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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](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:

- $f'(x) = \nabla f(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$

- $(uv)' = u'v + uv'$

- $\left(\frac{u}{v}\right)' = \frac{u'v - uv'}{v^2}$

- $(e^u)' = u'e^u$

- $(\log u)' = \frac{u'}{u}$

□ Multi-variate function  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  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  $\infty$  :

- $\frac{\partial u}{\partial x} = \frac{\partial u}{\partial v} \times \frac{\partial v}{\partial x}$

# 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  $u = \exp(x) + \exp(y) + \exp(z)$ .

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

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

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

□  $\nabla f = [f'_x, f'_y, f'_z] = \text{softmax}([x, y, z]).$

# Example (Forum discussion)

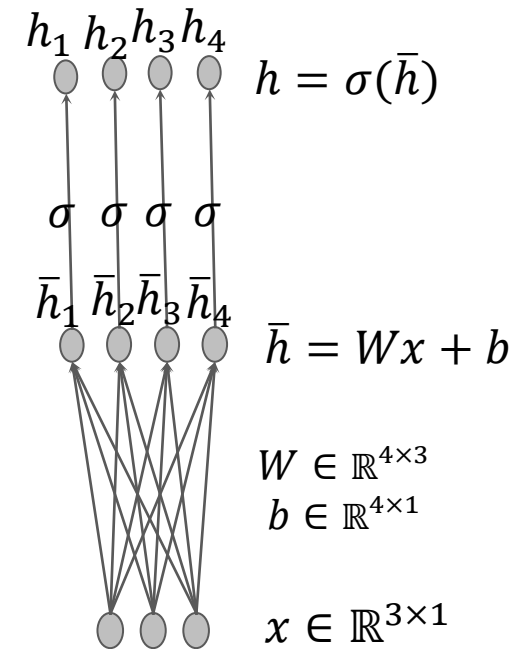
$$\square \quad \bar{h} = Wx + b \text{ and } h = \sigma(\bar{h})$$

- $h = \sigma(Wx + b)$
- $\sigma$  is the **activation function**

$$\square \quad \frac{\partial h}{\partial x} = \frac{\partial h}{\partial \bar{h}} \times \frac{\partial \bar{h}}{\partial x} = \text{diag}(\sigma'(\bar{h})) W$$

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

$$\square \quad \frac{\partial \bar{h}}{\partial x} = W$$



# How to code with numpy

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

```
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

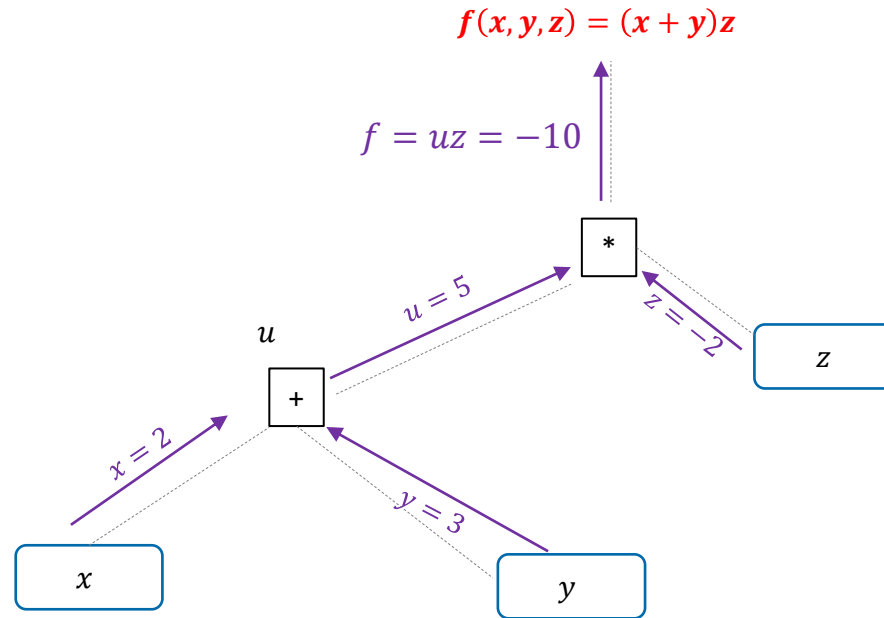
# Computational graph (used in TensorFlow)

Problem:  $f(x, y, z) = (x + y)z$

What are its partial derivatives, evaluated at  $x = 2, y = 3, z = -2$ ?

Step 1:

- construct computational graph
- forward propagation
- record value at each node

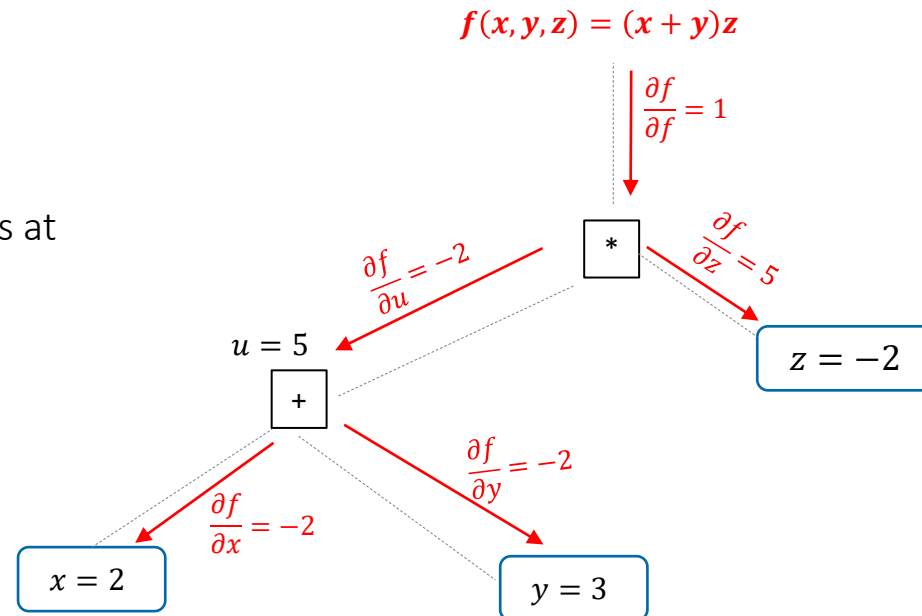




# Reverse Auto-Diff (used in TensorFlow)

Step 2:

- traverse backward
- apply chain rule
- record differential values at each node



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

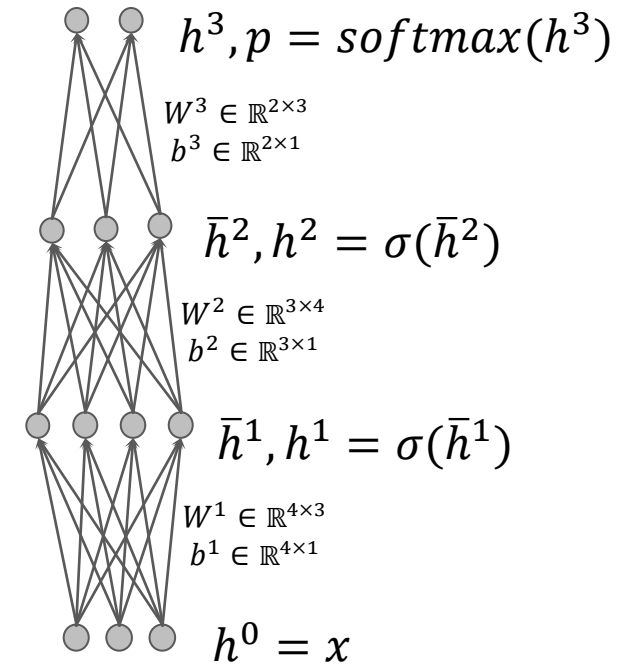
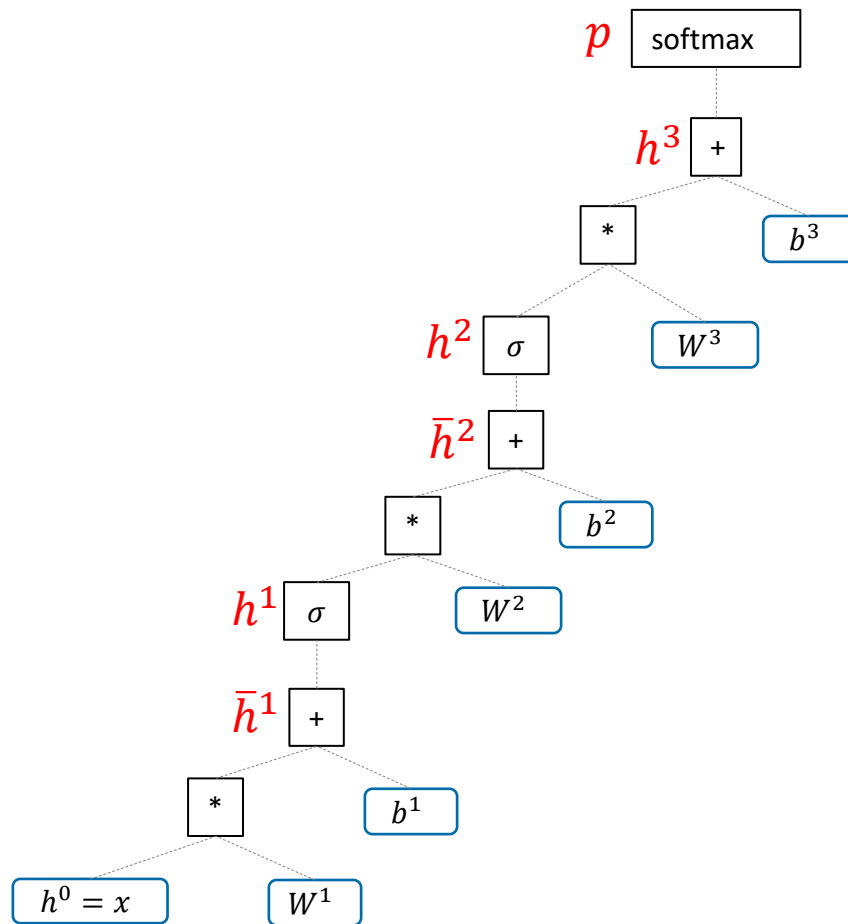
$$\frac{\partial f}{\partial u} = \frac{\partial f}{\partial f} \frac{\partial f}{\partial u} = 1 * z = -2$$

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

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

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

# Computational graph of feedforward nets (Forum discussion)



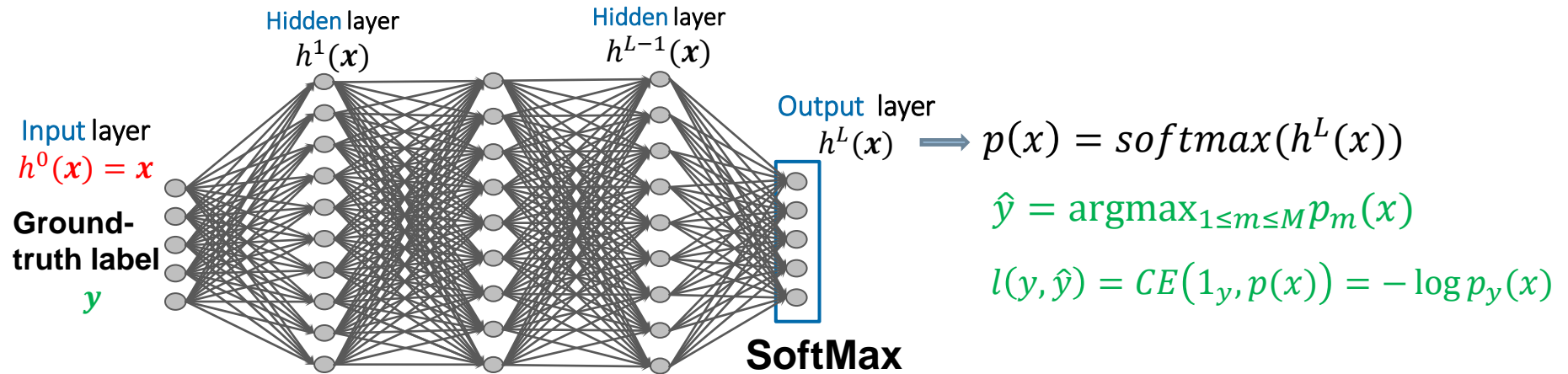
```

h0(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
 $h^3(x) = W^3 h^2(x) + b^3$ 
p(x) = softmax(h3(x)) //prediction probabilities
    
```



# Gradient descent and stochastic gradient descent

# Recall optimization problem in deep learning (Forum discussion)



**Training set**

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

**Loss function**

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

□ 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:

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

## Regularization term

- $\Omega(\theta) = \lambda \sum_k \sum_{i,j} (w_{i,j}^k)^2 = \lambda \sum_k \|w^k\|_F^2$
- 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)  $g = \nabla_{\theta} J(\theta)$  to update parameters

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

Use the **Hessian** matrix (second derivative)  $H = \nabla_{\theta}^2 J(\theta)$  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
    - $\theta$  includes **weight matrices**, **filters**, and **biases** which are trainable model parameters.
    - $P$  is the number of **trainable parameters** ( $P$  could be  $20 \times 10^6$ ).
    - $J(\theta)$  is the loss function over a training set.

- Gradient  $g = \nabla J(\theta)$  is the **first order derivative** and defined as

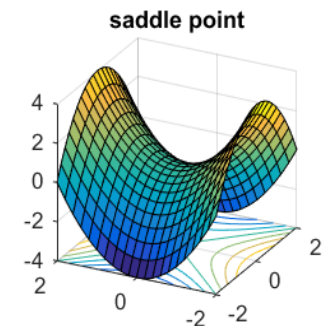
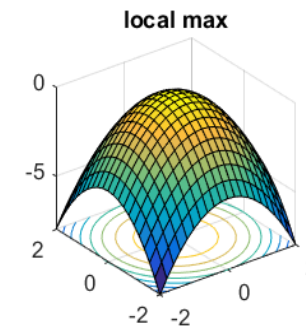
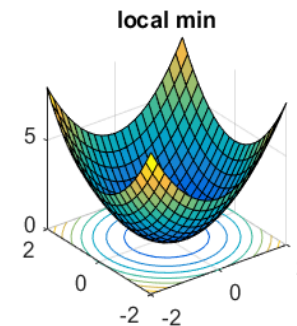
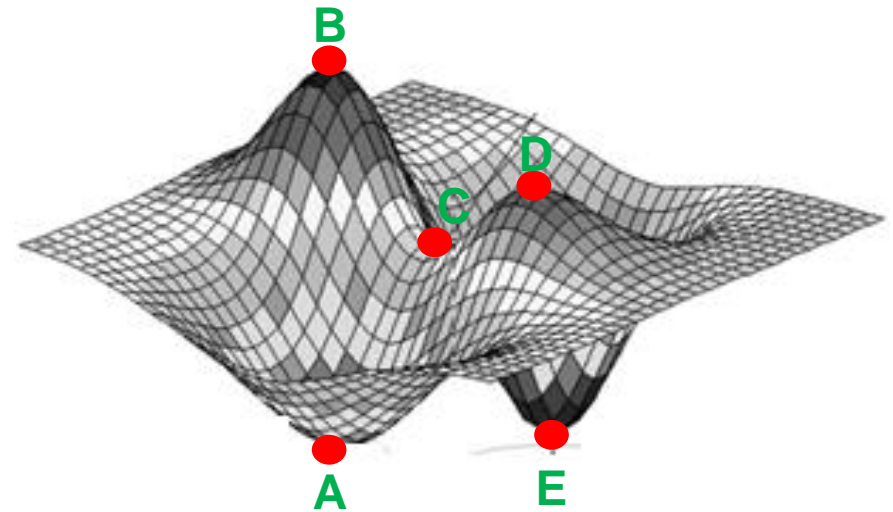
- $$\nabla J(\theta) = g = \begin{bmatrix} \frac{\partial J}{\partial \theta_1}(\theta) \\ \dots \dots \dots \\ \frac{\partial J}{\partial \theta_P}(\theta) \end{bmatrix}$$

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

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

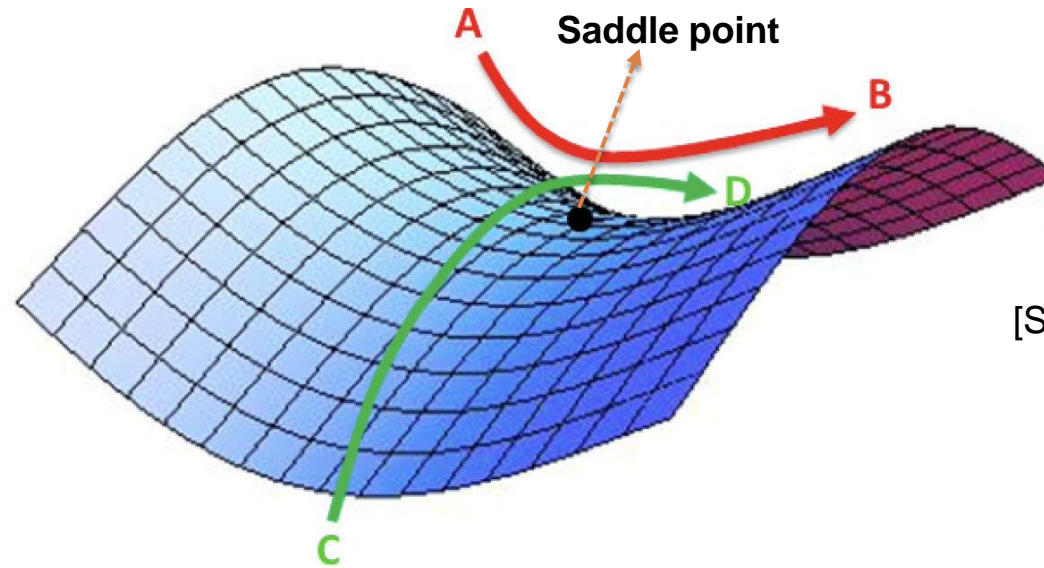
# Local minima-maxima and saddle point

- Given an **objective function**  $J(\theta)$  with  $\theta = [\theta_1, \theta_2, \dots, \theta_p]$ 
  - $\theta$  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
  - $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_p$
- **Local minima**
  - $\nabla J(\theta) = \mathbf{0}$  and  $\nabla^2 J(\theta) = H(\theta) \succ 0$  (positive semi-definite matrix)
  - $0 \leq \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_p$
- **Local maxima**
  - $\nabla J(\theta) = \mathbf{0}$  and  $\nabla^2 J(\theta) = H(\theta) \prec 0$  (negative semi-definite matrix)
  - $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_p \leq 0$
- **Saddle point**
  - $\nabla J(\theta) = \mathbf{0}$  and  $\nabla^2 J(\theta) = H(\theta) \prec 0$  (indefinite matrix)
  - $\lambda_1 \leq \lambda_2 \leq \dots < 0 < \dots \leq \lambda_p$





# More on saddle point (Forum discussion)



[Source: Internet]

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

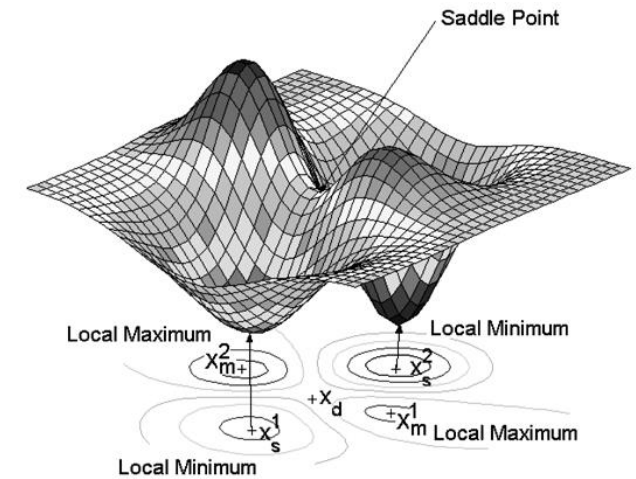
$$\text{Gradient } g = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 \\ -2x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \rightarrow \text{a critical point } \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

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

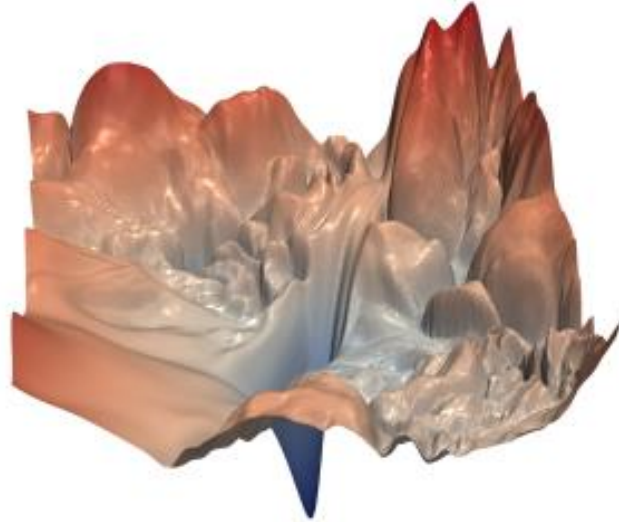
Two eigenvalues  $\lambda_1 = -2 < 0 < 2 = \lambda_2 \rightarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix}$  is a **saddle point**.

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

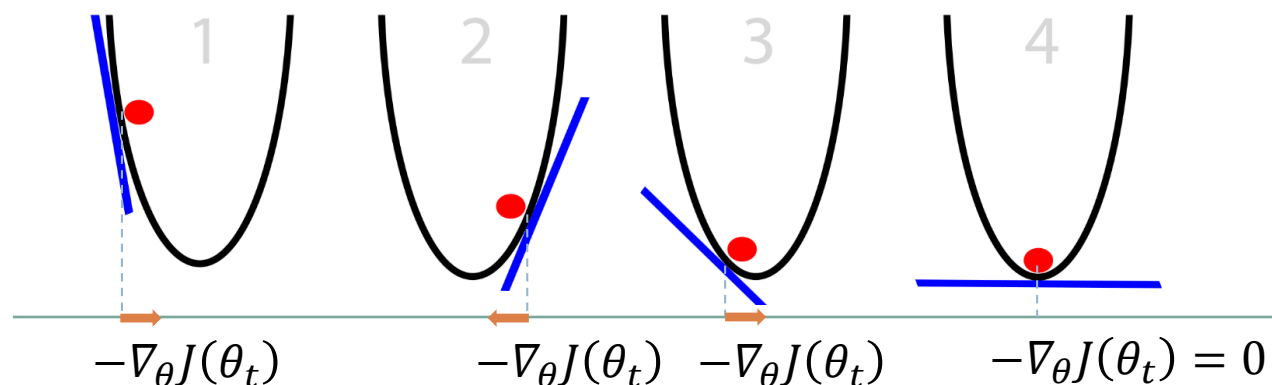
## □ The optimization problem in deep learning:

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

## □ 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)



□ We need to solve

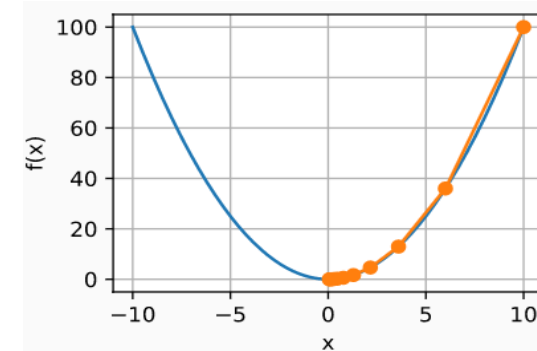
- $\min_{\theta} J(\theta)$

□ Follow to **the opposite side** of the current gradient

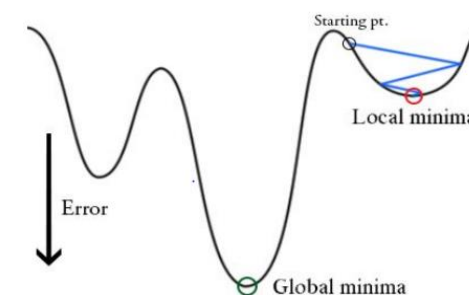
- $\theta_{t+1} = \theta_t - \eta \nabla_{\theta} J(\theta_t)$  where  $\eta > 0$  is the **learning rate**.

□ Guarantee to converge to a **global minima** if  $J(\cdot)$  is **convex**.

□ Get stuck in a **local minima** or **saddle points** if  $J(\cdot)$  is non-convex.

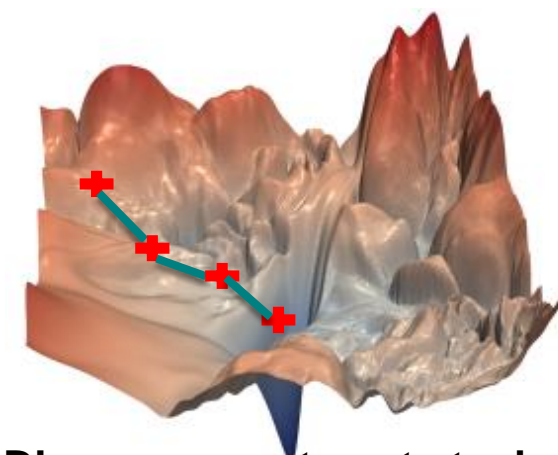


**Convex case**



(Source: [www.cs.ubc.ca](http://www.cs.ubc.ca))

**Non-convex case**



**DL case: easy to get stuck in saddle points**

# Gradient descend

## Algorithm

- ❑ **Input:** objective function  $J(\theta)$
- ❑ **Output:** optimal solution  $\theta^*$
- 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  $\theta^* = \theta_{T+1}$

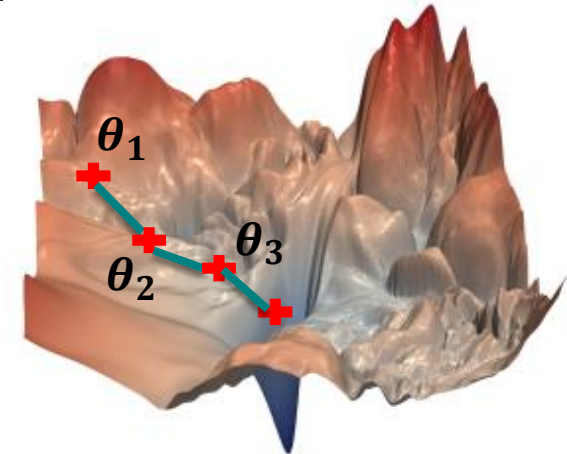


```
import tensorflow as tf

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
```



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

Define  $f(x) = x^2$  and solve  $\min_x f(x)$

```
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

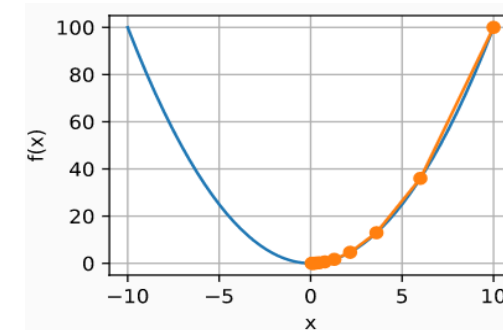
results = gd(0.2, f_grad)
```

epoch 10, x: 0.060466

```
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)
```

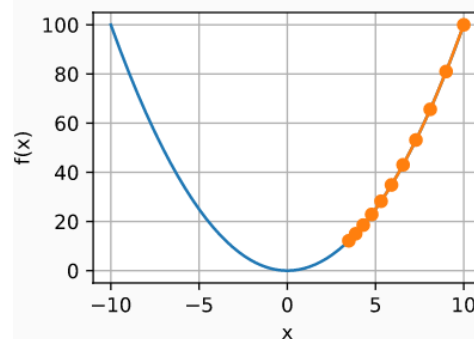
Show trace of  
gradient descent



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

epoch 10, x: 3.486784

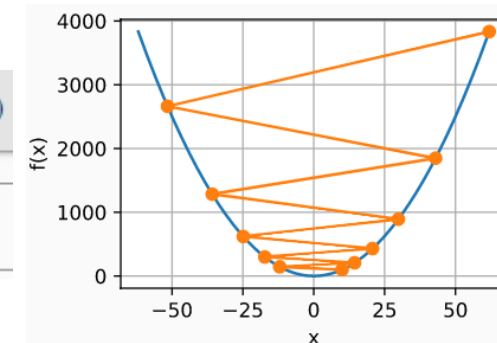
Good learning rate  $\eta$



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

epoch 10, x: 61.917364

Too high rate  $\eta$



# 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  $D \rightarrow$  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)

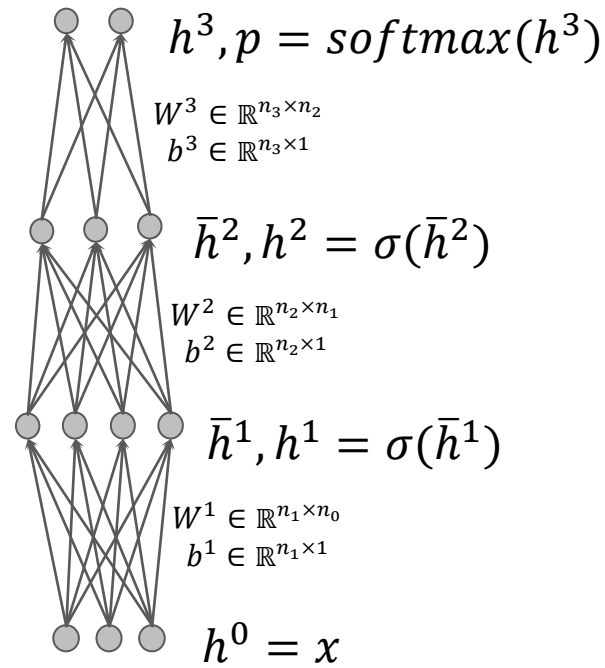
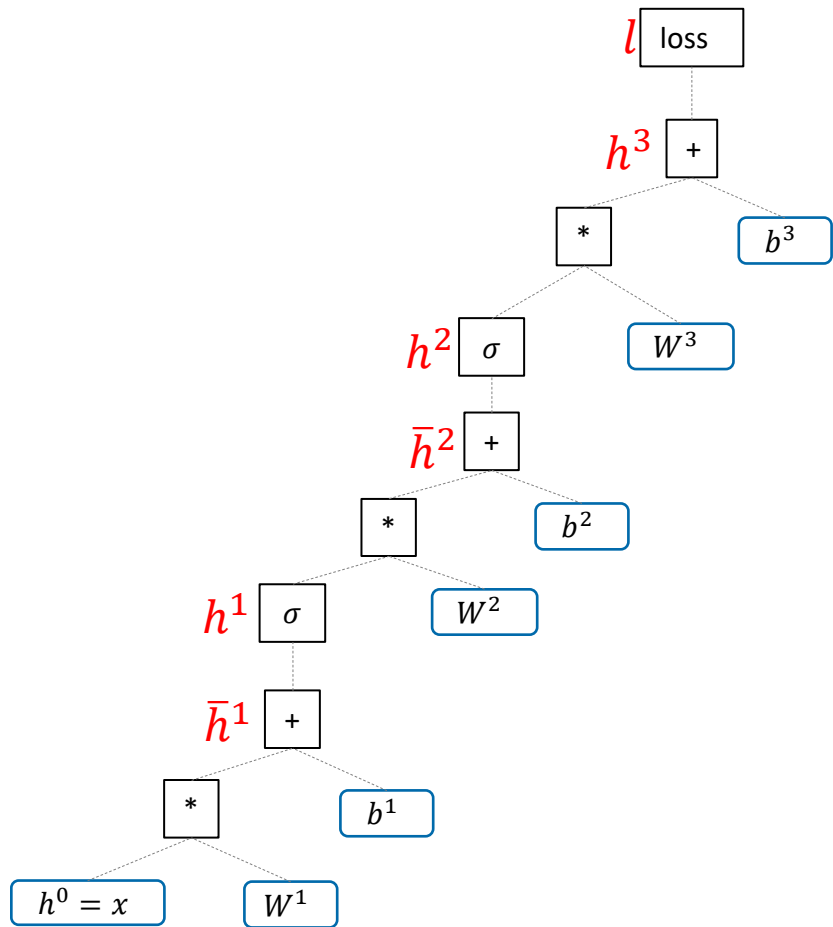
- The **optimization problem** in **deep learning** has the form
  - $\min_{\theta} L(D; \theta) := \frac{1}{N} \sum_{i=1}^N l(x_i, y_i; \theta)$
- Evaluation of the **full gradient** is **expensive**. We want to just **estimate** this gradient
  - Sample a mini-batch  $\mathbf{i}_1, \mathbf{i}_2, \dots, \mathbf{i}_b \sim \text{Uni}(\{1, 2, \dots, N\})$  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  $\eta_t \propto O(\frac{1}{t})$
  - 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**?





# Back propagation in feed-forward neural networks

# Back propagation



- 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.

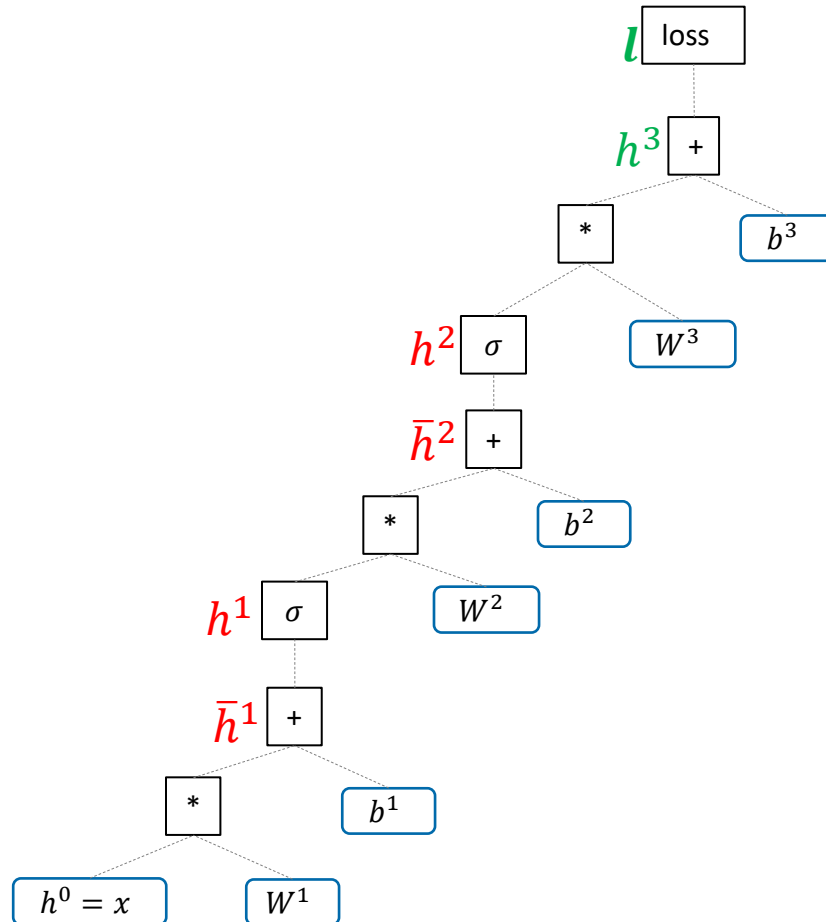
# Back propagation

From loss to  $h^3$



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

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



$$\square \quad l(x, y; \theta) = -\log \frac{\exp\{h_y^3(x)\}}{\sum_{m=1}^M \exp\{h_m^3(x)\}} =$$

$$-h_y^3(x) + \log[\sum_{m=1}^M \exp\{h_m^3(x)\}] =$$

$$-\sum_{m=1}^M \mathbf{1}_{m=y} h_m^3 + \log[\sum_{m=1}^M \exp\{h_m^3\}]$$

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

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

$$\square \quad g^3 = \frac{\partial l}{\partial h^3} = -\mathbf{1}_y + \text{softmax}(h^3) =$$

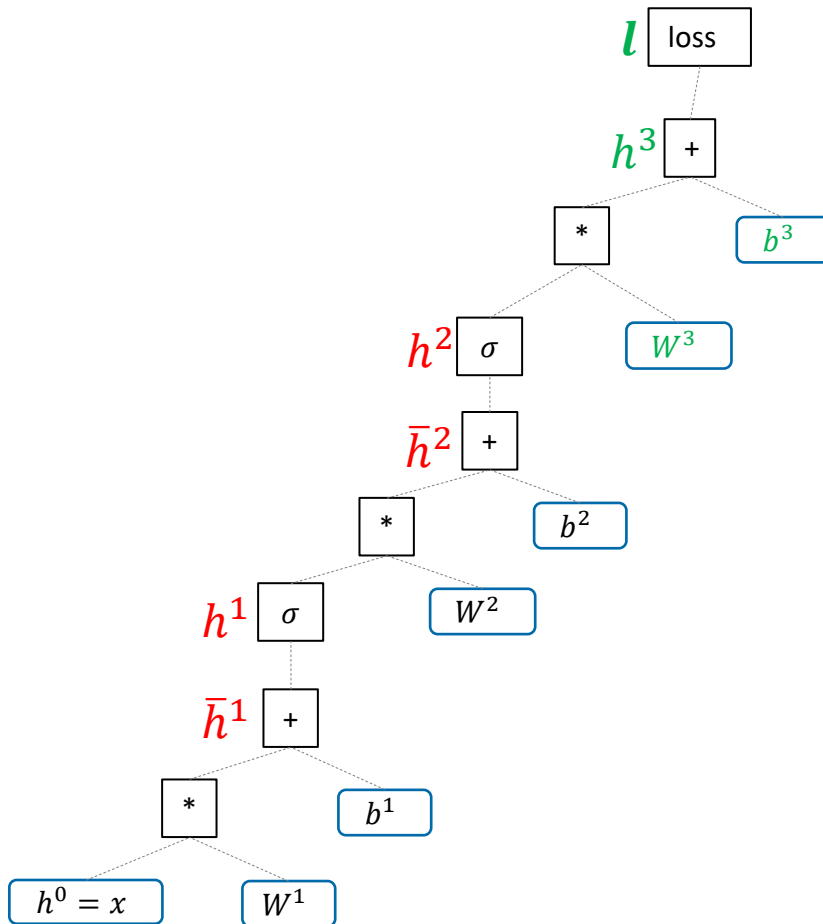
$$= \mathbf{p}^T - \mathbf{1}_y$$

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

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

# Back propagation

From loss to  $W^3, b^3$



$$\square \quad h^3 = W^3 h^2 + b^3$$

$$\square \quad \frac{\partial l}{\partial W^3} = \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial W^3} = (g^3)^T (h^2)^T$$

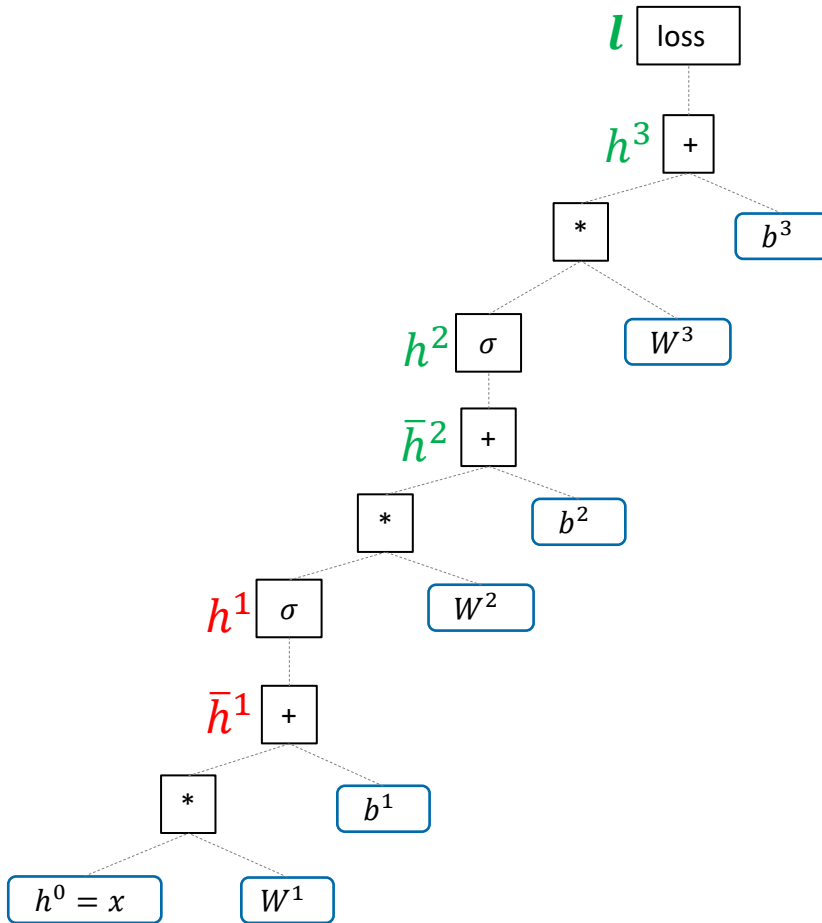
- $[n_3 \times 1] \times [1 \times n_2] \rightarrow [n_3 \times n_2]$

$$\square \quad \frac{\partial l}{\partial b^3} = \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial b^3} = g^3$$

- $[1 \times n_3]$

# Back propagation

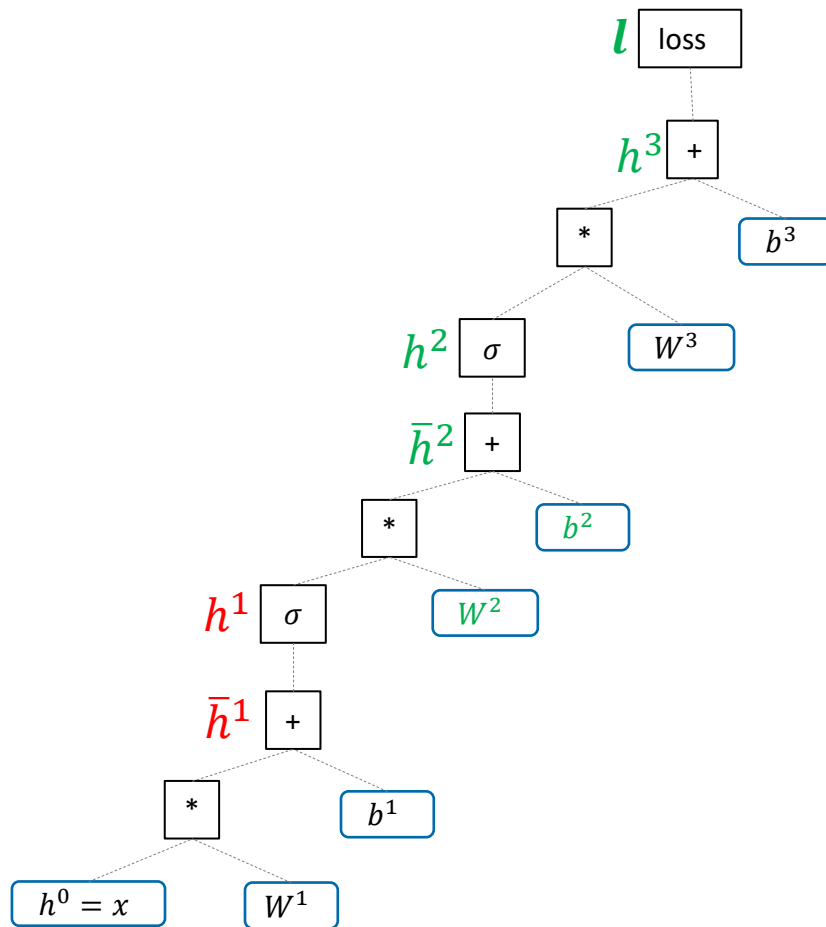
From loss to  $h^2$  and  $\bar{h}^2$



- $h^3 = W^3 h^2 + b^3$
- $g^2 = \frac{\partial l}{\partial h^2} = \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial h^2} = \mathbf{g^3 W^3}$ 
  - $[1 \times n_3] \times [n_3 \times n_2] \rightarrow [1 \times n_2]$
- $h^2 = \sigma(\bar{h}^2)$  (element-wise activation)
- $\frac{\partial h^2}{\partial \bar{h}^2} = \mathbf{diag}(\sigma'(\bar{h}^2))$ 
  - $\sigma'(\bar{h}^2)$  is **element-wise derivative** and  $\mathbf{diag}(u)$  is the **diagonal matrix** corresponding to the **vector  $u$**  (the diagnose is  $u$  and others are zeros).
- $\bar{g}^2 = \frac{\partial l}{\partial \bar{h}^2} = \frac{\partial l}{\partial h^2} \cdot \frac{\partial h^2}{\partial \bar{h}^2} = \mathbf{g^2 diag}(\sigma'(\bar{h}^2))$ 
  - $[1 \times n_2] \times [n_2 \times n_2] \rightarrow [1 \times n_2]$

# Back propagation

From loss to  $W^2$  and  $b^2$



$$\bar{h}^2 = W^2 h^1 + b^2$$

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

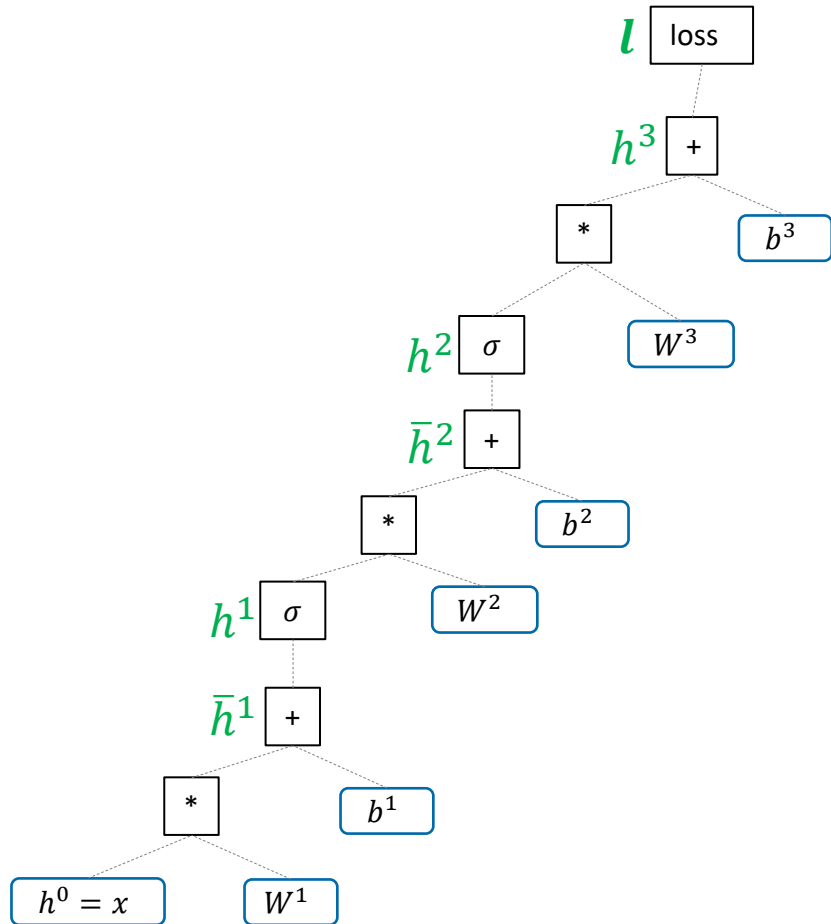
◦  $[n_2 \times 1] \times [1 \times n_1] \rightarrow [n_2 \times n_1]$

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

◦  $[1 \times n_2]$

# Back propagation

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

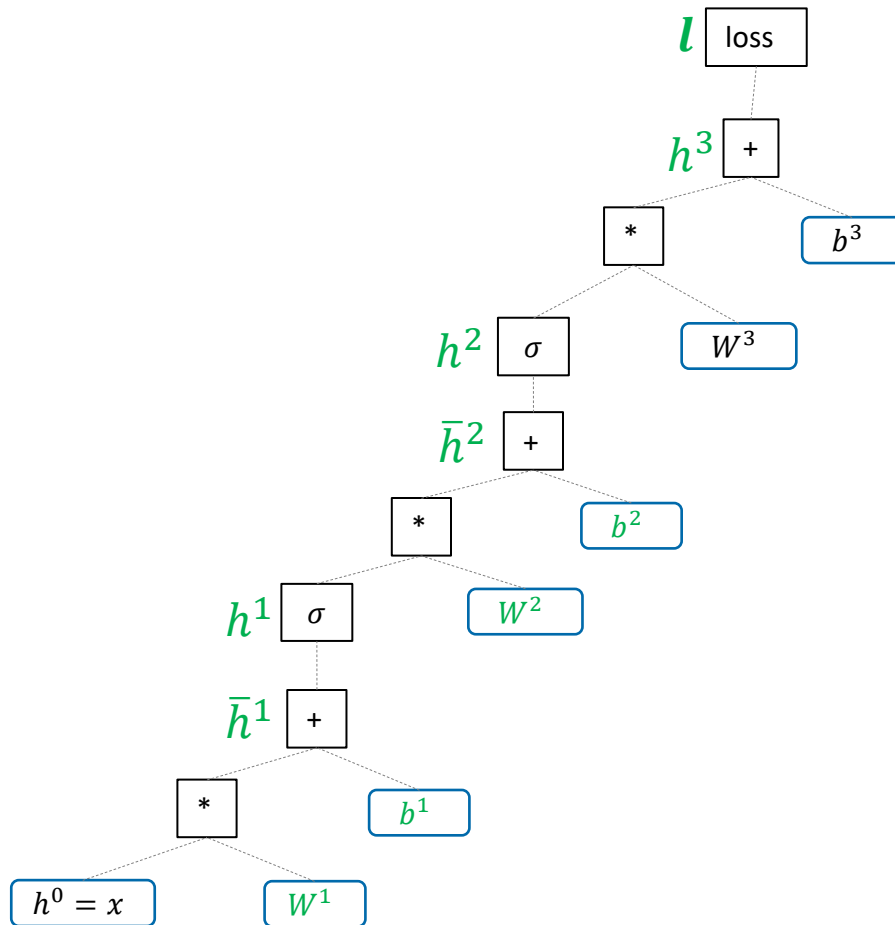


- $\bar{h}^2 = W^2 h^1 + b^2$
- $g^1 = \frac{\partial l}{\partial h^1} = \frac{\partial l}{\partial \bar{h}^2} \cdot \frac{\partial \bar{h}^2}{\partial h^1} = \bar{g}^2 W^2$ 
  - $[1 \times n_2] \times [n_2 \times n_1] \rightarrow [1 \times n_1]$
- $h^1 = \sigma(\bar{h}^1)$  (element-wise activation)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



# Back propagation

From loss to  $W^1$  and  $b^1$



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

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

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

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

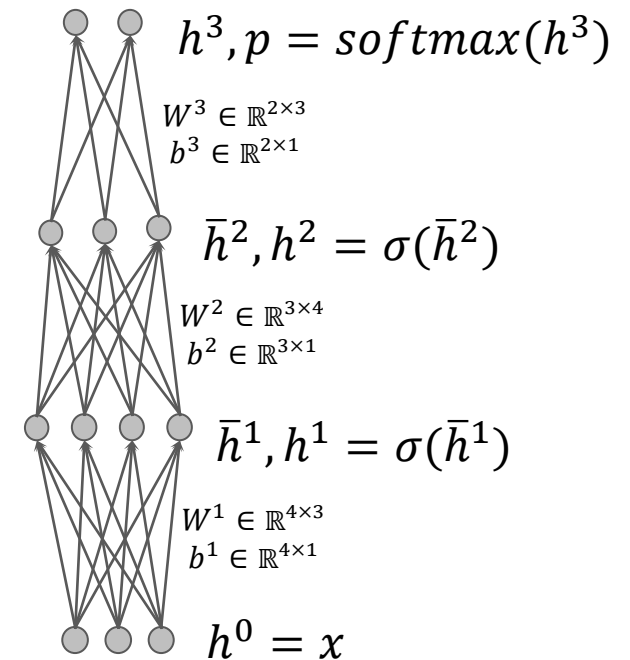
- $[1 \times n_1]$

**?** 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  $B = \{(x_{i_j}, y_{i_j})\}_{j=1}^b$  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
       $W_k = W_k - \eta \frac{\partial l}{\partial W^k}$ 
       $b_k = b_k - \eta \frac{\partial l}{\partial b^k}$ 
  
```



# Mini-batch feed-forward

## Input

- Tensor  $X$ :  $[n_0 = d, b]$  ( $b$  is the batch size)

## Hidden layer 1

- Tensor  $[n_1, b]$

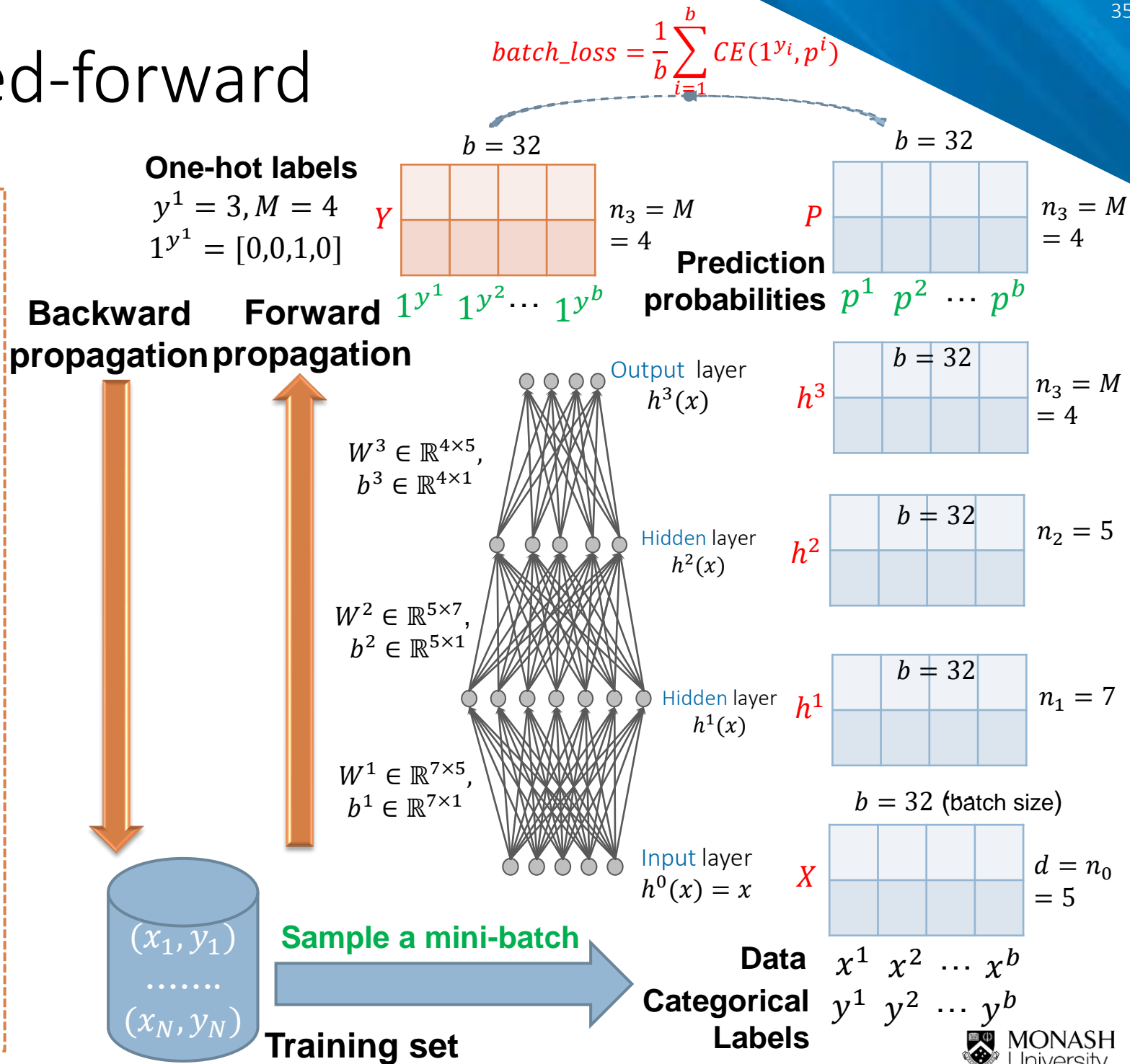
.....

## Output layer

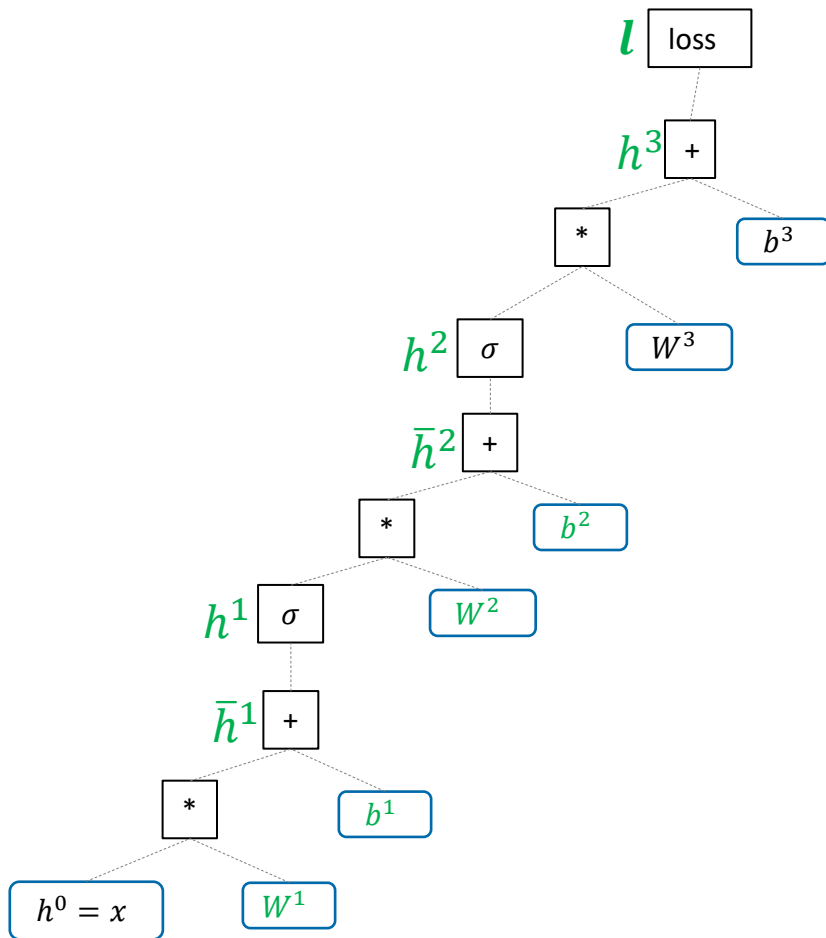
- Tensor  $P$ :  $[n_L = M, b]$

## 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**.



# Why does deep learning need GPU and TPU?



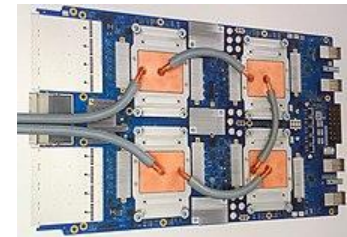
- Let consider

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

- 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)

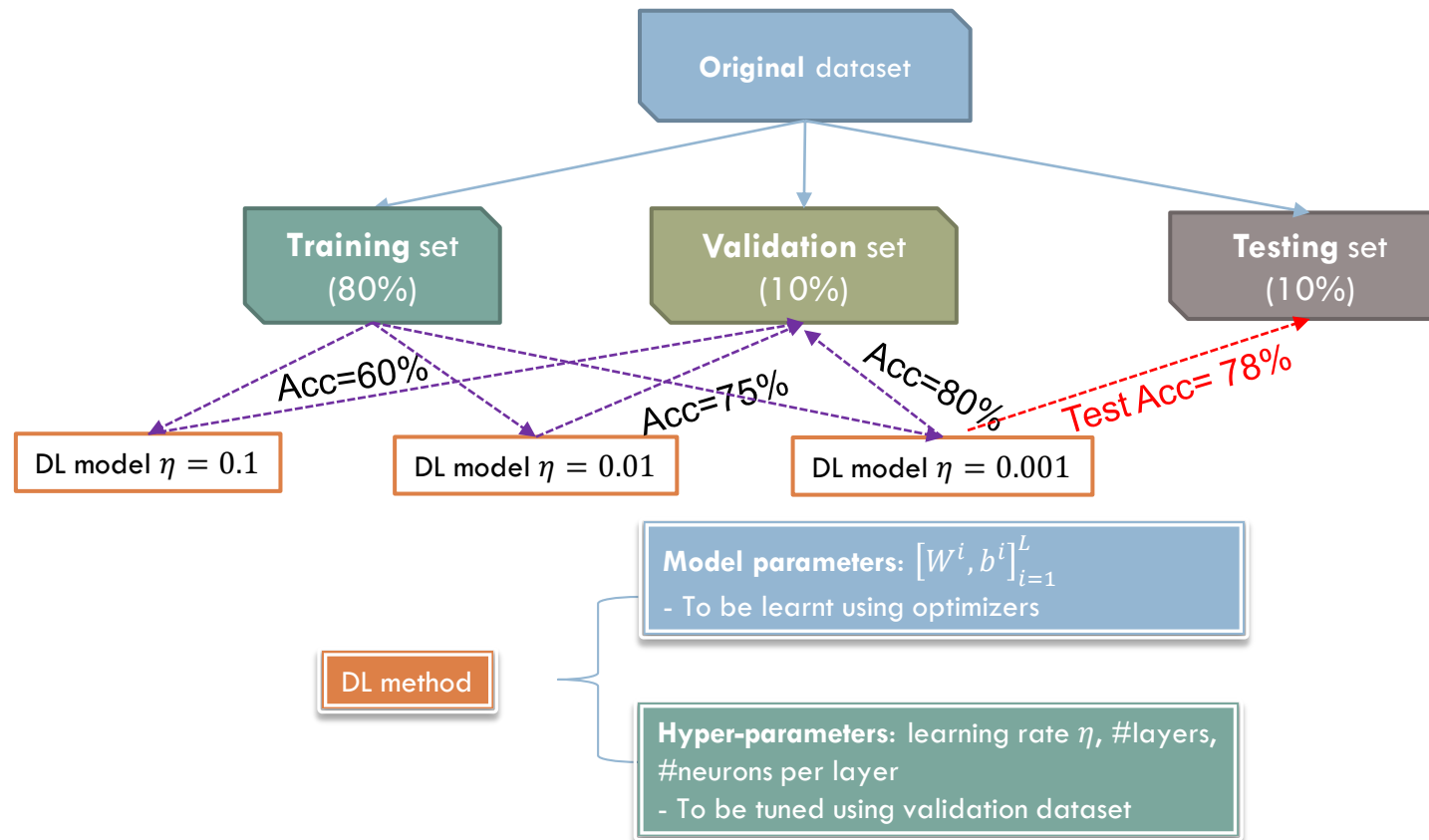


**TPU** (Source: Wikipedia)

# 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**.





# Optimizers for deep learning



# Challenges of optimization for Deep Learning (Forum discussion)

## □ The **optimization problem** in **deep learning**:

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






## □ A very **complex** and **complicated** objective function

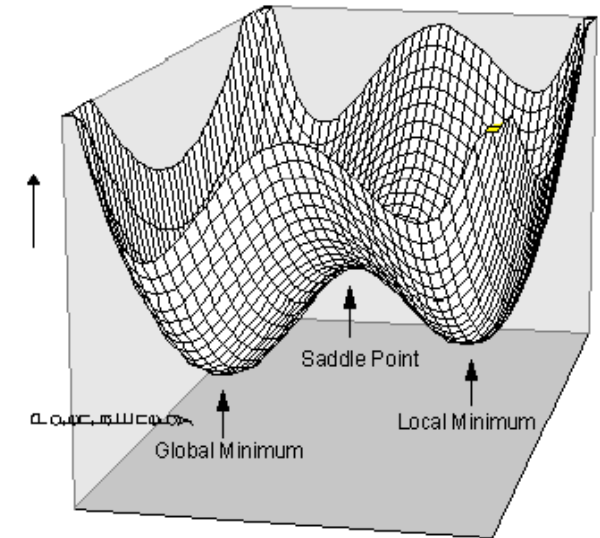
- Highly **non-linear** and **non-convex** function
- The **loss surface** is very **complex**
- Many local minima points, but the number of saddle points is even **exponentially much more**

## □ Need **efficient optimizers** to solve

- SGD with momentum, Adagrad, Adadelta, RMSProp, Adam, and Nadam
- They are **built-in optimizers** of TF.

### TF Implementation

	<code>tf.keras.optimizers.SGD</code>
	<code>tf.keras.optimizers.Adam</code>
	<code>tf.keras.optimizers.Adadelta</code>
	<code>tf.keras.optimizers.Adagrad</code>
	<code>tf.keras.optimizers.RMSProp</code>



(Source: Jan Jakubik)



# 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  $\theta$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient estimate:  $\hat{\mathbf{g}} \leftarrow +\frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Apply update:  $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$

**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.

---

**Algorithm 8.2** Stochastic gradient descent (SGD) with momentum

---

**Require:** Learning rate  $\epsilon$ , momentum parameter  $\alpha$ .

**Require:** Initial parameter  $\theta$ , initial velocity  $\mathbf{v}$ .

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient estimate:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Compute velocity update:  $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$

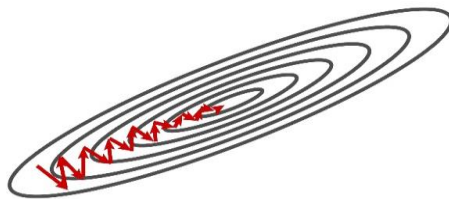
    Apply update:  $\theta \leftarrow \theta + \mathbf{v}$

**end while**

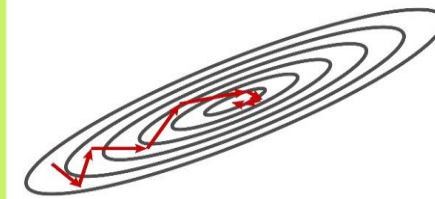
---

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

Without Momentum



Momentum



(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  $\theta$ , initial velocity  $v$ .

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{x^{(1)}, \dots, x^{(m)}\}$  with corresponding labels  $y^{(i)}$ .

    Apply interim update:  $\tilde{\theta} \leftarrow \theta + \alpha v$

    Compute gradient (at interim point):  $g \leftarrow \frac{1}{m} \nabla_{\tilde{\theta}} \sum_i L(f(x^{(i)}; \tilde{\theta}), y^{(i)})$

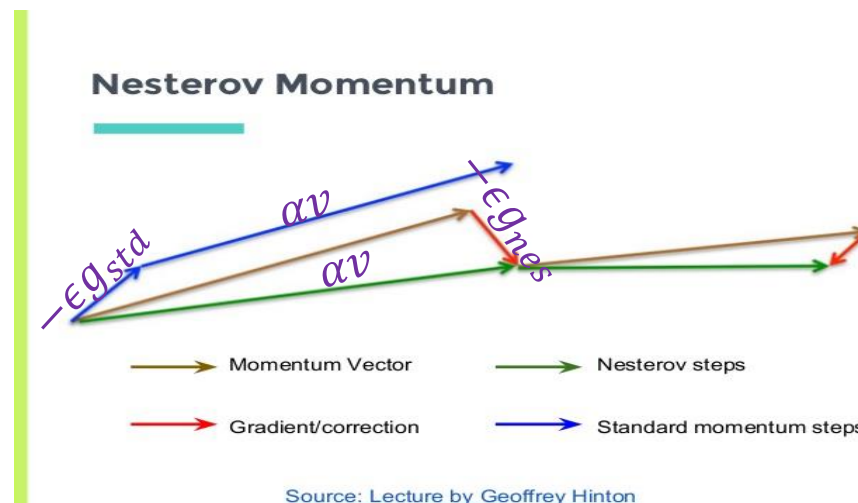
    Compute velocity update:  $v \leftarrow \alpha v - \epsilon g$

    Apply update:  $\theta \leftarrow \theta + v$

**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  $\theta$

**Require:** Small constant  $\delta$ , perhaps  $10^{-7}$ , for numerical stability

Initialize gradient accumulation variable  $\mathbf{r} = \mathbf{0}$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Accumulate squared gradient:  $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g} \odot \mathbf{g}$

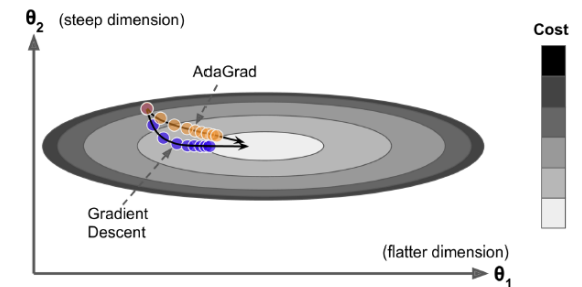
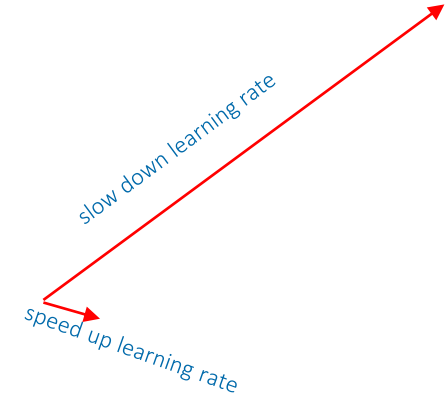
    Compute update:  $\Delta\theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{\mathbf{r}}} \odot \mathbf{g}$ . (Division and square root applied element-wise)

    Apply update:  $\theta \leftarrow \theta + \Delta\theta$

**end while**

---

- 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

---

**Algorithm 8.5** The RMSProp algorithm

---

**Require:** Global learning rate  $\epsilon$ , decay rate  $\rho$ .

**Require:** Initial parameter  $\theta$

**Require:** Small constant  $\delta$ , usually  $10^{-6}$ , used to stabilize division by small numbers.

Initialize accumulation variables  $\mathbf{r} = 0$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Accumulate squared gradient:  $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \mathbf{g} \odot \mathbf{g}$

    Compute parameter update:  $\Delta \theta = -\frac{\epsilon}{\sqrt{\delta + \mathbf{r}}} \odot \mathbf{g}$ . ( $\frac{1}{\sqrt{\delta + \mathbf{r}}}$  applied element-wise)

    Apply update:  $\theta \leftarrow \theta + \Delta \theta$

**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.

- 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  $\theta$

Initialize 1st and 2nd moment variables  $\mathbf{s} = \mathbf{0}$ ,  $\mathbf{r} = \mathbf{0}$

Initialize time step  $t = 0$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

$t \leftarrow t + 1$

    Update biased first moment estimate:  $\mathbf{s} \leftarrow \rho_1 \mathbf{s} + (1 - \rho_1) \mathbf{g}$

    Update biased second moment estimate:  $\mathbf{r} \leftarrow \rho_2 \mathbf{r} + (1 - \rho_2) \mathbf{g} \odot \mathbf{g}$

    Correct bias in first moment:  $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \rho_1^t}$

    Correct bias in second moment:  $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1 - \rho_2^t}$

    Compute update:  $\Delta \theta = -\epsilon \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}} + \delta}}$  (operations applied element-wise)

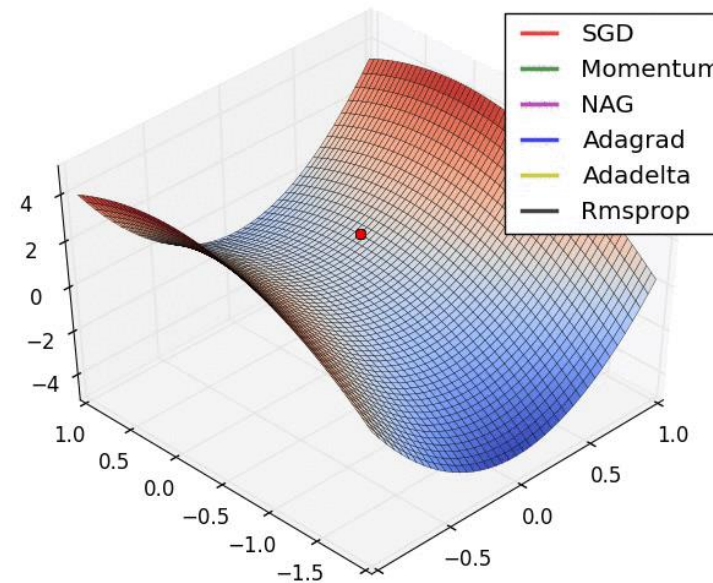
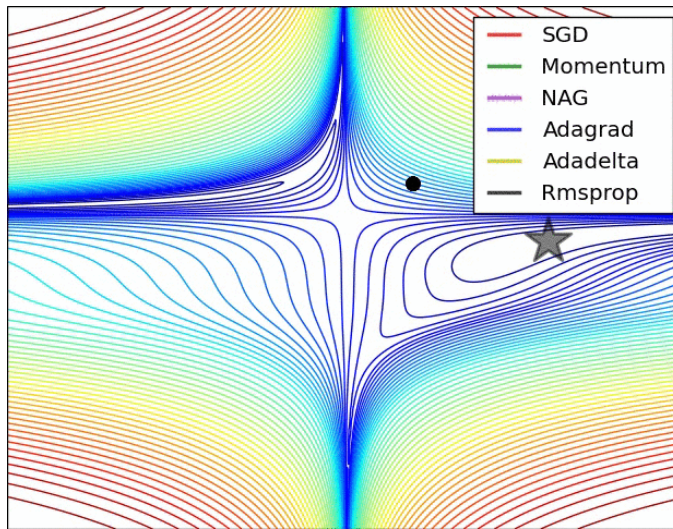
    Apply update:  $\theta \leftarrow \theta + \Delta \theta$

**end while**

---



# Visual comparison of all optimizers



[Source: Sebastian Ruder]

# TensorFlow optimizers

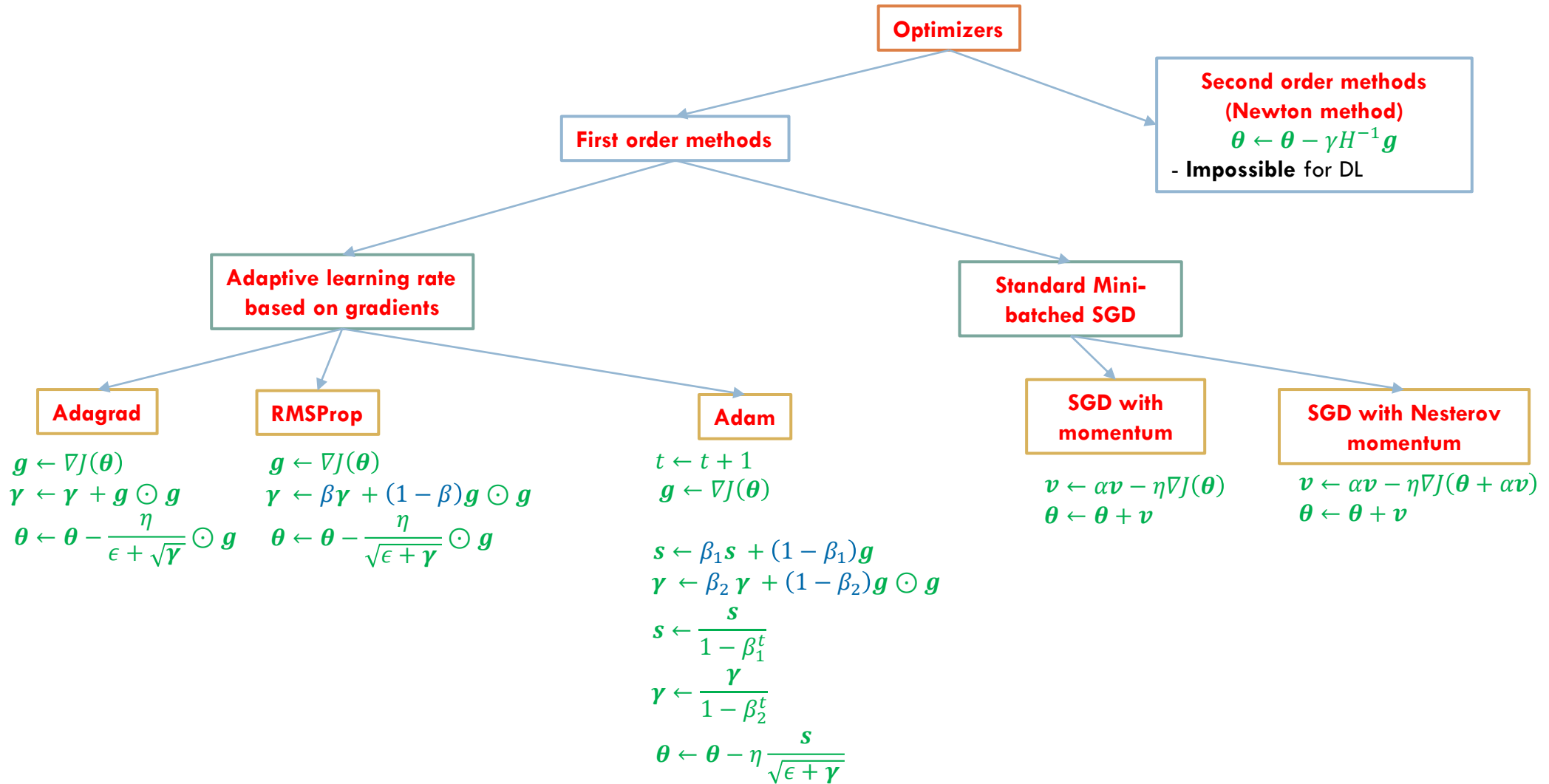
## □ TensorFlow pre-implemented methods for TF 1.x:

- `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", "Adadelata", "Adagrad", "RMSprop", "SGD"]
optimizer_list = [keras.optimizers.Nadam(learning_rate=0.001), keras.optimizers.Adam(learning_rate=0.001), keras.optimizers.Adadelata(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 {}".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 {}".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





# 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

- $\frac{1}{b} \sum_{i=1}^b CE(1^{y_i}, p^i) = -\frac{1}{b} \sum_{i=1}^b \log p_{y_i}^i$

