Lecture Notes for

# Machine Learning in Python

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## Optimization Techniques for Logistic Regression

## Demo Lecture

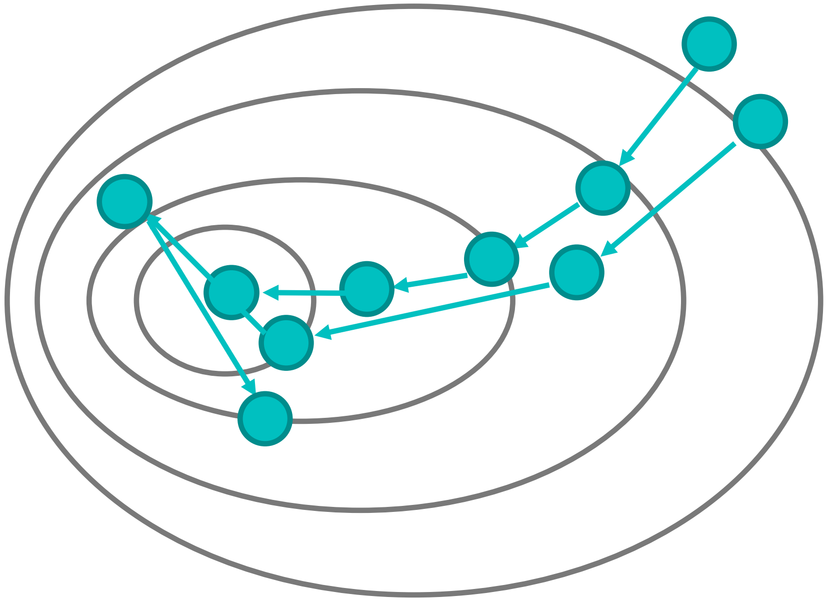
06. Optimization

## Optimization: gradient descent

- What we know thus far:

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

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

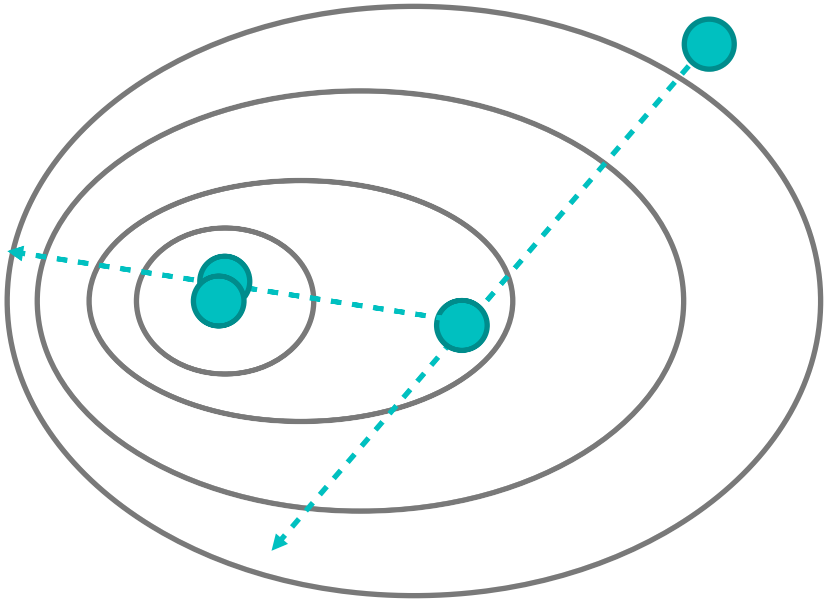


## Line Search: a better method

- Line search in direction of gradient:

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

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



## 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 + 1 add/subtract

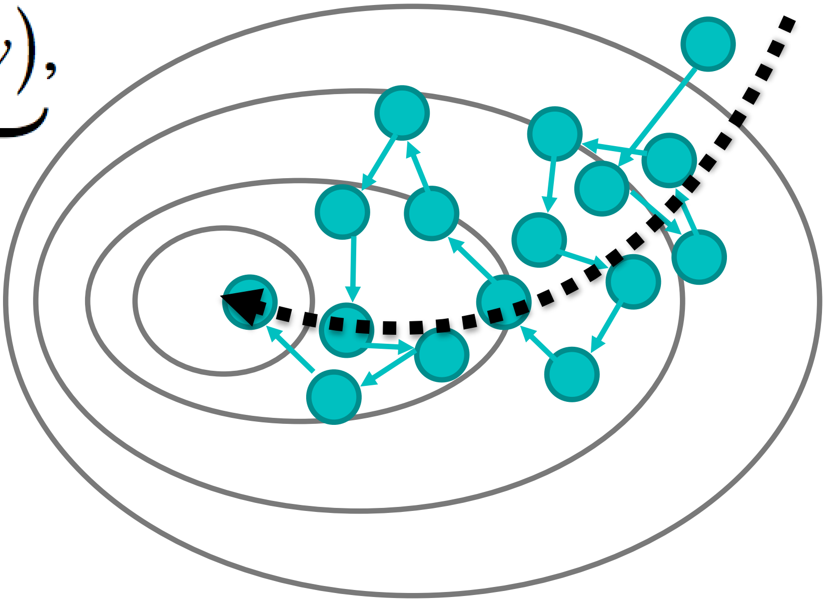
$$w \leftarrow w + \eta \underbrace{\left((y^{(i)} - \hat{y}^{(i)})x^{(i)} - 2C \cdot w\right)}_{\text{approx. gradient}},$$

$i$ chosen at random

**Per iteration:**

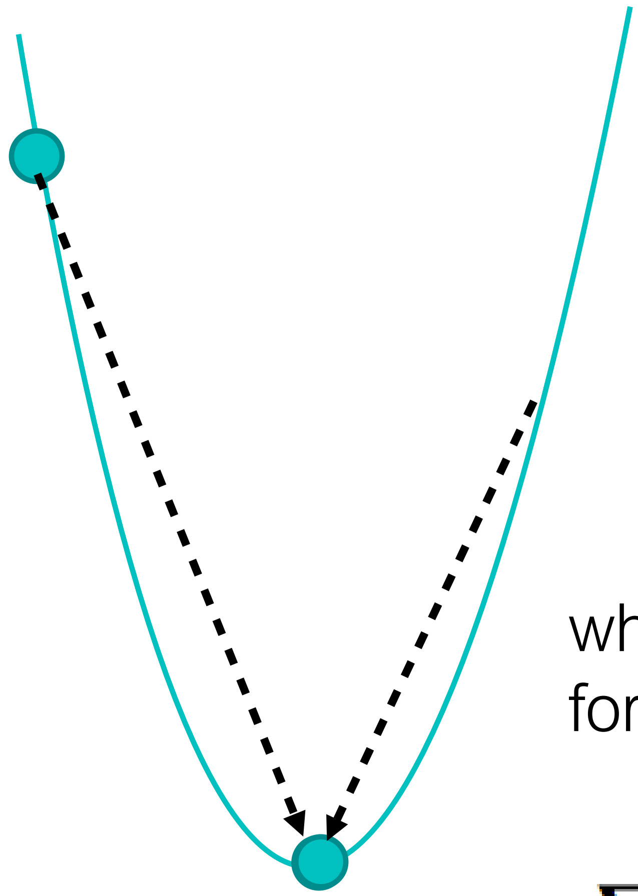
N+1 multiplications

2 add/subtract



## 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!

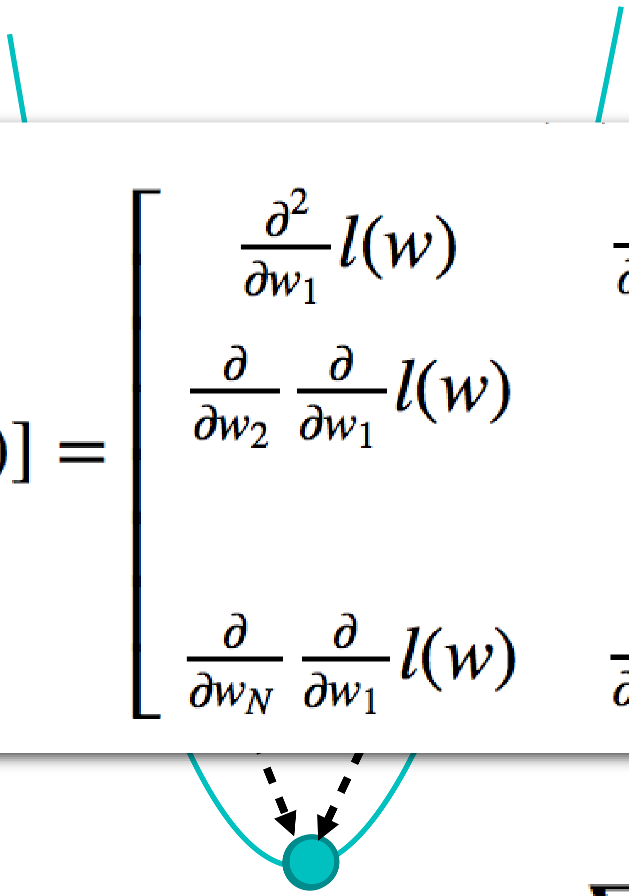
what is the second order derivative for a multivariate function?

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

# The Hessian

- Assume function is quadratic:

function of one variable:



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

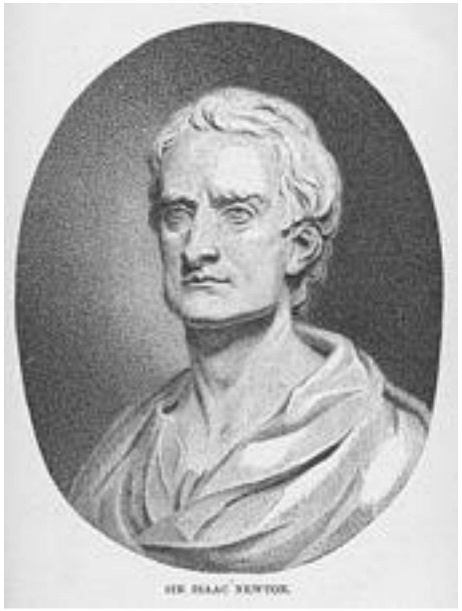
$$\nabla^2 l(w) = \mathbf{H}[l(w)]$$

# The Newton Update Method

- Assume function is quadratic (in high dimensions):

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

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



Is. Newton

# The Hessian for Logistic Regression

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

$$\begin{tikzcd}
& w \leftarrow w + \eta \cdot \underbrace{\mathbf{H}[l(w)]^{-1}}_{\text{inverse Hessian}} \cdot \underbrace{\nabla l(w)}_{\text{gradient}} \arrow[dl] \arrow[dr] & \\
\mathbf{H}_{j,k}[l(w)] = -\sum_{i=1}^{M} g(x^{(i)})(1 - g(x^{(i)})x_k{}^{(i)} x_j{}^{(i)} \arrow[d] & & \underbrace{\sum_{i=1}^{M} (y^{(i)} - \hat{y}^{(i)})x_j^{(i)}}_{\text{gradient}} \arrow[d] \\
\mathbf{H}[l(w)] = X^T \cdot \text{diag}[g(x^{(i)})(1 - g(x^{(i)}))] \cdot X \arrow[dr] & & X * y_{diff} \arrow[dl] \\
& w \leftarrow w + \eta[X^T \cdot \text{diag}[g(x^{(i)})(1 - g(x^{(i)}))] \cdot X]^{-1} \cdot X * y_{diff} &
\end{tikzcd}$$