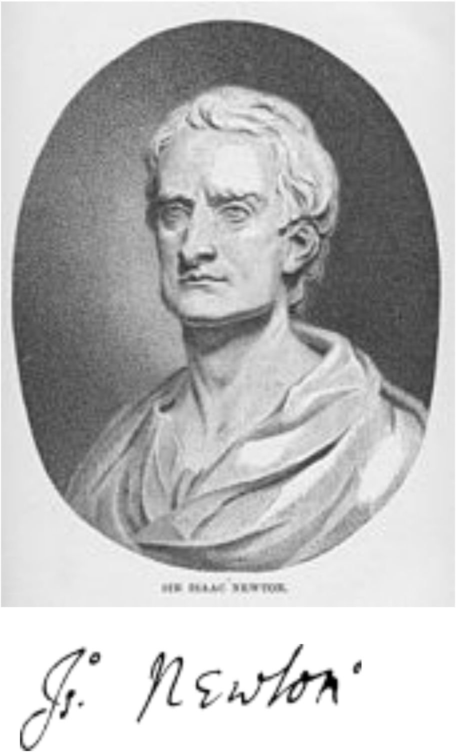
$$\nabla^2 l(w) = \mathbf{H}[l(w)]$$

The Newton Update Method

- Assume function is quadratic (in high dimensions):

$$w \leftarrow w - \underbrace{[\frac{\partial^2}{\partial w} l(w)]^{-1}}_{\text{inverse 2nd deriv}} \underbrace{\frac{\partial}{\partial w} l(w)}_{\text{derivative}}$$

$$w \leftarrow w + \eta \cdot \underbrace{\mathbf{H}[l(w)]^{-1}}_{\text{inverse Hessian}} \cdot \underbrace{\nabla l(w)}_{\text{gradient}}$$



I do not know what I may appear to the world, but to myself I seem to have been only like a boy playing on the sea-shore, and diverting myself in now and then finding a smoother pebble or a prettier shell than ordinary, whilst the great ocean of truth lay all undiscovered before me.

The Hessian for Logistic Regression

- The hessian is easy to calculate from the gradient for logistic regression

$$w \leftarrow w + \eta \cdot \underbrace{\mathbf{H}[l(w)]^{-1}}_{\text{inverse Hessian}} \cdot \underbrace{\nabla l(w)}_{\text{gradient}}$$

$$\mathbf{H}_{j,k}[l(w)] = -\sum_{i=1}^{M} g(x^{(i)})(1 - g(x^{(i)})x_k{}^{(i)} x_j{}^{(i)}$$

$$\underbrace{\sum_{i=1}^{M} (y^{(i)} - \hat{y}^{(i)})x_j^{(i)}}_{\text{gradient}}$$

$$\mathbf{H}[l(w)] = X^T \cdot \text{diag}[g(x^{(i)})(1 - g(x^{(i)}))] \cdot X$$

$$X * y_{diff}$$

$$w \leftarrow w + \eta[X^T \cdot \text{diag}[g(x^{(i)})(1 - g(x^{(i)}))] \cdot X]^{-1} \cdot X * y_{diff}$$

Numerical Optimization

Newton's method

Problems with Newton's Method

- **Quadratic** isn't always a great assumption:
  - highly dependent on starting point
    - jumps can get **really random**!
  - near saddle points, inverse hessian **unstable**
  - hessian **not** always **invertible**…
    - or invertible with correct numerical precision

The solution: quasi Newton methods

- In general:
  - **approximate** the **Hessian** with something numerically sound and readily invertible
  - **back off to gradient** descent when the approximate hessian is **not stable**
  - use **momentum** to update approximate hessian
- **A popular approach**: use Broyden-Fletcher-Goldfarb-Shanno (BFGS)
  - which you can look up if you are interested …

https://en.wikipedia.org/wiki/Broyden–Fletcher–Goldfarb–Shanno_algorithm

BFGS (if time)

$\mathbf{H}_0 = \mathbf{I}$	init
$p_k = -\mathbf{H}_k^{-1} \nabla l(w_k)$	get update direction
$w_{k+1} \leftarrow w_k + \eta \cdot p_k$	find next w
$s_k = \eta \cdot p_k$	get scaled direction
$v_k = \nabla l(w_{k+1}) - \nabla l(w_k)$	approx gradient change
$\mathbf{H}_{k+1} = \mathbf{H}_k + \frac{v_k v_k^T}{v_k^T s_k} - \frac{\mathbf{H}_k s_k s_k^T \mathbf{H}_k}{s_k^T \mathbf{H}_k s_k}$	update Hessian and inverse Hessian approx
$\mathbf{H}_{k+1}^{-1} = \mathbf{H}_k^{-1} + \frac{(s_k^T v_k + \mathbf{H}_k^{-1})(s_k s_k^T)}{(s_k^T v_k)^2} - \frac{\mathbf{H}_k^{-1} v_k s_k^T + s_k v_k^T \mathbf{H}_k^{-1}}{s_k^T v_k}$	
$k = k + 1$	increment k and repeat

invertibility of H well defined / only matrix operations

`06. Optimization.ipynb` **Demo**

Numerical Optimization

BFGS (if time)

parallelization

For Next Lecture

- **Next time**: SVMs via in class assignment
- **Next Next time**: Neural Networks

Scratch Paper

Scratch Paper

Scratch Paper