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FIT3181 Deep Learning

Week 03: Stochastic Gradient Descent and Optimization for Deep Learning

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Outline

- □ Revision of calculus.
- □ Computational graph and forward/backward propagations.
- □ Gradient descent and stochastic gradient descent.
- □ Backpropagation in feed-forward neural networks.
- □ Optimizers for deep learning.

- □ **Further reading recommendations**
  - ○ Deep Learning – Chapter 8
  - ○ Dive into Deep Learning – Chapter 11 (https://d2l.ai/chapter_optimization/index.html)
  - ○ Ruder’s blog: https://ruder.io/optimizing-gradient-descent/index.html

A small detour to calculus

- Calculus = **mathematics of change** (very important for deep learning)
- Properties of derivative:
  - $f'(x) = \nabla f(x) = \lim_{h \to 0} \frac{f(x+h)-f(x)}{h}$
  - $(uv)' = u'v + uv'$
  - $\left(\frac{u}{v}\right)' = \frac{u'v-uv'}{v^2}$
  - $(e^u)' = u'e^u$
  - $(\log u)' = \frac{u'}{u}$
- Multi-variate function $f: \mathbb{R}^n \to \mathbb{R}$ with $y = f(x) = f(x_1, \dots, x_n)$.
  - Gradient/derivative: $\frac{\partial f}{\partial x}(a) = \nabla_x f(a) = [\nabla_{x_1} f(a), \nabla_{x_2} f(a), \dots, \nabla_{x_n} f(a)]$.
- Chain rule 🔗 :
  - $\frac{\partial u}{\partial x} = \frac{\partial u}{\partial v} \times \frac{\partial v}{\partial x}$

Example

❑ Consider the function $f(x, y, z) = \log(\exp(x) + \exp(y) + \exp(z))$. What are $f'_x = \nabla_x f$, $f'_y = \nabla_y f$, and $f'_z = \nabla_z f$?

❑ $f(x, y, z) = \log(u)$ with $u = \exp(x) + \exp(y) + \exp(z)$.

❑ $f'_x = \frac{u'_x}{u} = \frac{\exp(x)}{\exp(x)+\exp(y)+\exp(z)}$.

❑ $f'_y = \frac{u'_y}{u} = \frac{\exp(y)}{\exp(x)+\exp(y)+\exp(z)}$.

❑ $f'_z = \frac{u'_z}{u} = \frac{\exp(z)}{\exp(x)+\exp(y)+\exp(z)}$.

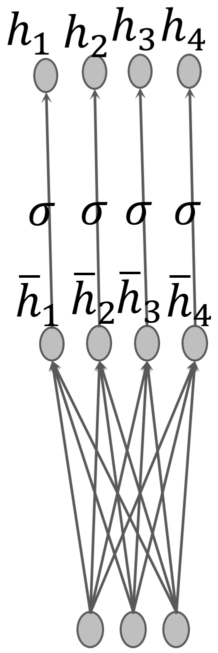
❑ $\nabla f = [f'_x, f'_y, f'_z] = softmax([x, y, z])$.

Example (Forum discussion)

- $\bar{h} = Wx + b$ and $h = \sigma(\bar{h})$
  - $h = \sigma(Wx + b)$
  - σ is the activation function
- $\dfrac{\partial h}{\partial x} = \dfrac{\partial h}{\partial \bar{h}} \times \dfrac{\partial \bar{h}}{\partial x} = diag\left(\sigma'(\bar{h})\right)W$

- $$\frac{\partial h}{\partial \bar{h}} = \begin{bmatrix} \frac{\partial h_1}{\partial \bar{h}_1} & \frac{\partial h_1}{\partial \bar{h}_2} & \frac{\partial h_1}{\partial \bar{h}_3} & \frac{\partial h_1}{\partial \bar{h}_4} \\ \frac{\partial h_2}{\partial \bar{h}_1} & \frac{\partial h_2}{\partial \bar{h}_2} & \frac{\partial h_2}{\partial \bar{h}_3} & \frac{\partial h_2}{\partial \bar{h}_4} \\ \frac{\partial h_3}{\partial \bar{h}_1} & \frac{\partial h_3}{\partial \bar{h}_2} & \frac{\partial h_3}{\partial \bar{h}_3} & \frac{\partial h_3}{\partial \bar{h}_4} \\ \frac{\partial h_4}{\partial \bar{h}_1} & \frac{\partial h_4}{\partial \bar{h}_2} & \frac{\partial h_4}{\partial \bar{h}_3} & \frac{\partial h_4}{\partial \bar{h}_4} \end{bmatrix} = \begin{bmatrix} \sigma'(\bar{h}_1) & 0 & 0 & 0 \\ 0 & \sigma'(\bar{h}_2) & 0 & 0 \\ 0 & 0 & \sigma'(\bar{h}_3) & 0 \\ 0 & 0 & 0 & \sigma'(\bar{h}_4) \end{bmatrix} = diag(\sigma'(\bar{h}))$$

- $\dfrac{\partial \bar{h}}{\partial x} = W$



h_1 h_2 h_3 h_4
σ σ σ σ
$\bar{h}_1$ $\bar{h}_2$ $\bar{h}_3$ $\bar{h}_4$

$h = \sigma(\bar{h})$

$\bar{h} = Wx + b$

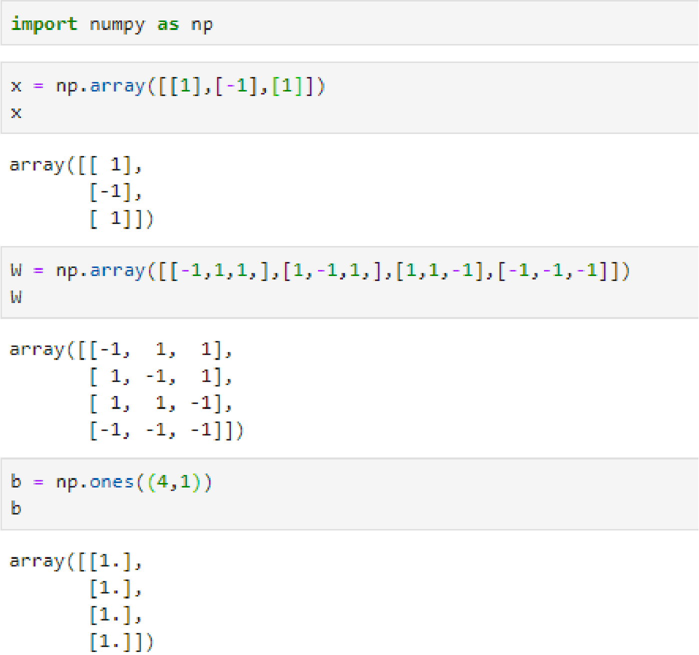
$W \in \mathbb{R}^{4\times3}$

$b \in \mathbb{R}^{4\times1}$

$x \in \mathbb{R}^{3\times1}$

How to code with numpy

- □ $\bar{h} = Wx + b$ and $h = sigmoid(\bar{h})$
  - ○ $h = sigmoid(Wx + b)$
  - ○ $\sigma = sigmoid$ is the activation function
- □ $\frac{\partial h}{\partial x} = \frac{\partial h}{\partial \bar{h}} \times \frac{\partial \bar{h}}{\partial x} = diag\left(\sigma'(\bar{h})\right)W = diag(\sigma(\bar{h})[1 - \sigma(\bar{h})])W = diag(h(1-h))W$



```
import numpy as np
```

```
x = np.array([[1],[-1],[1]])
x
```

```
array([[ 1],
       [-1],
       [ 1]])
```

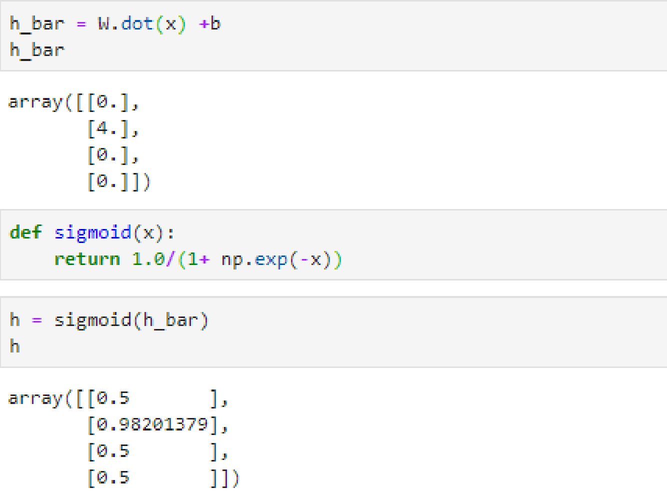
```
W = np.array([[-1,1,1,],[1,-1,1,],[1,1,-1],[-1,-1,-1]])
W
```

```
array([[-1,  1,  1],
       [ 1, -1,  1],
       [ 1,  1, -1],
       [-1, -1, -1]])
```

```
b = np.ones((4,1))
b
```

```
array([[1.],
       [1.],
       [1.],
       [1.]])
```

Declare W, x, b



```
h_bar = W.dot(x) +b
h_bar
```

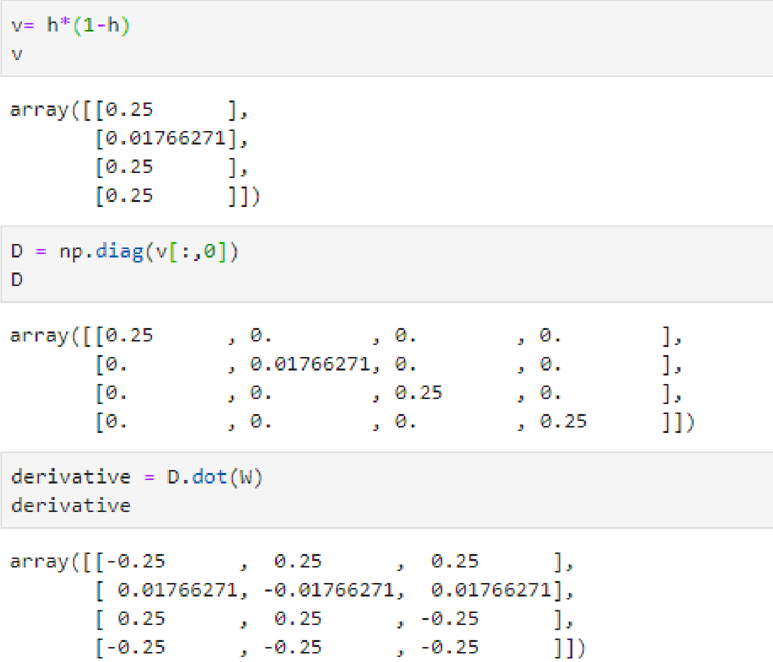
```
array([[0.],
       [4.],
       [0.],
       [0.]])
```

```
def sigmoid(x):
    return 1.0/(1+ np.exp(-x))
```

```
h = sigmoid(h_bar)
h
```

```
array([[0.5       ],
       [0.98201379],
       [0.5       ],
       [0.5       ]])
```

Forward propagation



```
v= h*(1-h)
v
```

```
array([[0.25      ],
       [0.01766271],
       [0.25      ],
       [0.25      ]])
```

```
D = np.diag(v[:,0])
D
```

```
array([[0.25      , 0.        , 0.        , 0.        ],
       [0.        , 0.01766271, 0.        , 0.        ],
       [0.        , 0.        , 0.25      , 0.        ],
       [0.        , 0.        , 0.        , 0.25      ]])
```

```
derivative = D.dot(W)
derivative
```

```
array([[-0.25      ,  0.25      ,  0.25      ],
       [ 0.01766271, -0.01766271,  0.01766271],
       [ 0.25      ,  0.25      , -0.25      ],
       [-0.25      , -0.25      , -0.25      ]])
```

Backward propagation

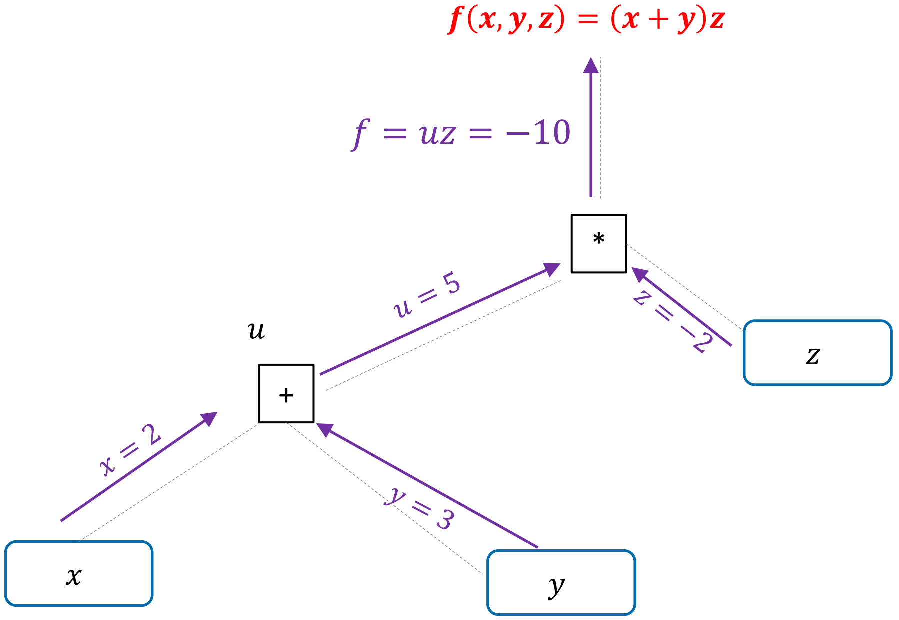
Computational graph

Computational graph (used in TensorFlow)

Problem: $f(x, y, z) = (x + y)z$
What are its partial derivatives, evaluated at $x = 2, y = 3, z = -2$?

Step 1:

a) construct computational graph
b) forward propagation
c) record value at each node



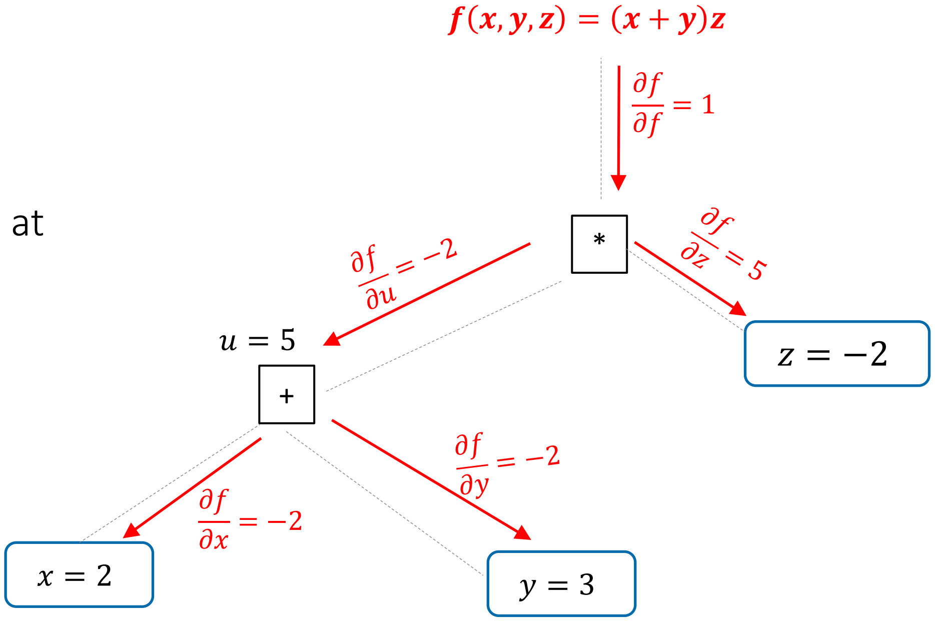
Reverse Auto-Diff (used in TensorFlow)

Step 2:

a) traverse backward

b) apply chain rule

c) record differential values at each node


$f(x,y,z)=(x+y)z$
$\frac{\partial f}{\partial f}=1$
$*$
$\frac{\partial f}{\partial u}=-2$
$\frac{\partial f}{\partial z}=5$
$u=5$
$+$
$z=-2$
$\frac{\partial f}{\partial y}=-2$
$\frac{\partial f}{\partial x}=-2$
$x=2$
$y=3$

$$\frac{\partial f}{\partial f}=1$$

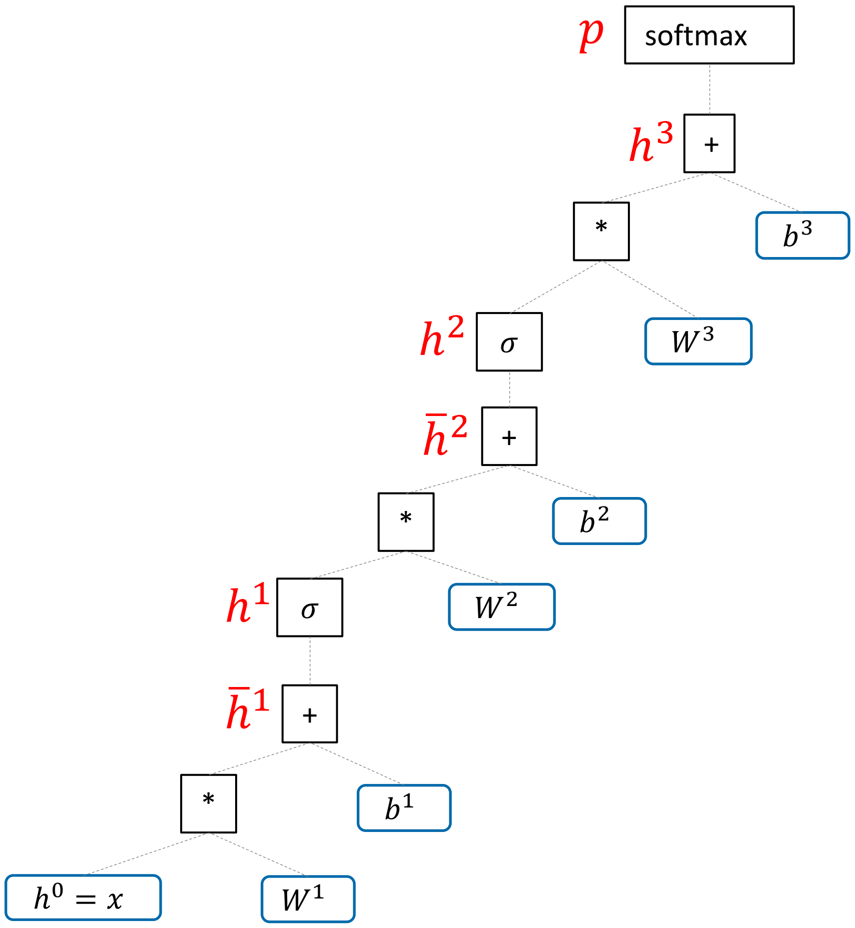
$$\frac{\partial f}{\partial u}=\frac{\partial f}{\partial f}\frac{\partial f}{\partial u}=1*z=-2$$

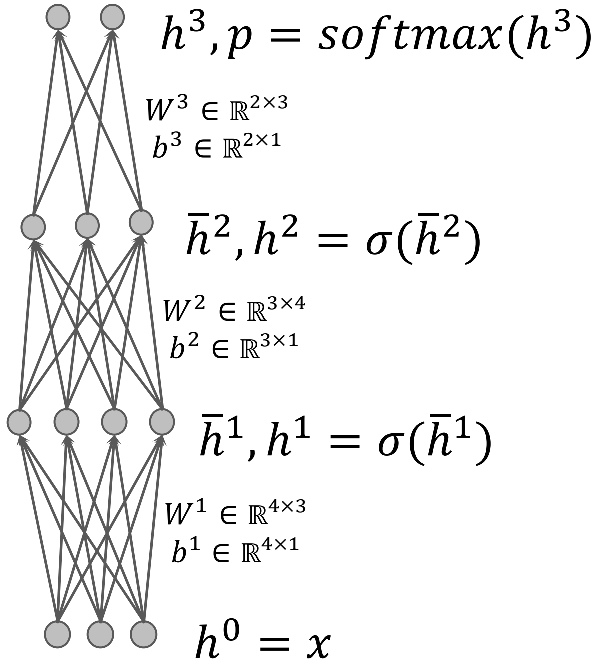
$$\frac{\partial f}{\partial x}=\frac{\partial f}{\partial u}\frac{\partial u}{\partial x}=-2*1=-2$$

$$\frac{\partial f}{\partial z}=\frac{\partial f}{\partial f}\frac{\partial f}{\partial z}=1*u=5$$

$$\frac{\partial f}{\partial y}=\frac{\partial f}{\partial u}\frac{\partial u}{\partial y}=-2*1=-2$$

Computational graph of feedforward nets (Forum discussion)



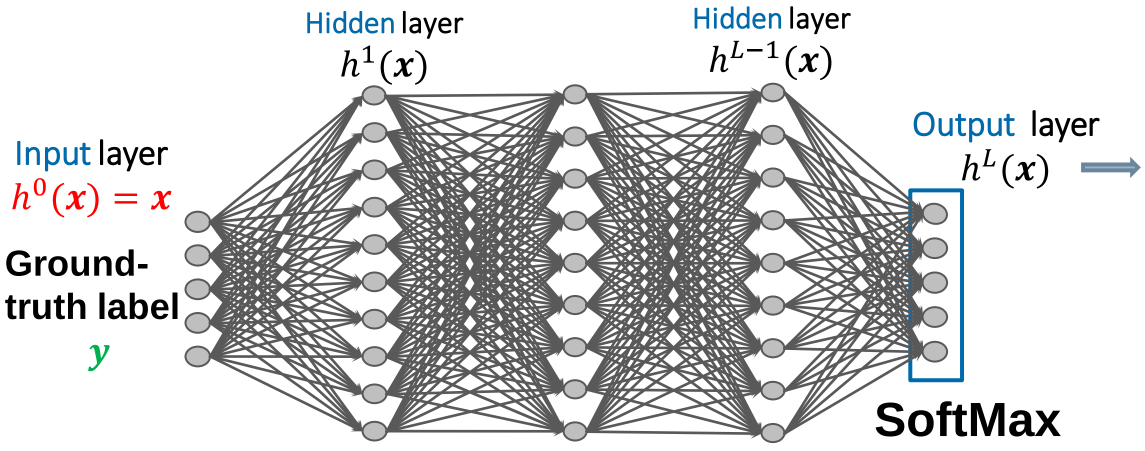


$h^3, p = softmax(h^3)$
$W^3 \in \mathbb{R}^{2\times3}$
$b^3 \in \mathbb{R}^{2\times1}$
$\bar{h}^2, h^2 = \sigma(\bar{h}^2)$
$W^2 \in \mathbb{R}^{3\times4}$
$b^2 \in \mathbb{R}^{3\times1}$
$\bar{h}^1, h^1 = \sigma(\bar{h}^1)$
$W^1 \in \mathbb{R}^{4\times3}$
$b^1 \in \mathbb{R}^{4\times1}$
$h^0 = x$

```
$h^0(x) = x$
for $k = 1$ to 2 do
    $\bar{h}^k = W^k h^{k-1}(x) + b^k$        //linear operation
    $h^k(x) = \sigma(\bar{h}^k(x))$        //activation
$h^3(x) = W^3 h^2(x) + b^2$
$p(x) = softmax(h^3(x))$        //prediction probabilities
```

Gradient descent and stochastic gradient descent

Recall optimization problem in deep learning (Forum discussion)



$\Longrightarrow p(x) = softmax(h^L(x))$

$\hat{y} = \mathrm{argmax}_{1\le m\le M}\, p_m(x)$

$l(y, \hat{y}) = CE\big(1_y, p(x)\big) = -\log p_y(x)$

Training set

$$D = \{(x_1, y_1), \ldots (x_N, y_N)\}$$

Loss function

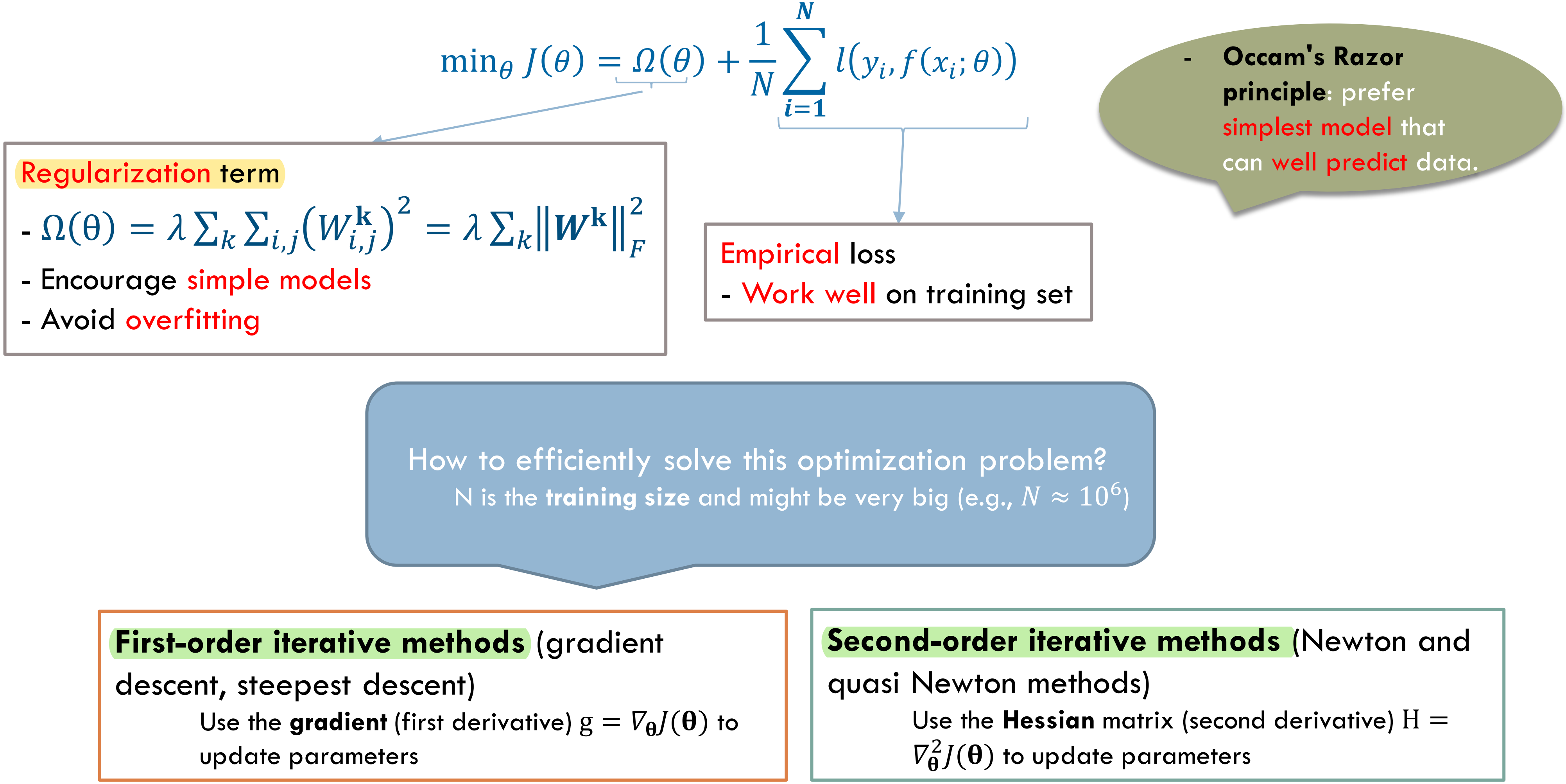
$$L(D;\theta) := \frac{1}{N}\sum_{i=1}^{N} CE\left(1_{y_i}, p(x_i)\right) = -\frac{1}{N}\sum_{i=1}^{N} \log p_{y_i}(x_i)$$

□ How to **solve** the **optimization problem** efficiently ($\theta := \{(W^l, b^l)\}_{l=1}^{L}$)?

- ○ $\min_\theta L(D;\theta) := -\frac{1}{N}\sum_{i=1}^{N}\log p_{y_i}(x_i) = -\frac{1}{N}\sum_{i=1}^{N}\log\frac{\exp\{h_{y_i}^L(x_i)\}}{\sum_{m=1}^{M}\exp\{h_m^L(x_i)\}}$
- ○ Generalize: $\min_\theta J(\theta) := \frac{1}{N}\sum_{i=1}^{N} l(f(x_i;\theta), y_i)$

Optimization problem in ML and DL

□ Most of optimization problems (OP) in machine learning (deep learning) has the following form:



$$\min_\theta J(\theta) = \underbrace{\Omega(\theta)} + \underbrace{\frac{1}{N}\sum_{i=1}^{N} l(y_i, f(x_i;\theta))}$$

Regularization term

- $\Omega(\theta) = \lambda \sum_k \sum_{i,j} \left(W^{\mathbf{k}}_{i,j}\right)^2 = \lambda \sum_k \left\|\boldsymbol{W}^{\mathbf{k}}\right\|_F^2$
- Encourage simple models
- Avoid overfitting

Empirical loss

- Work well on training set

- **Occam's Razor principle**: prefer simplest model that can well predict data.

How to efficiently solve this optimization problem?

N is the **training size** and might be very big (e.g., $N \approx 10^6$)

First-order iterative methods (gradient descent, steepest descent)

Use the **gradient** (first derivative) $\mathrm{g} = \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ to update parameters

Second-order iterative methods (Newton and quasi Newton methods)

Use the **Hessian** matrix (second derivative) $\mathrm{H} = \nabla^2_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ to update parameters

Gradient and Hessian matrix

□ Given an **objective function** $J(\theta)$ with $\theta = [\theta_1, \theta_2, \dots, \theta_P]$

- For DL models
  - θ includes **weight matrices**, **filters**, and **biases** which are trainable model parameters.
  - P is the number of **trainable parameters** (P could be 20×10^6).
  - $J(\theta)$ is the loss function over a training set.

□ Gradient $\mathrm{g} = \nabla J(\theta)$ is the **first order derivative** and defined as

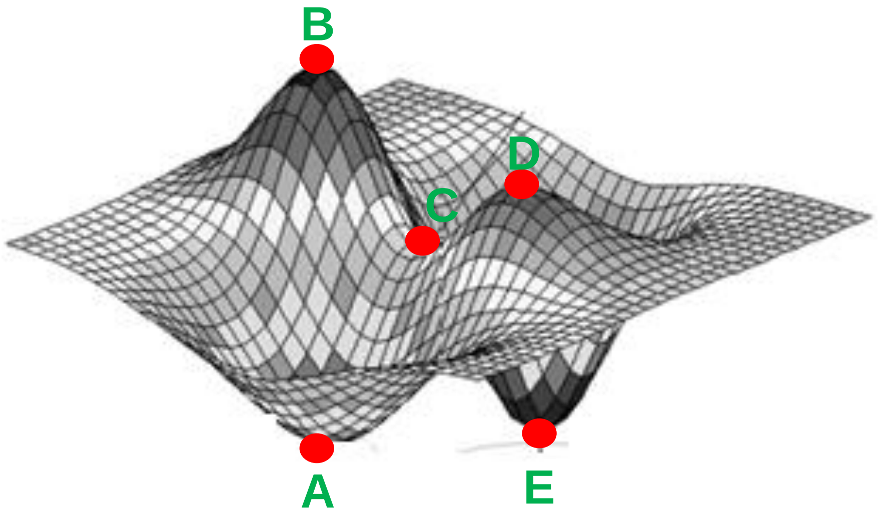
- $$\nabla J(\theta) = g = \begin{bmatrix} \frac{\partial J}{\partial \theta_1}(\theta) \\ \dots\ \dots\ \dots\ . \\ \frac{\partial J}{\partial \theta_P}(\theta) \end{bmatrix}$$

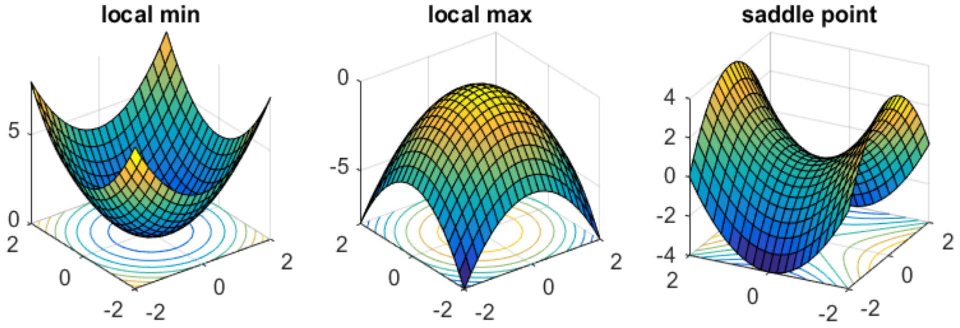
□ Hessian matrix $H(\theta)$ is the **second order derivative** $\nabla^2 J(\theta)$ and defined as

- $$\nabla^2 J(\theta) = H(\theta) = \begin{bmatrix} \frac{\partial^2 J}{\partial \theta_1 \partial \theta_1}(\theta) & \dots & \dots & \frac{\partial^2 J}{\partial \theta_1 \partial \theta_j}(\theta) & \dots & \frac{\partial^2 J}{\partial \theta_1 \partial \theta_P}(\theta) \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \frac{\partial^2 J}{\partial \theta_i \partial \theta_1}(\theta) & \dots & \dots & \frac{\partial^2 J}{\partial \theta_i \partial \theta_j}(\theta) & \dots & \frac{\partial^2 J}{\partial \theta_i \partial \theta_P}(\theta) \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \frac{\partial^2 J}{\partial \theta_P \partial \theta_1}(\theta) & \dots & \dots & \frac{\partial^2 J}{\partial \theta_P \partial \theta_j}(\theta) & \dots & \frac{\partial^2 J}{\partial \theta_P \partial \theta_P}(\theta) \end{bmatrix}$$

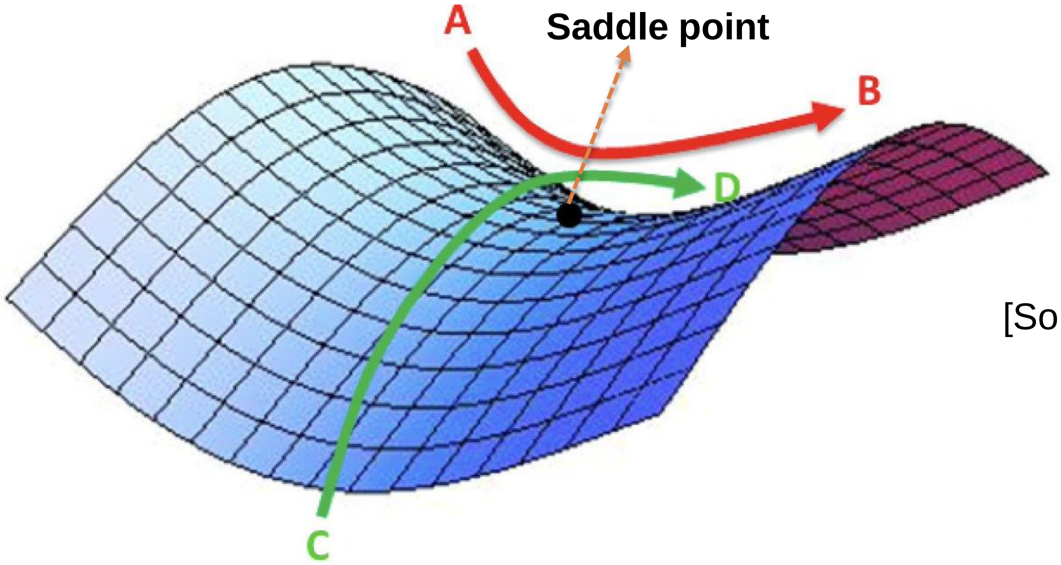
Local minima-maxima and saddle point

- Given an **objective function** $J(\theta)$ with $\theta = [\theta_1, \theta_2, \dots, \theta_P]$
  - θ is said to be a **critical point** if $\nabla J(\theta) = \mathbf{0}$ (vector $\mathbf{0}$)
- Let us denote the **set of eigenvalues** of Hessian matrix $\nabla^2 J(\theta) = H(\theta)$ by
  - $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_P$
- **Local minima**
  - $\nabla J(\theta) = \mathbf{0}$ and $\nabla^2 J(\theta) = H(\theta) \succ 0$ (positive semi-definite matrix)
  - $0 \le \lambda_1 \le \lambda_2 \le \cdots \le \lambda_P$
- **Local maxima**
  - $\nabla J(\theta) = \mathbf{0}$ and $\nabla^2 J(\theta) = H(\theta) \prec 0$ (negative semi-definite matrix)
  - $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_P \le 0$
- **Saddle point**
  - $\nabla J(\theta) = \mathbf{0}$ and $\nabla^2 J(\theta) = H(\theta) \prec 0$ (indefinite matrix)
  - $\lambda_1 \le \lambda_2 \le \cdots < 0 < \cdots \le \lambda_P$





More on saddle point (Forum discussion)



[Source: Internet]

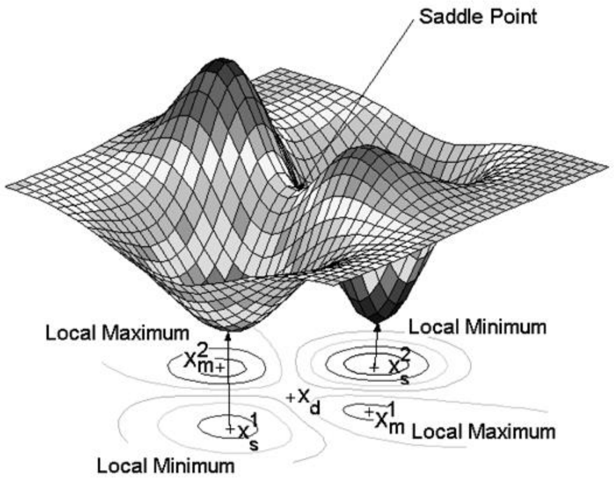
$$f(x) = f(x_1, x_2) = x_1^2 - x_2^2$$

Gradient $g = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 \\ -2x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ → a **critical point** $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

Hessian matrix is $H = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$

Two eigenvalues $\lambda_1 = -2 < 0 < 2 = \lambda_2 \rightarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ is a **saddle point**.

Numbers of local minima vs saddle points

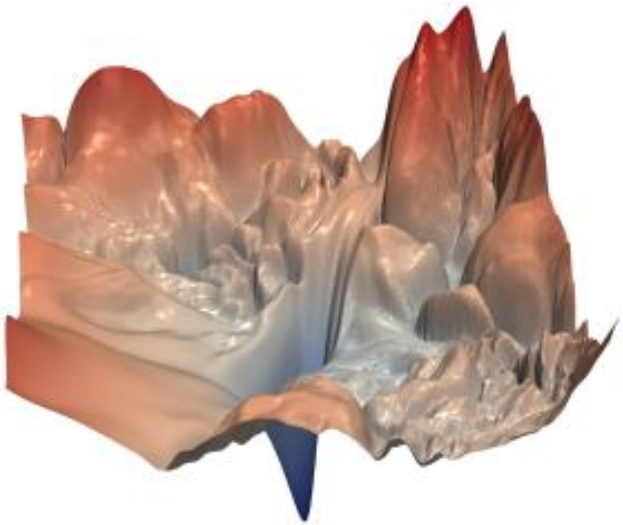


- We assume to pick randomly a training set
  - The Hessian matrix $H(\theta)$ is a random matrix with **random eigenvalues** $\lambda_1, \lambda_2, \dots, \lambda_P$
  - We assume that $\mathbb{P}(\lambda_1 \geq 0) = \mathbb{P}(\lambda_2 \geq 0) = \cdots = \mathbb{P}(\lambda_P \geq 0) = 0.5$

- Therefore, we have
  - $\mathbb{P}(minima) = \mathbb{P}(\lambda_1 \geq 0)\mathbb{P}(\lambda_2 \geq 0) \dots \mathbb{P}(\lambda_P \geq 0) = 0.5^P$
  - $\mathbb{P}(maxima) = \mathbb{P}(\lambda_1 \leq 0)\mathbb{P}(\lambda_2 \leq 0) \dots \mathbb{P}(\lambda_P \leq 0) = 0.5^P$
  - $\mathbb{P}(saddle\ point) = 1 - \mathbb{P}(minima) - \mathbb{P}(maxima) = 1 - 0.5^{P-1}$

- The ratio of **#local minima/maxima against #saddle points**
  - **#local-minima:#local-maxima:#saddle-point=**$1: 1: (2^P - 2)$
  - Number of **saddle points** is even **exponentially much more** than that of **local minima/maxima**

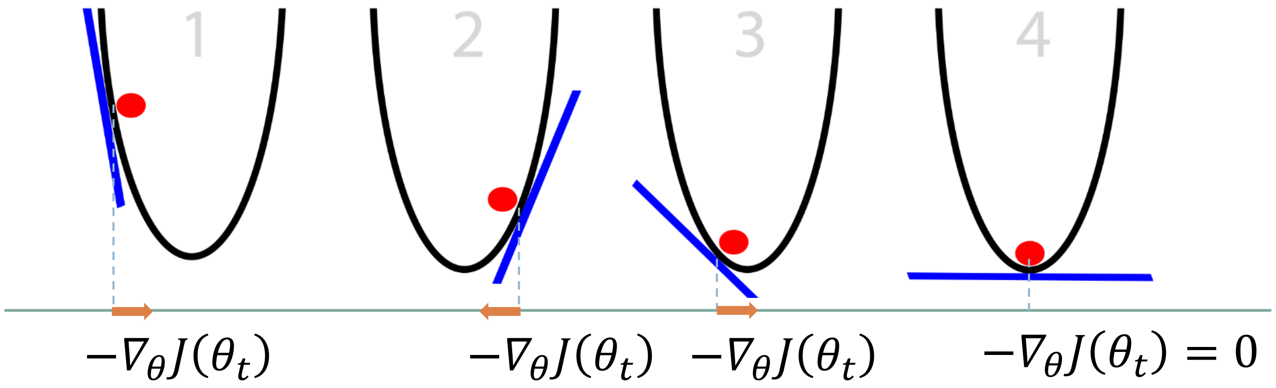
The loss surface of DL optimization problem



Loss surface of a ResNet without skip connection [Hao Li et al., NeurIPS 2017]

- □ The **optimization problem** in **deep learning:**
  - ○ $\min_{\theta} J(\theta) \coloneqq L(D;\theta) \coloneqq \frac{1}{N}\sum_{i=1}^{N} \ell(f(x_i;\theta), y_i) = -\frac{1}{N}\sum_{n=1}^{N} \log \frac{\exp\{h_{y_i}^{L}(x_i)\}}{\sum_{m=1}^{M} \exp\{h_{m}^{L}(x_i)\}}$
- □ A very **complex** and **complicated** objective function
  - ○ Highly **non-linear** and **non-convex** function
  - ○ The **loss surface** is very **complex**
  - ○ Many local minima points, but the number of saddle points is even **exponentially much more**

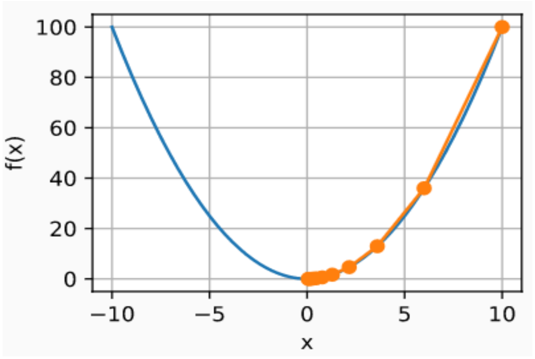
Gradient descend (Forum discussion)


1
2
3
4
$-\nabla_\theta J(\theta_t)$
$-\nabla_\theta J(\theta_t)$
$-\nabla_\theta J(\theta_t)$
$-\nabla_\theta J(\theta_t) = 0$

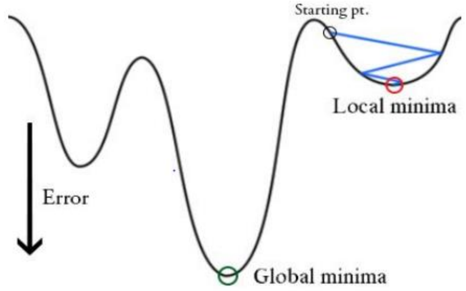
- ❑ We need to solve
  - ○ $\min_{\theta} J(\theta)$

we are updating the parameter to the opposute direction of the gradient!!

- ❑ Follow to **the opposite side** of the current gradient
  - ○ $\theta_{t+1} = \theta_t - \eta \nabla_\theta J(\theta_t)$ where $\boldsymbol{\eta > 0}$ is the **learning rate**.
- ❑ Guarantee to converge to a **global minima** if $J(.)$ is **convex**.
- ❑ Get stuck in a **local minima** or **saddle points** if $J(.)$ is non-convex.

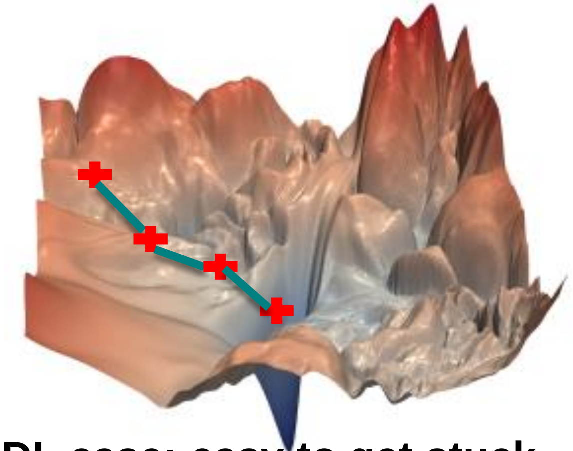


Convex case



(Source: www.cs.ubc.ca)

Non-convex case



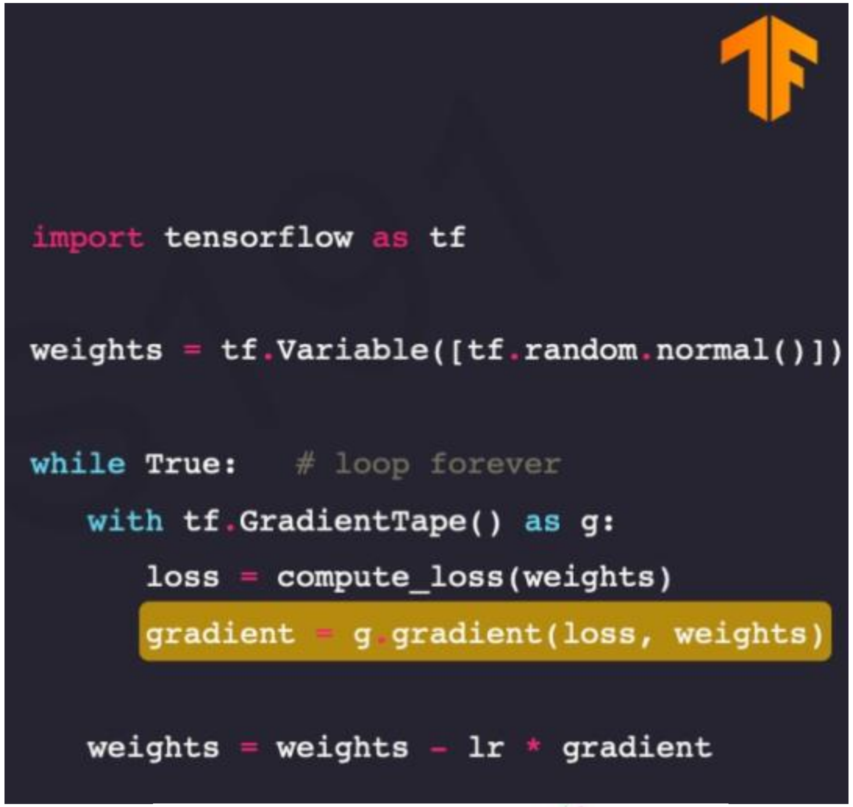
DL case: easy to get stuck in saddle points

Gradient descend

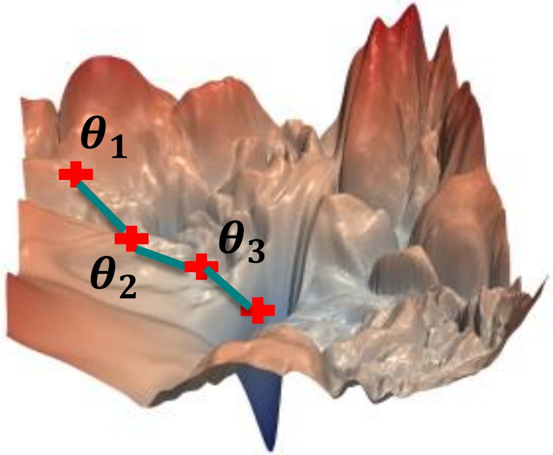
Algorithm

- ❑ **Input**: objective function $\boldsymbol{J(\theta)}$
- ❑ **Output**: optimal solution $\boldsymbol{\theta}^*$

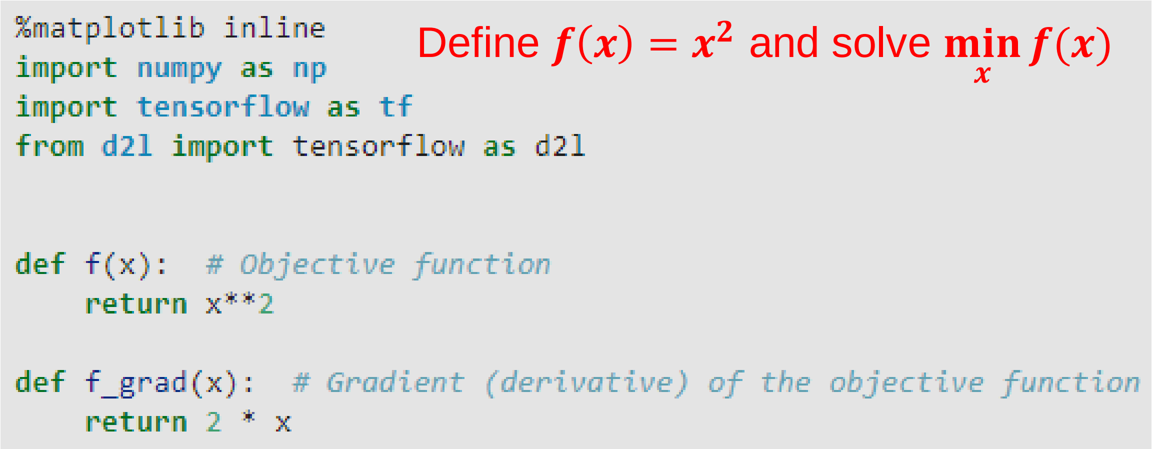
```
1.  Initialize parameters $\theta_0$ randomly $\sim N(0, \sigma^2)$.
2.  for t=1 to T
3.          Compute gradients $\nabla_\theta J(\theta_t) = \frac{\partial J}{\partial \theta}(\theta_t)$
4.          Update $\theta_{t+1} = \theta_t - \eta_t \nabla_\theta J(\theta_t)$
5.  Return $\theta^* = \theta_{T+1}$
```



```
import tensorflow as tf

weights = tf.Variable([tf.random.normal()])

while True:   # loop forever
    with tf.GradientTape() as g:
        loss = compute_loss(weights)
        gradient = g.gradient(loss, weights)

    weights = weights - lr * gradient
```

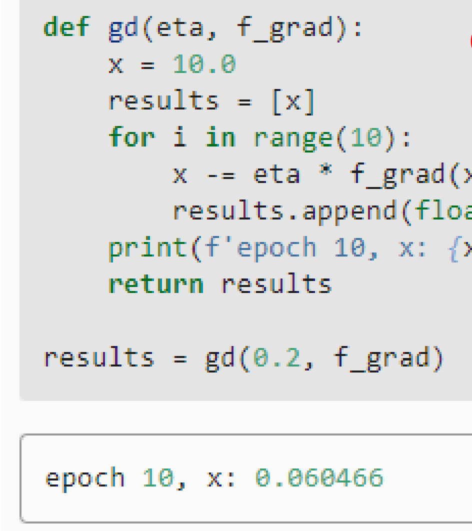


Gradient descent with TF



Define $f(x) = x^2$ and solve $\min_{x} f(x)$

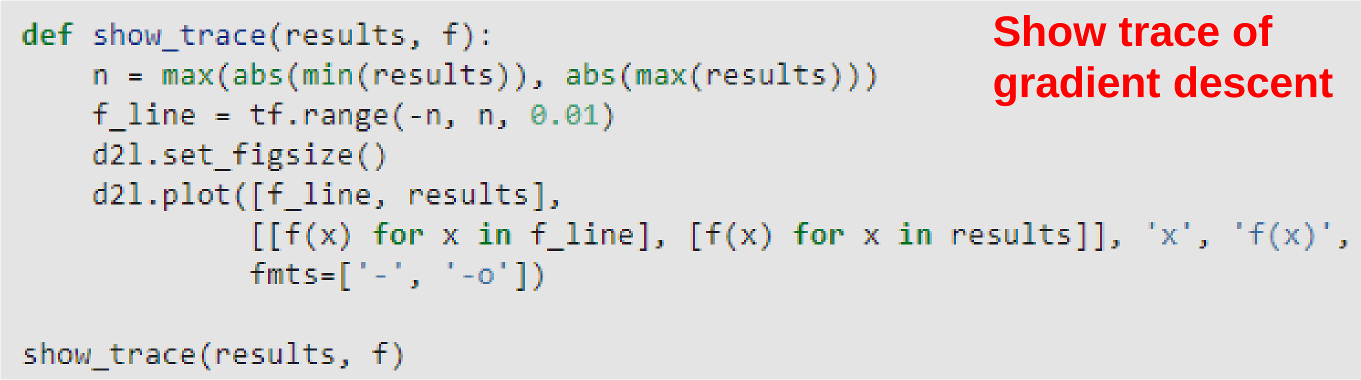
```
%matplotlib inline
import numpy as np
import tensorflow as tf
from d2l import tensorflow as d2l


def f(x):  # Objective function
    return x**2

def f_grad(x):  # Gradient (derivative) of the objective function
    return 2 * x
```



Gradient descent

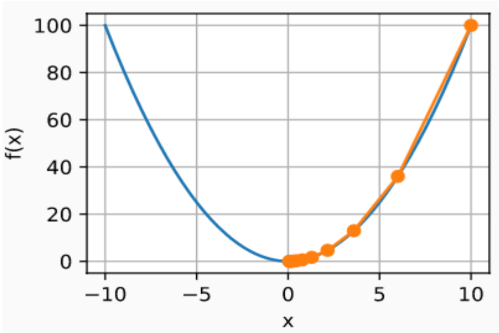
```
def gd(eta, f_grad):
    x = 10.0
    results = [x]
    for i in range(10):
        x -= eta * f_grad(x)
        results.append(float(x))
    print(f'epoch 10, x: {x:f}')
    return results

results = gd(0.2, f_grad)
```

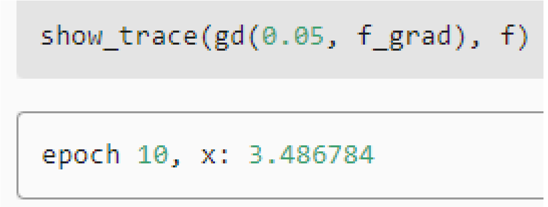
```
epoch 10, x: 0.060466
```



Show trace of gradient descent

```
def show_trace(results, f):
    n = max(abs(min(results)), abs(max(results)))
    f_line = tf.range(-n, n, 0.01)
    d2l.set_figsize()
    d2l.plot([f_line, results],
             [[f(x) for x in f_line], [f(x) for x in results]], 'x', 'f(x)',
             fmts=['-', '-o'])

show_trace(results, f)
```

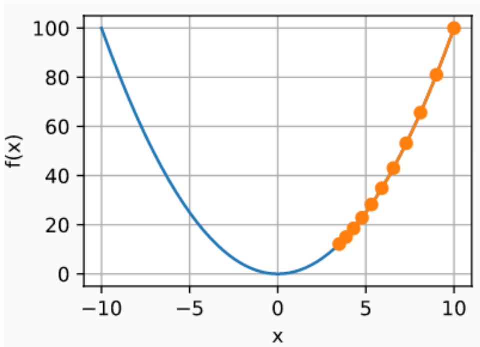


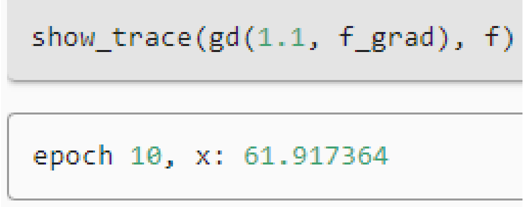


```
show_trace(gd(0.05, f_grad), f)
```

```
epoch 10, x: 3.486784
```

Good learning rate η

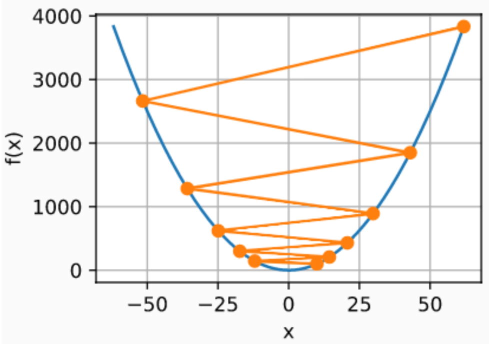




```
show_trace(gd(1.1, f_grad), f)
```

```
epoch 10, x: 61.917364
```

Too high rate η



[Source: Dive into Deep Learning]

Gradient descent for deep learning

- For **training deep nets**, we need to solve
  - $\min_{\theta} L(D;\theta) := \frac{1}{N}\sum_{i=1}^{N} l(x_i, y_i; \theta)$

  where $l(x_i, y_i; \theta) = -\log p(y = y_i | x_i) = -\log \frac{\exp\{h_{y_i}^{L}(x_i)\}}{\sum_{m=1}^{M} \exp\{h_m^{L}(x_i)\}}$ is the loss incurred by (x_i, y_i).
- Gradient descent update
  - $\theta_{t+1} = \theta_t - \eta \nabla_\theta L(D;\theta_t) = \theta_t - \frac{\eta}{N}\sum_{i=1}^{N} \nabla_\theta\, l(x_i, y_i; \theta_t)$ where $\boldsymbol{\eta} > \mathbf{0}$ is a learning rate.
  - To compute the gradient $\nabla_\theta L(D;\theta_t) = \frac{1}{N}\sum_{i=1}^{N} \nabla_\theta\, l(x_i, y_i; \theta_t)$, we need to go through **all data points** in D → the **computational cost** is $O(N)$.
- This is very **computationally expensive** for big datasets ($N \approx 10^6$).
- How to **estimate the gradient** $\nabla_\theta L(D;\theta_t)$ more efficiently?

Stochastic gradient descent (Forum discussion)

- The **optimization problem** in **deep learning** has the form
  - $\min_{\theta} L(D;\theta) := \frac{1}{N}\sum_{i=1}^{N} l(x_i, y_i; \theta)$
- Evaluation of the **full gradient** is **expensive**. We want to just **estimate** this gradient
  - Sample a mini-batch $\boldsymbol{i_1, i_2, \ldots, i_b \sim Uni(\{1, 2, \ldots, N\})}$ where b is the mini-batch (batch) size.
    - The batch size is usually $32, 64, 128, 256$, and so on.
  - Construct $\tilde{L}(\theta) := \frac{1}{b}\sum_{k=1}^{b} l(x_{i_k}, y_{i_k}; \theta)$ as the average loss of those in the current batch.
  - $E[\nabla_\theta \tilde{L}(\theta_t)] = \nabla_\theta L(D;\theta_t)$
    - $\nabla_\theta \tilde{L}(\theta_t) = \frac{1}{b}\sum_{k=1}^{b} \nabla_\theta l(x_{i_k}, y_{i_k}; \theta_t)$ is **unbiased** estimation of $\nabla_\theta L(D;\theta_t)$
    - $O(b)$ compares to $O(N)$.
- The update rule of SGD
  - $\theta_{t+1} = \theta_t - \eta_t \nabla_\theta \tilde{L}(\theta_t)$ with learning rate $\boldsymbol{\eta_t \propto O(\frac{1}{t})}$
  - We use $\nabla_\theta \tilde{L}(\theta_t)$ as an **unbiased estimate** of the full gradient $\nabla_\theta L(D;\theta)$
  - How to compute $\nabla_\theta \tilde{L}(\theta_t)$ efficiently for **deep networks**?

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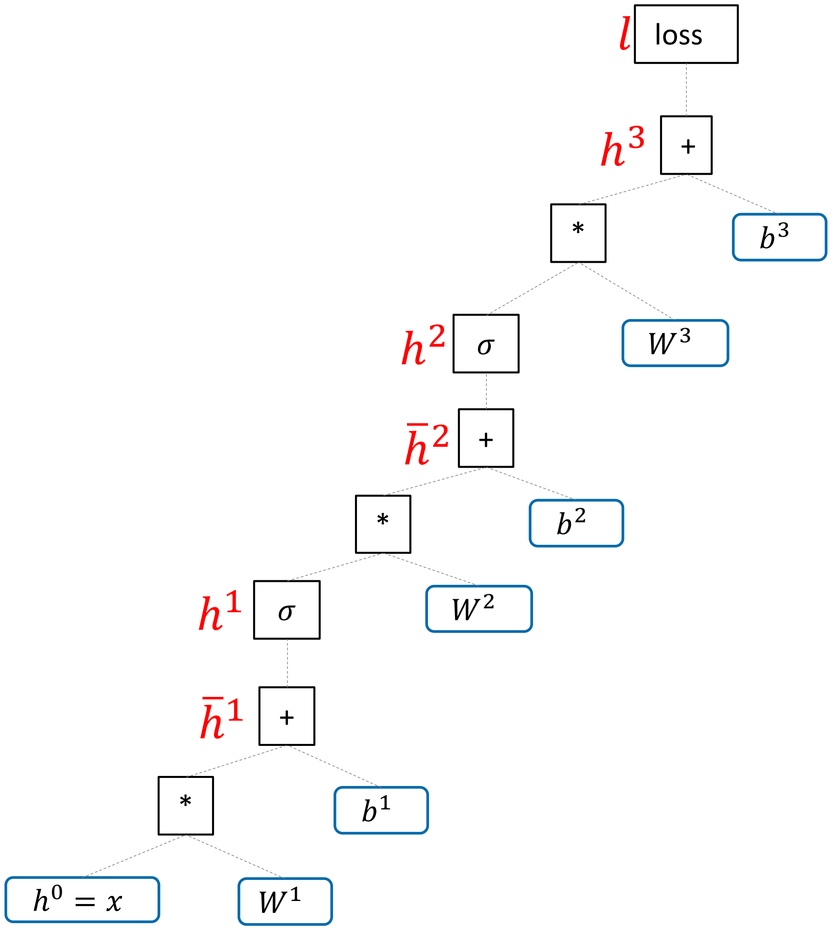
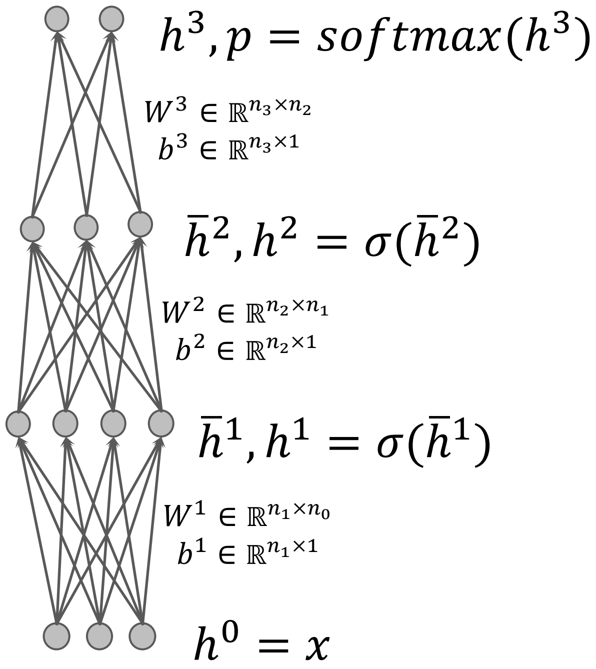
Back propagation in feed-forward neural networks

Back propagation




$h^3, p = softmax(h^3)$
$W^3 \in \mathbb{R}^{n_3 \times n_2}$
$b^3 \in \mathbb{R}^{n_3 \times 1}$
$\bar{h}^2, h^2 = \sigma(\bar{h}^2)$
$W^2 \in \mathbb{R}^{n_2 \times n_1}$
$b^2 \in \mathbb{R}^{n_2 \times 1}$
$\bar{h}^1, h^1 = \sigma(\bar{h}^1)$
$W^1 \in \mathbb{R}^{n_1 \times n_0}$
$b^1 \in \mathbb{R}^{n_1 \times 1}$
$h^0 = x$

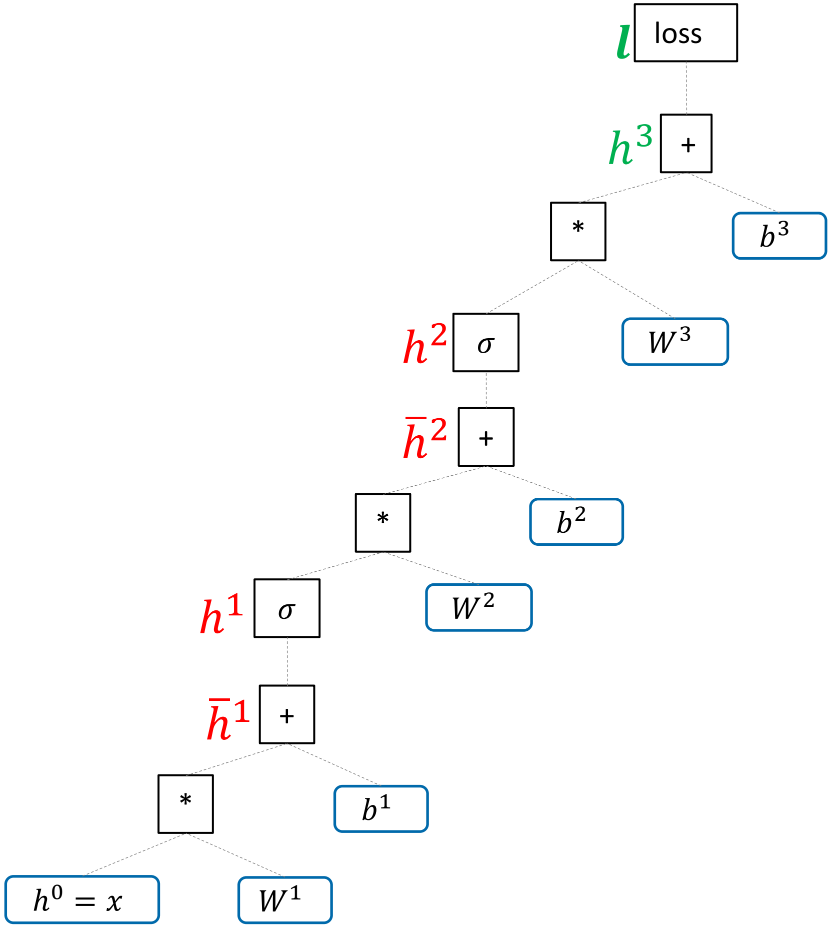
- □ Given a data point and label pair (x, y)
  - ○ $l(x, y; \theta) = -\log \frac{\exp\{h_y^3(x)\}}{\sum_{m=1}^{M} \exp\{h_m^3(x)\}}$
- □ What are the derivatives?
  - ○ $\nabla_{W^k} l(x, y; \theta)$ and $\nabla_{b^k} l(x, y; \theta)$ for $k = 1,2,3$?
  - ○ Using **back propagation** to compute these derivatives conveniently.
- □ Update the model using SGD with the derivatives.

Back propagation

From loss to h^3

$f(x,y,z) = \log(\exp(x) + \exp(y) + \exp(z))$

$\nabla f = [f'_x, f'_y, f'_z] = softmax([x,y,z])$



□ $l(x,y;\theta) = -\log \frac{\exp\{h_y^3(x)\}}{\sum_{m=1}^{M} \exp\{h_m^3(x)\}} =$
$-h_y^3(x) + \log[\sum_{m=1}^{M} \exp\{h_m^3(x)\}] =$
$-\sum_{m=1}^{M} \mathbf{1}_{m=y} h_m^3 + \log[\sum_{m=1}^{M} \exp\{h_m^3\}]$

where $\mathbf{1}_{m=y} = \mathbf{1}$ if $\boldsymbol{m} = \boldsymbol{y}$ and $\mathbf{0}$ otherwise.

□ $\frac{\partial l}{\partial h_m^3} = -\mathbf{1}_{m=y} + \frac{exp\{h_m^3\}}{\sum_{k=1}^{M} exp\{h_k^3\}}$

□ $g^3 = \frac{\partial l}{\partial h^3} = -\mathbf{1}_y + softmax(h^3) =$
$= p^T - \mathbf{1}_y$

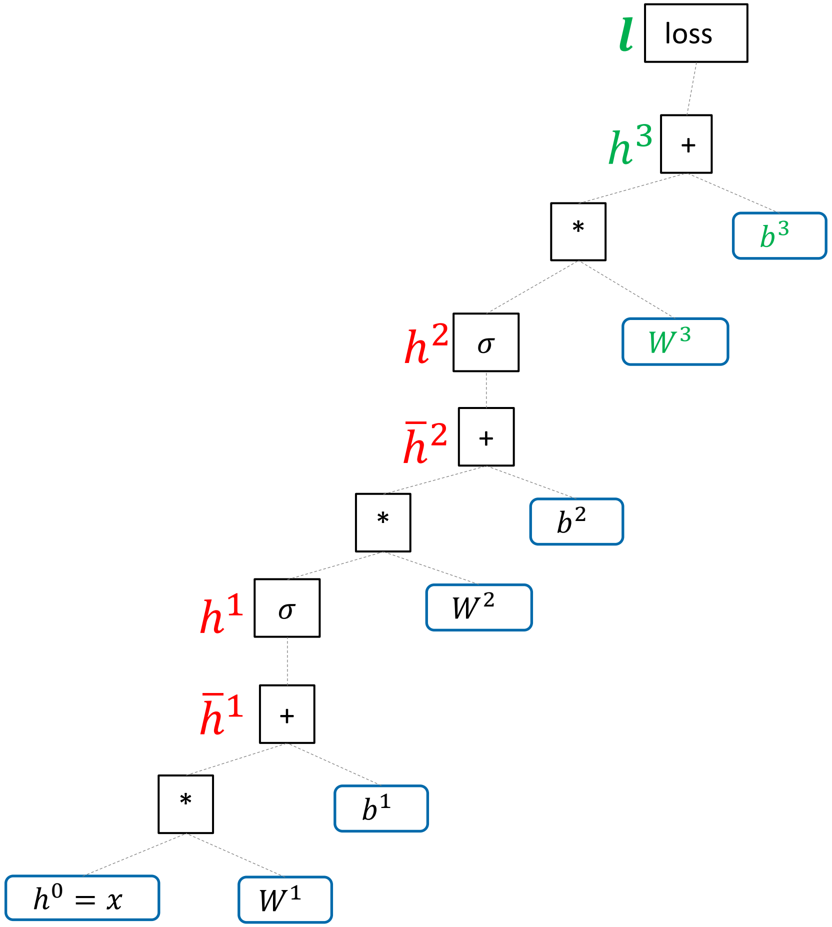
where $\mathbf{1}_y$ is the corresponding one-hot vector.

- g^3 has a shape $[1 \times n_3]$.

one hot vector of the true ground label, e.g. [0,0,1]

Back propagation

From loss to W^3, b^3



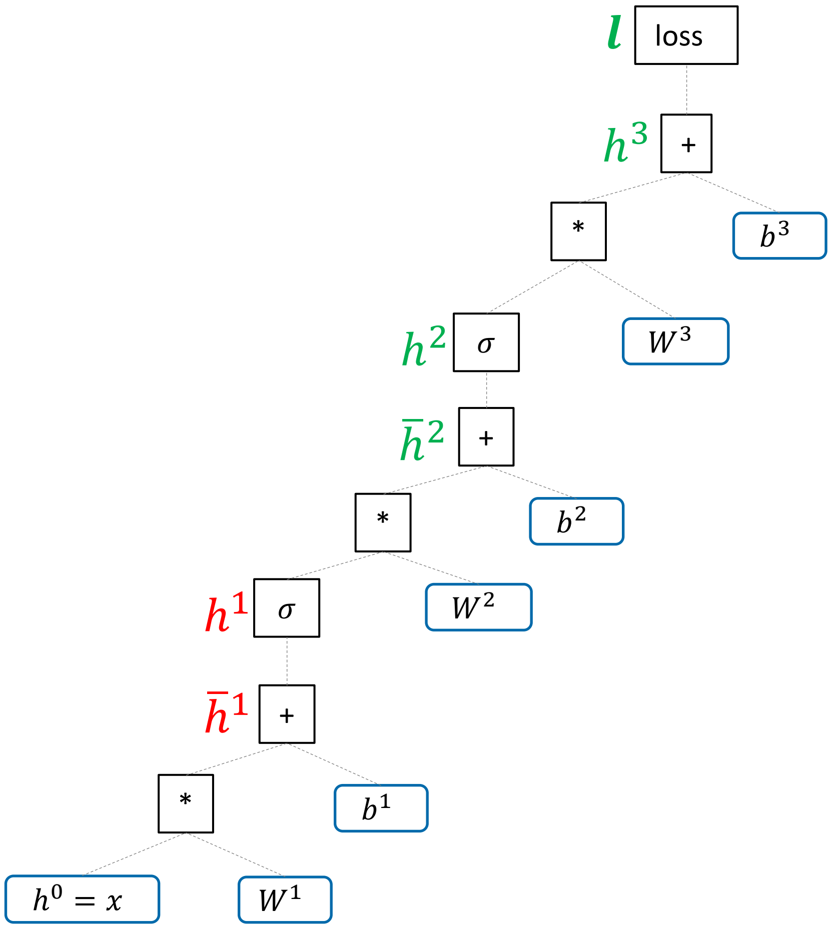
- □ $h^3 = W^3 h^2 + b^3$

- □ $$\frac{\partial l}{\partial W^3} = \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial W^3} = (g^3)^T (h^2)^T$$
  - ○ $[n_3 \times 1] \times [1 \times n_2] \rightarrow [n_3 \times n_2]$

- □ $$\frac{\partial l}{\partial b^3} = \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial b^3} = g^3$$
  - ○ $[1 \times n_3]$

Back propagation

From loss to h^2 and $\bar{h}^2$



□ $h^3 = W^3 h^2 + b^3$

□ $\boldsymbol{g^2 = \frac{\partial l}{\partial h^2} = \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial h^2} = g^3 W^3}$

- ○ $[1 \times n_3] \times [n_3 \times n_2] \to [1 \times n_2]$

□ $\boldsymbol{h^2 = \sigma(\bar{h}^2)}$ (element-wise activation)

□ $\boldsymbol{\frac{\partial h^2}{\partial \bar{h}^2} = diag(\sigma'(\bar{h}^2))}$

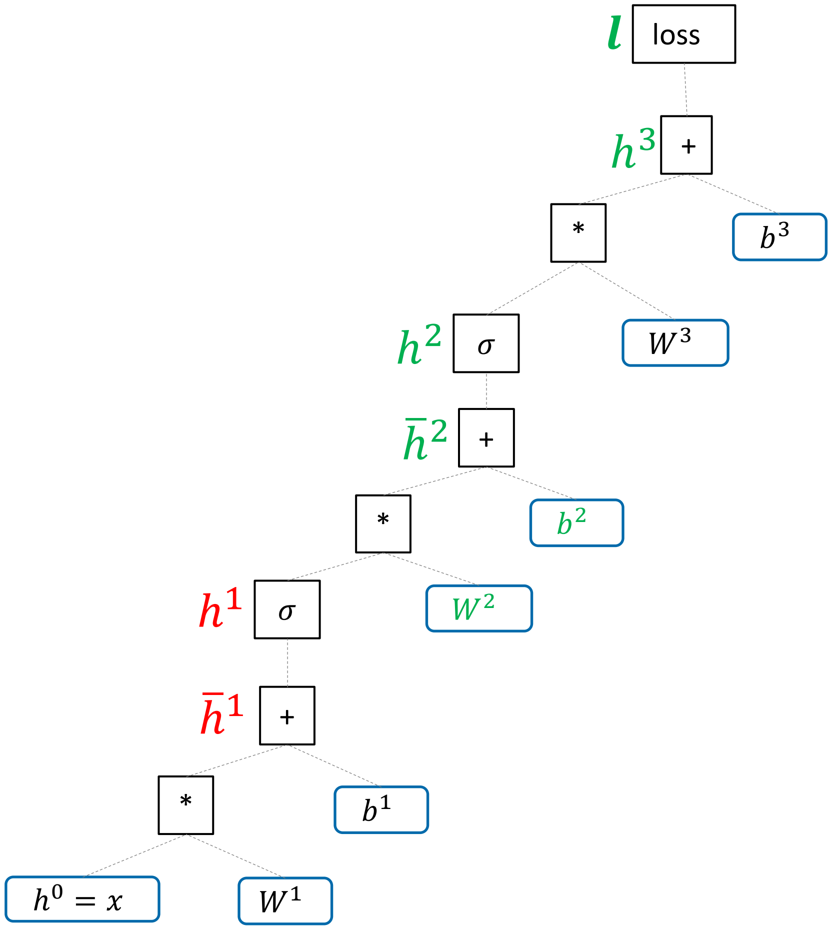
- ○ $\sigma'(\bar{h}^2)$ is **element-wise derivative** and $diag(u)$ is the **diagonal matrix** corresponding to the **vector** $\boldsymbol{u}$ (the diagnose is u and others are zeros).

□ $\boldsymbol{\bar{g}^2 = \frac{\partial l}{\partial \bar{h}^2} = \frac{\partial l}{\partial h^2} \cdot \frac{\partial h^2}{\partial \bar{h}^2} = g^2 diag(\sigma'(\bar{h}^2))}$

- ○ $[1 \times n_2] \times [n_2 \times n_2] \to [1 \times n_2]$

Back propagation

From loss to W^2 and b^2



□ $\bar{h}^2 = W^2 h^1 + b^2$

□ $$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{W^2}} = \frac{\partial \boldsymbol{l}}{\partial \bar{\boldsymbol{h}}^2} \cdot \frac{\partial \bar{\boldsymbol{h}}^2}{\partial \boldsymbol{W^2}} = \left(\bar{\boldsymbol{g}}^2\right)^T \left(\boldsymbol{h}^1\right)^T$$

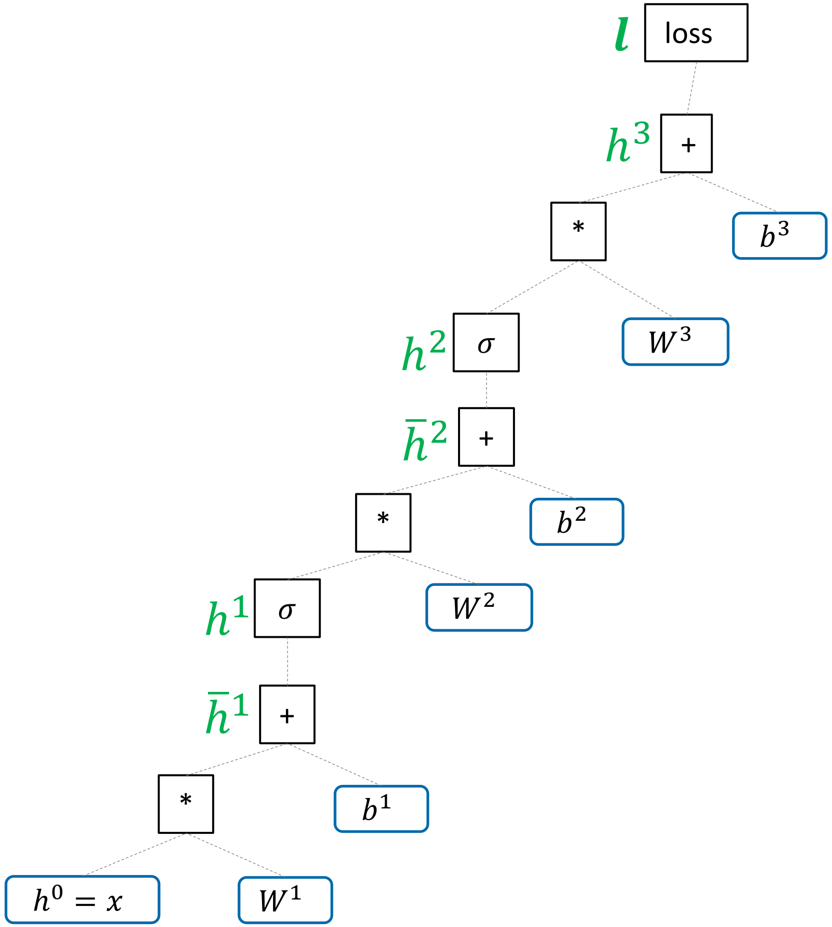
- ○ $[n_2 \times 1] \times [1 \times n_1] \rightarrow [n_2 \times n_1]$

□ $$\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{b^2}} = \frac{\partial \boldsymbol{l}}{\partial \bar{\boldsymbol{h}}^2} \cdot \frac{\partial \bar{\boldsymbol{h}}^2}{\partial \boldsymbol{b^2}} = \bar{\boldsymbol{g}}^2$$

- ○ $[1 \times n_2]$

Back propagation

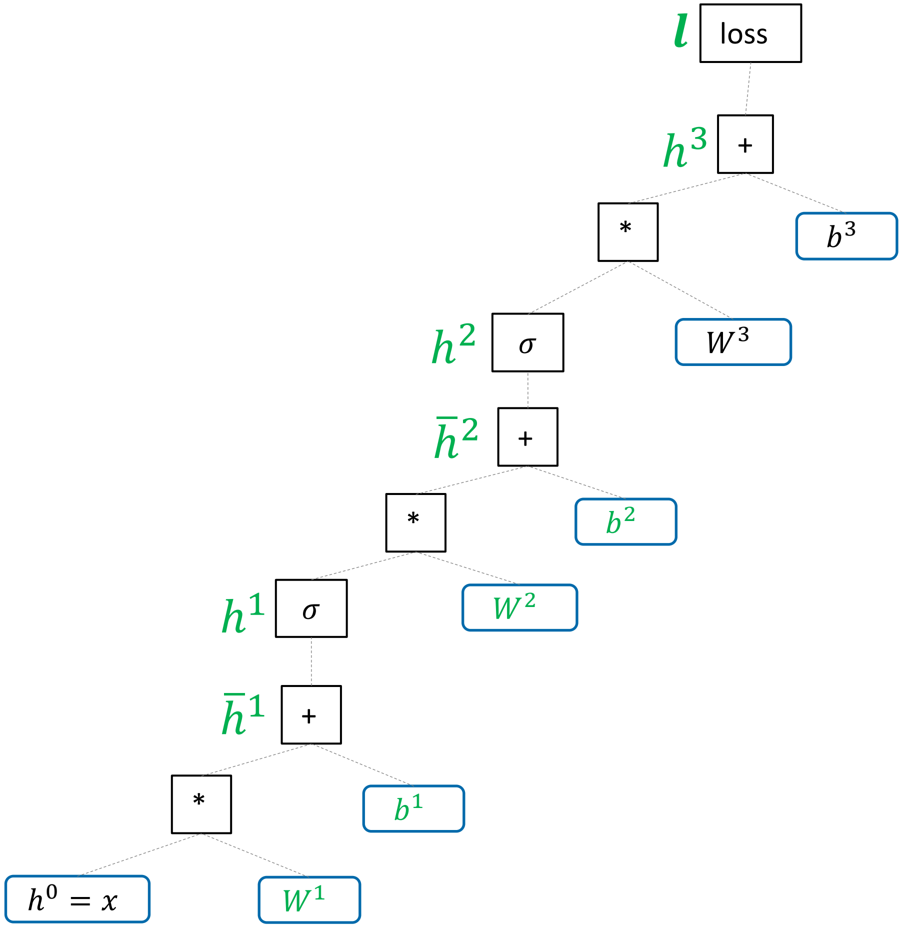
From loss to h^1 and $\bar{h}^1$



- □ $\bar{h}^2 = W^2 h^1 + b^2$
- □ $\boldsymbol{g^1 = \frac{\partial l}{\partial h^1} = \frac{\partial l}{\partial \bar{h}^2} . \frac{\partial \bar{h}^2}{\partial h^1}} = \boldsymbol{\bar{g}^2 W^2}$
  - ○ $[1 \times n_2] \times [n_2 \times n_1] \rightarrow [1 \times n_1]$
- □ $\boldsymbol{h^1 = \sigma(\bar{h}^1)}$ (element-wise activation)
- □ $\boldsymbol{\frac{\partial h^1}{\partial \bar{h}^1}} = \boldsymbol{diag(\sigma'(\bar{h}^1))}$
  - ○ $\sigma'(\bar{h}^1)$ is **element-wise derivative** and $diag(u)$ is the **diagonal matri**x corresponding to the **vector $\boldsymbol{u}$** (the diagnose is u and others are zeros).
- □ $\boldsymbol{\bar{g}^1 = \frac{\partial l}{\partial \bar{h}^1} = \frac{\partial l}{\partial h^1} . \frac{\partial h^1}{\partial \bar{h}^1}} = \boldsymbol{g^1 diag(\sigma'(\bar{h}^1))}$
  - ○ $[1 \times n_1] \times [n_1 \times n_1] \rightarrow [1 \times n_1]$

Back propagation

From loss to W^1 and b^1



□ $\bar{h}^1 = W^1 h^0 + b^1 \quad (h^0 = x)$

□ $\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{W^1}} = \frac{\partial \boldsymbol{l}}{\partial \bar{\boldsymbol{h}}^1} \cdot \frac{\partial \bar{\boldsymbol{h}}^1}{\partial \boldsymbol{W^1}} = (\bar{\boldsymbol{g}}^1)^T (\boldsymbol{h}^0)^T$

- ○ $[n_1 \times 1] \times [1 \times d] \rightarrow [n_1 \times d]$

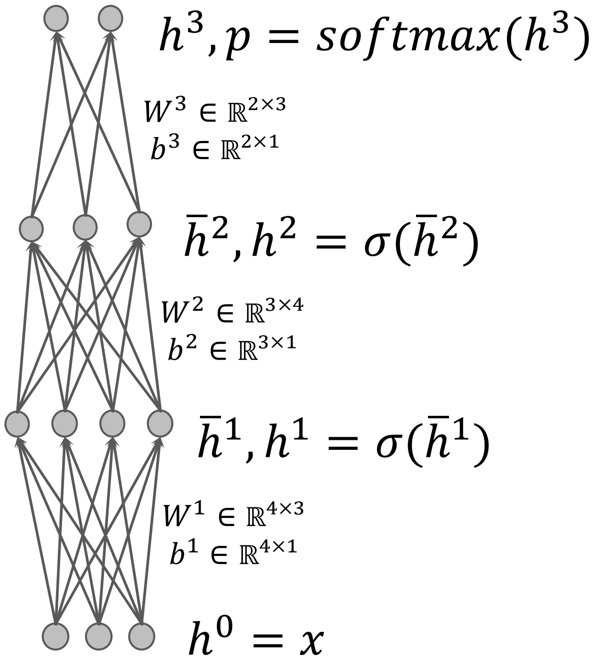
□ $\frac{\partial \boldsymbol{l}}{\partial \boldsymbol{b^1}} = \frac{\partial \boldsymbol{l}}{\partial \bar{\boldsymbol{h}}^1} \cdot \frac{\partial \bar{\boldsymbol{h}}^1}{\partial \boldsymbol{b^1}} = \bar{\boldsymbol{g}}^1$

- ○ $[1 \times n_1]$

? Exercise: How to compute $\frac{\partial l}{\partial x}$?

SGD for deep learning

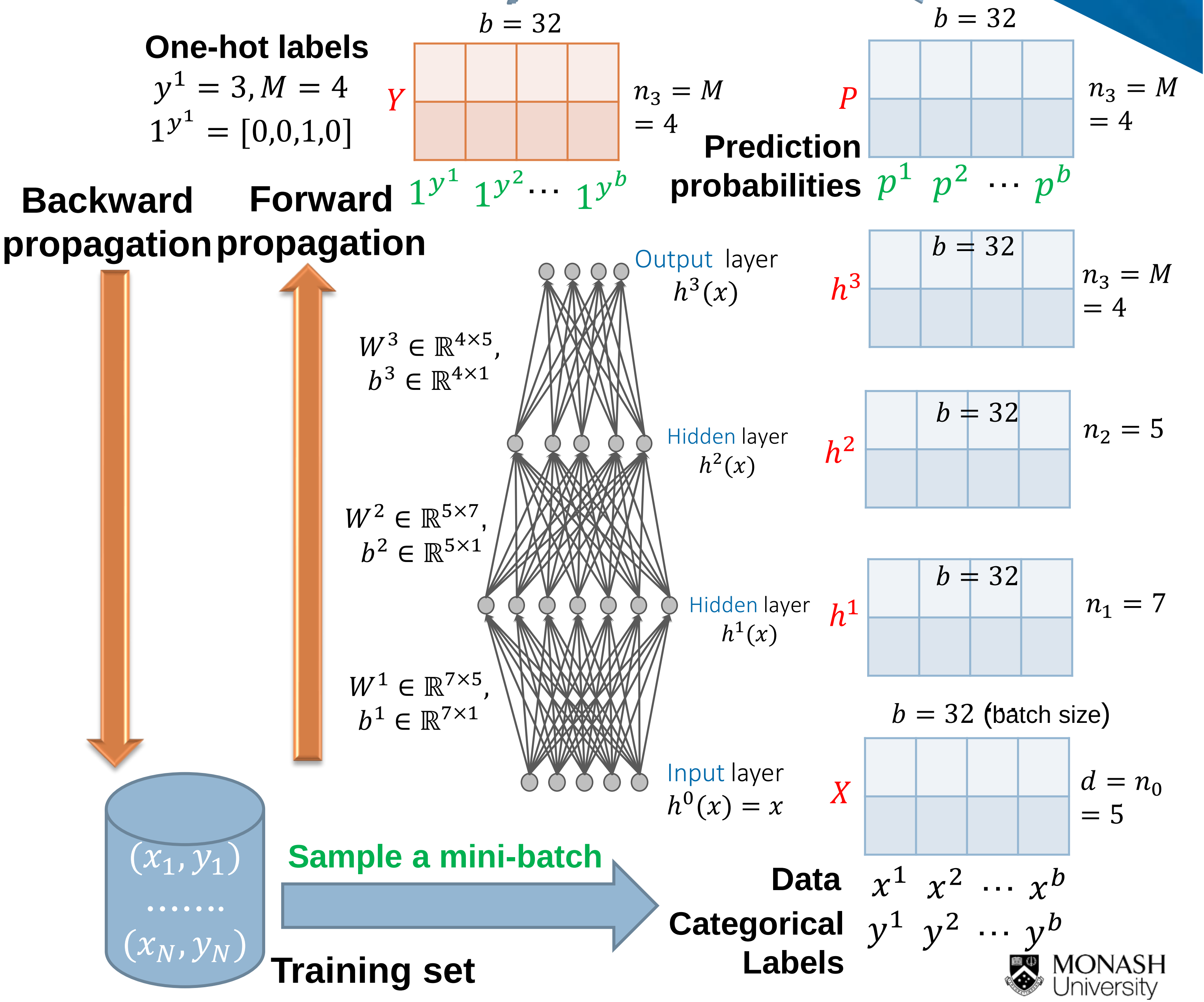
```
b = 32                              //batch size
iter_per_epoch = N/b                //epoch means one round going
                                     through all data points
n_epoch = 50                        //number of epochs
for epoch=1 to n_epoch do
    for i=1 to iter_per_epoch do
        Sample a minibatch $B = \left\{\left(x_{i_j}, y_{i_j}\right)\right\}_{j=1}^{b}$ from the training set
        Do forward propagation for B
        Do back propagation to compute $\left(\frac{\partial l}{\partial W^k}, \frac{\partial l}{\partial b^k}\right)_{k=1}^{L}$
        for k=1 to L do
            $W_k = W_k - \eta \frac{\partial l}{\partial W^k}$
            $b_k = b_k - \eta \frac{\partial l}{\partial b^k}$
```


$h^3, p = softmax(h^3)$
$W^3 \in \mathbb{R}^{2\times 3}$
$b^3 \in \mathbb{R}^{2\times 1}$
$\bar{h}^2, h^2 = \sigma(\bar{h}^2)$
$W^2 \in \mathbb{R}^{3\times 4}$
$b^2 \in \mathbb{R}^{3\times 1}$
$\bar{h}^1, h^1 = \sigma(\bar{h}^1)$
$W^1 \in \mathbb{R}^{4\times 3}$
$b^1 \in \mathbb{R}^{4\times 1}$
$h^0 = x$

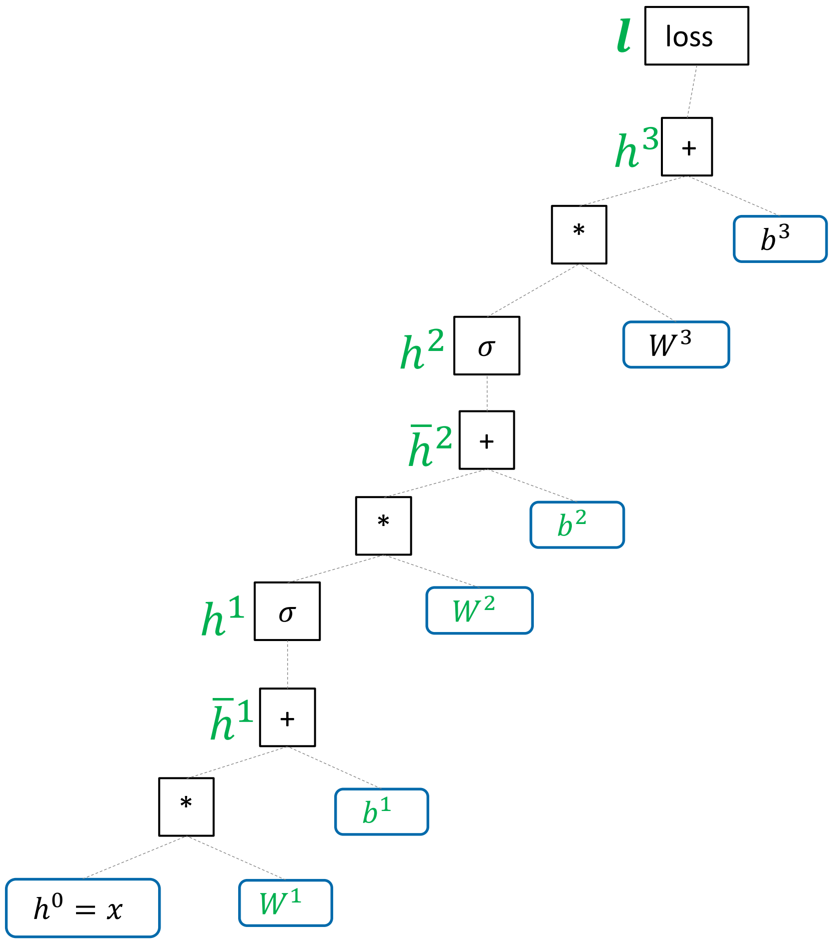
Mini-batch feed-forward

- □ Input
  - ○ Tensor X: $[n_0 = d, b]$ (b is the batch size)
- □ Hidden layer 1
  - ○ Tensor $[n_1, b]$
- □ ……………..
- □ Output layer
  - ○ Tensor P: $[n_L = M, b]$
- □ The loss of the batch
  - ○ $\frac{1}{b}\sum_{i=1}^{b} CE(1^{y_i}, p^i) = -\frac{1}{b}\sum_{i=1}^{b} \log p_{y_i}^i$
  - ○ Update **weight matrices** and **biases** to **minimize** the batch loss using back **propagation**.

$$batch\_loss = \frac{1}{b}\sum_{i=1}^{b} CE(1^{y_i}, p^i)$$



Why does deep learning need GPU and TPU?



□ Let consider

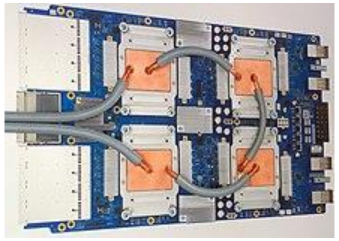
$$\frac{\partial l}{\partial W^1} = \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial h^2} \cdot \frac{\partial h^2}{\partial \bar{h}^2} \cdot \frac{\partial \bar{h}^2}{\partial h^1} \cdot \frac{\partial h^1}{\partial \bar{h}^1} \cdot \frac{\partial \bar{h}^1}{\partial W^1}$$

$$= \left[(p - 1_y) W^3 diag\left(\sigma'\left(\bar{h}^2\right)\right) W^2 diag\left(\sigma'\left(\bar{h}^1\right)\right) \right]^T \left(h^0\right)^T$$

□ For a really deep net, this **back propagation** requires many **matrix multiplications**

- ○ We need specific hardware that can parallel and significantly speed up matrix multiplication operation
- ○ **GPU** (Graphic Processing Unit) and **TPU** (Tensor Processing Unit)

GPU (Source: HelloTech)

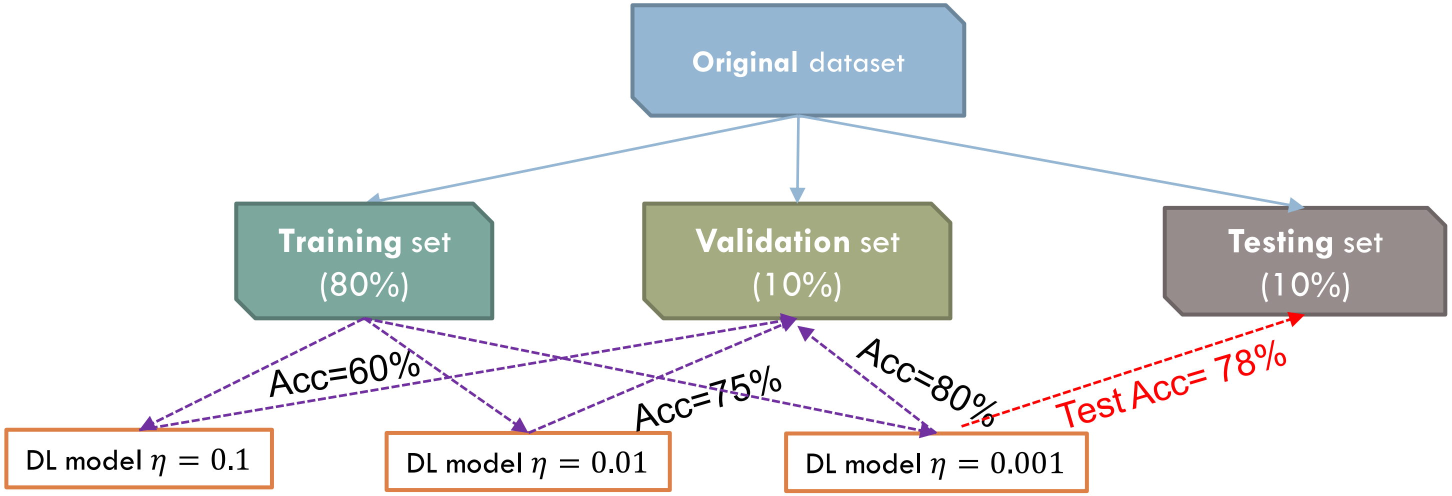


TPU (Source: Wikepedia)

Deep learning pipeline

Tuning hyper-parameters

□ We want to train our DL model on a **training set** such that the **trained model** can predict well **unseen data** in a **separate testing set**.



Original dataset

Training set (80%)

Validation set (10%)

Testing set (10%)

Acc=60%

Acc=75%

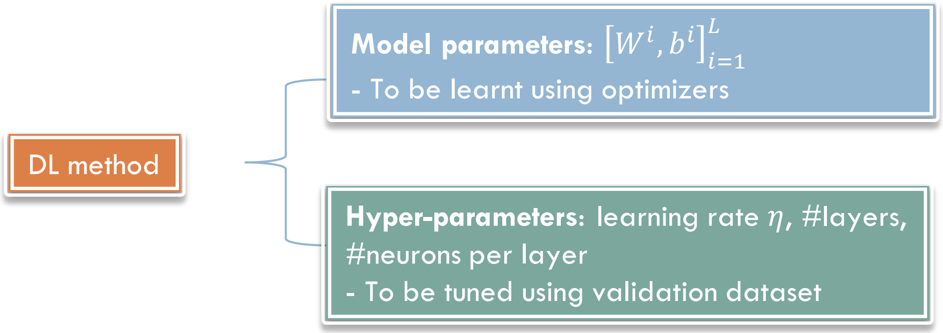
Acc=80%

Test Acc= 78%

DL model $\eta = 0.1$

DL model $\eta = 0.01$

DL model $\eta = 0.001$



DL method

Model parameters: $\left[W^i, b^i\right]_{i=1}^{L}$

- To be learnt using optimizers

Hyper-parameters: learning rate η, #layers, #neurons per layer

- To be tuned using validation dataset

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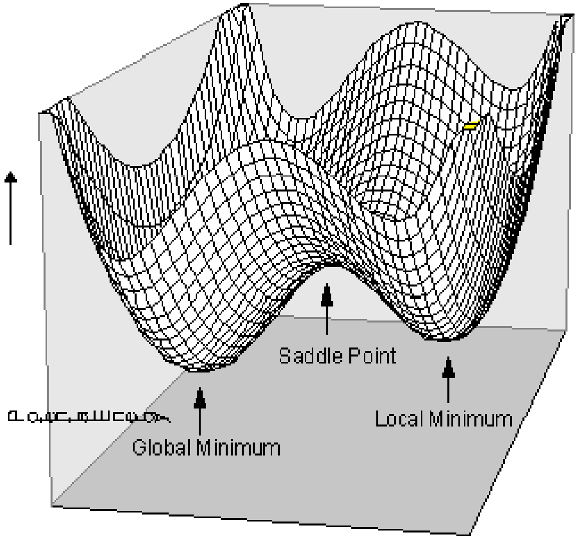
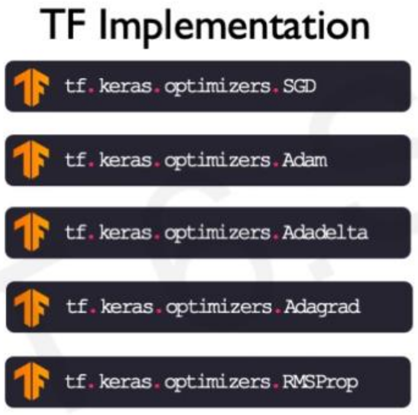
Optimizers for deep learning

Challenges of optimization for Deep Learning (Forum discussion)

- The **optimization problem** in **deep learning:**
  - $\min_{\theta} J(\theta) := L(D;\theta) := \frac{1}{N}\sum_{i=1}^{N} l(x_i, y_i; \theta) = -\frac{1}{N}\sum_{n=1}^{N} \log \frac{\exp\{h^L_{y_i}(x_i)\}}{\sum_{m=1}^{M} \exp\{h^L_m(x_i)\}}$
- A very **complex** and **complicated** objective function
  - Highly **non-linear** and **non-convex** function
  - The **loss surface** is very **complex**
  - Many local minima points, but the number of saddle points is even **exponentially much more**
- Need **efficient optimizers** to solve
  - SGD with momentum, Adagrad, Adadelta, RMSProp, Adam, and Nadam
  - They are **built-in optimizers** of TF.



(Source: Jan Jakubik)

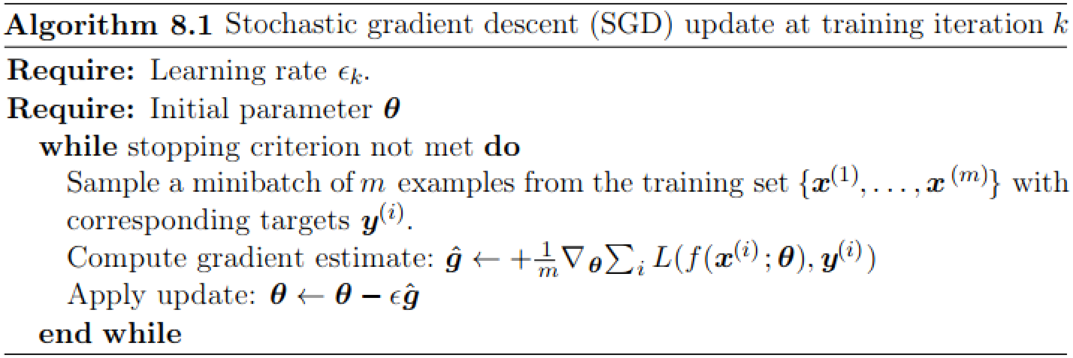


TF Implementation

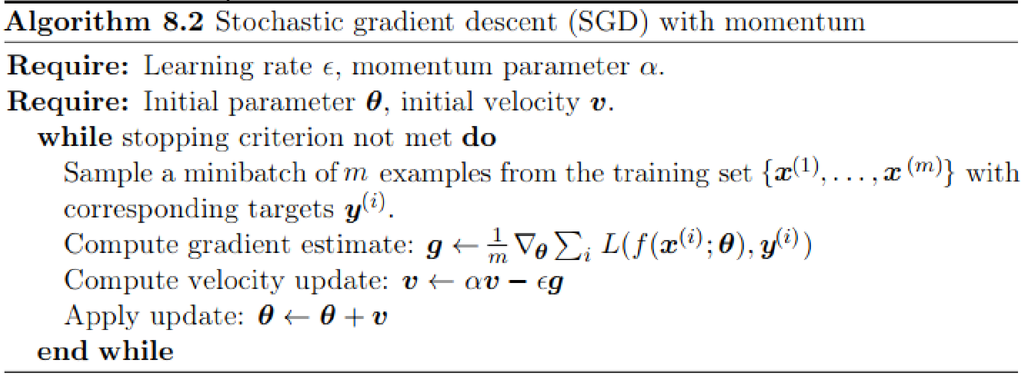
```
tf.keras.optimizers.SGD
tf.keras.optimizers.Adam
tf.keras.optimizers.Adadelta
tf.keras.optimizers.Adagrad
tf.keras.optimizers.RMSProp
```

SGD and SGD with momentum

(Source: DL book, Ch. 8)



```
Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration $k$
Require: Learning rate $\epsilon_k$.
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m}\nabla_{\boldsymbol{\theta}}\sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon\hat{\boldsymbol{g}}$
  end while
```



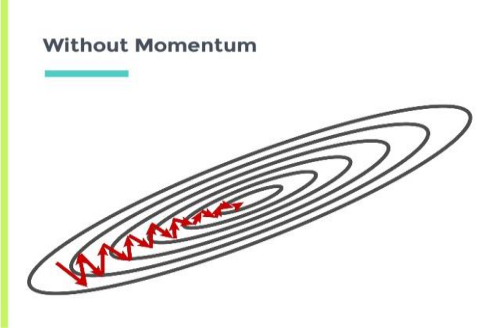
```
Algorithm 8.2 Stochastic gradient descent (SGD) with momentum
Require: Learning rate $\epsilon$, momentum parameter $\alpha$.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\boldsymbol{g} \leftarrow \frac{1}{m}\nabla_{\boldsymbol{\theta}}\sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Compute velocity update: $\boldsymbol{v} \leftarrow \alpha\boldsymbol{v} - \epsilon\boldsymbol{g}$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
  end while
```

□ SGD uses only the **gradient of the mini-batch** to update the model

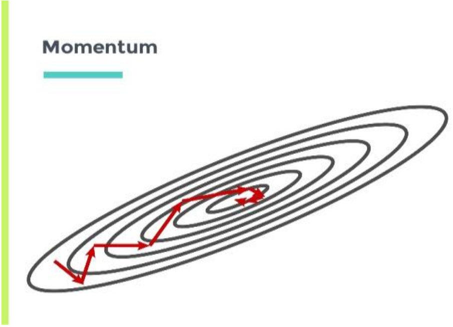
□ It is fast at first several epochs and becomes **much slower** later.

□ SGD with momentum uses a **velocity vector $\boldsymbol{v}$** which **stores the past gradients** together with the **current gradient** to speed up SGD

- ○ α is a hyper-parameter that indicates how quickly the contributions of previous gradients. In practice, this is usually set to 0.5, 0.9, and 0.99.
- ○ The momentum primarily solves 2 problems: **poor conditioning** of the Hessian matrix and **variance** in the stochastic gradient.

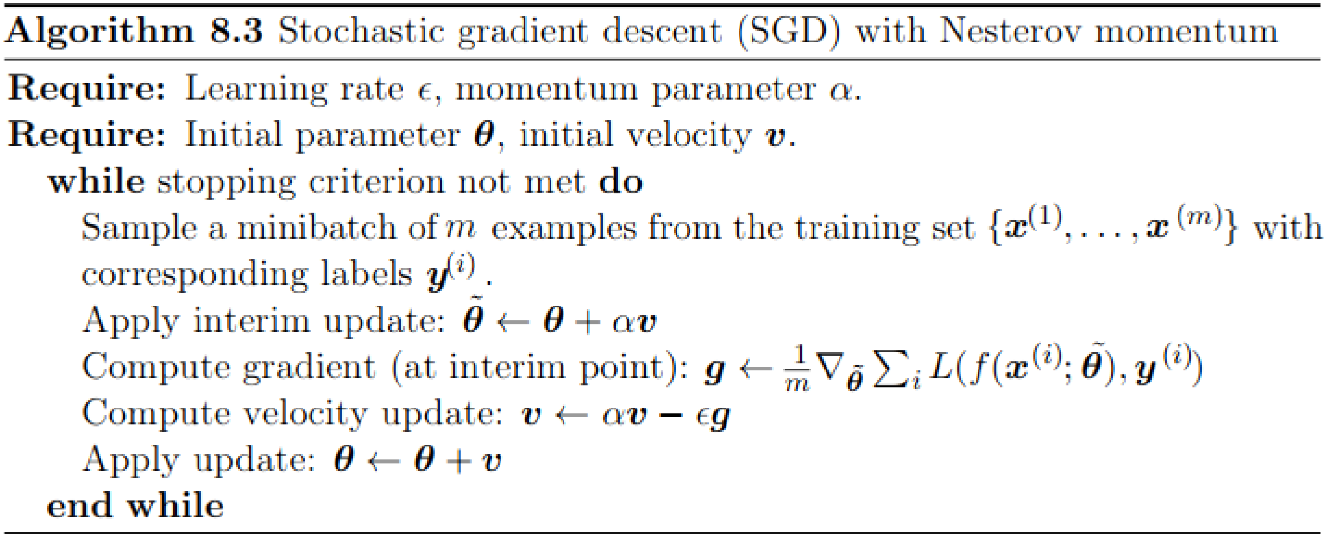


(Source: Sebastian Ruder)



SGD with Nesterov Momentum

Not in assessment

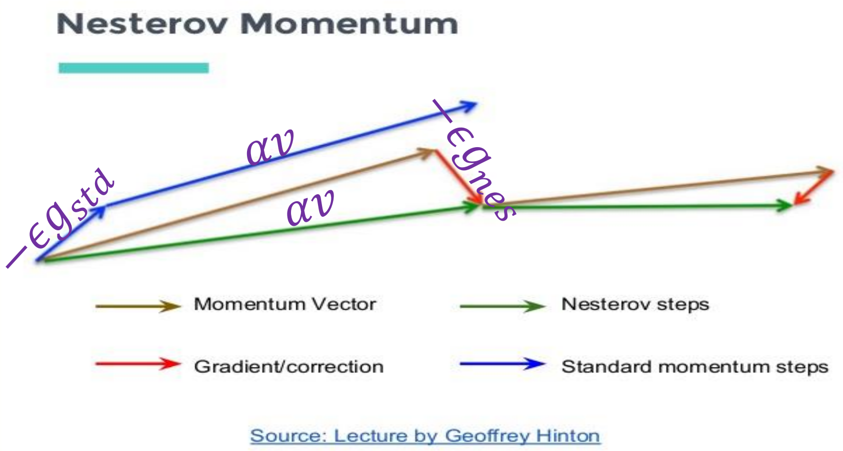


Algorithm 8.3 Stochastic gradient descent (SGD) with Nesterov momentum

```
Require: Learning rate $\epsilon$, momentum parameter $\alpha$.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ with
    corresponding labels $\boldsymbol{y}^{(i)}$.
    Apply interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \alpha \boldsymbol{v}$
    Compute gradient (at interim point): $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\tilde{\boldsymbol{\theta}}} \sum_i L(f(\boldsymbol{x}^{(i)}; \tilde{\boldsymbol{\theta}}), \boldsymbol{y}^{(i)})$
    Compute velocity update: $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \boldsymbol{g}$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
  end while
```

(Source: DL book, Ch. 8)

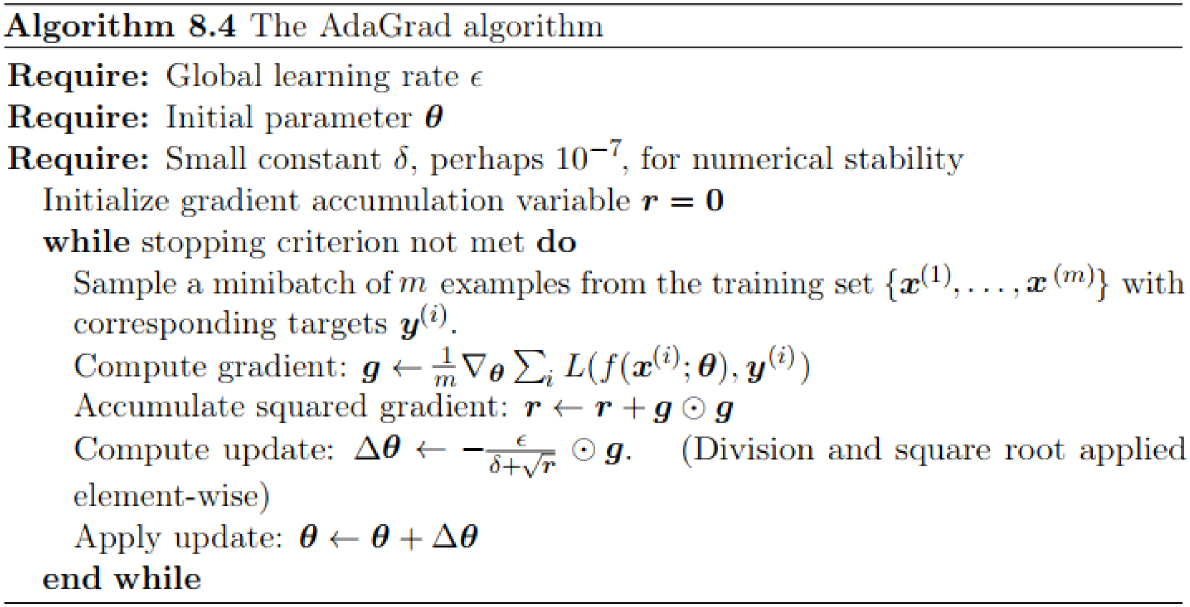
- □ The only difference between **Nesterov momentum** and **standard momentum** is how the gradient is computed.
  - ○ With Nesterov momentum the gradient is computed after the velocity is applied
- □ For **convex batch gradient**, Nesterov momentum **improves** the convergence rate from $\mathcal{O}(1/k)$ to $\mathcal{O}(1/k^2)$.
- □ Unfortunately, this result **does not** hold for stochastic gradient.



(Source: lecture of Geoffrey Hinton)

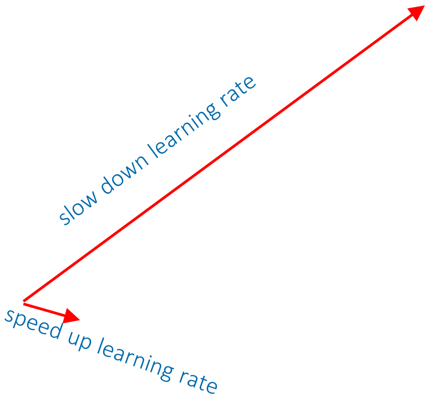
AdaGrad

Not in assessment



Algorithm 8.4 The AdaGrad algorithm

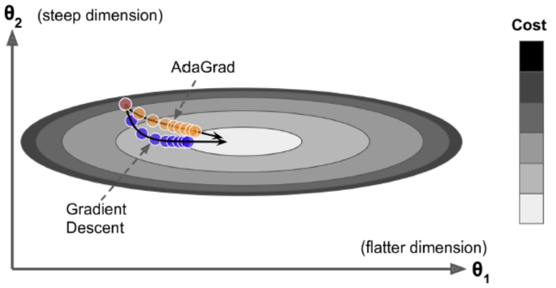
```
Require: Global learning rate $\epsilon$
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant $\delta$, perhaps $10^{-7}$, for numerical stability
  Initialize gradient accumulation variable $\boldsymbol{r} = \boldsymbol{0}$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Accumulate squared gradient: $\boldsymbol{r} \leftarrow \boldsymbol{r} + \boldsymbol{g} \odot \boldsymbol{g}$
    Compute update: $\Delta\boldsymbol{\theta} \leftarrow -\frac{\epsilon}{\delta + \sqrt{\boldsymbol{r}}} \odot \boldsymbol{g}$.   (Division and square root applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
  end while
```



slow down learning rate

speed up learning rate

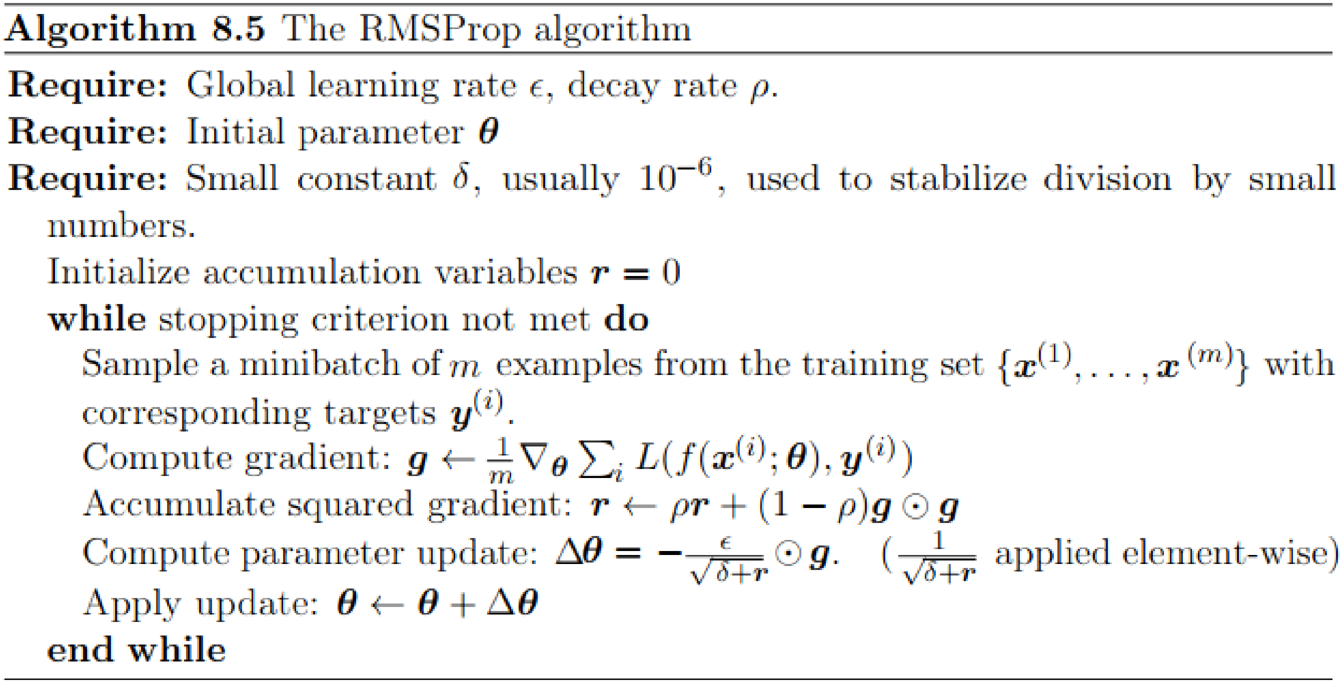
- □ Learning rates are scaled by the square root of the cumulative sum of squared gradients
- □ Direction with large partial derivatives
  - ○ Thus, rapid decrease in their learning rates
- □ Direction with small partial derivatives
  - ○ Hence relatively small decrease in their learning rates
- □ Weakness: always decrease the learning rate!
  - ○ Excellent for convex problems
  - ○ But not so good for DL (with non-convex problems)



(Source: Hands. On, Ch. 11)

RMSProp

Not in assessment



```
Algorithm 8.5 The RMSProp algorithm
Require: Global learning rate $\epsilon$, decay rate $\rho$.
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant $\delta$, usually $10^{-6}$, used to stabilize division by small numbers.
  Initialize accumulation variables $\boldsymbol{r} = 0$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m}\nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Accumulate squared gradient: $\boldsymbol{r} \leftarrow \rho \boldsymbol{r} + (1 - \rho)\boldsymbol{g} \odot \boldsymbol{g}$
    Compute parameter update: $\Delta\boldsymbol{\theta} = -\frac{\epsilon}{\sqrt{\delta + \boldsymbol{r}}} \odot \boldsymbol{g}$.   ($\frac{1}{\sqrt{\delta + \boldsymbol{r}}}$ applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
  end while
```

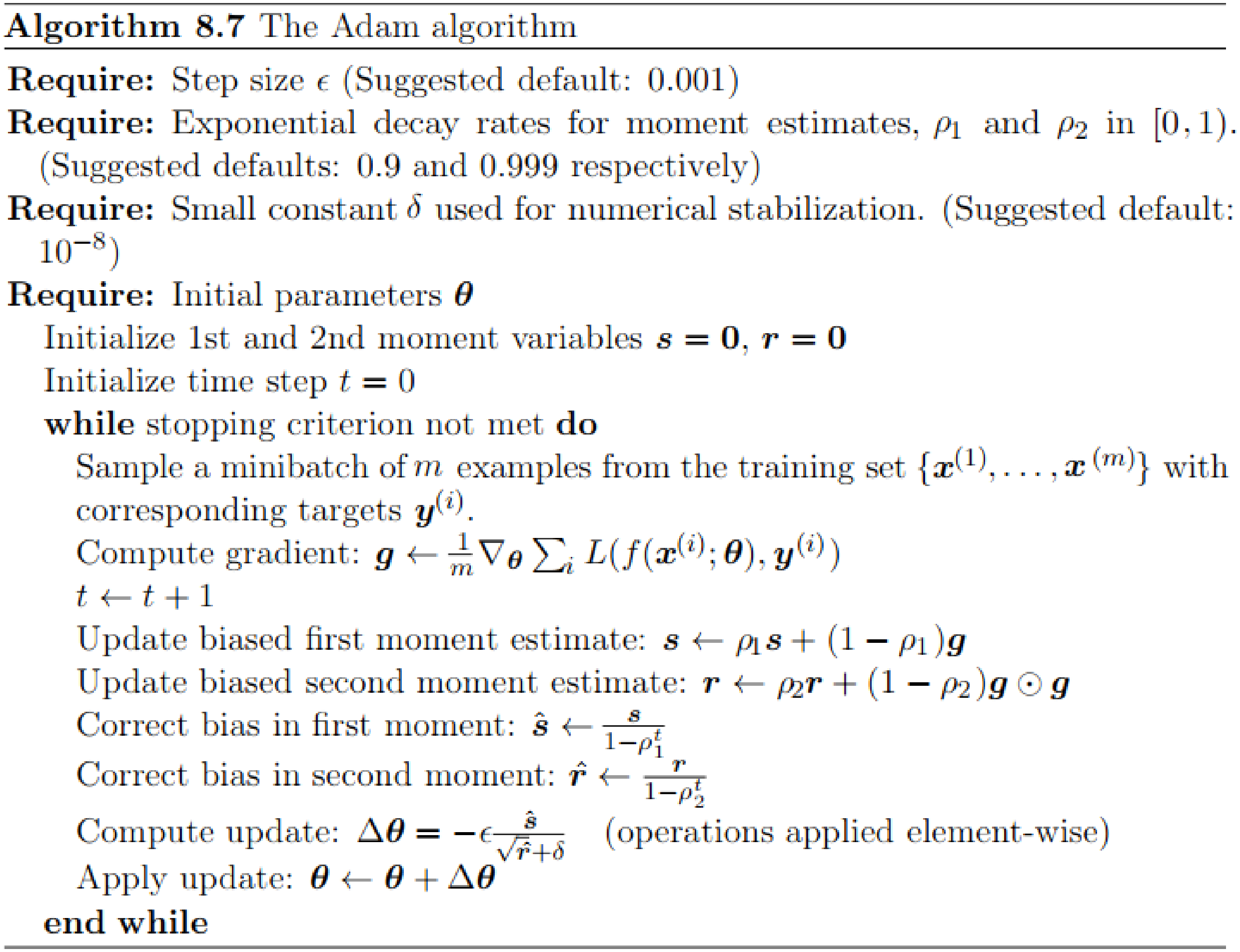
(Source: DL book, Ch. 8)

- □ A modification of AdaGrad to work better for **non-convex** setting.
- □ Instead of cumulative sum, use exponential moving/smoothing average.
- □ RMSProp has been shown to be an effective and practical optimization algorithm for DNN.
  - ○ Currently one of the go-to optimization methods being employed routinely by DL applications.

Adam

Not in assessment

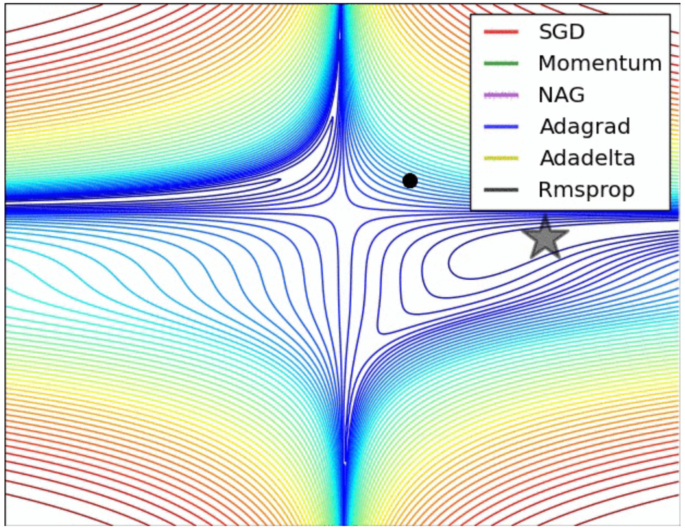
- □ The best variant that essentially combines RMSProp with momentum
- □ Suggested default values: $\eta = 0.001, \beta_1 = 0.9, \beta_2 = 0.999$ and $\epsilon = 10^{-8}$.

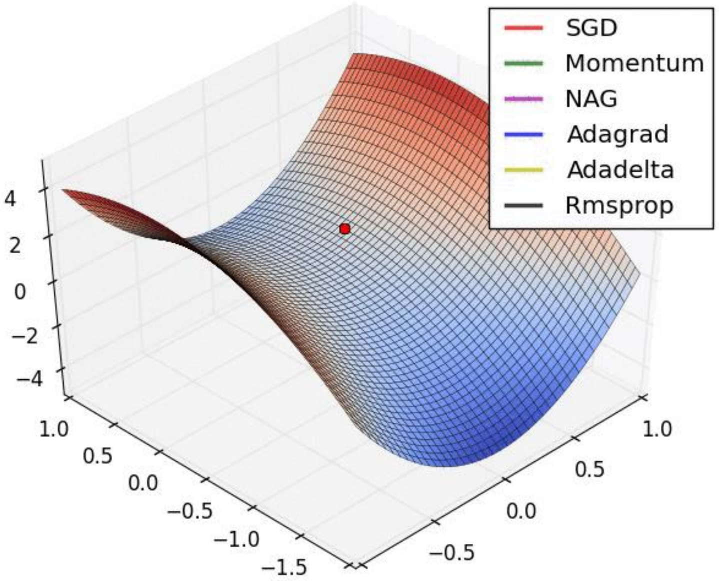


Algorithm 8.7 The Adam algorithm

```
Require: Step size $\epsilon$ (Suggested default: 0.001)
Require: Exponential decay rates for moment estimates, $\rho_1$ and $\rho_2$ in $[0, 1)$.
  (Suggested defaults: 0.9 and 0.999 respectively)
Require: Small constant $\delta$ used for numerical stabilization. (Suggested default:
  $10^{-8}$)
Require: Initial parameters $\boldsymbol{\theta}$
  Initialize 1st and 2nd moment variables $\boldsymbol{s} = \boldsymbol{0}$, $\boldsymbol{r} = \boldsymbol{0}$
  Initialize time step $t = 0$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with
    corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    $t \leftarrow t + 1$
    Update biased first moment estimate: $\boldsymbol{s} \leftarrow \rho_1 \boldsymbol{s} + (1 - \rho_1) \boldsymbol{g}$
    Update biased second moment estimate: $\boldsymbol{r} \leftarrow \rho_2 \boldsymbol{r} + (1 - \rho_2) \boldsymbol{g} \odot \boldsymbol{g}$
    Correct bias in first moment: $\hat{\boldsymbol{s}} \leftarrow \frac{\boldsymbol{s}}{1 - \rho_1^t}$
    Correct bias in second moment: $\hat{\boldsymbol{r}} \leftarrow \frac{\boldsymbol{r}}{1 - \rho_2^t}$
    Compute update: $\Delta \boldsymbol{\theta} = -\epsilon \frac{\hat{\boldsymbol{s}}}{\sqrt{\hat{\boldsymbol{r}}} + \delta}$   (operations applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$
  end while
```

Visual comparison of all optimizers

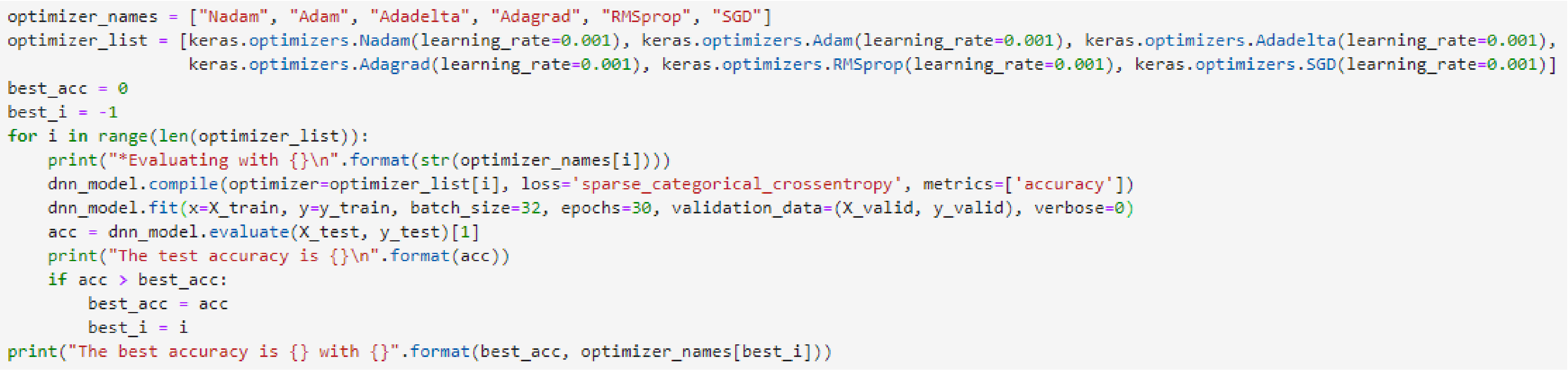




[Source: Sebastian Ruder]

TensorFlow optimizers

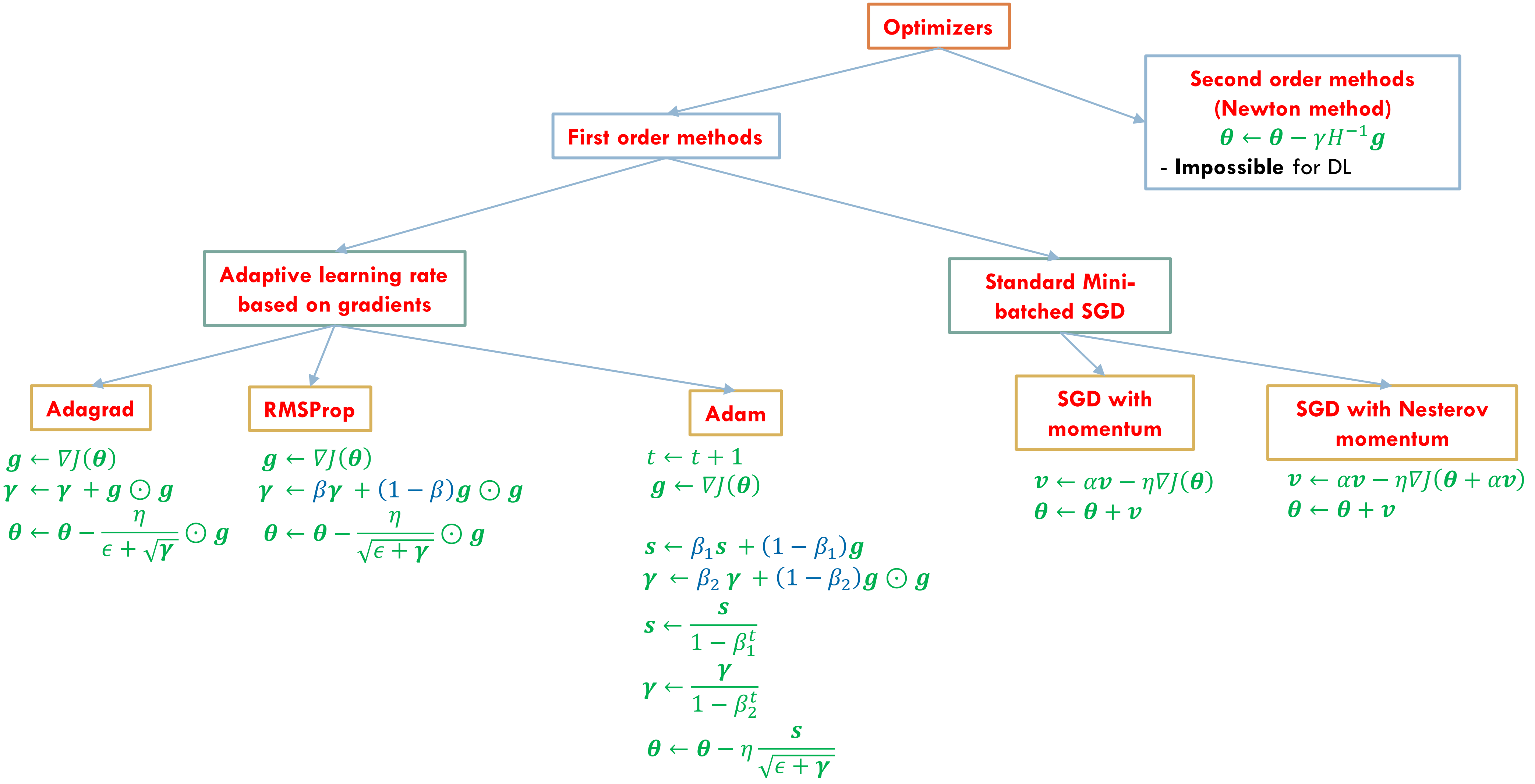
- TensorFlow pre-implemented methods for **TF 1.x**:
  - ☐ `tf.train.GradientDescentOptimizer` (Standard SGD)
  - ☐ `tf.train.MomentumOptimizer` (SGD with momentum)
  - ☐ `tf.train.AdaGradOptimizer` (AdaGrad)
  - ☐ `tf.train.RMSPropOptimizer` (RMSProp)
  - ☐ `tf.train.AdamOptimizer` (Adam)



```
optimizer_names = ["Nadam", "Adam", "Adadelta", "Adagrad", "RMSprop", "SGD"]
optimizer_list = [keras.optimizers.Nadam(learning_rate=0.001), keras.optimizers.Adam(learning_rate=0.001), keras.optimizers.Adadelta(learning_rate=0.001),
                  keras.optimizers.Adagrad(learning_rate=0.001), keras.optimizers.RMSprop(learning_rate=0.001), keras.optimizers.SGD(learning_rate=0.001)]
best_acc = 0
best_i = -1
for i in range(len(optimizer_list)):
    print("*Evaluating with {}\n".format(str(optimizer_names[i])))
    dnn_model.compile(optimizer=optimizer_list[i], loss='sparse_categorical_crossentropy', metrics=['accuracy'])
    dnn_model.fit(x=X_train, y=y_train, batch_size=32, epochs=30, validation_data=(X_valid, y_valid), verbose=0)
    acc = dnn_model.evaluate(X_test, y_test)[1]
    print("The test accuracy is {}\n".format(acc))
    if acc > best_acc:
        best_acc = acc
        best_i = i
print("The best accuracy is {} with {}".format(best_acc, optimizer_names[best_i]))
```

For TF 2.x

Optimizers in deep learning



Optimizers

First order methods

Second order methods (Newton method)

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma H^{-1} \boldsymbol{g}$

- **Impossible** for DL

Adaptive learning rate based on gradients

Standard Mini-batched SGD

Adagrad

$\boldsymbol{g} \leftarrow \nabla J(\boldsymbol{\theta})$

$\boldsymbol{\gamma} \leftarrow \boldsymbol{\gamma} + \boldsymbol{g} \odot \boldsymbol{g}$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \frac{\eta}{\epsilon + \sqrt{\boldsymbol{\gamma}}} \odot \boldsymbol{g}$

RMSProp

$\boldsymbol{g} \leftarrow \nabla J(\boldsymbol{\theta})$

$\boldsymbol{\gamma} \leftarrow \beta \boldsymbol{\gamma} + (1 - \beta) \boldsymbol{g} \odot \boldsymbol{g}$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \frac{\eta}{\sqrt{\epsilon + \boldsymbol{\gamma}}} \odot \boldsymbol{g}$

Adam

$t \leftarrow t + 1$

$\boldsymbol{g} \leftarrow \nabla J(\boldsymbol{\theta})$

$\boldsymbol{s} \leftarrow \beta_1 \boldsymbol{s} + (1 - \beta_1) \boldsymbol{g}$

$\boldsymbol{\gamma} \leftarrow \beta_2 \boldsymbol{\gamma} + (1 - \beta_2) \boldsymbol{g} \odot \boldsymbol{g}$

$\boldsymbol{s} \leftarrow \frac{\boldsymbol{s}}{1 - \beta_1^t}$

$\boldsymbol{\gamma} \leftarrow \frac{\boldsymbol{\gamma}}{1 - \beta_2^t}$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \frac{\boldsymbol{s}}{\sqrt{\epsilon + \boldsymbol{\gamma}}}$

SGD with momentum

$\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \eta \nabla J(\boldsymbol{\theta})$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$

SGD with Nesterov momentum

$\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \eta \nabla J(\boldsymbol{\theta} + \alpha \boldsymbol{v})$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$

Not in assessment

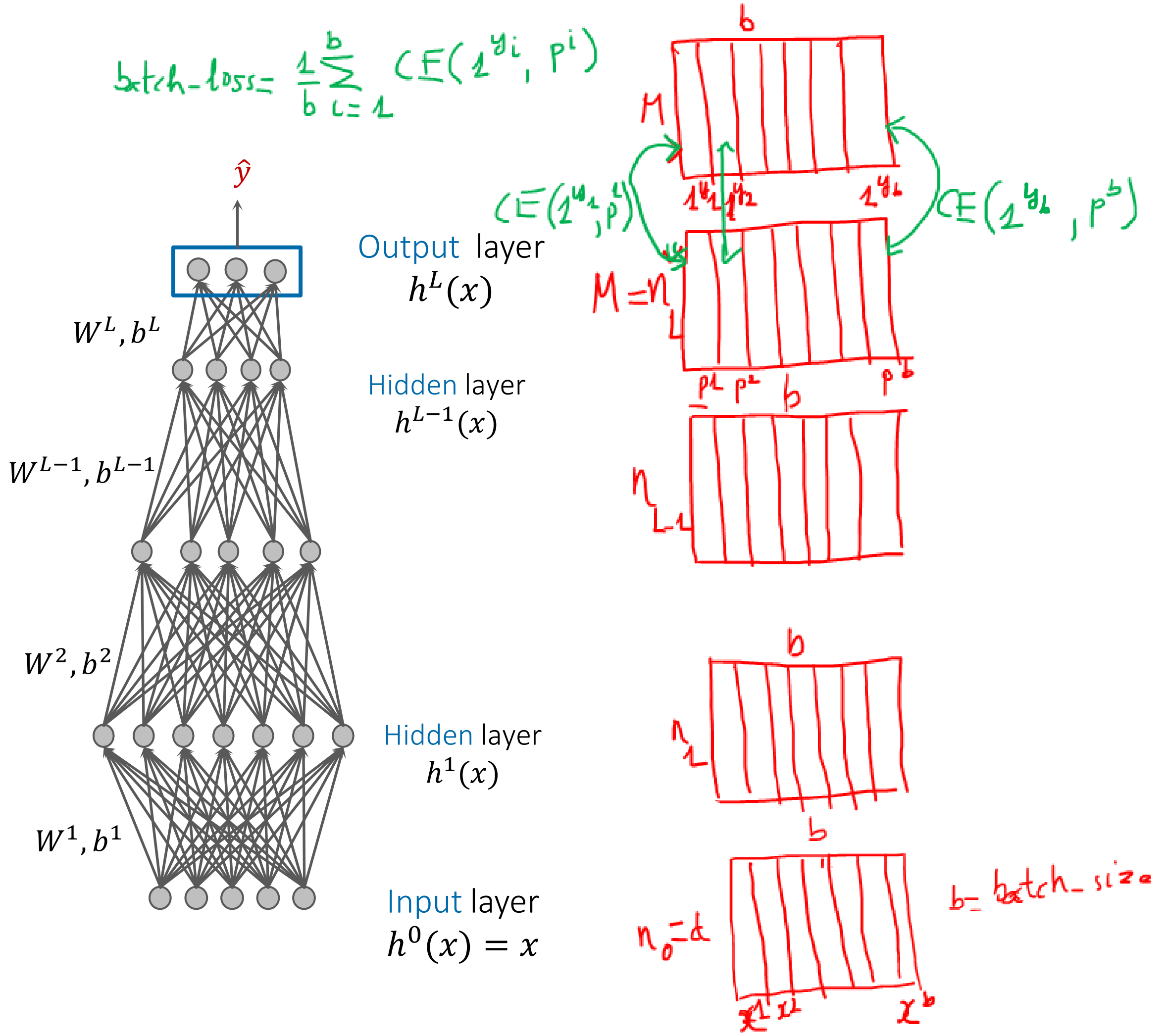
Summary

- □ Optimization problem in DL and ML
  - ○ Regularization term + Empirical loss term
- □ Gradient descent
- □ Stochastic gradient descent
- □ Backward propagation
- □ Other optimizers in DL
  - ○ SGD with momentum, Adagrad, RMSProp, and Adam
- □ First order methods and second order methods

Thanks for your attention!

Mini-batch feed-forward

- □ Input
  - ○ Tensor X: $[n_0 = d, b]$ (b is the batch size)
- □ Hidden layer 1
  - ○ Tensor $[n_1, b]$
- □ ……………..
- □ Output layer
  - ○ Tensor P: $[n_L = M, b]$
- □ The loss of the batch
  - ○ $\frac{1}{b}\sum_{i=1}^{b} CE(1^{y_i}, p^i) = -\frac{1}{b}\sum_{i=1}^{b} \log p_{y_i}^i$


batch_loss = $\frac{1}{b}\sum_{i=1}^{b} CE(1^{y_i}, p^i)$
$\hat{y}$
Output layer
$h^L(x)$
W^L, b^L
Hidden layer
$h^{L-1}(x)$
W^{L-1}, b^{L-1}
W^2, b^2
Hidden layer
$h^1(x)$
W^1, b^1
Input layer
$h^0(x) = x$
b
M
$CE(1^{y_1}, p^1)$
1^{y_1} 1^{y_2}
1^{y_b}
$CE(1^{y_b}, p^b)$
$M = n_L$
p^1 p^2
p^b
b
n_{L-1}
b
n_1
b
$n_0 = d$
x^1 x^2
x^b
b = batch_size