Lecture Notes for

Machine Learning in Python

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Professor Eric Larson

Logistic Regression

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Machine Learning in Python

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Optimization Techniques for Logistic Regression

Class Logistics and Agenda

- Logistic: grading!
- Agenda
  - Finish Logistic Regression
  - Numerical Optimization Techniques
    - Types of Optimization
    - Programming the Optimization
- **Whirlwind Lecture Alert**
  - Get an intuition, program it, maybe you don’t follow every mathematical concept in lecture
  - But you know how to approach it outside lecture

Class Overview, by topic

Table Data Visualization
Numpy, Pandas, Seaborn
Overviews with some in-depth discussion

Dimension Reduction and Image Processing
Scikit-learn, Scikit Image,
Intuition only, Some mathematics

Linear and Logistic Regression
Numpy, Recreate API for Scikit-learn
Detailed mathematics for simple optimization
intuition for advanced optimization

Neural Networks and Back Prop.
Numpy
Detailed mathematics for NN operations

Wide and Deep Networks

Convolutional Networks

Recurrent Networks

Keras, Tensorflow
Intuition, Detailed implement.

Ethics in Language Models

ConceptNet
Case studies

Review

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

now $\mathbf{x}$, $\mathbf{w}$ are vectors

$$\underbrace{\mathbf{w}}_{\text{new vect}} \leftarrow \underbrace{\mathbf{w}}_{\text{old vect}} + \frac{\eta}{M}\sum_{i=1}^{M}(y^{(i)} - g(\mathbf{w}^T\mathbf{x}^{(i)})) \cdot \mathbf{x}^{(i)}$$

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \cdot \text{mean}(\mathbf{y}_{diff} \odot \mathbf{X})_{columns}$$

$$\mathbf{y}_{diff} = \begin{bmatrix} y^{(1)} - g(\mathbf{w}^T\mathbf{x}^{(1)}) \\ y^{(2)} - g(\mathbf{w}^T\mathbf{x}^{(2)}) \\ \vdots \\ y^{(M)} - g(\mathbf{w}^T\mathbf{x}^{(M)}) \end{bmatrix} = \begin{bmatrix} y_{diff}^{(1)} \\ y_{diff}^{(2)} \\ \vdots \\ y_{diff}^{(M)} \end{bmatrix}$$

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \cdot \text{mean}\left(\begin{bmatrix} y_{diff}^{(1)} \\ y_{diff}^{(2)} \\ \vdots \\ y_{diff}^{(M)} \end{bmatrix} \odot \begin{bmatrix} \leftarrow & \mathbf{x}^{(1)} & \rightarrow \\ \leftarrow & \mathbf{x}^{(2)} & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}^{(M)} & \rightarrow \end{bmatrix}\right)_{columns}$$

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \cdot \text{mean}\left(\begin{bmatrix} (\leftarrow & \mathbf{x}^{(1)} & \rightarrow) \cdot y_{diff}^{(1)} \\ (\leftarrow & \mathbf{x}^{(2)} & \rightarrow) \cdot y_{diff}^{(2)} \\ & \vdots & \\ (\leftarrow & \mathbf{x}^{(M)} & \rightarrow) \cdot y_{diff}^{(M)} \end{bmatrix}\right)_{columns}$$

Demo

`05. Logistic Regression.ipynb`

“Finish”

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

Demo Lecture

`06. Optimization`

Scratch Paper

Back Up Slides

Last time

$$p(y^{(i)} = 1 \mid x^{(i)}, w) = \frac{1}{1 + \exp\left(w^T x^{(i)}\right)}$$

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

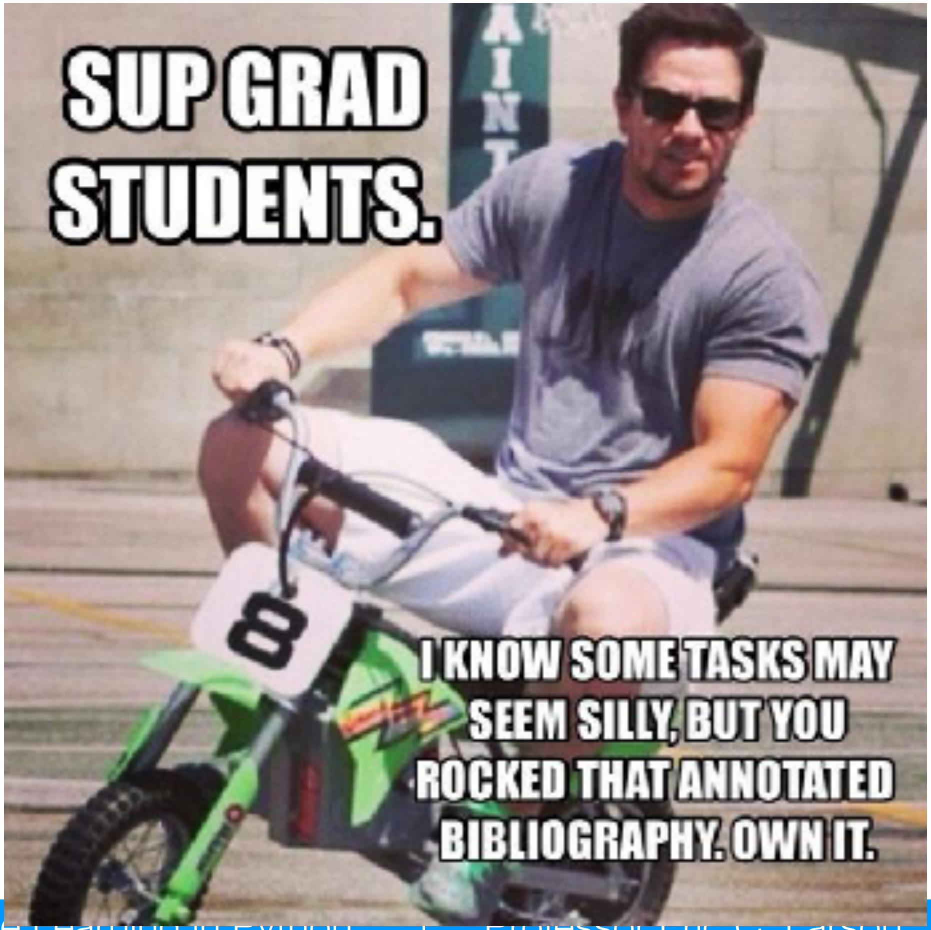
$$\underbrace{w_j}_{\text{new value}} \leftarrow \underbrace{w_j}_{\text{old value}} + \underbrace{\eta \sum_{i=1}^{M} (y^{(i)} - g(x^{(i)}))x_j^{(i)}}_{\text{gradient}}$$

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

$$w \leftarrow w + \eta \left[\underbrace{\nabla l(w)_{old}}_{\text{old gradient}} - C \cdot 2w \right]$$

```
def _get_gradient(self,X,y):
    # programming \sum_i (yi-g(xi))xi
    gradient = np.zeros(self.w_.shape) # set
    for (xi,yi) in zip(X,y):
        # the actual update inside of sum
        gradi = (yi - self.predict_proba(xi,
        # reshape to be column vector and ad
        gradient += gradi.reshape(self.w_.sh

    return gradient/float(len(y))
```

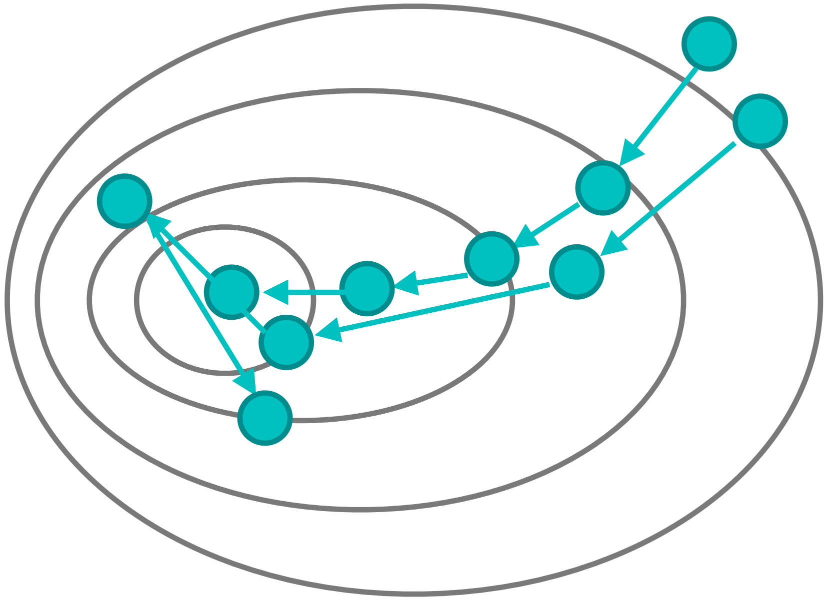

SUP GRAD
STUDENTS.
I KNOW SOME TASKS MAY
SEEM SILLY, BUT YOU
ROCKED THAT ANNOTATED
BIBLIOGRAPHY. OWN IT.

Optimization: gradient descent

- What we know thus far:

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

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

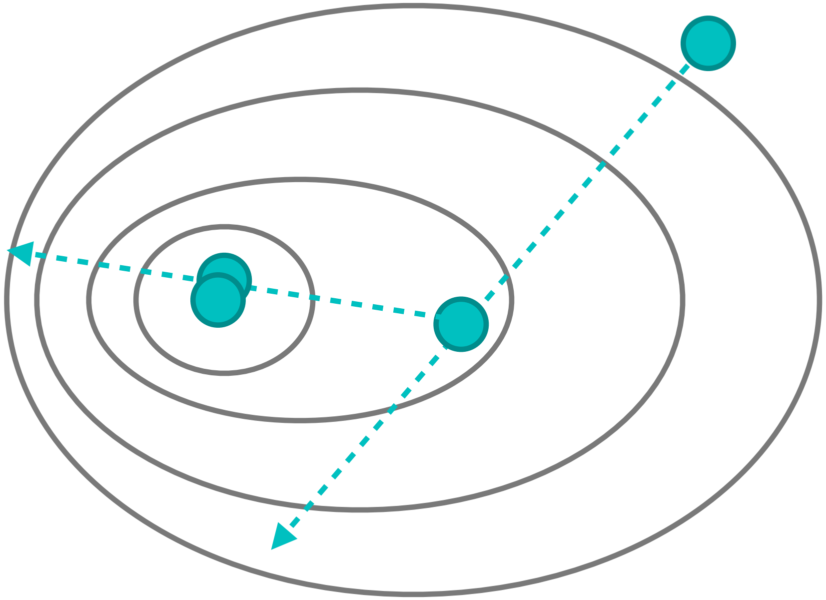


Line Search: a better method

- Line search in direction of gradient:

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

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



Revisiting the Gradient

- 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+1 multiplications
B. (M+1)*N multiplications
C. 2N multiplications
D. 2N-M multiplications

Stochastic Methods

- How much computation is required (for gradient)?

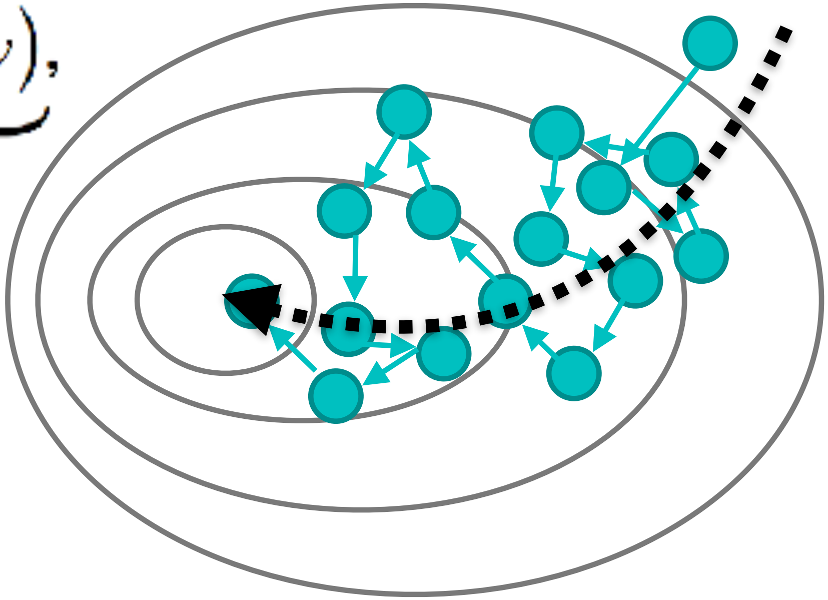
$$\sum_{i=1}^{M}(y^{(i)} - \hat{y}^{(i)})x^{(i)} - 2C \cdot w$$

Per iteration:

(M+1)*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+1 multiplications

1 add/subtract

06. Optimization.ipynb

Demo

Gradient Descent (with line search)

Stochastic Gradient Descent

Hessian

Quasi-Newton Methods

Multi-processing

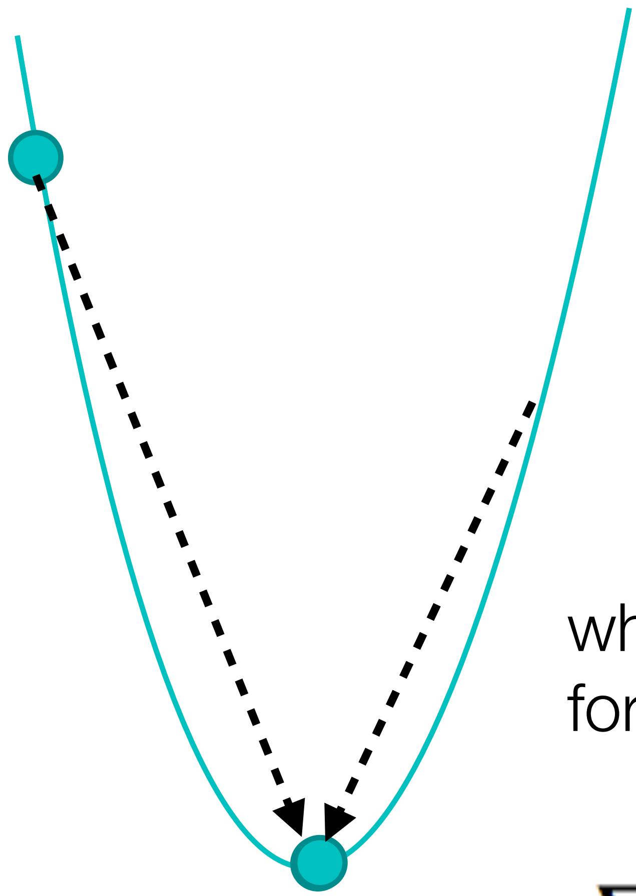
For Next Lecture

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


SUP. HAVE YOU HEARD THE LATEST STATS JOKE?
PROBABLY.

Can we do better than the gradient?

- 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:

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

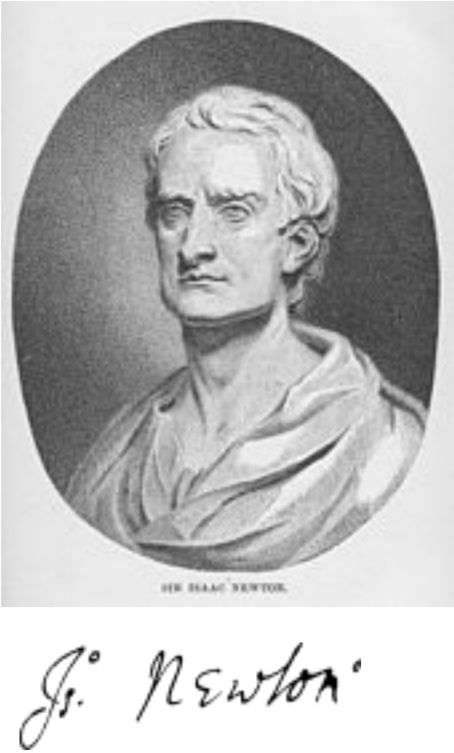
$$\nabla^2 l(w) = \mathbf{H}[l(w)]$$

The Newton Update Method

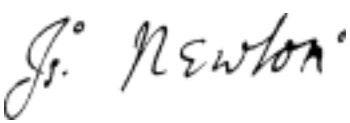
- Assume function is quadratic (in high dimensions):

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

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



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.



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$$\frac{\partial}{\partial w_j} l(w) = \sum_i \left(y^{(i)} - g(x^{(i)})\right) x_j^{(i)}$$

PLUG IN

H[k,j]= $$\frac{\partial}{\partial w_k}\frac{\partial}{\partial w_j} l = \frac{\partial}{\partial w_k}\left(\sum_i \left(y^{(i)} - g(x^{(i)})\right) x_j^{(i)}\right)$$

$$= \sum_i \overset{\nearrow 0}{\frac{\partial}{\partial w_k} y^{(i)}} x_j^{(i)} - \frac{\partial}{\partial w_k} g(x^{(i)}) x_j^{(i)}$$

LEFT OVER TERM

$$= -\sum_i \frac{\partial}{\partial w_k} g(x^{(i)}) x_j^{(i)}$$

Already know $\frac{\partial}{\partial w_k} g(w^T x^{(i)})$ side calculation

$$= g(x^{(i)})\left(1 - g(x^{(i)})\right) \frac{\partial}{\partial w_k}\left(w^T x^{(i)}\right)$$

$$= g(x^{(i)})\left(1 - g(x^{(i)})\right) x_k^{(i)}$$

PLUG IN

$$\therefore = -\sum_i g(x^{(i)})\left(1 - g(x^{(i)})\right) x_k^{(i)} x_j^{(i)}$$

THAT'S THE HESSIAN!

H(k,j) = This is a valid equation for the Hessian, but we want to represent it using linear algebra

$$\boxed{= -\sum_i g(x^{(i)})\left(1 - g(x^{(i)})\right) x_k^{(i)} x_j^{(i)}}$$

SIGMOID

The Hessian for Logistic Regression

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

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

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

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

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

$$X * y_{diff}$$

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

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 efficiently 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

$$\mathbf{H}_0 = \mathbf{I}$$ init

$$p_k = -\mathbf{H}_k^{-1} \nabla l(w_k)$$ get update direction

find next w $$w_{k+1} \leftarrow w_k + \eta \cdot p_k$$

get scaled direction $$s_k = \eta \cdot p_k$$

$$v_k = \nabla l(w_{k+1}) - \nabla l(w_k)$$ approx gradient change

$$\mathbf{H}_{k+1} = \mathbf{H}_k + \underbrace{\frac{v_k v_k^T}{v_k^T s_k}}_{\text{approx. Hessian}} - \underbrace{\frac{\mathbf{H}_k s_k s_k^T \mathbf{H}_k}{s_k^T \mathbf{H}_k s_k}}_{\text{momentum}}$$

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

BFGS (if time)

parallelization