Optimization

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Outline of the lecture

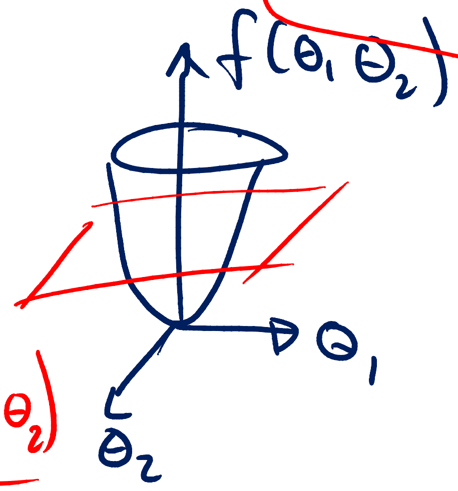
Many machine learning problems can be cast as optimization problems. This lecture introduces optimization. The objective is for you to learn:

- ❑ The definitions of gradient and Hessian.
- ❑ The gradient descent algorithm.
- ❑ Newton's algorithm.
- ❑ Stochastic gradient descent (SGD) for online learning.
- ❑ Popular variants, such as AdaGrad and Asynchronous SGD.
- ❑ Improvements such as momentum and Polyak averaging.
- ❑ How to apply all these algorithms to linear regression.

Calculus background: Partial derivatives and gradient

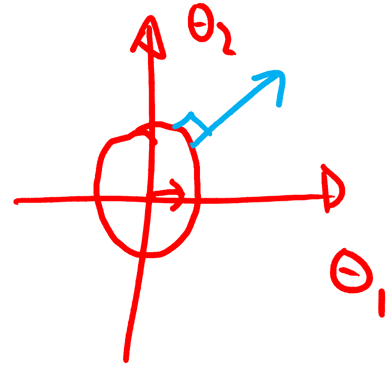
∇

$$f(\theta) = f(\theta_1, \theta_2) = \theta_1^2 + \theta_2^2$$



$$\frac{\partial f(\theta_1, \theta_2)}{\partial \theta_1} = \lim_{\Delta\theta_1 \to 0} \frac{f(\theta_1 + \Delta\theta_1, \theta_2) - f(\theta_1, \theta_2)}{\Delta\theta_1}$$

$$\frac{\partial f(\theta)}{\partial \theta_1} = \boxed{2\theta_1} \qquad \frac{\partial f(\theta)}{\partial \theta_2} = 2\theta_2$$



$$\nabla J(\theta) = \begin{bmatrix} 2\theta_1 \\ 2\theta_2 \end{bmatrix}$$

$$(\theta_1 = 1, \theta_2 = 1)$$

$$\nabla J(\theta_1, \theta_2) = (2, 2)$$

Necessary calculus background: Hessian

$$\frac{\partial}{\partial \theta_1}\left(\frac{\partial f(\theta)}{\partial \theta_1}\right) = \frac{\partial^2 f(\theta)}{\partial \theta_1^2} = 2$$

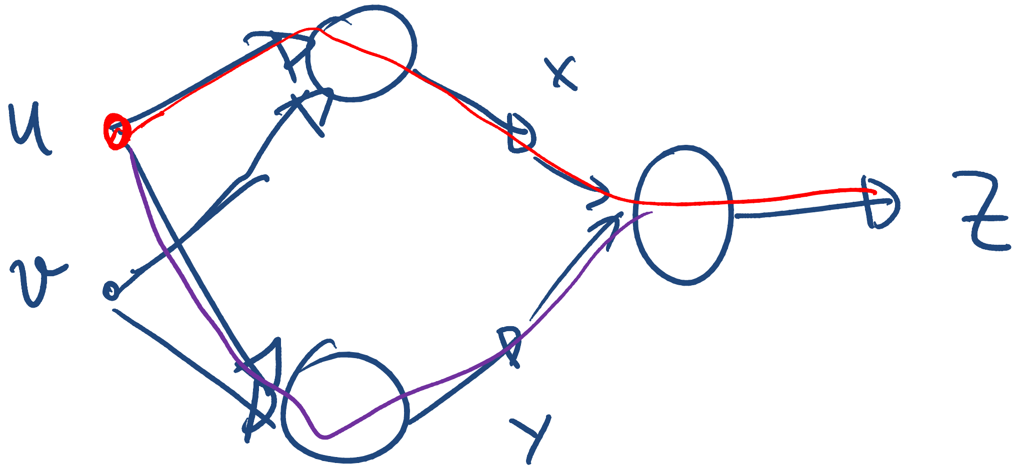
$$\frac{\partial^2 f(\theta)}{\partial \theta_2^2} = 2$$

$$H = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

$$\frac{\partial^2 f(\theta)}{\partial \theta_1 \partial \theta_2} = \frac{\partial^2 f(\theta)}{\partial \theta_2 \partial \theta_1} = 0$$

Necessary calculus background: Chain rule

$$z = f(x(u,v), y(u,v))$$



$$\frac{\partial z}{\partial u} = \frac{\partial z}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial z}{\partial y}\frac{\partial y}{\partial u}$$

Necessary calculus background: Linear regression

$$y_i = \theta_0 + \theta_1 x_i \qquad i = 1, 2, \ldots, n$$

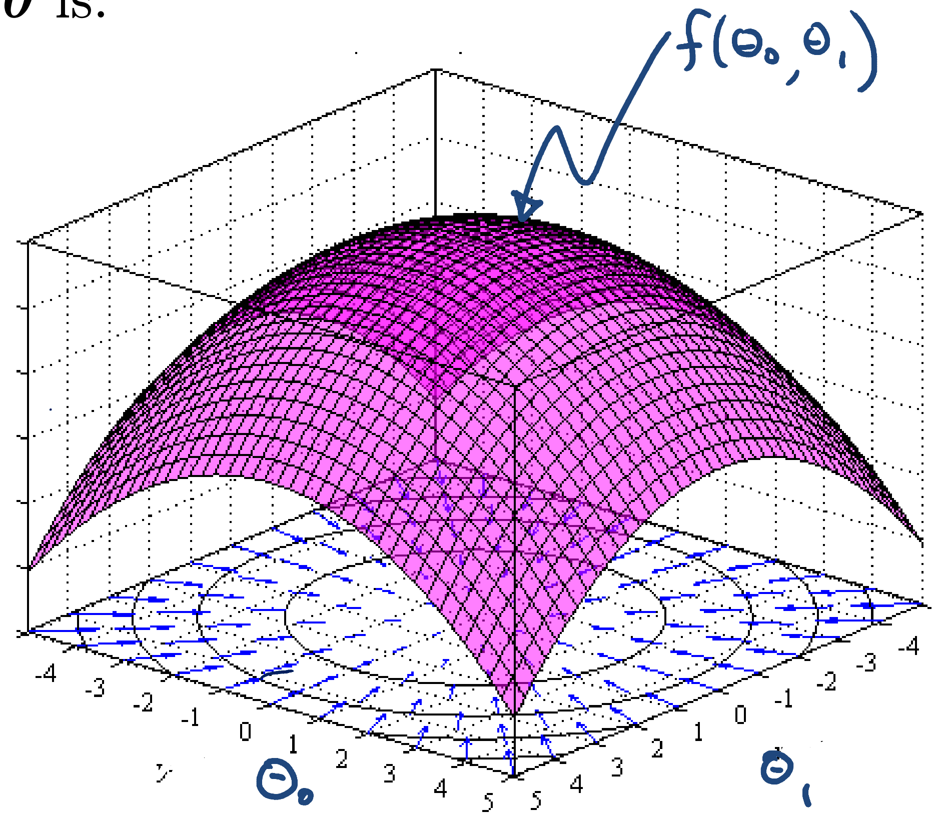
$$\boxed{J(\underline{\theta}) = \sum_{i=1}^{n} \left(y_i - \theta_0 - \theta_1 x_i\right)^2 + \delta^2 \theta_1^2}$$

$$\nabla J = \begin{bmatrix} \sum_{i=1}^{n} 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-1) \\ \sum_{i=1}^{n} 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-x_i) + 2\delta^2 \theta_1 \end{bmatrix}$$

Gradient vector

Let $\boldsymbol{\theta}$ be an d-dimensional vector and $f(\boldsymbol{\theta})$ a scalar-valued function. The gradient vector of $f(\cdot)$ with respect to $\boldsymbol{\theta}$ is:

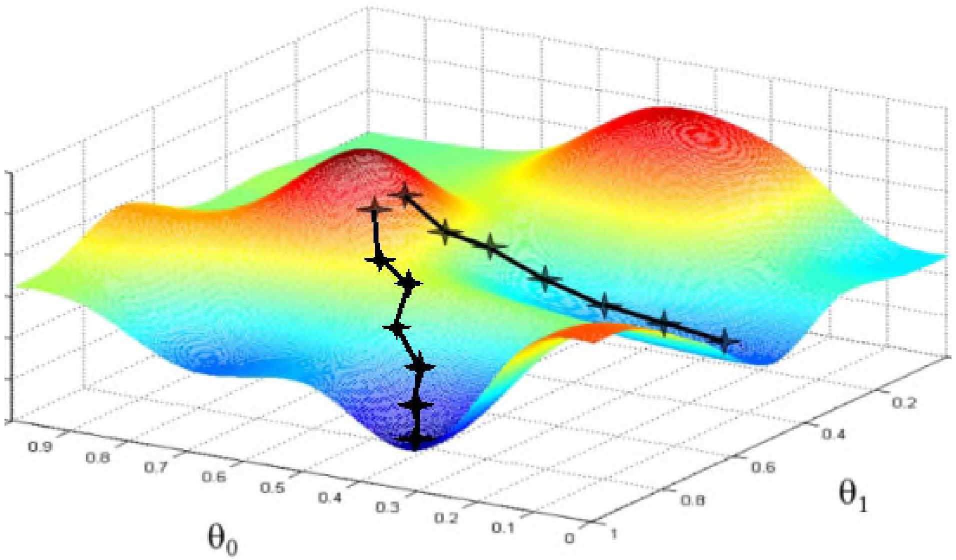
$$\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial f(\boldsymbol{\theta})}{\partial \theta_1} \\ \frac{\partial f(\boldsymbol{\theta})}{\partial \theta_2} \\ \vdots \\ \frac{\partial f(\boldsymbol{\theta})}{\partial \theta_n} \end{bmatrix}$$



e.g.

$$f(\theta_0, \theta_1) = -\sum_{i=1}^{n} \underline{(y_i - \underline{x}_i \underline{\theta})^2}$$

$$\underline{\theta} = (\theta_0, \theta_1)$$



Hessian matrix

The **Hessian** matrix of $f(\cdot)$ with respect to $\boldsymbol{\theta}$, written $\nabla^2_{\boldsymbol{\theta}} f(\boldsymbol{\theta})$ or simply as $\mathbf{H}$, is the $d \times d$ matrix of partial derivatives,

$$\nabla^2_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_1^2} & \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_1 \partial \theta_n} \\ \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_2^2} & \cdots & \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_2 \partial \theta_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_d \partial \theta_1} & \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_d \partial \theta_2} & \cdots & \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_d^2} \end{bmatrix}$$

In **offline** learning, we have a **batch** of data $\mathbf{x}_{1:n} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$. We typically optimize cost functions of the form

$$\boxed{f(\boldsymbol{\theta}) = f(\boldsymbol{\theta}, \mathbf{x}_{1:n}) = \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{\theta}, \mathbf{x}_i)} \approx \int f(\theta, x) p(x) dx$$

The corresponding gradient is

$$g(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) = \boxed{\frac{1}{n}\sum_{i=1}^{n} \underbrace{\nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}, \mathbf{x}_i)}}$$

For linear regression with training data $\{\mathbf{x}_i, y_i\}_{i=1}^{n}$, we have have the quadratic cost

$$f(\boldsymbol{\theta}) = f(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = \underbrace{(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})} = \underbrace{\sum_{i=1}^{n}(y_i - \mathbf{x}_i\boldsymbol{\theta})^2}$$

Gradient vector and Hessian matrix

$$f(\boldsymbol{\theta}) = f(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) = \sum_{i=1}^{n} (y_i - \mathbf{x}_i\boldsymbol{\theta})^2$$

$$\nabla f(\theta) = \frac{\partial}{\partial \theta}\left(y^T y - 2y^T X\theta + \theta^T X^T X \theta \right)$$

$$= -2X^T y + 2X^T X \theta$$

$$\nabla f(\theta) = -2\sum_{i=1}^{n} \underline{x}_i^T (y_i - \underline{x}_i \underline{\theta})$$

$$D^2 f(\theta) = 0 + 2X^T X$$

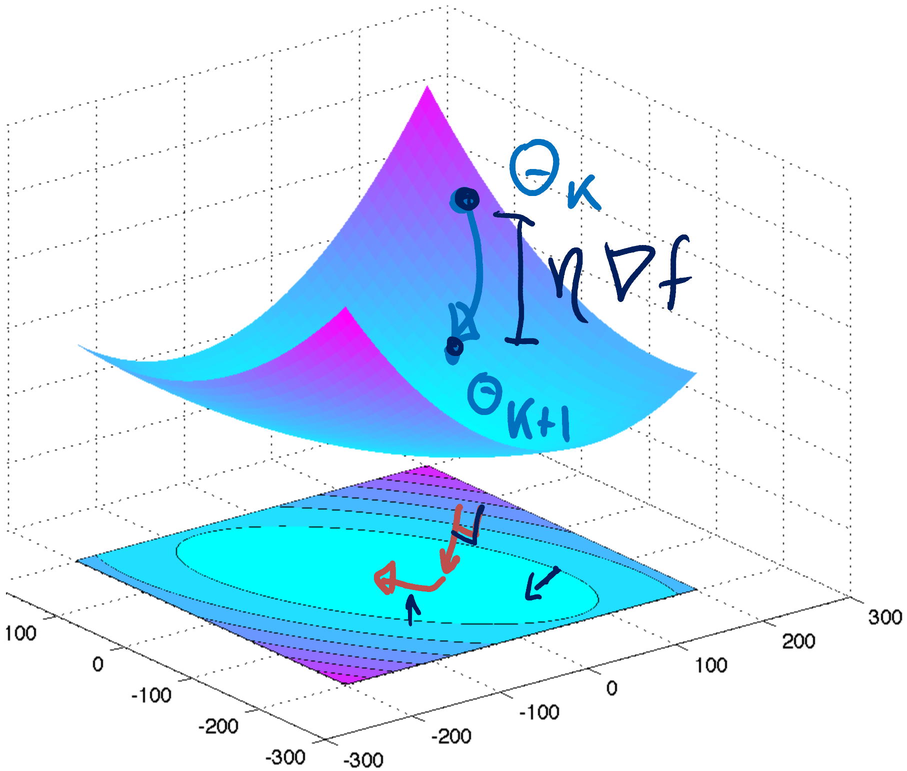
$$= 2\underset{d\times n}{X^T}\underset{n\times d}{X}$$

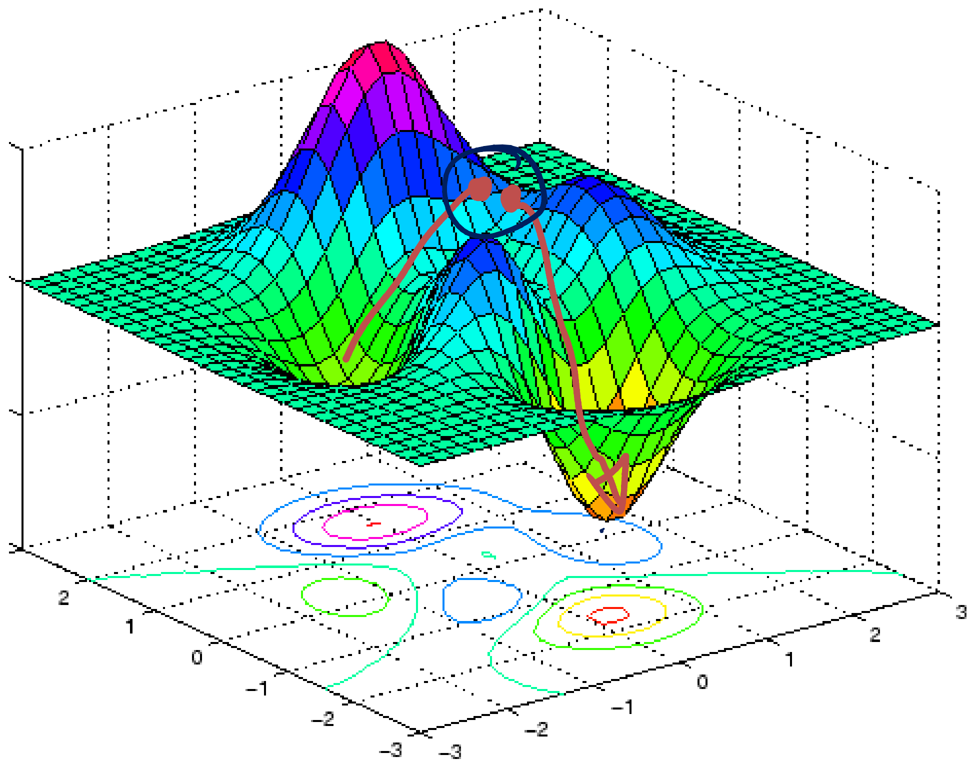
Steepest gradient descent algorithm

One of the simplest optimization algorithms is called **gradient descent** or **steepest descent**. This can be written as follows:

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta_k \mathbf{g}_k = \boldsymbol{\theta}_k - \eta_k \nabla f(\boldsymbol{\theta}_k)$$

where k indexes steps of the algorithm, $\mathbf{g}_k = \mathbf{g}(\boldsymbol{\theta}_k)$ is the gradient at step k, and $\eta_k > 0$ is called the **learning rate** or **step size**.





Steepest gradient descent algorithm for least squares

$$f(\boldsymbol{\theta}) = f(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) = \sum_{i=1}^{n}(y_i - \mathbf{x}_i\boldsymbol{\theta})^2$$

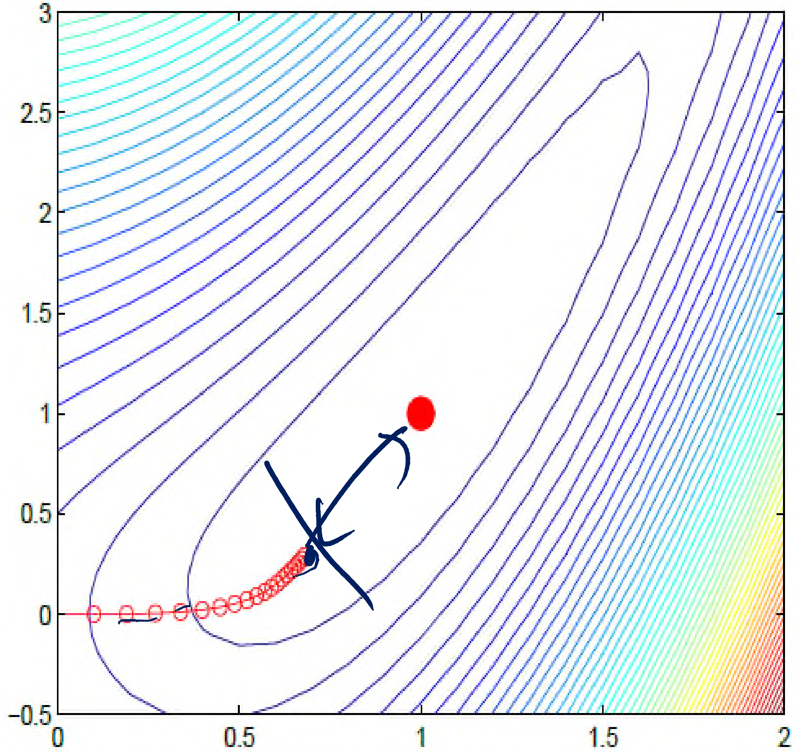
$$\nabla f(\theta) = -2X^T y + 2X^T X \theta$$

$$\theta_{k+1} = \theta_k - \eta \left[-2X^T y + 2X^T X \theta_k \right]$$

$$\theta_{k+1} = \theta_k - \eta \left[-2 \sum_{i=1}^{n} x_i^T \underbrace{(y_i - x_i \theta_k)}_{\text{Fit}} \right]$$

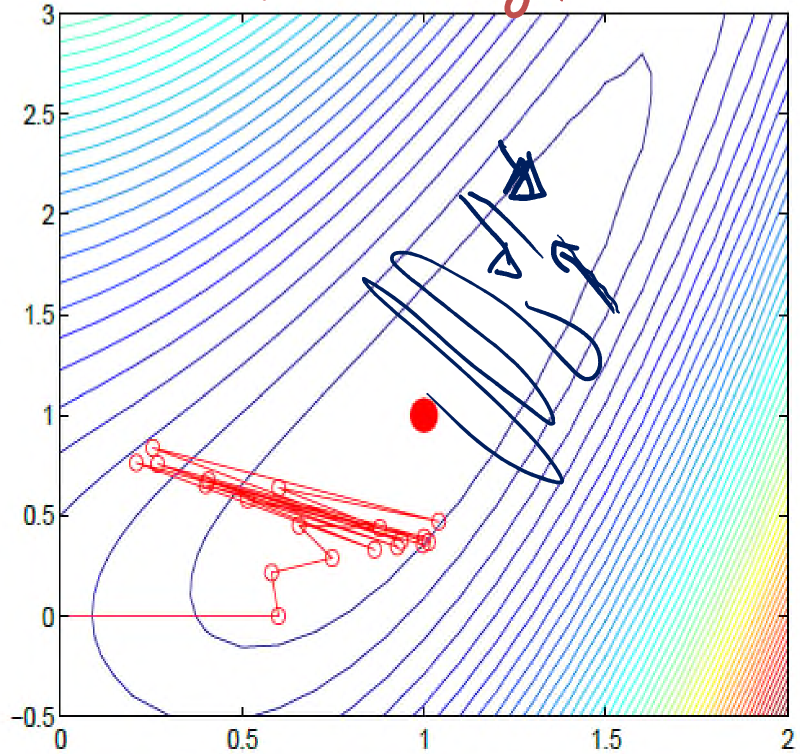
How to choose the step size ?

too small



$\eta = 0.1$

too large



$\eta = 0.6$

Newton's algorithm

The most basic second-order optimization algorithm is **Newton's algorithm**, which consists of updates of the form

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \overbrace{\mathbf{H}_K^{-1}\mathbf{g}_k}^{d_k}$$

This algorithm is derived by making a second-order Taylor series approximation of $f(\boldsymbol{\theta})$ around $\boldsymbol{\theta}_k$:

$$f_{quad}(\boldsymbol{\theta}) = f(\boldsymbol{\theta}_k) + \mathbf{g}_k^T(\boldsymbol{\theta} - \boldsymbol{\theta}_k) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_k)^T \mathbf{H}_k (\boldsymbol{\theta} - \boldsymbol{\theta}_k)$$

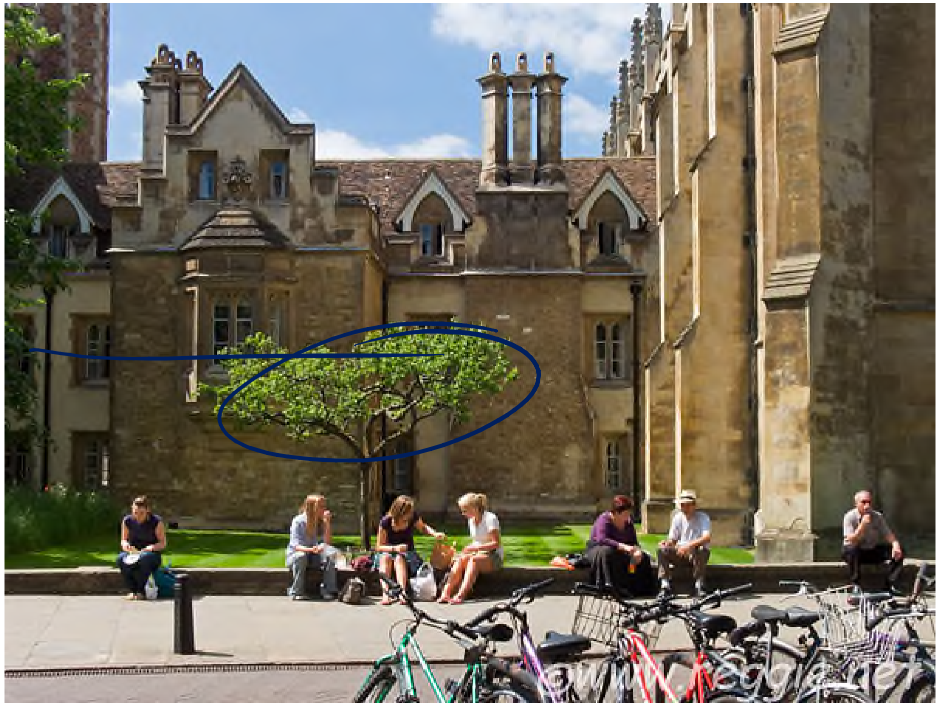
differentiating and equating to zero to solve for $\boldsymbol{\theta}_{k+1}$.

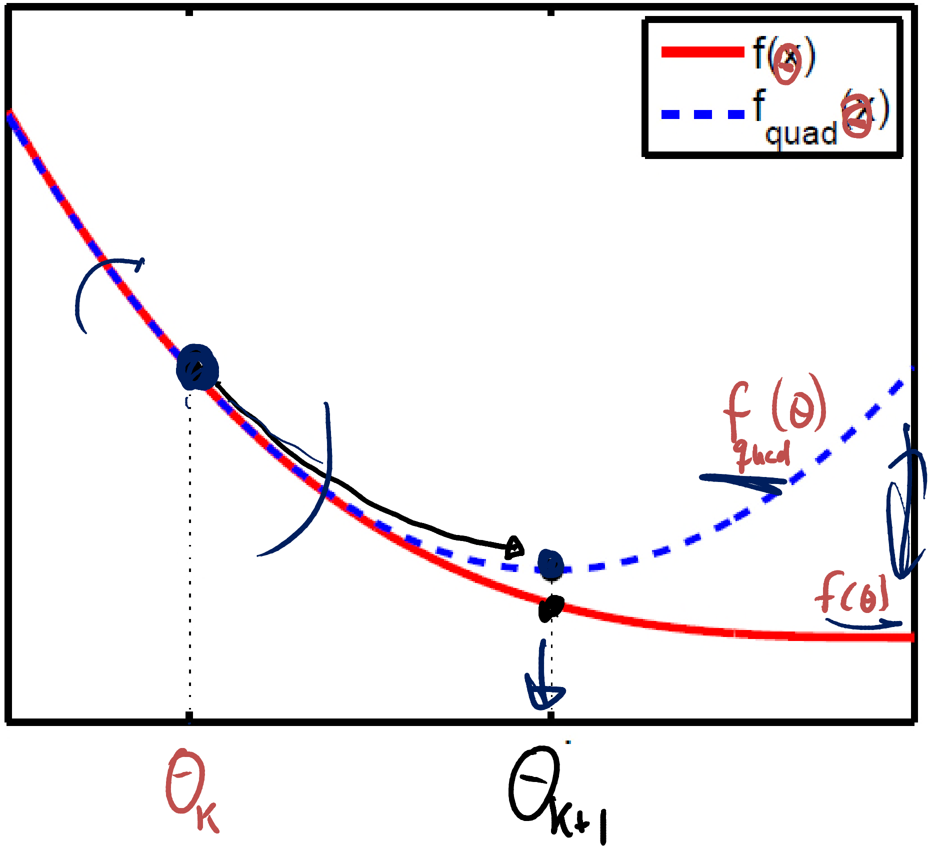
$$\nabla f_{quad}(\theta) = \cancel{0} + g_k + H_k(\theta - \theta_k) = 0$$

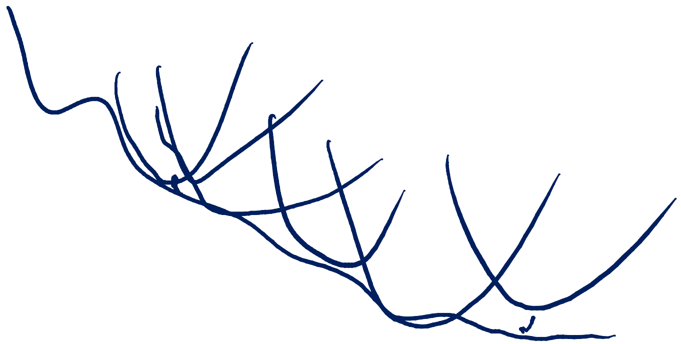
$$-g_k = H_k(\theta - \theta_k)$$

$$\boxed{\theta = \theta_k - H_k^{-1} g_k}$$

Newton as bound optimization





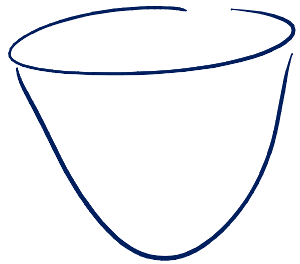


Newton's algorithm for linear regression

$$f(\boldsymbol{\theta}) = f(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) = \sum_{i=1}^{n}(y_i - \mathbf{x}_i\boldsymbol{\theta})^2$$

$g = \nabla f(\theta) = -2X^Ty + 2X^TX\theta$ ✓

$H = \nabla^2 f(\theta) = 2X^TX$ ✓



$$\theta_{k+1} = \theta_k - H_k^{-1} g_k$$

$$= \theta_k - (2X^TX)^{-1}\left[-2X^Ty + 2X^TX\theta_k\right]$$

$$= \cancel{\theta_k} + (X^TX)^{-1}X^Ty - \cancel{(X^TX)^{-1}X^TX\theta_k}$$

$$= (X^TX)^{-1}X^Ty$$

Advanced: Newton CG algorithm

Rather than computing $\mathbf{d}_k = -\mathbf{H}_k^{-1}\mathbf{g}_k$ directly, we can solve the linear system of equations $\mathbf{H}_k\mathbf{d}_k = -\mathbf{g}_k$ for $\mathbf{d}_k$.

One efficient and popular way to do this, especially if $\mathbf{H}$ is sparse, is to use a conjugate gradient method to solve the linear system.

Initialize $\boldsymbol{\theta}_0$

for $k = 1, 2, \ldots$ *until convergence* **do**

- Evaluate $\mathbf{g}_k = \nabla f(\boldsymbol{\theta}_k)$
- Evaluate $\mathbf{H}_k = \nabla^2 f(\boldsymbol{\theta}_k)$
- Solve $\mathbf{H}_k\mathbf{d}_k = -\mathbf{g}_k$ for $\mathbf{d}_k$
- Use line search to find stepsize η_k along $\mathbf{d}_k$
- $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k + \eta_k\mathbf{d}_k$

SGD

epoch

$$\nabla_\theta f(\theta) = \underbrace{\int \nabla_\theta f(x,\theta)\, p(x)\, dx}_{\mathbb{E}[\nabla f(x,\theta)]} \overset{\text{want}}{=} 0$$

$$\eta \times \mathbb{E}[\nabla f(x,\theta)] = 0 \times \eta = 0$$

$$\Theta + \eta\, \mathbb{E}[\nabla f(x,\theta)] = \Theta$$

$x^{(i)} \sim p(x)$

$$\Theta_{k+1} = \theta_k - \eta\, \mathbb{E}[\nabla f(x,\theta)]$$

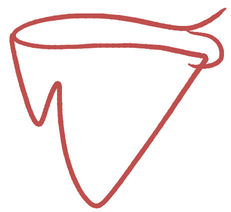
$$\approx \theta_k - \eta \frac{1}{n} \sum_{i=1}^{n} \nabla f(x^{(i)}, \theta_k)$$

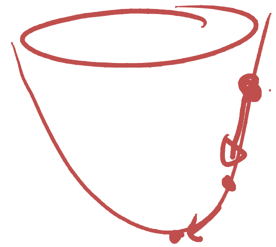
$$\approx \theta_k - \eta \nabla f(x^{(k)}, \theta_k)$$

$\alpha\ 1/k$

$$\theta_{k+1} = \cancel{\theta_k - \eta\, \mathbb{E}[\nabla f]} + \eta_k \underbrace{\left[\mathbb{E}[\nabla f] - \nabla f(x_k, \theta_k)\right]}_{\text{noise}}$$

Online learning with mini-batches





Batch

$$\theta_{k+1} = \theta_k + \eta \sum_{i=1}^{n} x_i^T (y_i - x_i \theta_t)$$

(n data points)

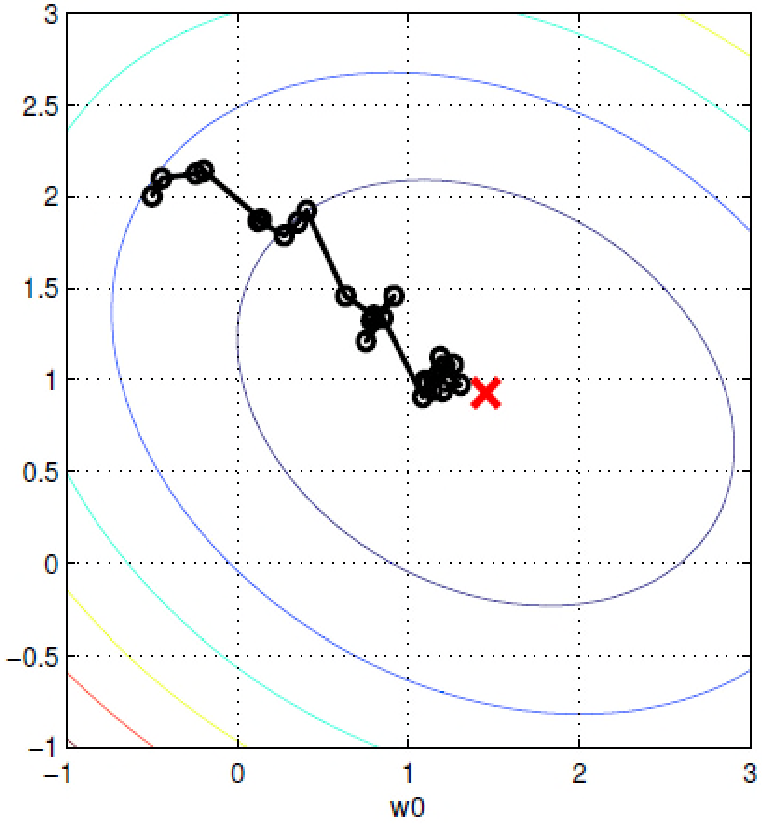
Online

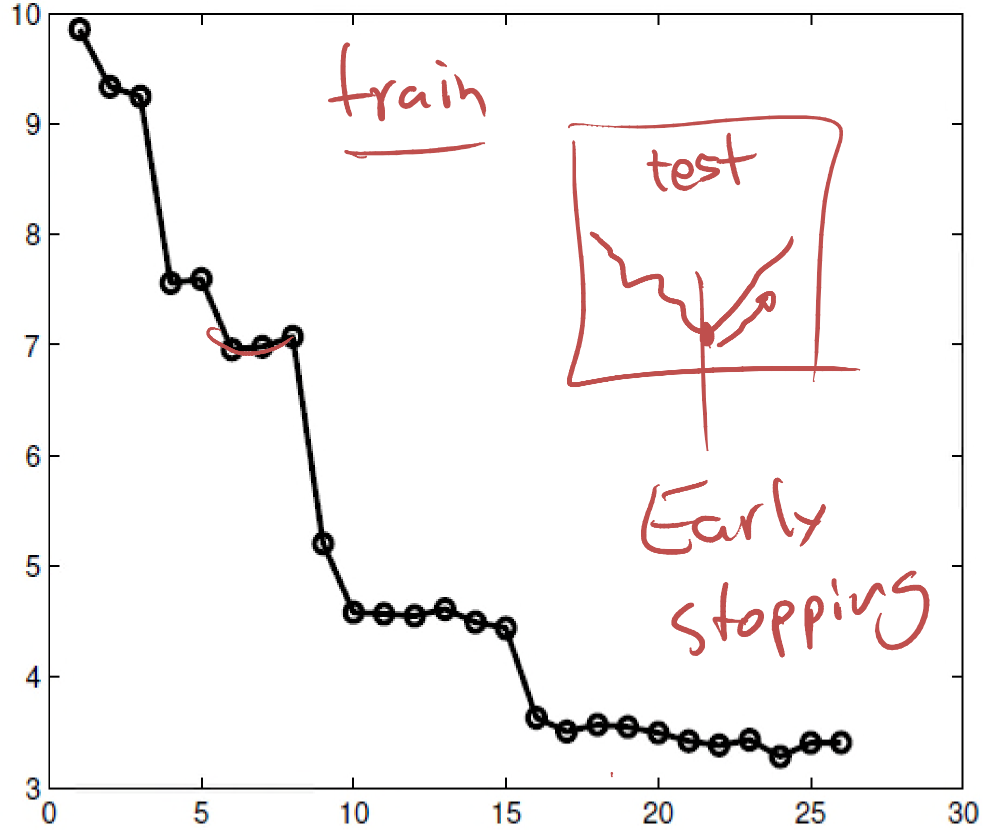
$$\theta_{k+1} = \theta_k + \eta\, x_k^T (y_k - x_k \theta_k)$$

mini-batch

$$\theta_{k+1} = \theta_k + \eta \sum_{j=1}^{20} x_j^T (y_j - x_j \theta_k)$$

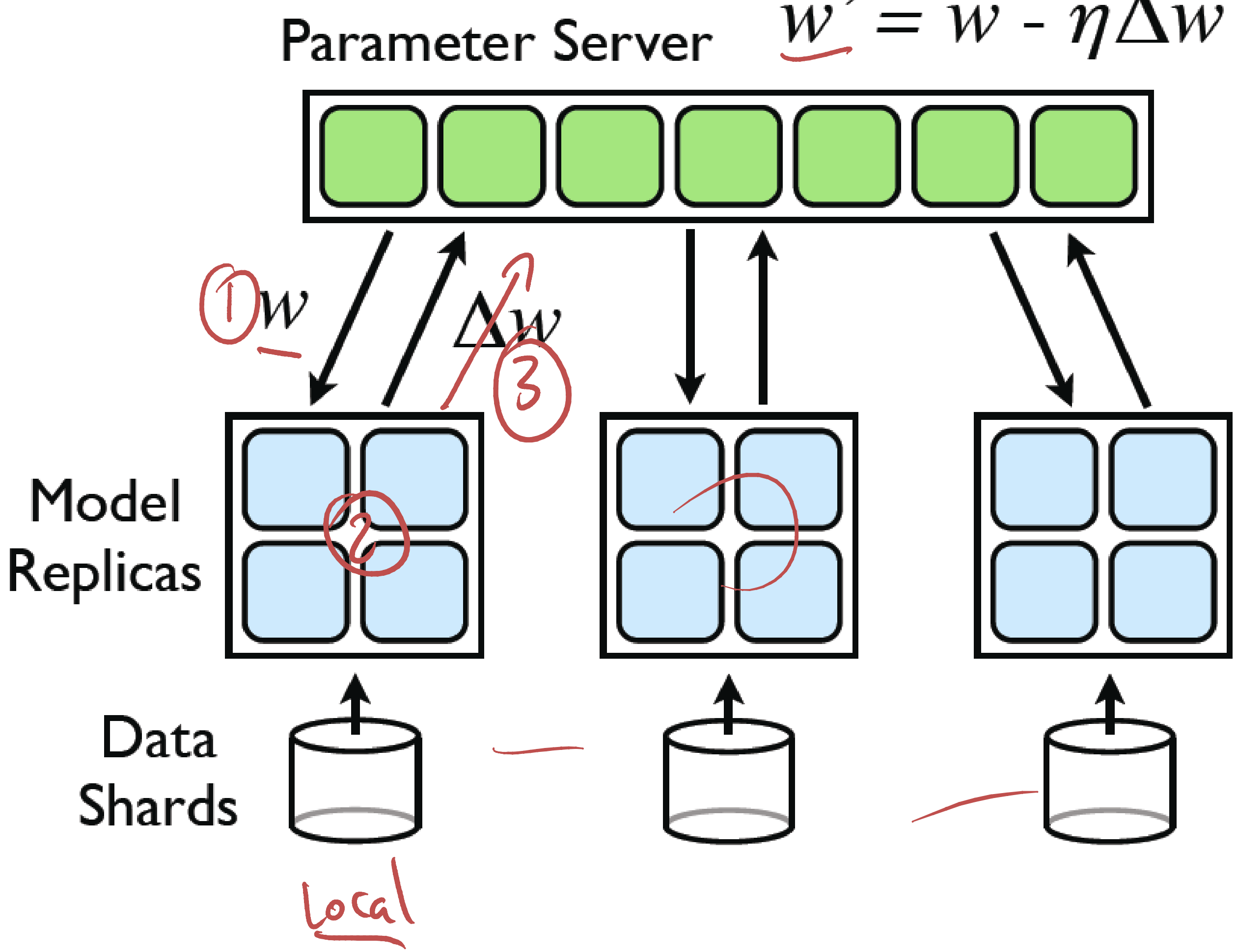
The online learning algorithm

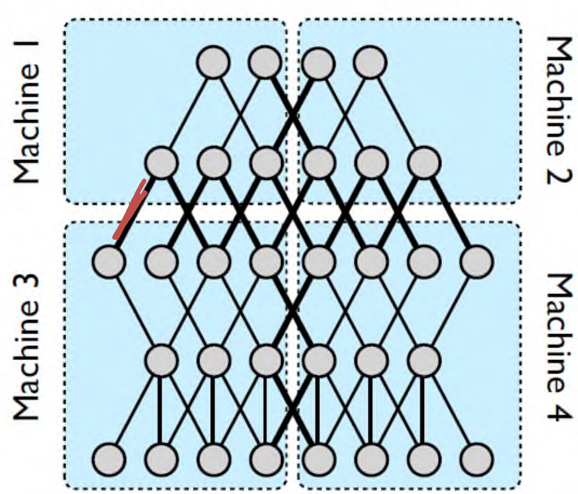




Downpour – Asynchronous SGD

$w' = w - \eta \Delta w$





[Jeff Dean et al.]

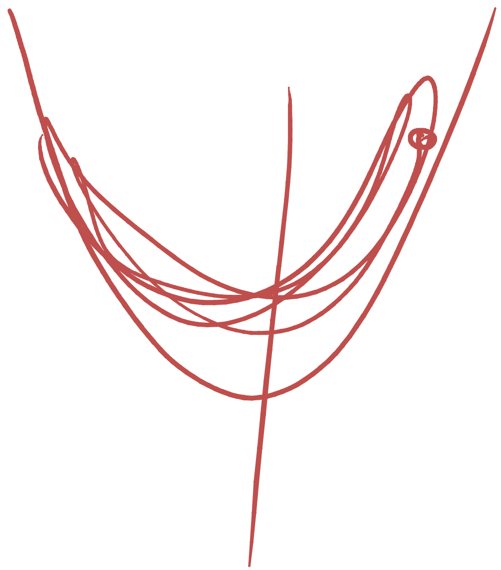
Polyak averaging

Polyak averaging (see papers of Mark Schmidt / Francis Bach)

$$\frac{1}{t+1}\sum_{i}^{t+1} w^{i} \rightarrow$$

$$\begin{aligned} W^{(t+1)} &= W^{(t)} - \gamma^{(t)} \nabla L(W^{(t)}, v^{(t)}) \\ \overline{W}^{(t+1)} &= \overline{W}^{(t)} - \frac{1}{t}(\overline{W}^{(t)} - W^{(t)}), \end{aligned}$$

See also predictive variance reduction (Tong Zhang, NIPS 2013)



Momentum

$$\underset{\Delta\theta_{t+1}}{\left[\theta_{t+1} - \theta_t\right]} = \alpha\underbrace{(\theta_t - \theta_{t-1})}_{\Delta\theta_t} + (1-\alpha)\left[-\eta\nabla J(\theta)\right]$$

Adagrad: Put more weight on rare features

y_t	$\phi_{t,1}$	$\phi_{t,2}$	$\phi_{t,3}$
1	1	0	0
-1	.5	0	1
1	-.5	1	0
-1	0	0	0
1	.5	0	0
-1	1	0	0
1	-1	1	0
-1	-.5	0	1

Text data:

The most unsung birthday in American business and technological history this year may be the 50th anniversary of the Xerox 914 photocopier.[a]

[a] *The Atlantic*, July/August 2010.

1. Frequent, irrelevant
2. Infrequent, predictive
3. Infrequent, predictive

gradient

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \frac{\eta}{\sqrt{\sum_{\tau=1}^{t} g_{\tau,i}^2}} g_{t,i}$$

[Duchi et al.]

Other useful optimization

- BFGS and limited-BFGS (Take e.g. Nick Trefethen's course)
- Nesterov's method (See Nesterov's book)
- Proximal methods (See Bertsekas book)
- Natural gradient (Yoshua Bengio et al – ICLR)
- Hessian-vector updates and automatic differentiation (Bishop's book and Nocedal & Wright)
- Convex optimization / constrained optimization (See Boy's book)

Next lecture

In the next lecture, we apply these ideas to learn a neural network with a single neuron (logistic regression).