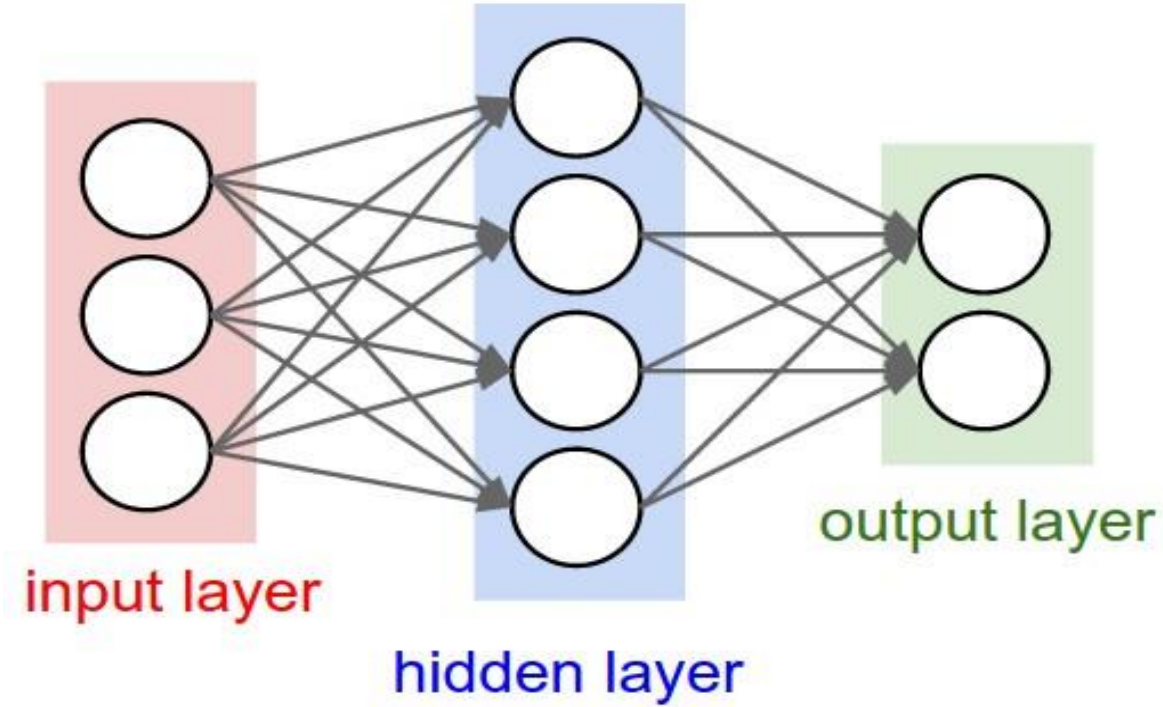
Scaling Optimization

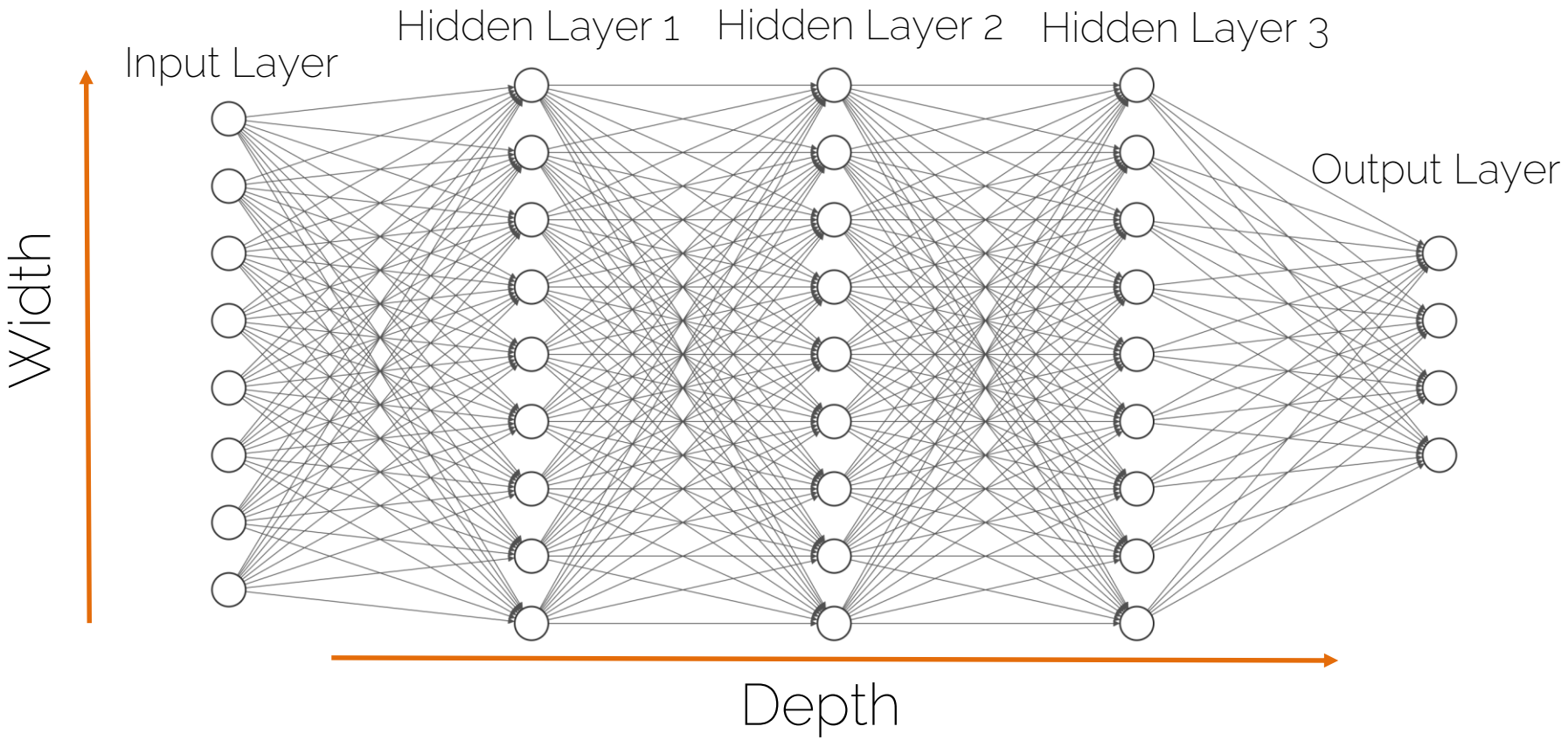
Lecture 4 Recap

Neural Network

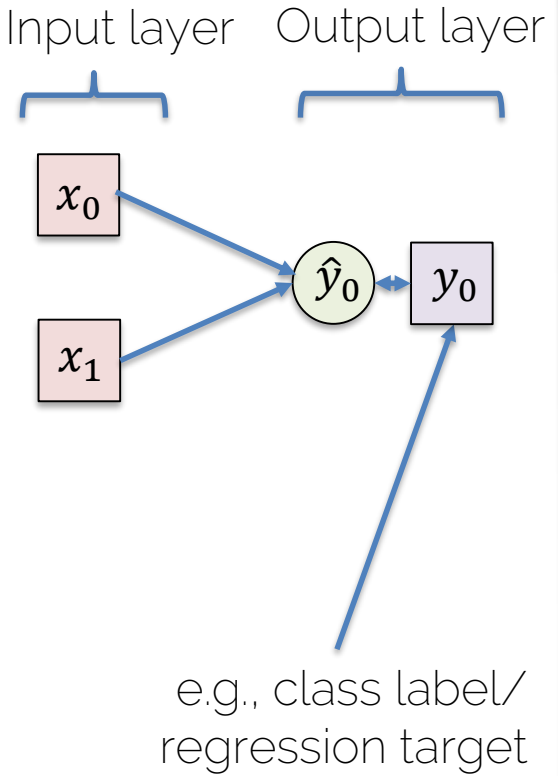


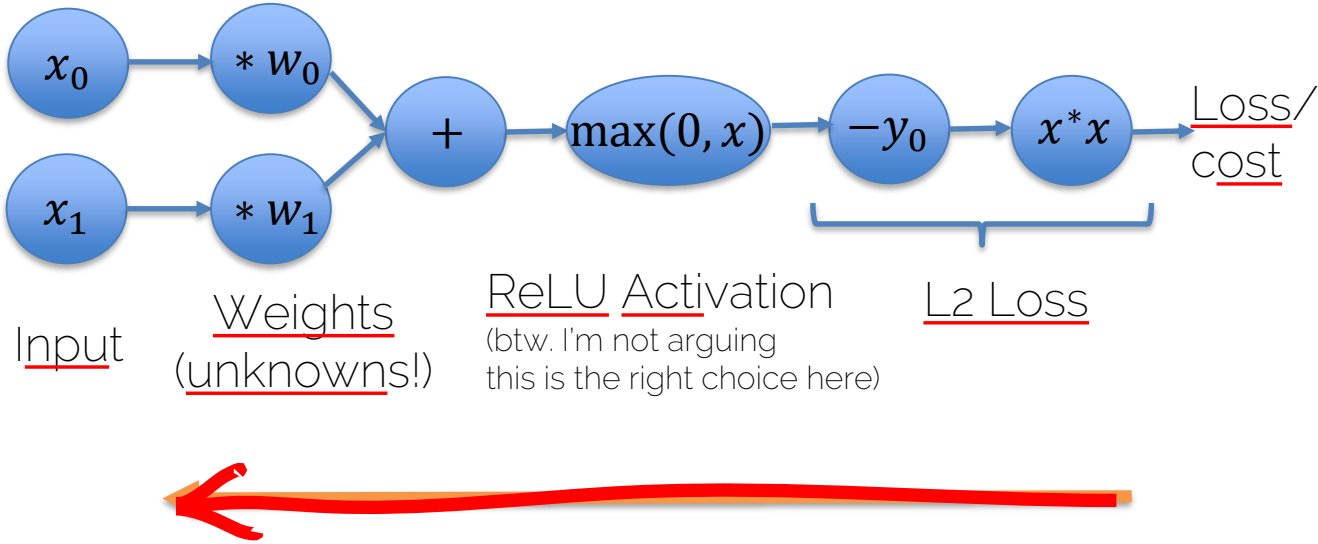
Source: http://cs231n.github.io/neural-networks-1/

Neural Network



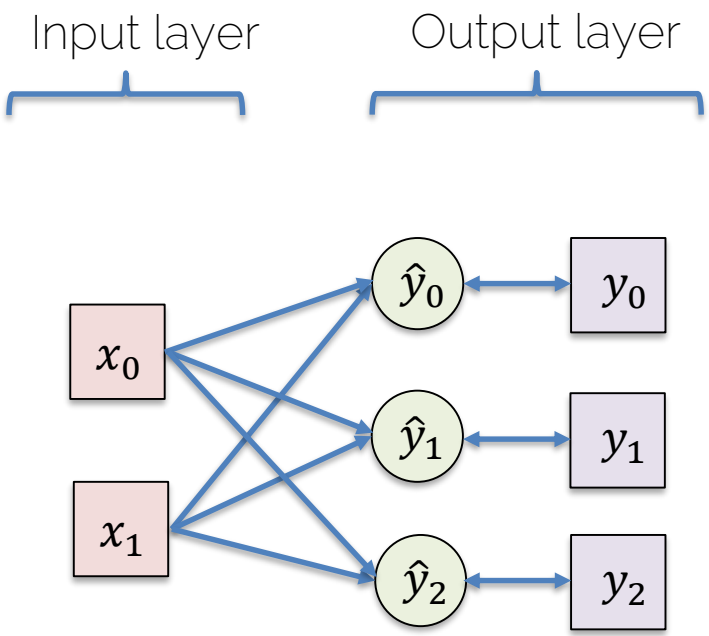
Compute Graphs → Neural Networks

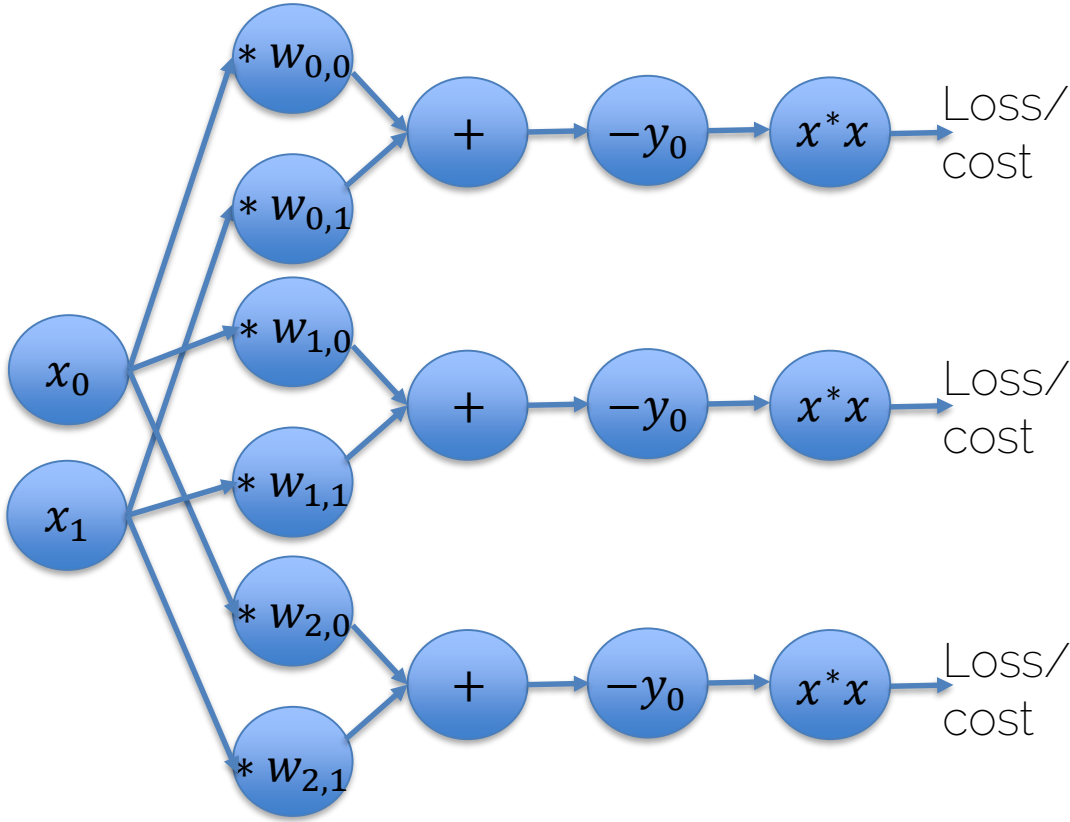




We want to compute gradients w.r.t. all weights $\boldsymbol{W}$

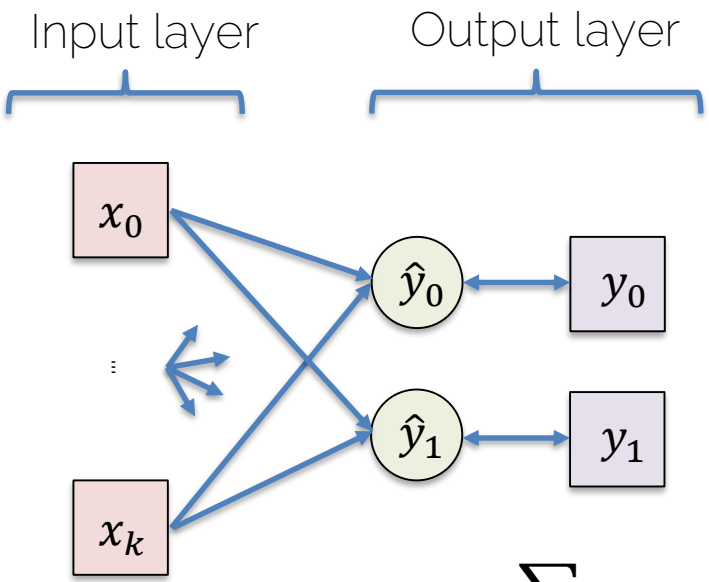
Compute Graphs → Neural Networks





We want to compute gradients w.r.t. all weights $\boldsymbol{W}$

Compute Graphs → Neural Networks



$$\hat{y}_i = A(b_i + \sum_k x_k w_{i,k})$$

Activation function

bias

Goal: We want to compute gradients of the loss function L w.r.t. all weights $\boldsymbol{w}$

$$L = \sum_i L_i$$

L: sum over loss per sample, e.g. L2 loss → simply sum up squares:

$$L_i = (\hat{y}_i - y_i)^2$$

→ use chain rule to compute partials

$$\frac{\partial L}{\partial w_{i,k}} = \frac{\partial L}{\partial \hat{y}_i} \cdot \frac{\partial \hat{y}_i}{\partial w_{i,k}}$$

NB

We want to compute gradients w.r.t. all weights $\boldsymbol{W}$ AND all biases $\boldsymbol{b}$

Summary

- We have
  - (Directional) compute graph
  - Structure graph into layers
  - Compute partial derivatives w.r.t. weights (unknowns)

$$\nabla_{\boldsymbol{W}} f_{\{\boldsymbol{x},\boldsymbol{y}\}}(\boldsymbol{W}) = \begin{bmatrix} \frac{\partial f}{\partial w_{0,0,0}} \\ \dots \\ \frac{\partial f}{\partial w_{l,m,n}} \\ \dots \\ \frac{\partial f}{\partial b_{l,m}} \end{bmatrix}$$

- Next
  - Find weights based on gradients

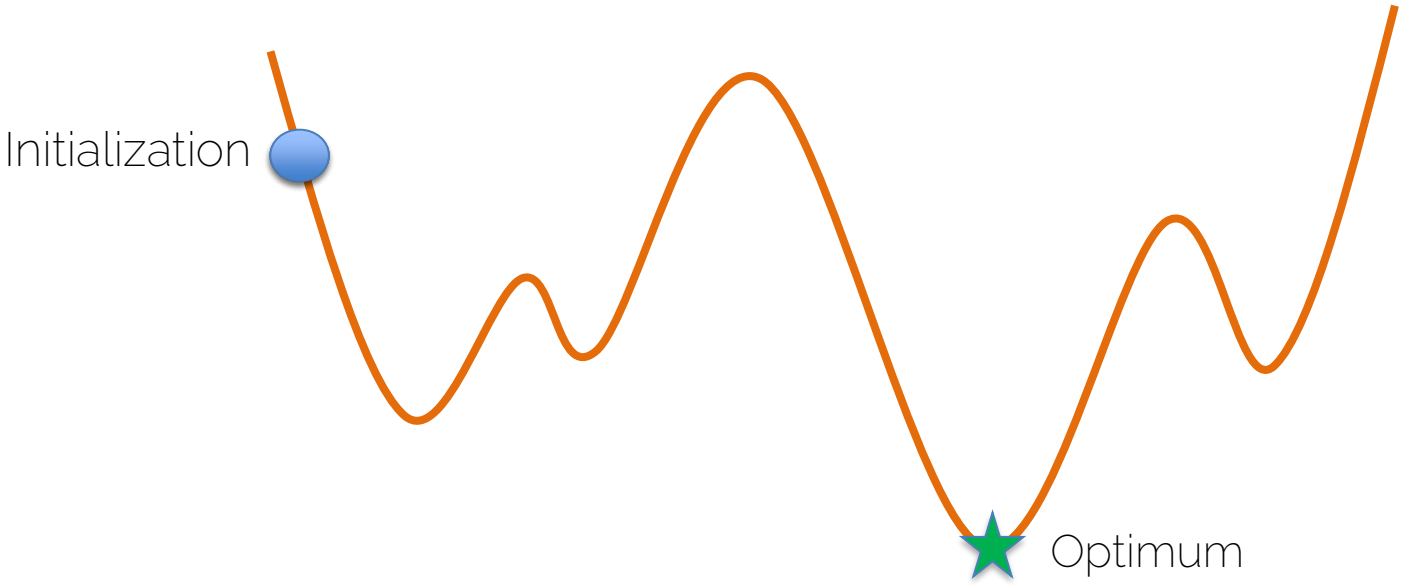
Gradient step:

$$\boldsymbol{W}' = \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} f_{\{\boldsymbol{x},\boldsymbol{y}\}}(\boldsymbol{W})$$

Optimization

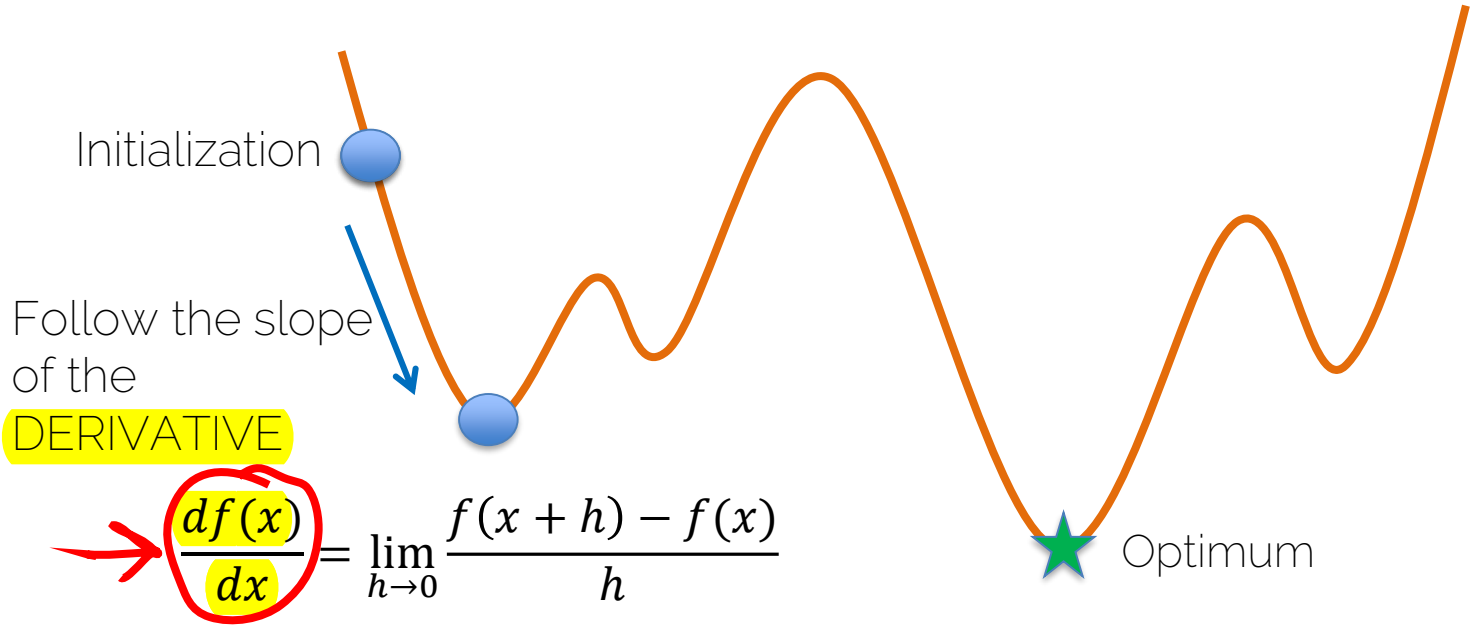
Gradient Descent

$$x^* = \arg\min f(x)$$



Gradient Descent

$$x^* = \arg\min f(x)$$



$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Understand

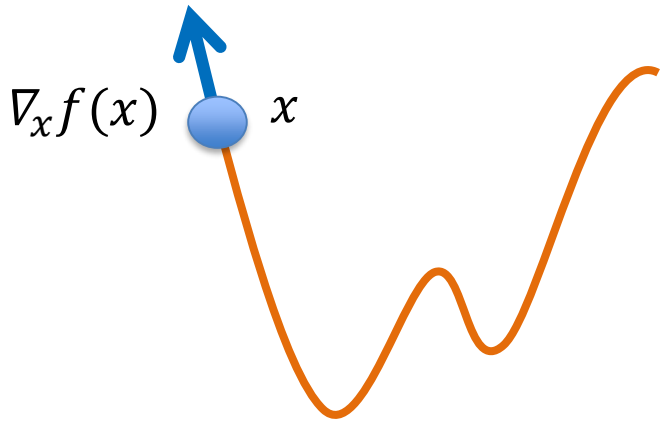
Gradient Descent

- From derivative to gradient

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} \longrightarrow \nabla_x f(x)$$

Direction of greatest increase of the function

- Gradient steps in direction of negative gradient



$$x' = x - \alpha \nabla_x f(x)$$

Learning rate

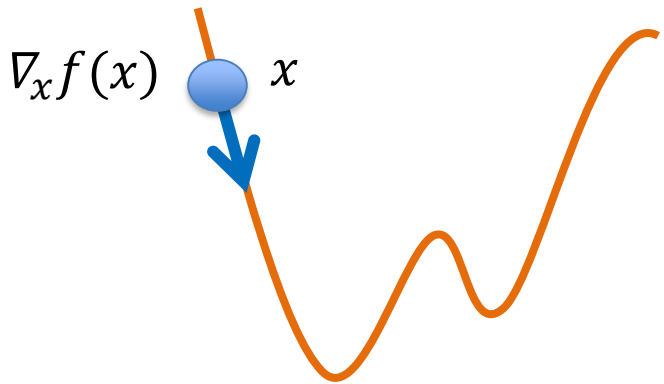
Gradient Descent

- From derivative to gradient

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} \longrightarrow \nabla_x f(x)$$

Direction of greatest increase of the function

- Gradient steps in direction of negative gradient



$$x' = x - \alpha \nabla_x f(x)$$

SMALL Learning rate

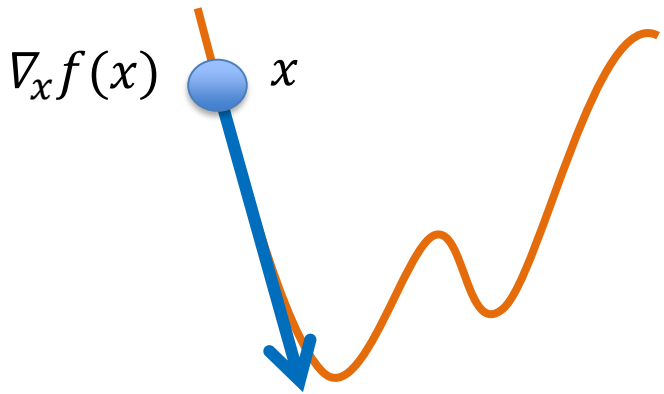
Gradient Descent

- From derivative to gradient

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} \longrightarrow \nabla_x f(x)$$

Direction of greatest increase of the function

- Gradient steps in direction of negative gradient

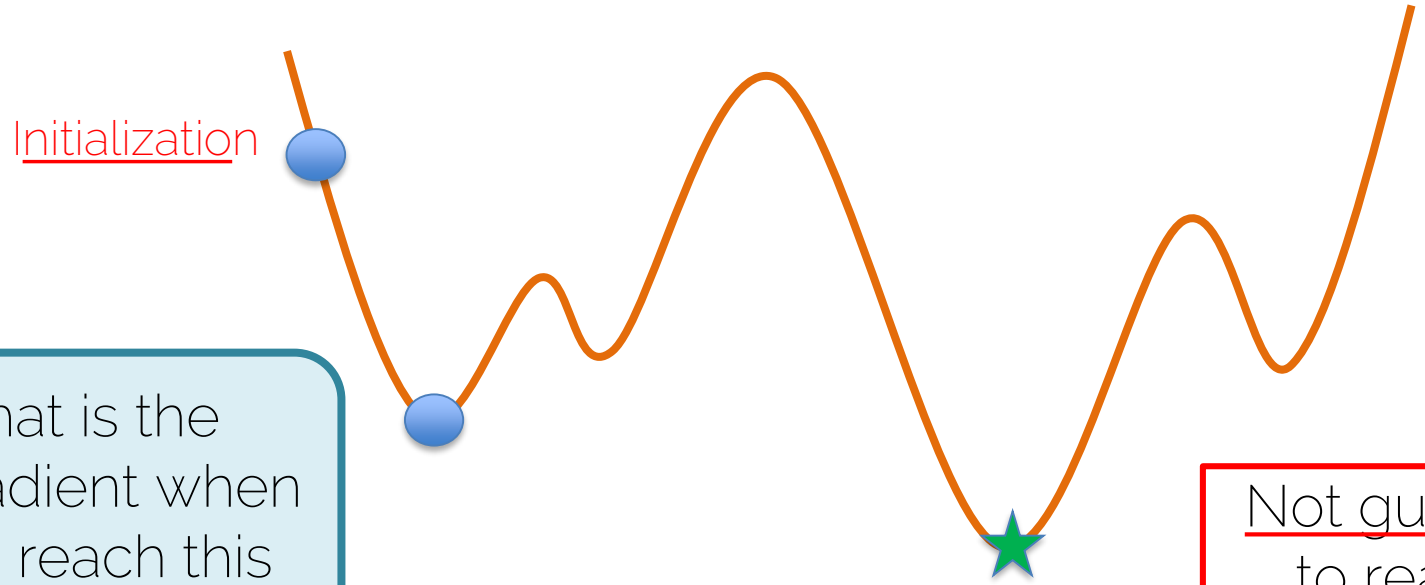


$$x' = x - \alpha \nabla_x f(x)$$

LARGE Learning rate

Gradient Descent

$$\boldsymbol{x}^* = \arg\min f(\boldsymbol{x})$$



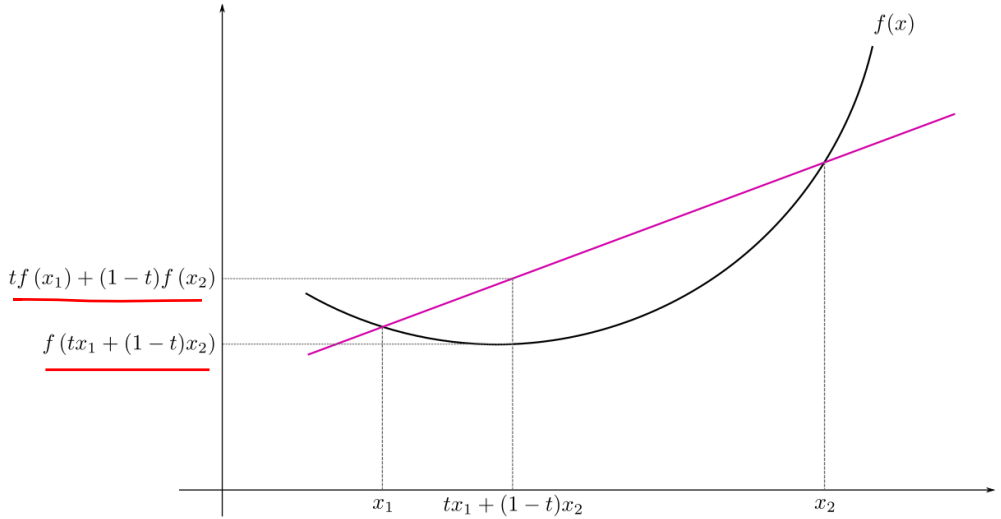
What is the gradient when we reach this point?

NB

Not guaranteed to reach the global optimum

Convergence of Gradient Descent

- Convex function: all local minima are global minima



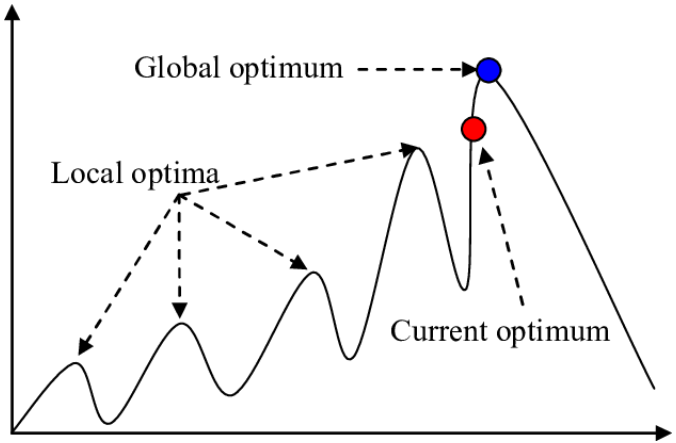
Source: https://en.wikipedia.org/wiki/Convex_function#/media/File:ConvexFunction.svg

If line/plane segment between any two points lies above or on the graph

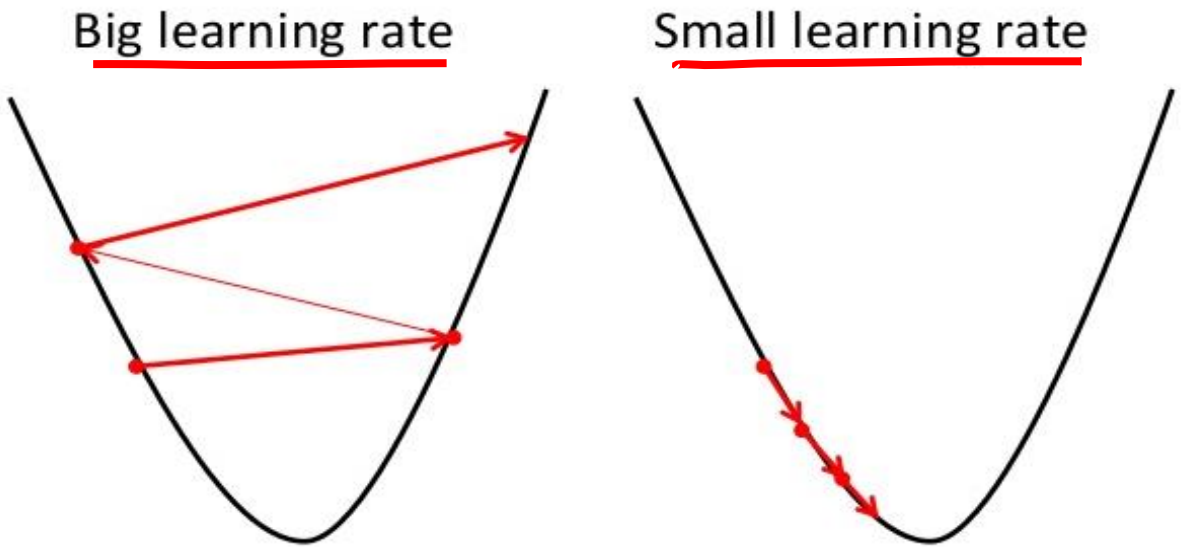
Understand

Neural networks are non-convex

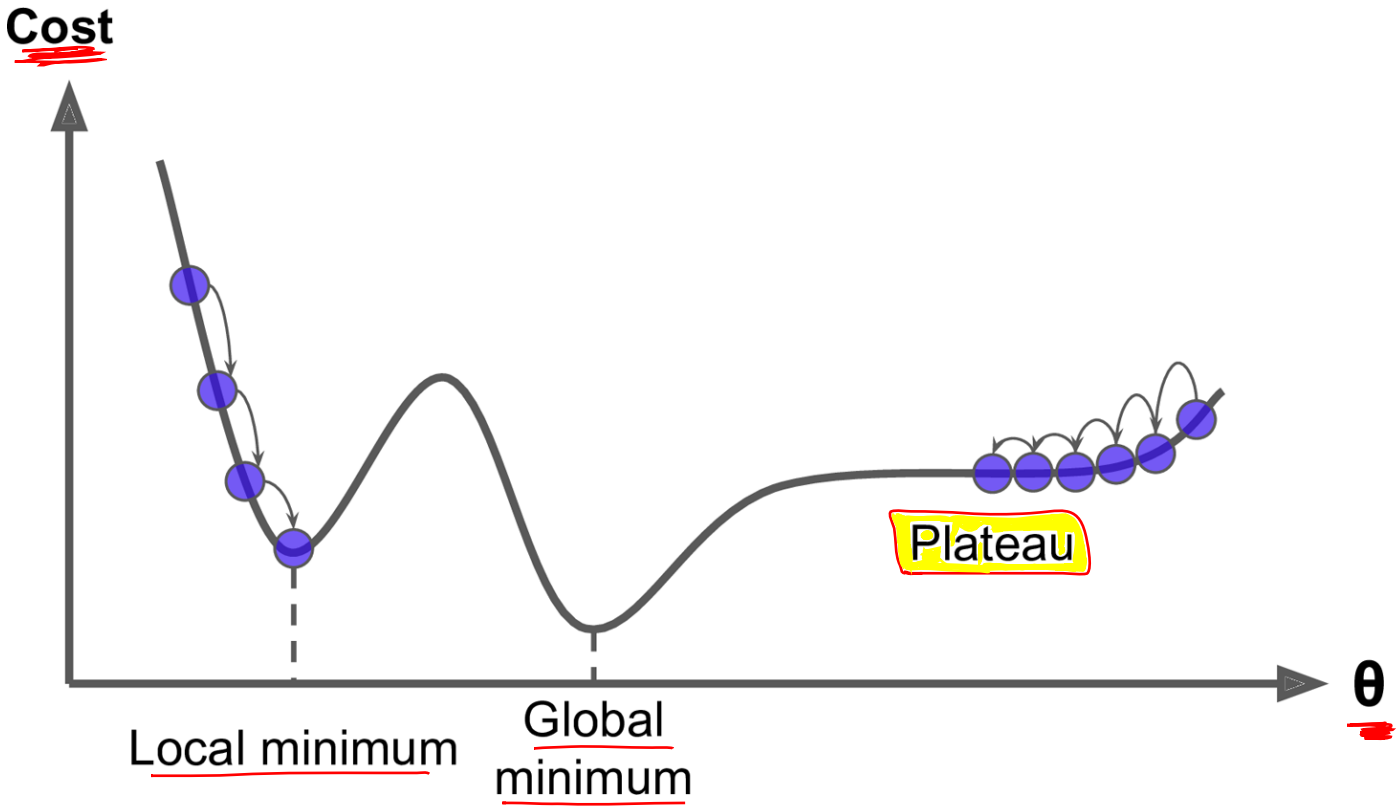
- many (different) local minima
- no (practical) way to say which is globally optimal



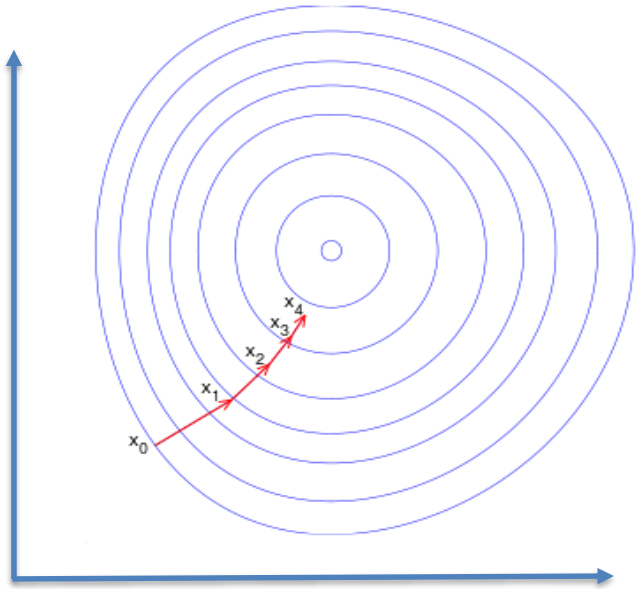
Source: Li, Qi. (2006). Challenging Registration of Geologic Image Data

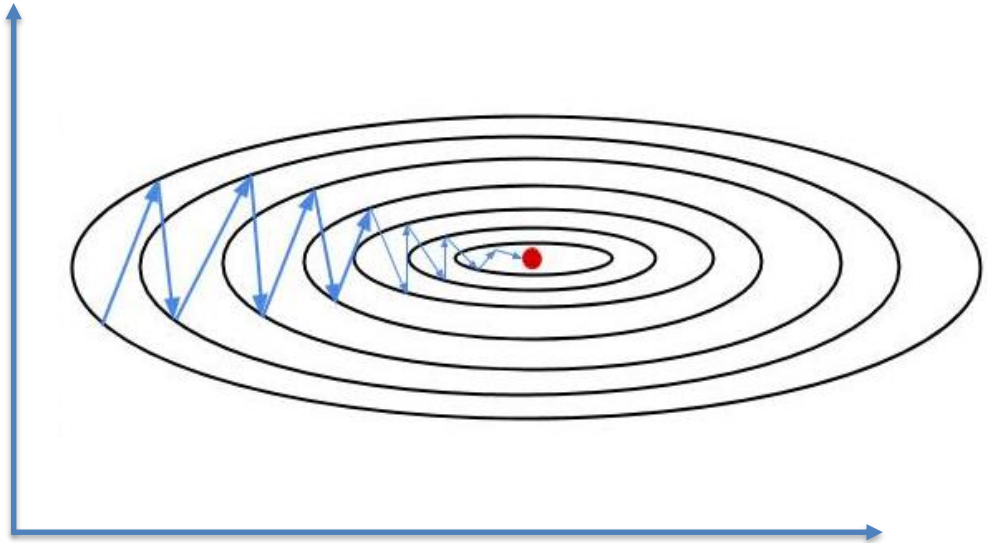


Source: https://builtin.com/data-science/gradient-descent


Cost
Plateau
θ
Local minimum
Global minimum

Gradient Descent: Multiple Dimensions



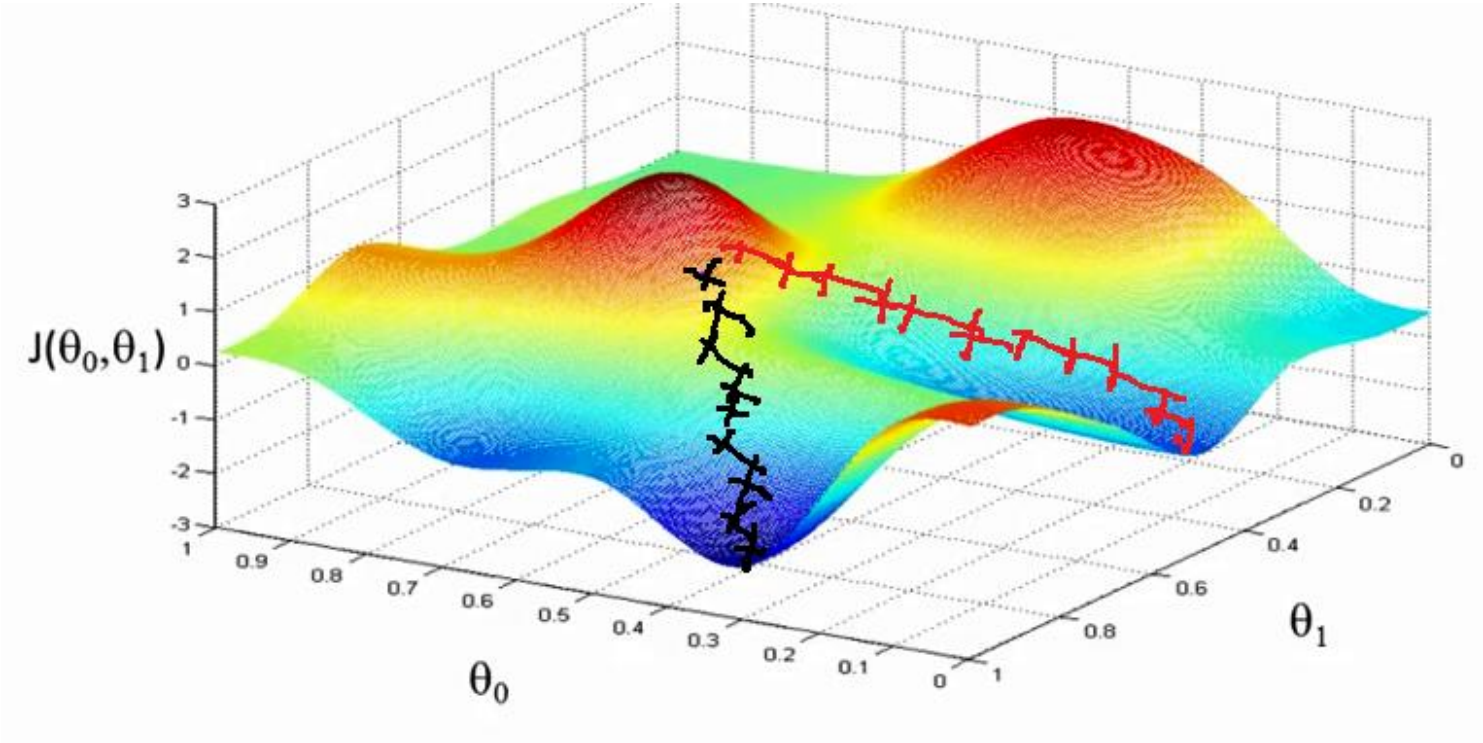


NB grad shall be orthogonal to isolines along the way

Source: builtin.com/data-science/gradient-descent

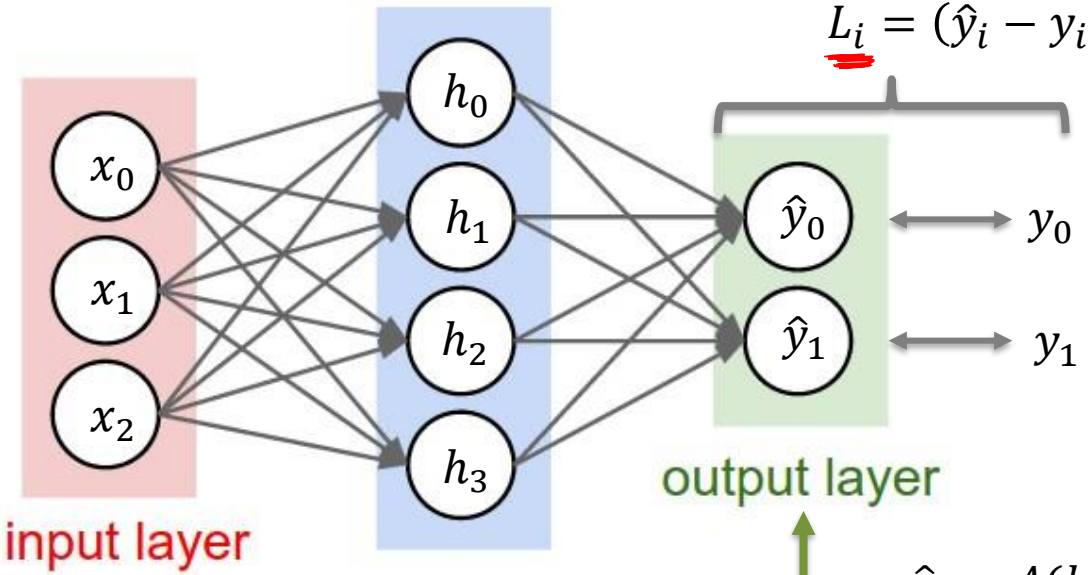
Various ways to visualize…

Gradient Descent: Multiple Dimensions



Source: http://blog.datumbox.com/wp-content/uploads/2013/10/gradient-descent.png

Gradient Descent for Neural Networks



Loss function

$$L_i = (\hat{y}_i - y_i)^2$$

$$\nabla_{\boldsymbol{W},\boldsymbol{b}} f_{\{\boldsymbol{x},\boldsymbol{y}\}}(\boldsymbol{W}) = \begin{bmatrix} \frac{\partial f}{\partial w_{0,0,0}} \\ \dots \\ \dots \\ \frac{\partial f}{\partial w_{l,m,n}} \\ \dots \\ \dots \\ \frac{\partial f}{\partial b_{l,m}} \end{bmatrix}$$

grad vec

$$\hat{y}_i = A(b_{1,i} + \sum_j h_j w_{1,i,j})$$

$$h_j = A(b_{0,j} + \sum_k x_k w_{0,j,k})$$

Just simple:

$$A(x) = \max(0, x)$$

Gradient Descent: Single Training Sample

- Given a loss function $\boldsymbol{L}$ and a single training sample $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}$
- Find best model parameters $\boldsymbol{\theta} = \{\boldsymbol{W}, \boldsymbol{b}\}$
- Cost $L_i(\boldsymbol{\theta}, \boldsymbol{x}_i, \boldsymbol{y}_i)$
  - $\boldsymbol{\theta} = \arg\min L_i(\boldsymbol{x}_i, \boldsymbol{y}_i)$
- Gradient Descent:
  - Initialize $\boldsymbol{\theta}^1$ with 'random' values (more to that later)
  - $\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \nabla_{\boldsymbol{\theta}} L_i(\boldsymbol{\theta}^k, \boldsymbol{x}_i, \boldsymbol{y}_i)$
  - Iterate until convergence: $\left|\boldsymbol{\theta}^{k+1} - \boldsymbol{\theta}^k\right| < \epsilon$

* Of course, it's less ideal to train simple sample!

Update step

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} - \alpha \nabla_{\boldsymbol{\theta}} L_i(\boldsymbol{\theta}^{k}, \boldsymbol{x}_i, \boldsymbol{y}_i)$$

- $\boldsymbol{\theta}^{k+1}$: Weights, biases after update step
- $\boldsymbol{\theta}^{k}$: Weights, biases at step k (current model)
- α: Learning rate
- $\nabla_{\boldsymbol{\theta}} L_i(\boldsymbol{\theta}^{k}, \boldsymbol{x}_i, \boldsymbol{y}_i)$: Gradient w.r.t. $\boldsymbol{\theta}$
- L_i: Loss Function
- $\boldsymbol{x}_i, \boldsymbol{y}_i$: Training sample

looping over all layers over all parameters

NB

- $\nabla_{\boldsymbol{\theta}} L_i(\boldsymbol{\theta}^{k}, \boldsymbol{x}_i, \boldsymbol{y}_i)$ computed via backpropagation
- Typically: $\dim\left(\nabla_{\boldsymbol{\theta}} L_i(\boldsymbol{\theta}^{k}, \boldsymbol{x}_i, \boldsymbol{y}_i)\right) = \dim(\boldsymbol{\theta}) \gg 1\ million$

Gradient Descent: Multiple Training Samples

- Given a loss function $\boldsymbol{L}$ and multiple ($\boldsymbol{n}$) training samples $\{\boldsymbol{x_i}, \boldsymbol{y_i}\}$
- Find best model parameters $\boldsymbol{\theta} = \{\boldsymbol{W}, \boldsymbol{b}\}$

- Cost $L = \frac{1}{n}\sum_{i=1}^{n} L_i(\boldsymbol{\theta}, \boldsymbol{x_i}, \boldsymbol{y_i})$
  - $\boldsymbol{\theta} = \arg\min L$

[Global Loss]

- Update step for multiple samples

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} - \alpha \nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^{k}, \boldsymbol{x}_{\{1..n\}}, \boldsymbol{y}_{\{1..n\}}\right)$$

- Gradient is average / sum over residuals

$$\nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^{k}, \boldsymbol{x}_{\{1..n\}}, \boldsymbol{y}_{\{1..n\}}\right) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{\theta}} L_i\left(\boldsymbol{\theta}^{k}, \boldsymbol{x}_i, \boldsymbol{y}_i\right)$$

Reminder: this comes from backprop.

Sum is over all training samples

NB

- Often people are lazy and just write: $\nabla L = \sum_{i=1}^{n} \nabla_{\boldsymbol{\theta}} L_i$
  - omitting $\frac{1}{n}$ is not 'wrong', it just means rescaling the learning rate

≠ An update step of the grad shall be repeated till convergence

Remember Side Note: Optimal Learning Rate

Can compute optimal learning rate α using Line Search (optimal for a given set)

1. Compute gradient: $\nabla_{\boldsymbol{\theta}} L = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{\theta}} L_i$
2. Optimize for optimal step α:

$$\arg\min_{\alpha} L(\underbrace{\boldsymbol{\theta}^k - \alpha \nabla_{\boldsymbol{\theta}} L}_{\boldsymbol{\theta}^{k+1}})$$

3. $\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \nabla_{\boldsymbol{\theta}} L$

Not that practical for DL since we need to solve huge system every step…

Gradient Descent on Train Set

- Given large train set with n training samples $\{x_i, y_i\}$
  - Let's say 1 million labeled images
  - Let's say our network has 500k parameters

- Gradient has 500k dimensions
- $n = 1\ million$

→ Extremely expensive to compute

Stochastic Gradient Descent (SGD)

- If we have $\boldsymbol{n}$ training samples we need to compute the gradient for all of them which is $\boldsymbol{O(n)}$

- If we consider the problem as empirical risk minimization, we can express the total loss over the training data as the expectation of all the samples

$$\frac{1}{n}\left(\sum_{i=1}^{n} L_i(\boldsymbol{\theta}, \boldsymbol{x_i}, \boldsymbol{y_i})\right) = \mathbb{E}_{i\sim[1,\dots,n]}[L_i(\boldsymbol{\theta}, \boldsymbol{x_i}, \boldsymbol{y_i})]$$

- The expectation can be approximated with a small subset of the data

$$\mathbb{E}_{i\sim[1,\dots,n]}[L_i(\boldsymbol{\theta}, \boldsymbol{x_i}, \boldsymbol{y_i})] \approx \frac{1}{|S|}\sum_{j\in S}\left(L_j(\boldsymbol{\theta}, \boldsymbol{x_j}, \boldsymbol{y_j})\right) \text{ with S} \subseteq \{1, \dots, n\}$$

Minibatch

choose subset of trainset $\boldsymbol{m} \ll \boldsymbol{n}$

$$B_i = \{\{\boldsymbol{x_1}, \boldsymbol{y_1}\}, \{\boldsymbol{x_2}, \boldsymbol{y_2}\}, \dots, \{\boldsymbol{x_m}, \boldsymbol{y_m}\}\}$$
$$\{B_1, B_2, \dots, B_{n/m}\}$$

Minibatch size is hyperparameter

- Typically power of 2 → 8, 16, 32, 64, 128…
- Smaller batch size means greater variance in the gradients

  → noisy updates
- Mostly limited by GPU memory (in backward pass)
- E.g.,
  - Train set has $\mathbf{n = 2^{20}}$ (about 1 million) images
  - With batch size $\mathbf{m = 64}$: $B_{1 \ldots n/m} = B_{1 \ldots 16{,}384}$ minibatches

(Epoch = complete pass through training set)

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{k}, \boldsymbol{x}_{\{1..m\}}, \boldsymbol{y}_{\{1..m\}})$$

$\boldsymbol{k}$ now refers to $\boldsymbol{k}$-th iteration

one forward & one backward for each batch size

$$\nabla_{\boldsymbol{\theta}} L = \frac{1}{m} \sum_{i=1}^{m} \nabla_{\boldsymbol{\theta}} L_i$$

$\boldsymbol{m}$ training samples in the current minibatch

Gradient for the $\boldsymbol{k}$-th minibatch

Note the terminology: iteration vs epoch

Convergence of SGD

Suppose we want to minimize the function $F(\theta)$ with the stochastic approximation

$$\theta^{k+1} = \theta^k - \alpha_k H(\theta^k, X)$$

where $\alpha_1, \alpha_2 \dots \alpha_n$ is a sequence of positive step-sizes and $H(\theta^k, X)$ is the unbiased estimate of $\nabla \mathrm{F}(\theta^k)$, i.e.

$$\mathbb{E}[H(\theta^k, X)] = \nabla \mathrm{F}(\theta^k)$$

Robbins, H. and Monro, S. "A Stochastic Approximation Method" 1951.

Mathematically, one can tell when it will converge

$$\theta^{k+1} = \theta^k - \alpha_k H(\theta^k, X)$$

converges to a local (global) minimum if the following conditions are met:

1) $\alpha_n \geq 0, \forall\, n \geq 0$
2) $\sum_{n=1}^{\infty} \alpha_n = \infty$
3) $\sum_{n=1}^{\infty} \alpha_n^2 < \infty$
4) $F(\theta)$ is strictly convex

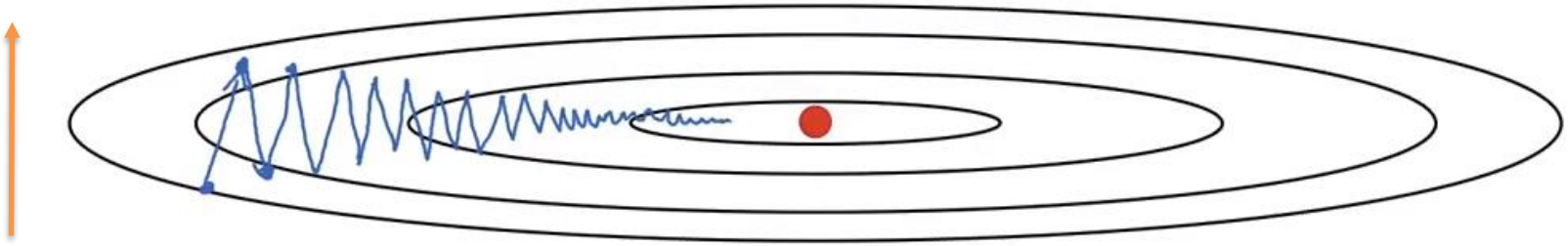
The proposed sequence by Robbins and Monro is $\alpha_n \propto \frac{\alpha}{n}, for\ n > 0$

Problems of SGD

- Gradient is scaled equally across all dimensions
  → i.e., cannot independently scale directions
  → need to have conservative min learning rate to avoid divergence
  → Slower than 'necessary'

- Finding good learning rate is an art by itself
  → More next lecture

Gradient Descent with Momentum



Source: A. Ng

We're making many steps back and forth along this dimension. Would love to track that this is averaging out over time.

Would love to go faster here…
I.e., accumulated gradients over time

i.e history of all grads

First Momentum

mean of grads

$$v^{k+1} = \beta \cdot v^k - \alpha \cdot \nabla_\theta L(\theta^k)$$

accumulation rate ('friction', momentum)

velocity

learning rate

Gradient of current minibatch

$$\theta^{k+1} = \theta^k + v^{k+1}$$

weights of model

around 0, if grad ↗↘

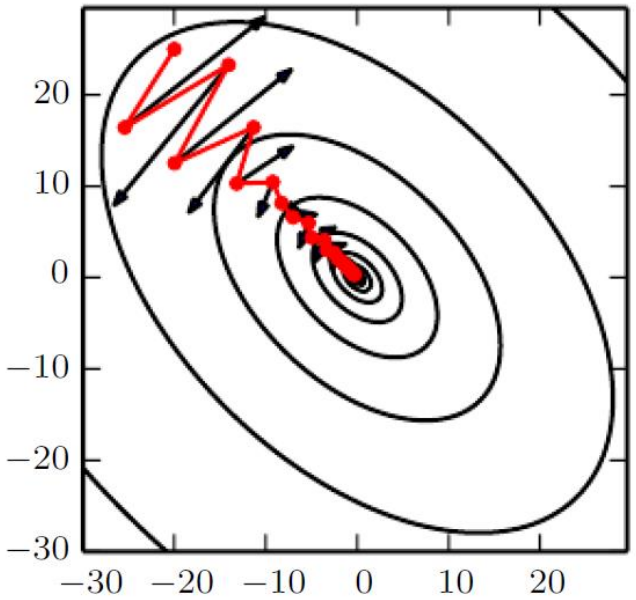
accumulate more, if grad → →

Exponentially-weighted average of gradient

Important: velocity v^k is vector-valued! → on partial deriv basis; in order to accumulate grad in each dim

[Sutskever et al., ICML'13] On the importance of initialization and momentum in deep learning

* Needless to say, setting β to Zero is just naive GD.



Source: I. Goodfellow

Very Important

idea

Step will be largest when a sequence of gradients all point to the same direction

Speeding things up

Hyperparameters are α, β

β is often set to 0.9

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} + \boldsymbol{v}^{k+1}$$

- Can it overcome local minima? YES.

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} + \boldsymbol{v}^{k+1}$$

Nesterov Momentum

- Look-ahead momentum

$$\tilde{\boldsymbol{\theta}}^{k+1} = \boldsymbol{\theta}^{k} + \beta \cdot \boldsymbol{v}^{k}$$

directly looking ahead from prev velo v^k

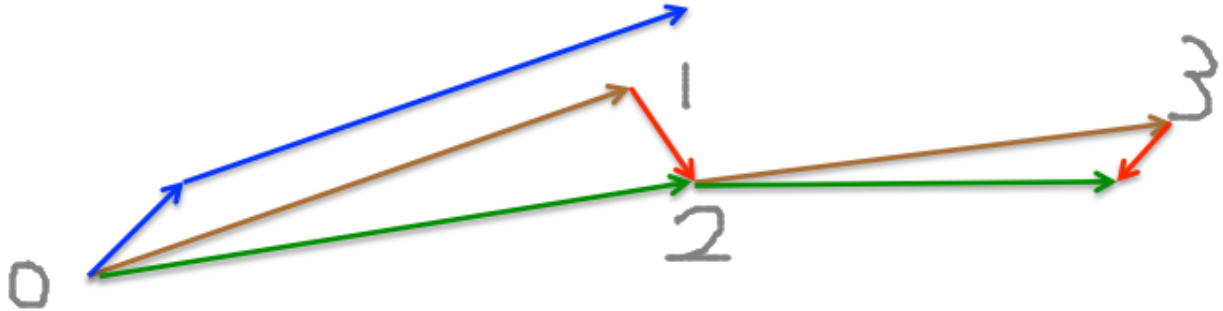
$$\boldsymbol{v}^{k+1} = \beta \cdot \boldsymbol{v}^{k} - \alpha \cdot \nabla_{\boldsymbol{\theta}} L(\tilde{\boldsymbol{\theta}}^{k+1})$$

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} + \boldsymbol{v}^{k+1}$$

Nesterov, Yurii E. "A method for solving the convex programming problem with convergence rate O (1/k^ 2)." *Dokl. akad. nauk Sssr*. Vol. 269. 1983.

* All those tricks are computationally inexpensive

- First make a big jump in the direction of the previous accumulated gradient.
- Then measure the gradient where you end up and make a correction.



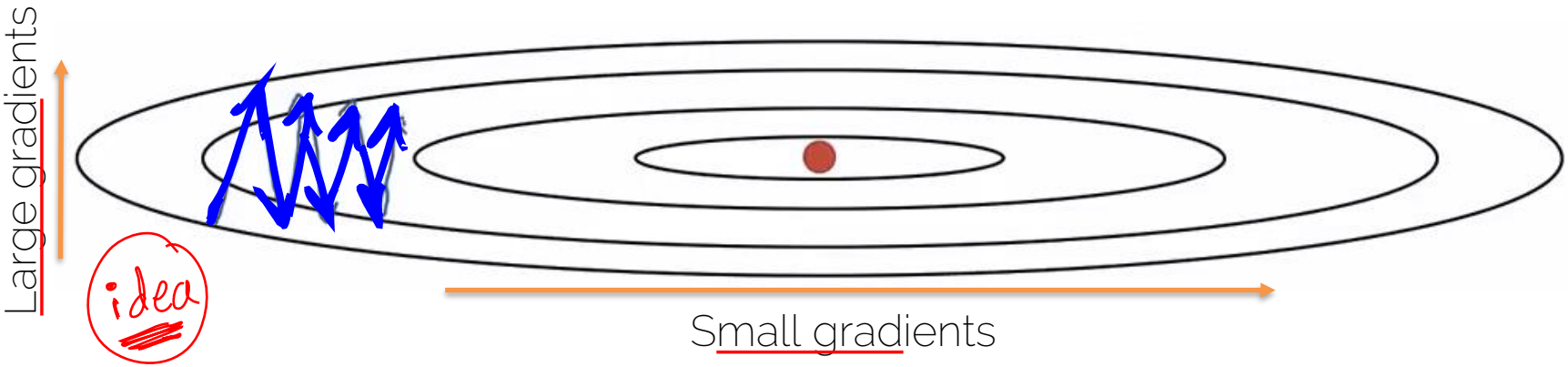
brown vector = jump, red vector = correction, green vector = accumulated gradient

blue vectors = standard momentum

Source: G. Hinton

$$\tilde{\boldsymbol{\theta}}^{k+1} = \boldsymbol{\theta}^{k} + \beta \cdot \boldsymbol{v}^{k}$$
$$\boldsymbol{v}^{k+1} = \beta \cdot \boldsymbol{v}^{k} - \alpha \cdot \nabla_{\boldsymbol{\theta}} L(\tilde{\boldsymbol{\theta}}^{k+1})$$
$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} + \boldsymbol{v}^{k+1}$$

Root Mean Squared Prop (RMSProp)



Source: Andrew. Ng

to dampen this jittering

- RMSProp divides the learning rate by an exponentially-decaying average of squared gradients.

Hinton et al. "Lecture 6.5-rmsprop: Divide the gradient by a running average of its recent magnitude." COURSERA: Neural networks for machine learning 4.2 (2012): 26-31.

$$s^{k+1} = \beta \cdot s^k + (1-\beta)[\nabla_\theta L \circ \nabla_\theta L]$$

Element-wise multiplication

$$\theta^{k+1} = \theta^k - \alpha \cdot \frac{\nabla_\theta L}{\sqrt{s^{k+1}} + \epsilon}$$

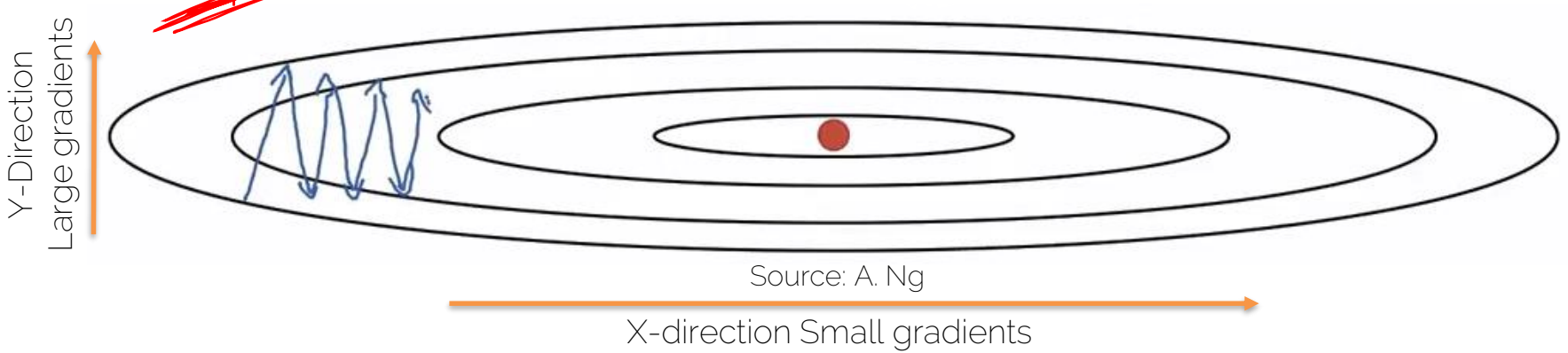
Hyperparameters: α, β, ϵ

Needs tuning!

Often 0.9

Typically 10^{-8}

Important



(Uncentered) variance of gradients
→ second momentum

$$\boldsymbol{s}^{k+1} = \beta \cdot \boldsymbol{s}^{k} + (1-\beta)[\nabla_{\boldsymbol{\theta}} L \circ \nabla_{\boldsymbol{\theta}} L]$$

We're dividing by square gradients:
- Division in Y-Direction will be large
- Division in X-Direction will be small

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} - \alpha \cdot \frac{\nabla_{\boldsymbol{\theta}} L}{\sqrt{\boldsymbol{s}^{k+1}} + \epsilon}$$

Can increase learning rate!

Dampening the oscillations for high-variance directions

- Can use faster learning rate because it is less likely to diverge
  → Speed up learning speed
  → Second moment

Adaptive Moment Estimation (Adam)

Idea : Combine Momentum and RMSProp

$$\boldsymbol{m}^{k+1} = \beta_1 \cdot \boldsymbol{m}^k + (1-\beta_1)\nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^k\right)$$

First momentum: mean of gradients

$$\boldsymbol{v}^{k+1} = \beta_2 \cdot \boldsymbol{v}^k + (1-\beta_2)[\nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^k\right) \circ \nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^k\right)]$$

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \cdot \frac{\boldsymbol{m}^{k+1}}{\sqrt{\boldsymbol{v}^{k+1}} + \epsilon}$$

Note : This is not the update rule of Adam

Second momentum: variance of gradients

Q. What happens at $\boldsymbol{k} = \mathbf{0}$?
A. We need bias correction as $\boldsymbol{m}^0 = 0$ and $\boldsymbol{v}^0 = 0$

[Kingma et al., ICLR'15] Adam: A method for stochastic optimization

Adam : Bias Corrected

- Combines Momentum and RMSProp

$$\boldsymbol{m}^{k+1} = \beta_1 \cdot \boldsymbol{m}^k + (1-\beta_1)\nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^k\right) \qquad \boldsymbol{v}^{k+1} = \beta_2 \cdot \boldsymbol{v}^k + (1-\beta_2)[\nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^k\right) \circ \nabla_{\boldsymbol{\theta}} L\left(\boldsymbol{\theta}^k\right)$$

$\boldsymbol{m}^k$ and $\boldsymbol{v}^k$ are initialized with zero

→ bias towards zero

→ Need bias-corrected moment updates

Update rule of Adam

$$\hat{\boldsymbol{m}}^{k+1} = \frac{\boldsymbol{m}^{k+1}}{1-\beta_1{}^{k+1}} \qquad \hat{\boldsymbol{v}}^{k+1} = \frac{\boldsymbol{v}^{k+1}}{1-\beta_2{}^{k+1}} \longrightarrow \boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \cdot \frac{\hat{\boldsymbol{m}}^{k+1}}{\sqrt{\hat{\boldsymbol{v}}^{k+1}}+\epsilon}$$

Exponentially-decaying mean and variance of gradients (combines first and second order momentum)

- Hyperparameters: α, β_1, β_2, ϵ

Needs tuning!

Often 0.9

Typically 10^{-8}

Often 0.999

Defaults in PyTorch

$$\boldsymbol{m}^{k+1} = \beta_1 \cdot \boldsymbol{m}^k + (1-\beta_1)\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k)$$

$$\boldsymbol{v}^{k+1} = \beta_2 \cdot \boldsymbol{v}^k + (1-\beta_2)\left[\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k) \circ \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k)\right]$$

$$\hat{\boldsymbol{m}}^{k+1} = \frac{\boldsymbol{m}^{k+1}}{1-{\beta_1}^{k+1}} \qquad \hat{\boldsymbol{v}}^{k+1} = \frac{\boldsymbol{v}^{k+1}}{1-{\beta_2}^{k+1}}$$

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \cdot \frac{\hat{\boldsymbol{m}}^{k+1}}{\sqrt{\hat{\boldsymbol{v}}^{k+1}} + \epsilon}$$

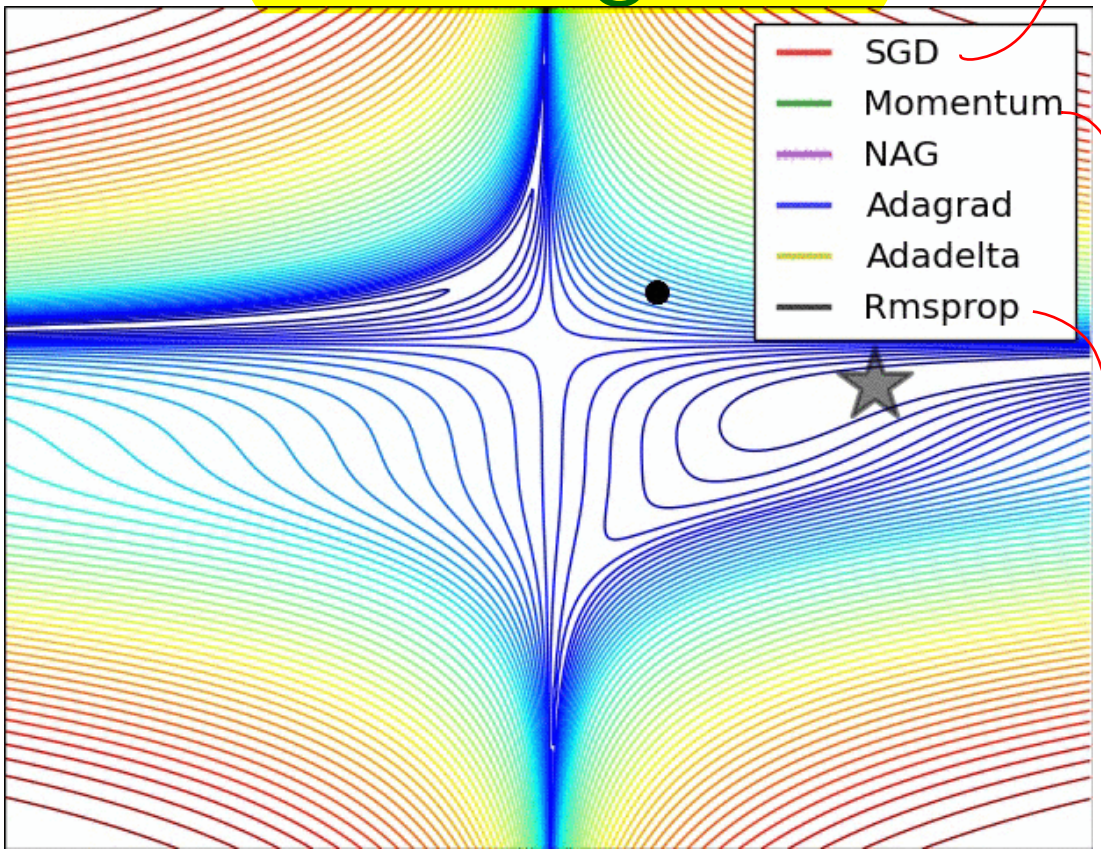
There are a few others…

- 'Vanilla' SGD
- Momentum
- RMSProp
- Adagrad
- Adadelta
- AdaMax
- Nada
- AMSGrad

Adam is mostly method of choice for neural networks!

It's actually fun to play around with SGD updates.
It's easy and you get pretty immediate feedback ☺

Convergence



slow, since there is no accumulation of grads

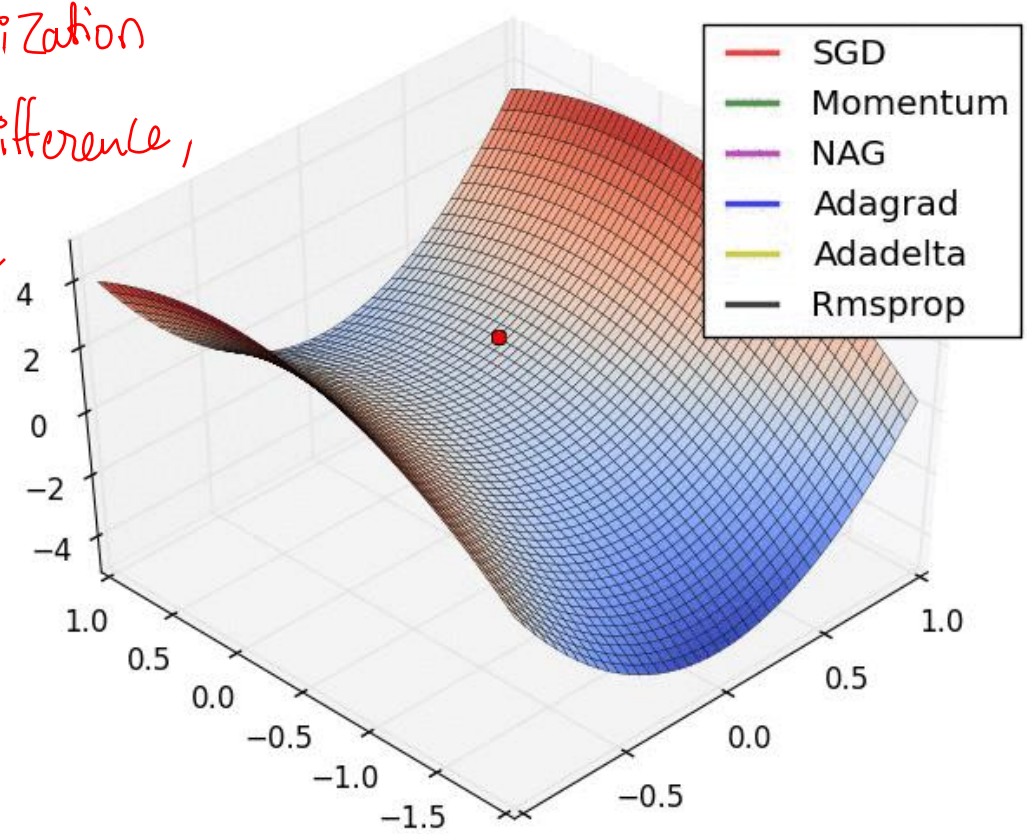
usually overshoots

pretty good, yet slower to make step in forward dir

Source: http://ruder.io/optimizing-gradient-descent/

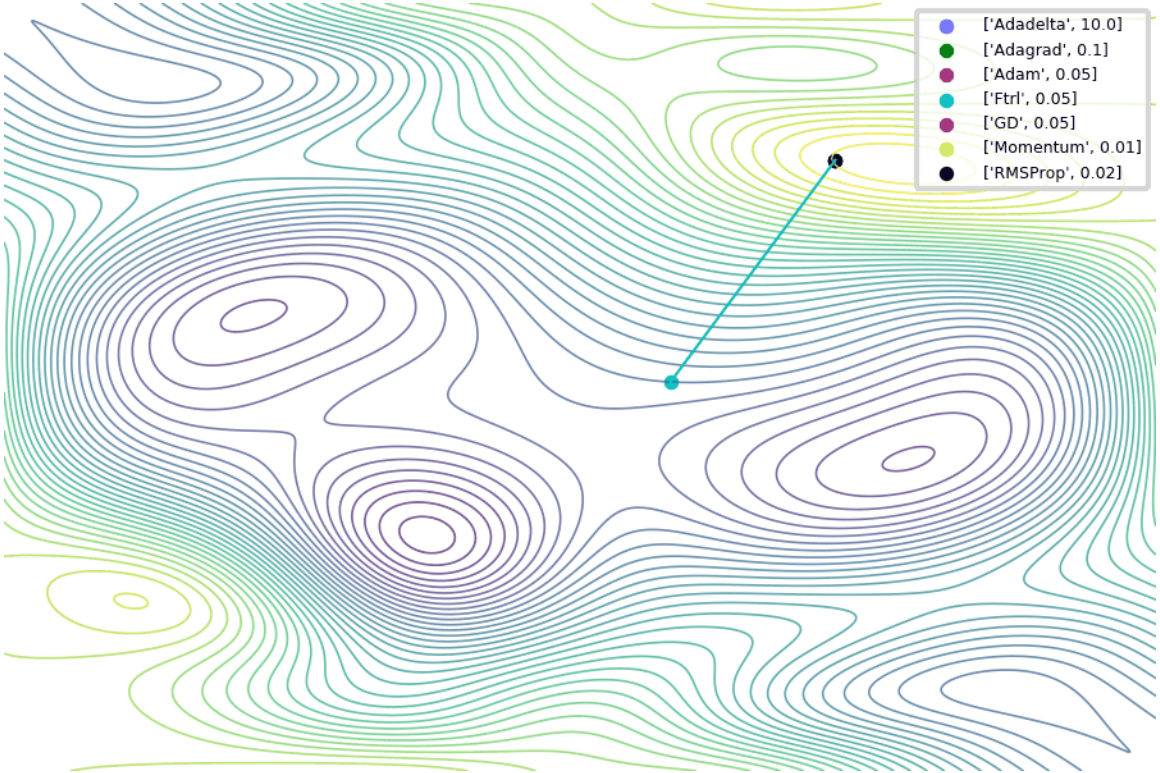
Convergence

* Choise of optimization makes huge difference, depending on the problem



Source: http://ruder.io/optimizing-gradient-descent/

Convergence



Source: https://github.com/Jaewan-Yun/optimizer-visualization

Jacobian and Hessian

- Derivative $\boldsymbol{f}: \mathbb{R} \rightarrow \mathbb{R}$ $\frac{df(x)}{dx}$
- Gradient $\boldsymbol{f}: \mathbb{R}^m \rightarrow \mathbb{R}$ $\nabla_x f(\boldsymbol{x})$ $\left(\frac{\mathrm{d}f(\boldsymbol{x})}{\mathrm{d}x_1}, \frac{\mathrm{d}f(\boldsymbol{x})}{\mathrm{d}x_2}\right)$
- Jacobian $\boldsymbol{f}: \mathbb{R}^m \rightarrow \mathbb{R}^n$ $\mathbf{J} \in \mathbb{R}^{n \times m}$
- Hessian $\boldsymbol{f}: \mathbb{R}^m \rightarrow \mathbb{R}$ $\mathbf{H} \in \mathbb{R}^{m \times m}$

SECOND DERIVATIVE

Important

Newton's Method

- Approximate our function by a second-order Taylor series expansion

$$L(\boldsymbol{\theta}) \approx L(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^T \boldsymbol{\nabla}_{\boldsymbol{\theta}} L(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^T \mathbf{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

First derivative

Second derivative (curvature)

More info: https://en.wikipedia.org/wiki/Taylor_series

- Differentiate and equate to zero

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \mathbf{H}^{-1}\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$

Update step

We got rid of the learning rate!

* **H** is somehow replacing learning rate, scaling grad across every parameter dim

Remember

SGD $\quad \boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}_k, \mathbf{x}_i, \mathbf{y}_i)$

NB 2nd_order optimizer will do much better than agrad optimizer.

- Differentiate and equate to zero

* No need to invert **H**, just solve the linear sys

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \mathbf{H}^{-1}\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$ Update step

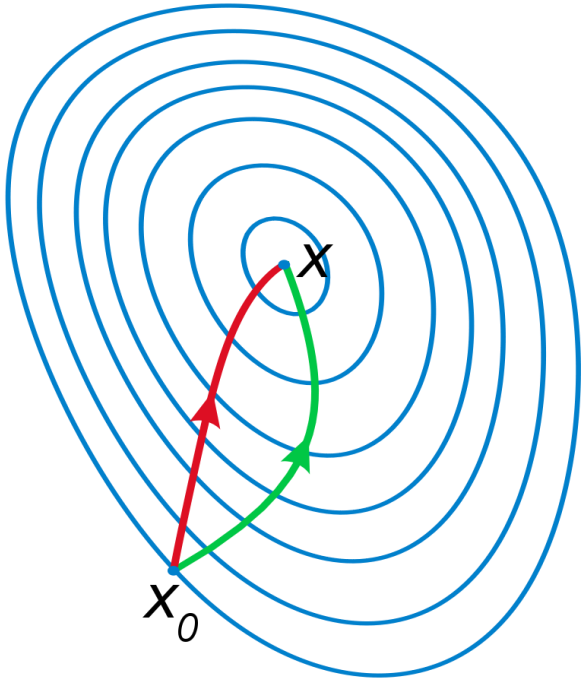
NB

Parameters of a network (millions)	Number of elements in the Hessian	Computational complexity of 'inversion' per iteration
k	k^2	$\mathcal{O}(k^3)$

- Gradient Descent (green)

* Newton's method exploits the curvature to take a more direct route

fewer, yet more expensive steps needed



Source: https://en.wikipedia.org/wiki/Newton%27s_method_in_optimization

$$J(\boldsymbol{\theta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$$

Can you apply Newton's method for linear regression? What do you get as a result?

YES.

it will solve it in one step!

Variations of Newton's

BFGS and L-BFGS

- Broyden-Fletcher-Goldfarb-Shanno algorithm
- Belongs to the family of quasi-Newton methods
- Have an approximation of the inverse of the Hessian

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \mathbf{H}^{-1} \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$

Computational Complexity

- BFGS $\mathcal{O}(n^2)$
- Limited memory: L-BFGS $\mathcal{O}(n)$

Gauss-Newton

- $x_{k+1} = x_k - H_f(x_k)^{-1} \nabla f(x_k)$
  - 'true' 2nd derivatives are often hard to obtain (e.g., numerics)
  - $H_f \approx 2J_F^T J_F$
- Gauss-Newton (GN):

$$x_{k+1} = x_k - [2J_F(x_k)^T J_F(x_k)]^{-1} \nabla f(x_k)$$

- Solve linear system (again, inverting a matrix is unstable):

$$2\big(J_F(x_k)^T J_F(x_k)\big)(x_k - x_{k+1}) = \nabla f(x_k)$$

Solve for delta vector

Levenberg

- Levenberg
  - "damped" version of Gauss-Newton:
  - $(J_F(x_k)^T J_F(x_k) + \lambda \cdot I) \cdot (x_k - x_{k+1}) = \nabla f(x_k)$

    Tikhonov regularization

  - The damping factor λ is adjusted in each iteration ensuring:

    $$f(x_k) > f(x_{k+1})$$

    - if the equation is not fulfilled increase λ
    - →Trust region

→ "Interpolation" between Gauss-Newton (small λ) and Gradient Descent (large λ)

Levenberg-Marquardt

- Levenberg-Marquardt (LM)

$$(J_F(x_k)^T J_F(x_k) + \lambda \cdot diag(J_F(x_k)^T J_F(x_k))) \cdot (x_k - x_{k+1}) = \nabla f(x_k)$$

- Instead of a plain Gradient Descent for large λ, scale each component of the gradient according to the curvature.
  - Avoids slow convergence in components with a small gradient

Which, What, and When?

- Standard: **Adam**

- Fallback option: **SGD with momentum**

- **Newton, L-BFGS, GN, LM** only if you can do full batch updates (doesn't work well for minibatches!!)

This practically never happens for DL
Theoretically, it would be nice though due to fast convergence

General Optimization

- Linear Systems (Ax = b)
  - LU, QR, Cholesky, Jacobi, Gauss-Seidel, CG, PCG, etc.
- Non-linear (gradient-based)
  - Newton, Gauss-Newton, LM, (L)BFGS ← second order
  - Gradient Descent, SGD ← first order
- Others
  - Genetic algorithms, MCMC, Metropolis-Hastings, etc.
  - Constrained and convex solvers (Langrage, ADMM, Primal-Dual, etc.)

Please Remember!

- Think about your problem and optimization at hand

SGD is specifically designed for minibatch

- When you can, use 2nd order method → it's just faster

GD or SGD is **not** a way to solve a linear system!

Next Lecture

- This week:
  - Check exercises
  - Check office hours ☺

- Next lecture
  - Training Neural networks

See you next week ☺

Some References to SGD Updates

- Goodfellow et al. “Deep Learning” (2016),
  - Chapter 8: Optimization
- Bishop “Pattern Recognition and Machine Learning” (2006),
  - Chapter 5.2: Network training (gradient descent)
  - Chapter 5.4: The Hessian Matrix (second order methods)
- https://ruder.io/optimizing-gradient-descent/index.html
- PyTorch Documetation (with further readings)
  - https://pytorch.org/docs/stable/optim.html