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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:

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

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

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

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

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

□ 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 \Rightarrow :

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

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)

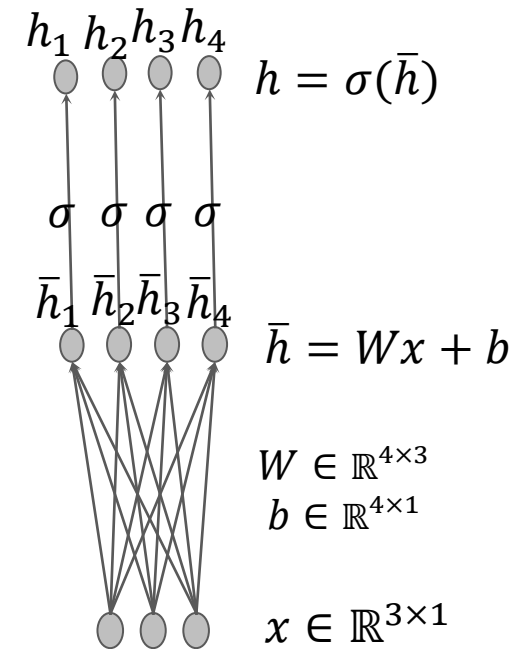
$$\square \quad \bar{h} = Wx + b \text{ and } h = \sigma(\bar{h})$$

- $h = \sigma(Wx + b)$
- σ 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

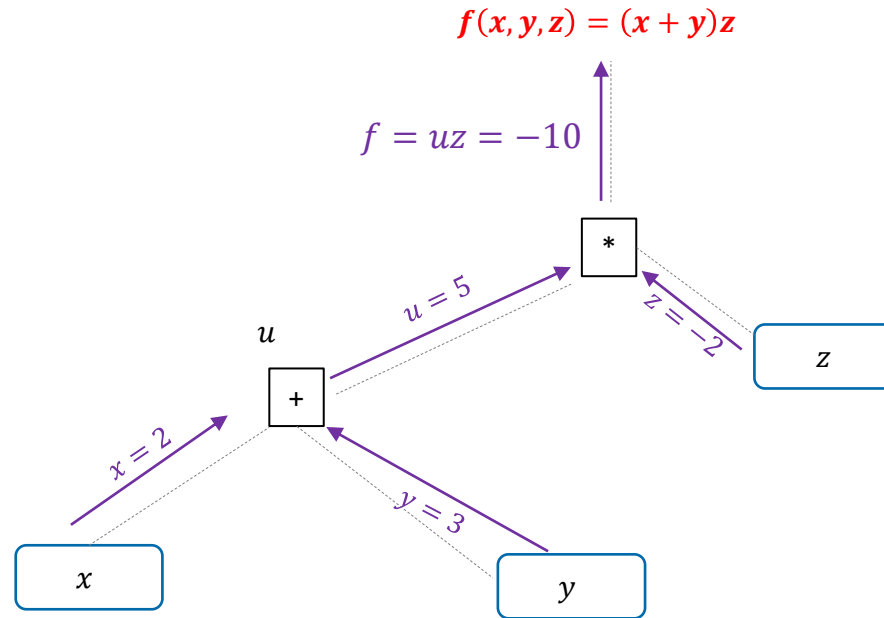
Computational graph (used in TensorFlow)

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

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

Step 1:

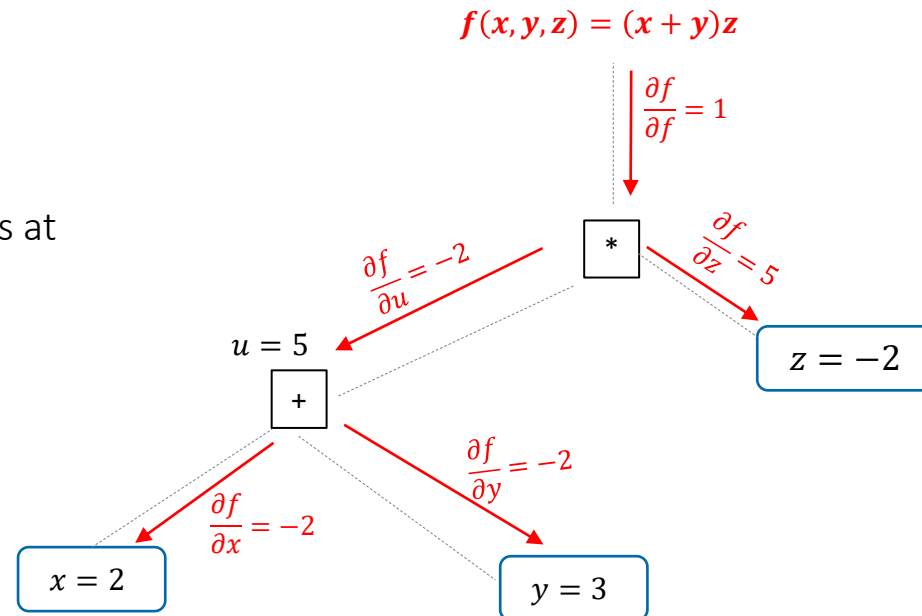
- construct computational graph
- forward propagation
- record value at each node



Reverse Auto-Diff (used in TensorFlow)

Step 2:

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



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

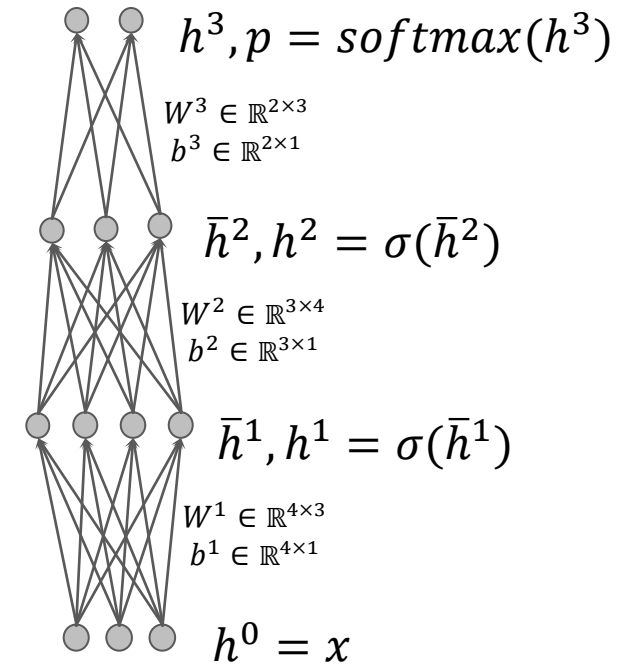
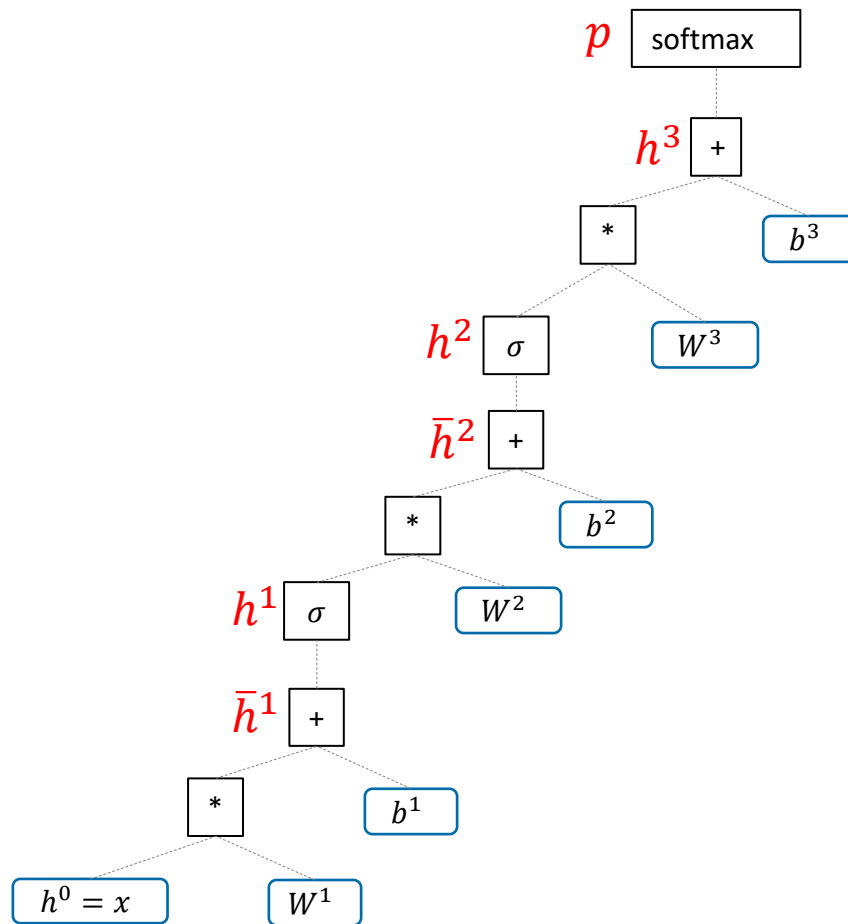
$$\frac{\partial f}{\partial u} = \frac{\partial f}{\partial f} \frac{\partial f}{\partial u} = 1 * z = -2$$

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

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

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

Computational graph of feedforward nets (Forum discussion)



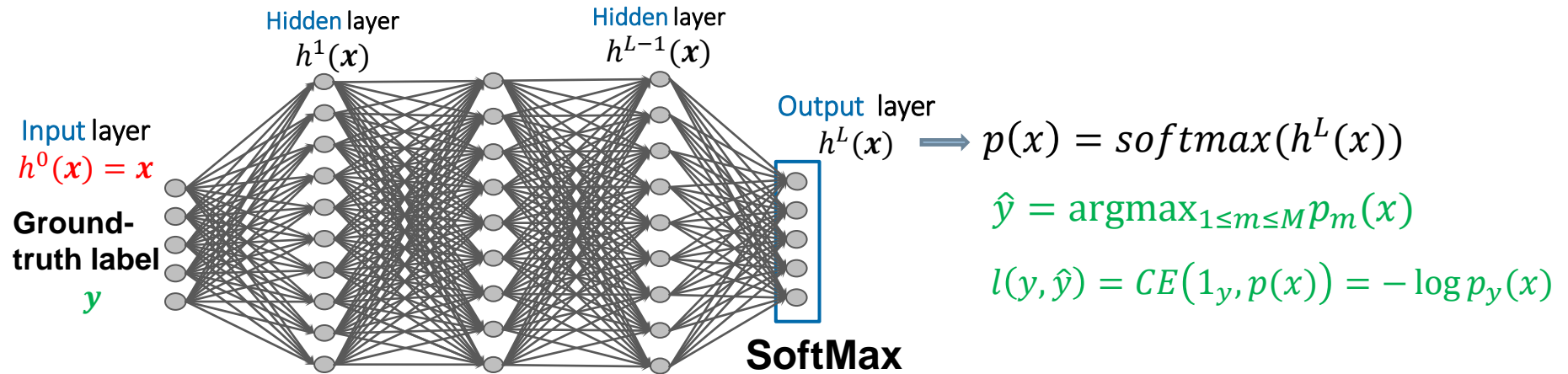
```

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
h3(x) = W3h2(x) + b2
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
 - 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 $g = \nabla J(\theta)$ is the **first order derivative** and defined as

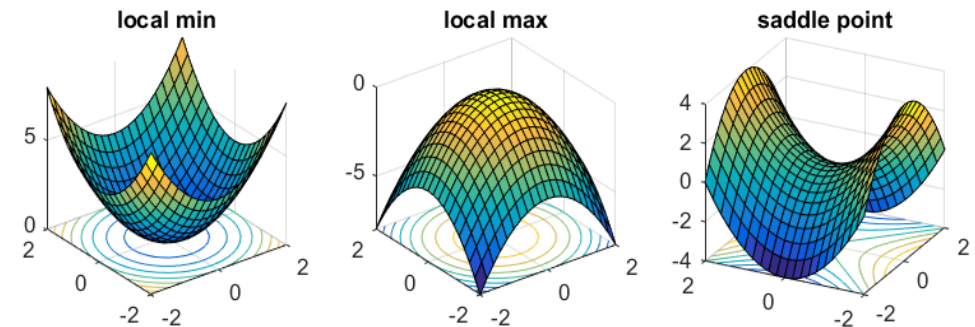
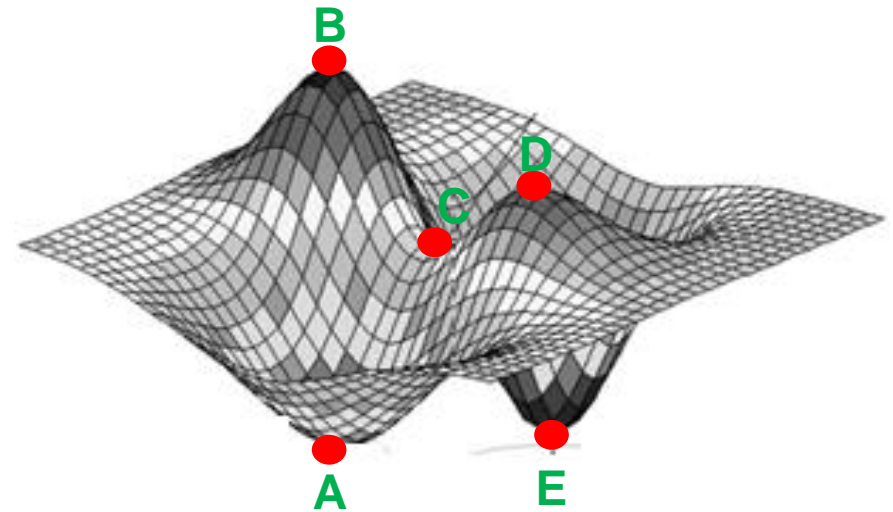
- $$\nabla J(\theta) = g = \begin{bmatrix} \frac{\partial J}{\partial \theta_1}(\theta) \\ \dots \dots \dots \\ \frac{\partial J}{\partial \theta_P}(\theta) \end{bmatrix}$$

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

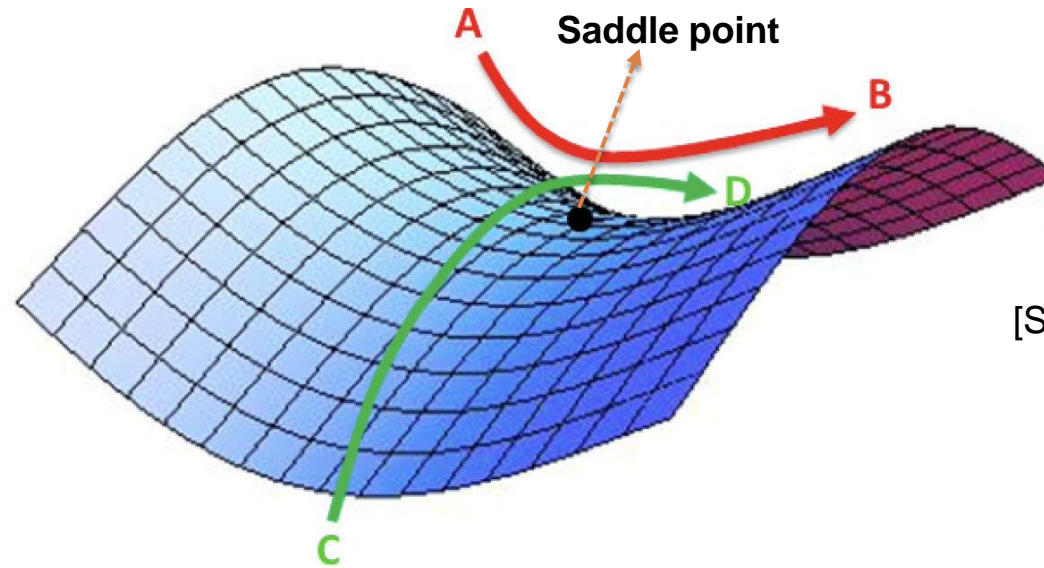
- $$\nabla^2 J(\theta) = H(\theta) = \begin{bmatrix} \frac{\partial^2 J}{\partial \theta_1 \partial \theta_1}(\theta) & \dots & \dots & \frac{\partial^2 J}{\partial \theta_1 \partial \theta_j}(\theta) & \dots & \frac{\partial^2 J}{\partial \theta_1 \partial \theta_P}(\theta) \\ \dots & \dots & \dots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

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
 - $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_p$
- **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]

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

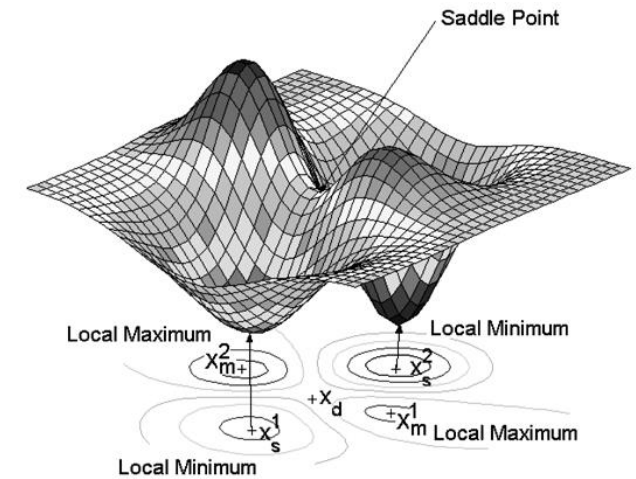
Gradient $g = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 \\ -2x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \rightarrow$ a critical point $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

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

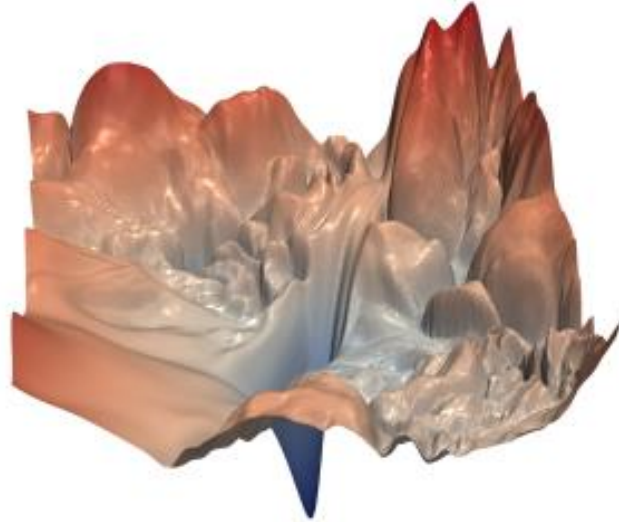
Two eigenvalues $\lambda_1 = -2 < 0 < 2 = \lambda_2 \rightarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ is a saddle point.

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 $\mathbb{P}(\lambda_1 \geq 0) = \mathbb{P}(\lambda_2 \geq 0) = \dots = \mathbb{P}(\lambda_P \geq 0) = 0.5$
- 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]

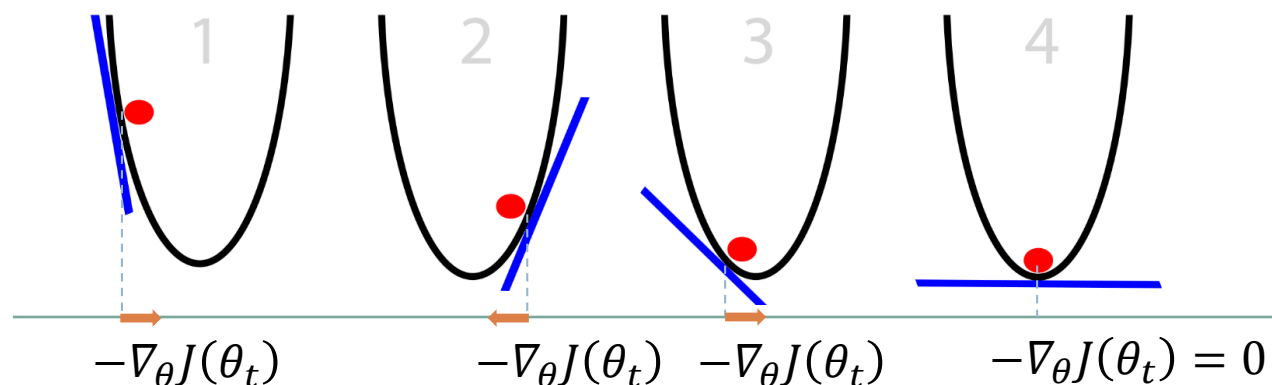
□ The optimization problem in deep learning:

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

□ 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

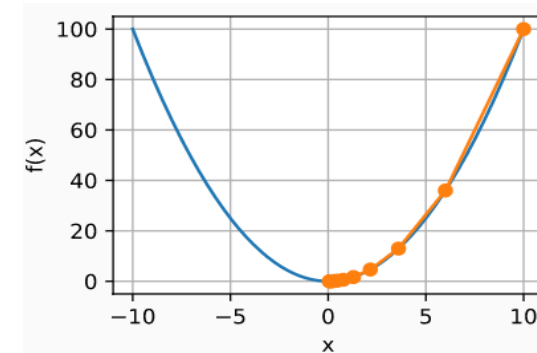
- $\min_{\theta} J(\theta)$

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

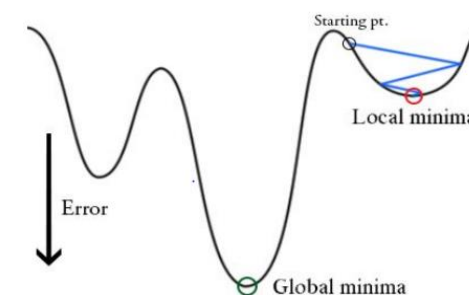
- $\theta_{t+1} = \theta_t - \eta \nabla_{\theta} J(\theta_t)$ where $\eta > 0$ is the **learning rate**.

□ 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.

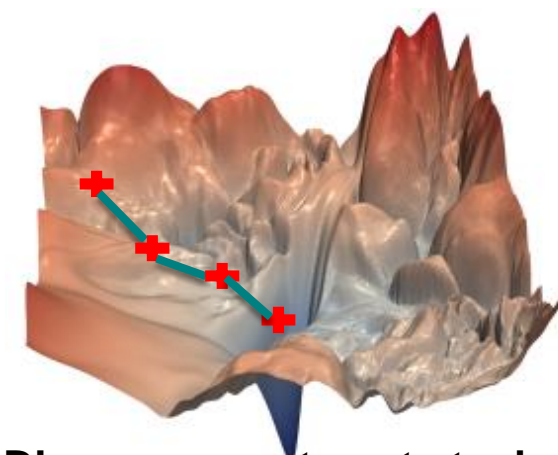


Convex case



(Source: www.cs.ubc.ca)

Non-convex case



DL case: easy to get stuck in saddle points

Gradient descend

Algorithm

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

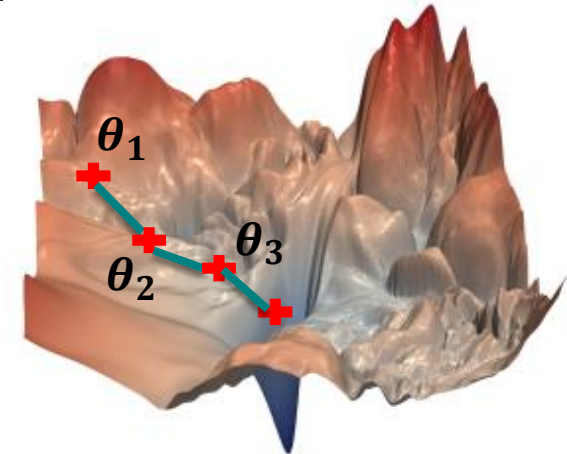


```
import tensorflow as tf

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

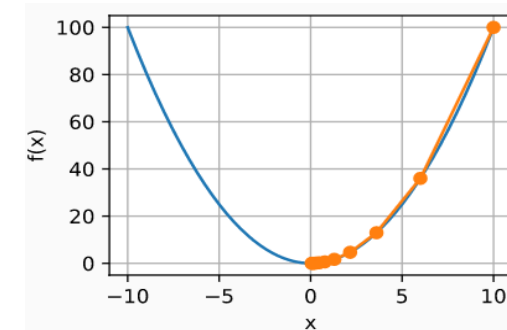
results = gd(0.2, f_grad)
```

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)
```

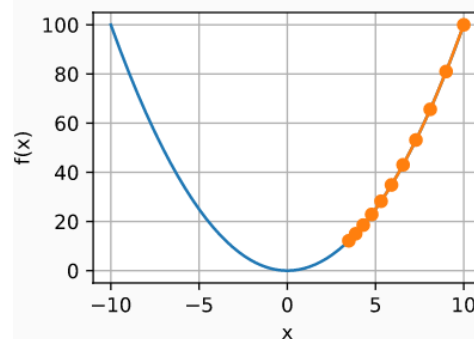
Show trace of
gradient descent



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

epoch 10, x: 3.486784

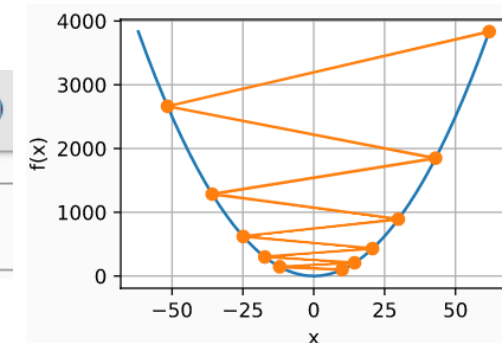
Good learning rate η



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

epoch 10, x: 61.917364

Too high rate η



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?

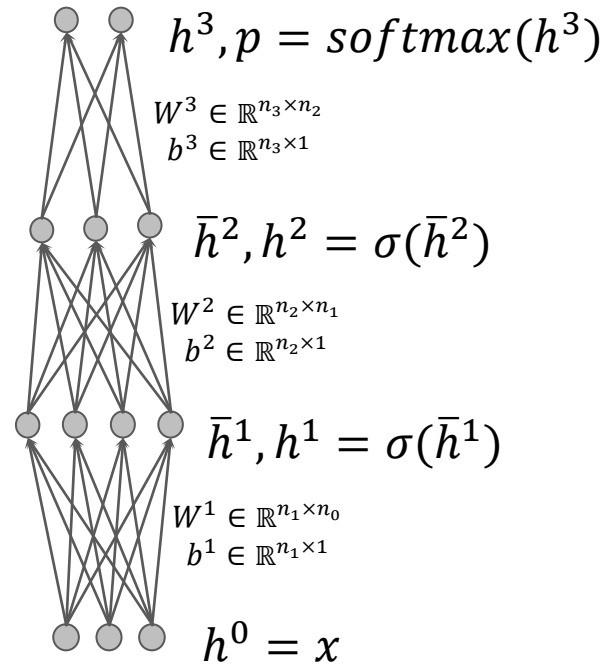
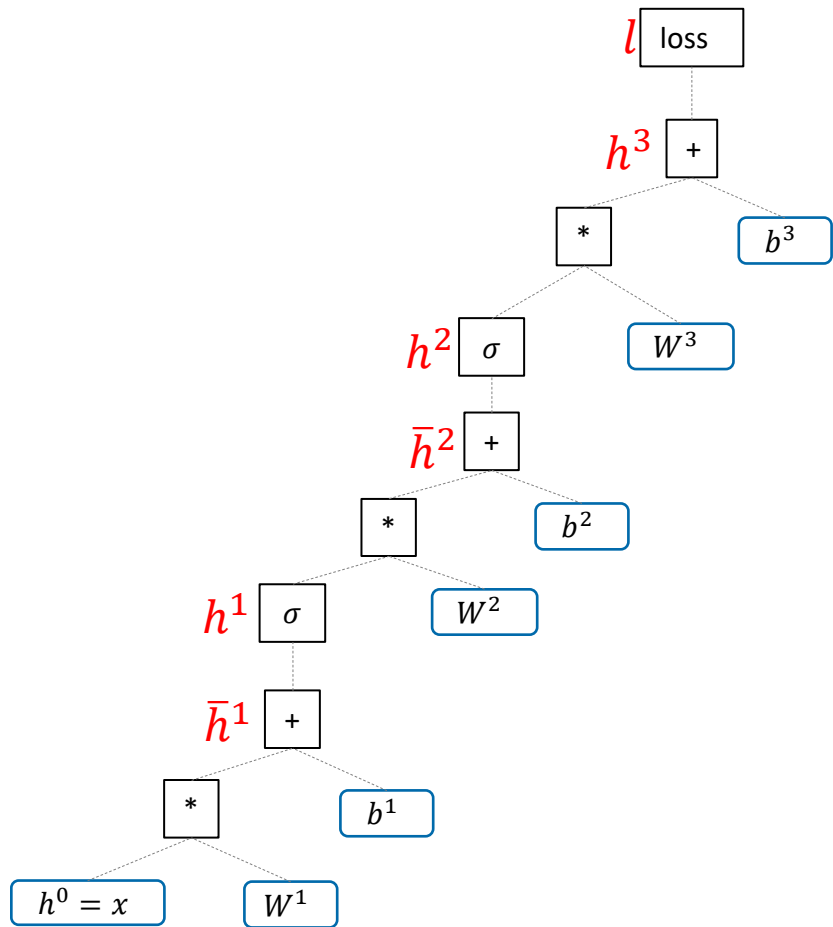
Stochastic gradient descent (Forum discussion)

- 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.

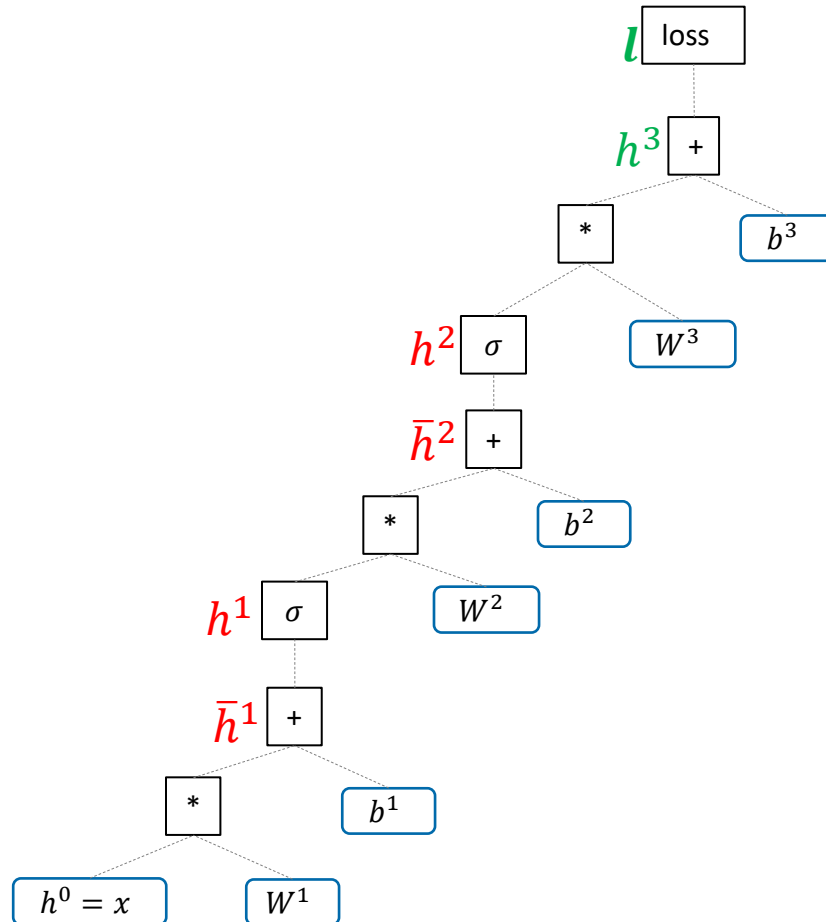
Back propagation

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.

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

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

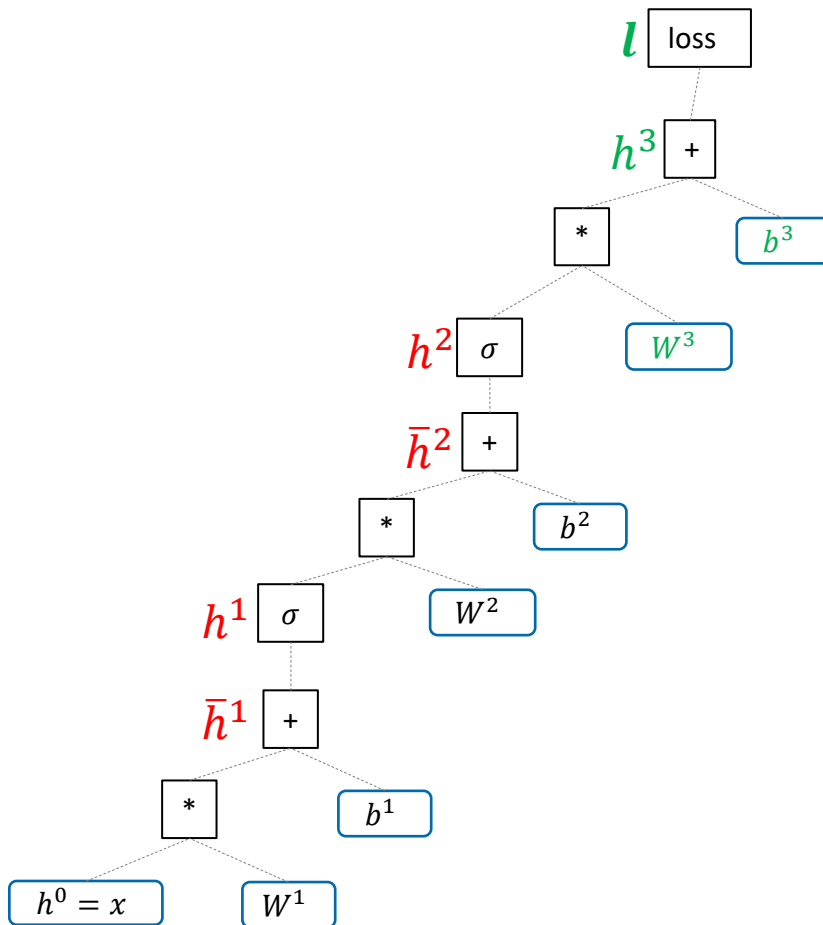
$$= \mathbf{p}^T - \mathbf{1}_y$$

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

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

Back propagation

From loss to W^3, b^3



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

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

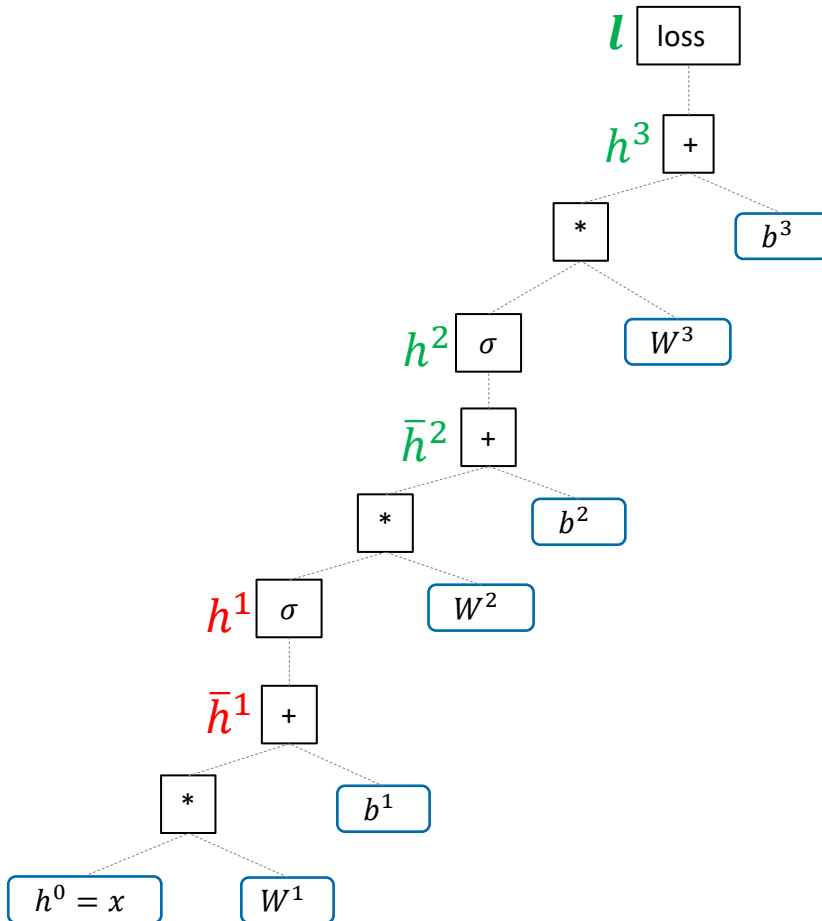
- $[n_3 \times 1] \times [1 \times n_2] \rightarrow [n_3 \times n_2]$

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

- $[1 \times n_3]$

Back propagation

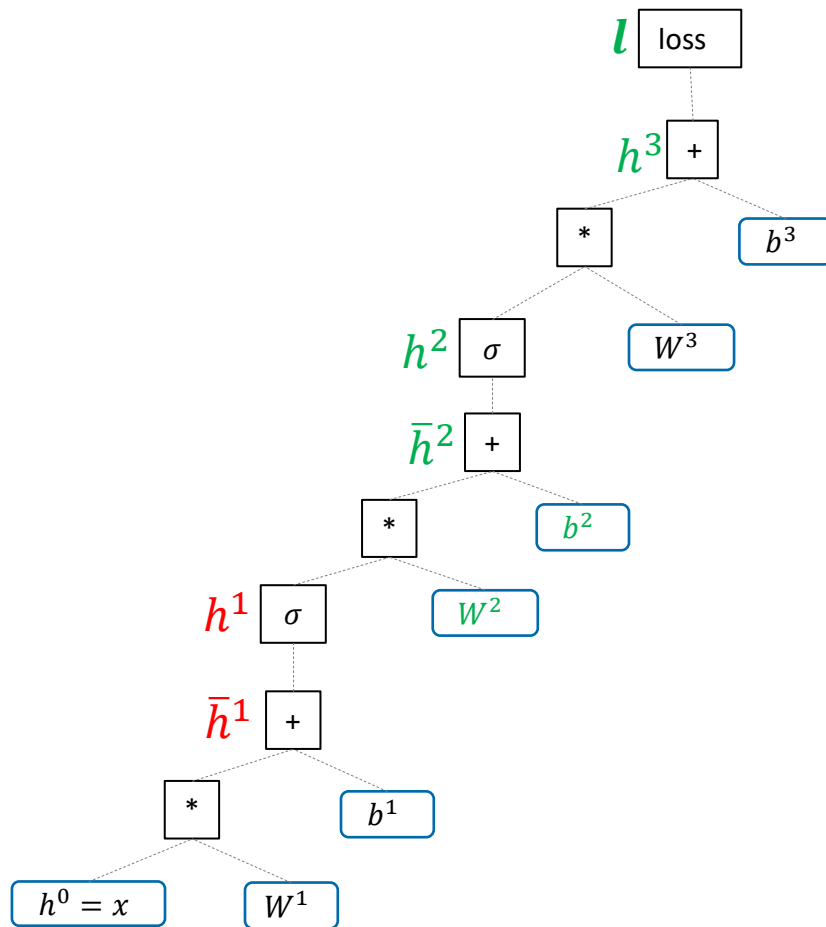
From loss to h^2 and \bar{h}^2



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

Back propagation

From loss to W^2 and b^2



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

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

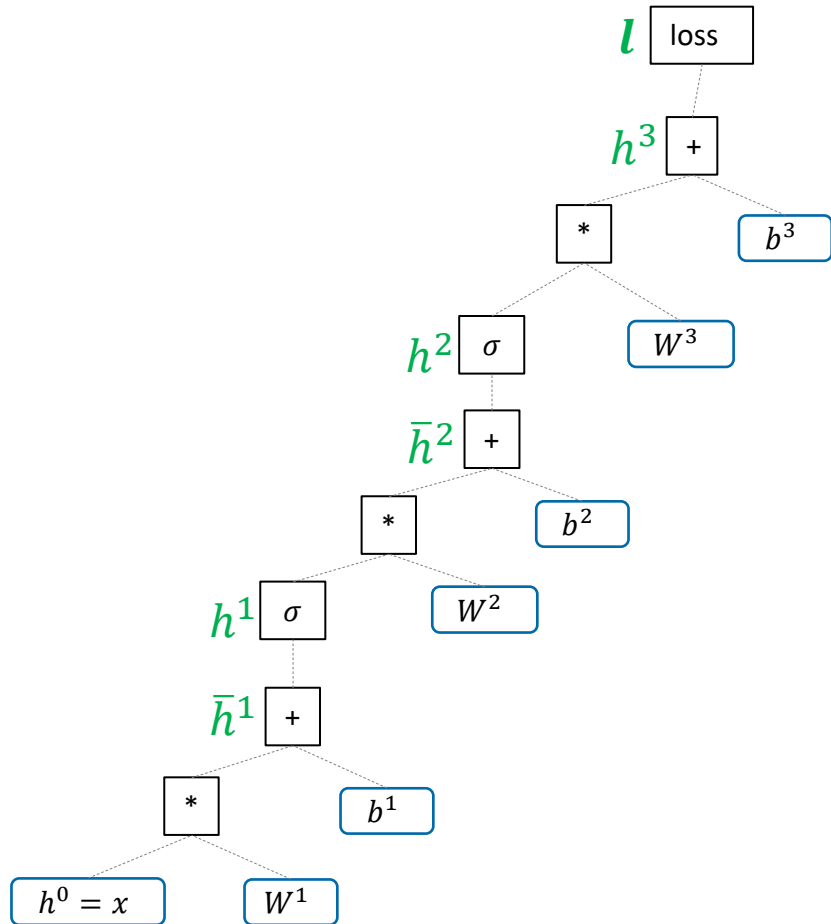
◦ $[n_2 \times 1] \times [1 \times n_1] \rightarrow [n_2 \times n_1]$

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

◦ $[1 \times n_2]$

Back propagation

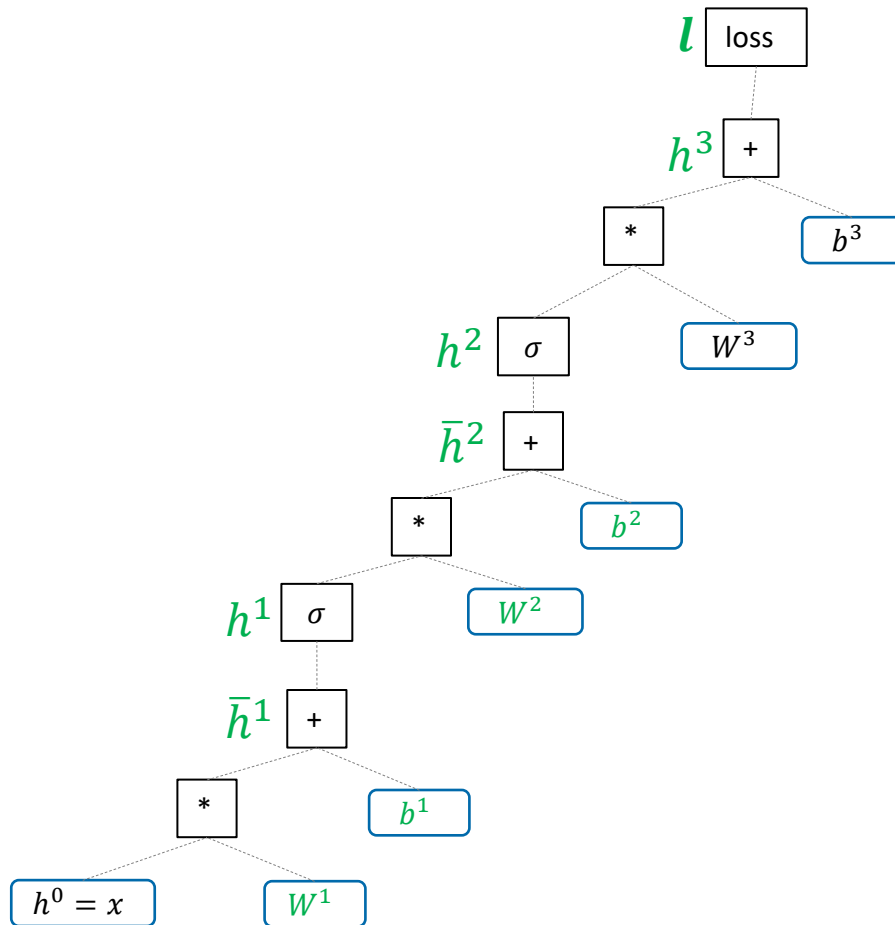
From loss to h^1 and \bar{h}^1



- $\bar{h}^2 = W^2 h^1 + b^2$
- $g^1 = \frac{\partial l}{\partial h^1} = \frac{\partial l}{\partial \bar{h}^2} \cdot \frac{\partial \bar{h}^2}{\partial h^1} = \bar{g}^2 W^2$
 - $[1 \times n_2] \times [n_2 \times n_1] \rightarrow [1 \times n_1]$
- $h^1 = \sigma(\bar{h}^1)$ (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



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

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

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

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

- $[1 \times n_1]$

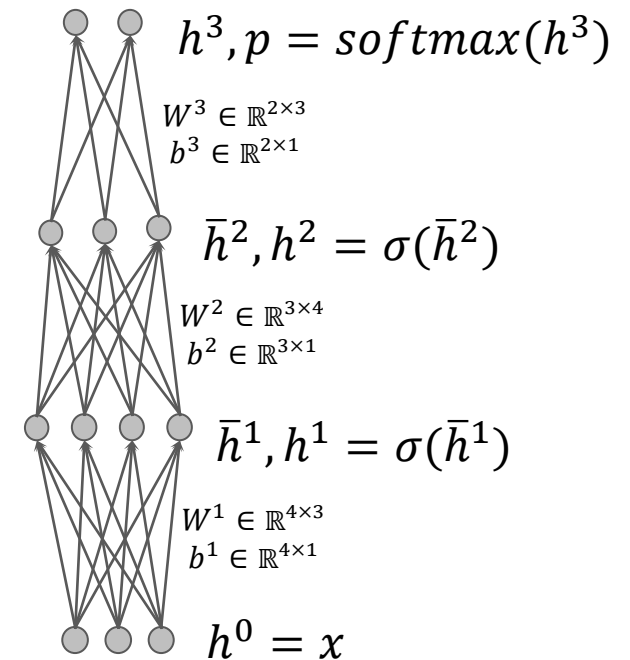


Exercise: How to compute $\frac{\partial l}{\partial x}$?

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 $[n_1, b]$

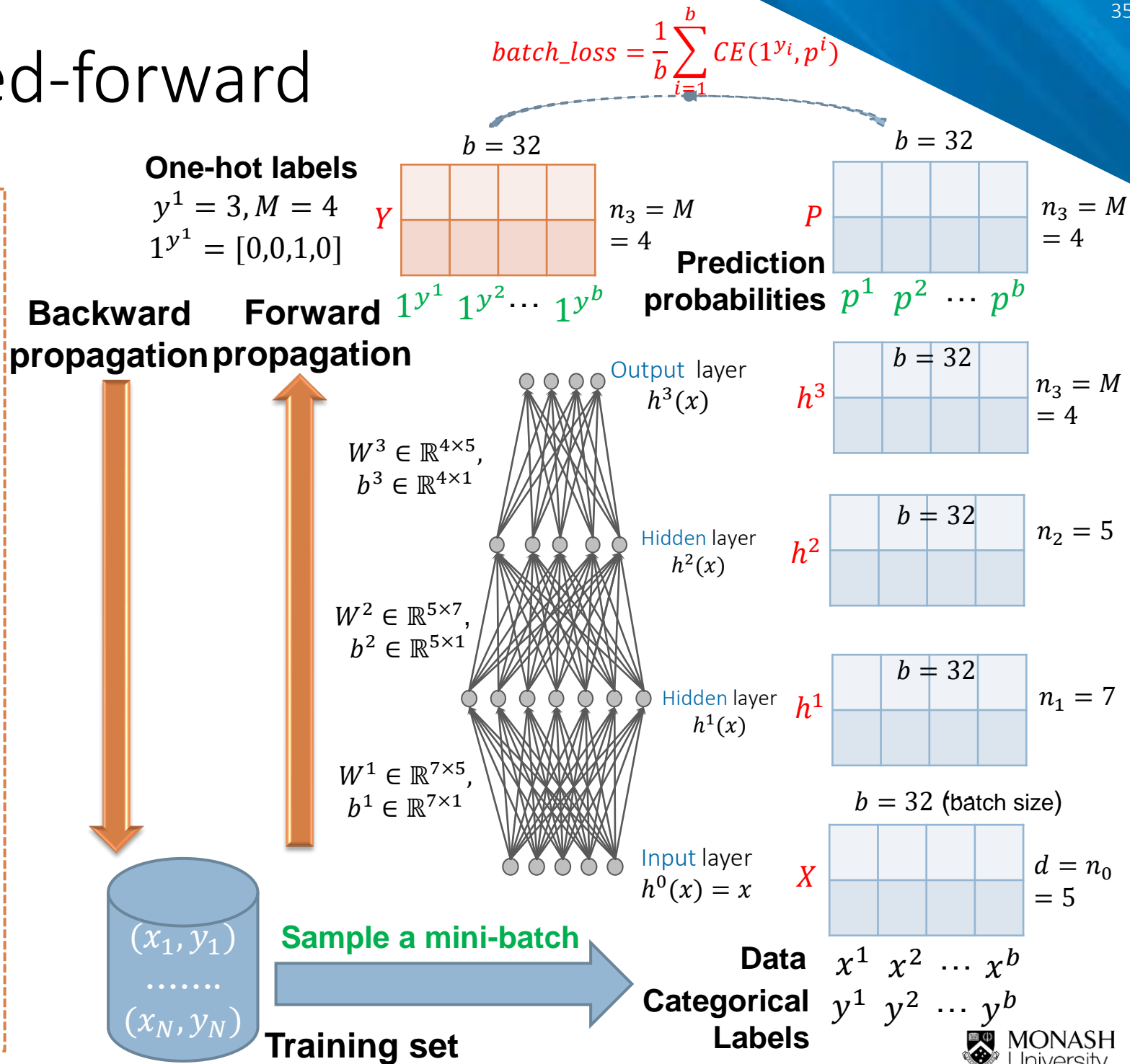
.....

Output layer

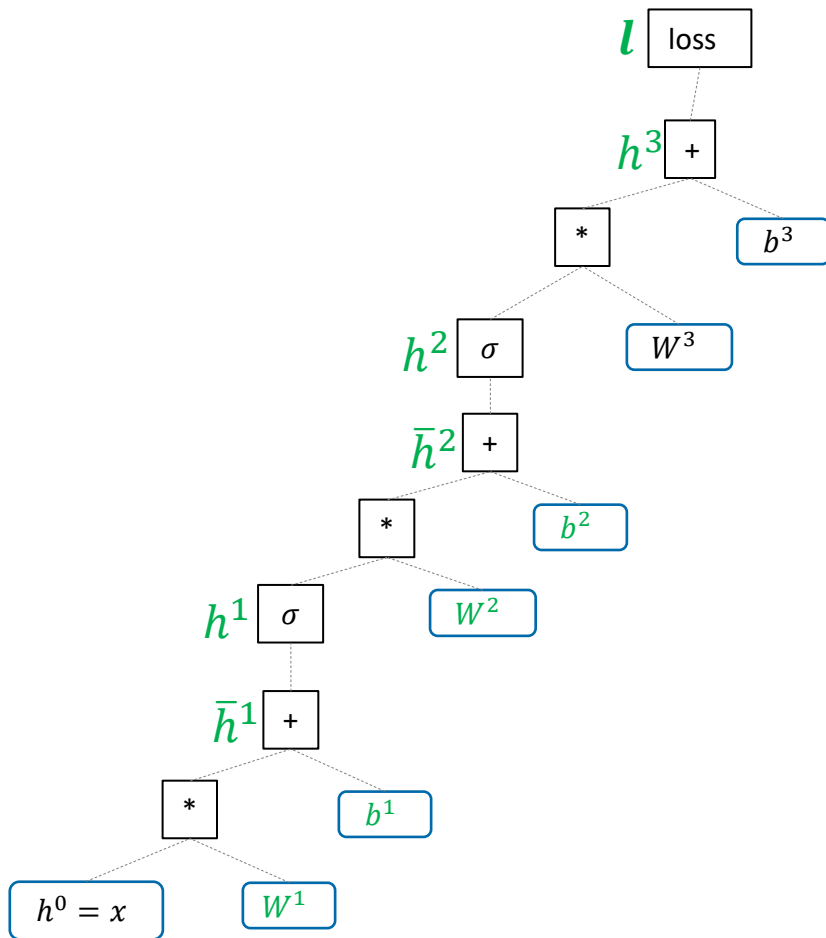
- Tensor P : $[n_L = M, b]$

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?



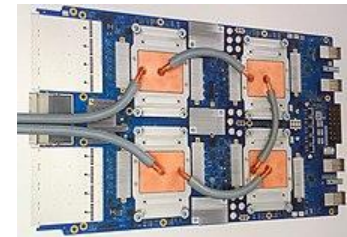
- Let consider

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

- 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)

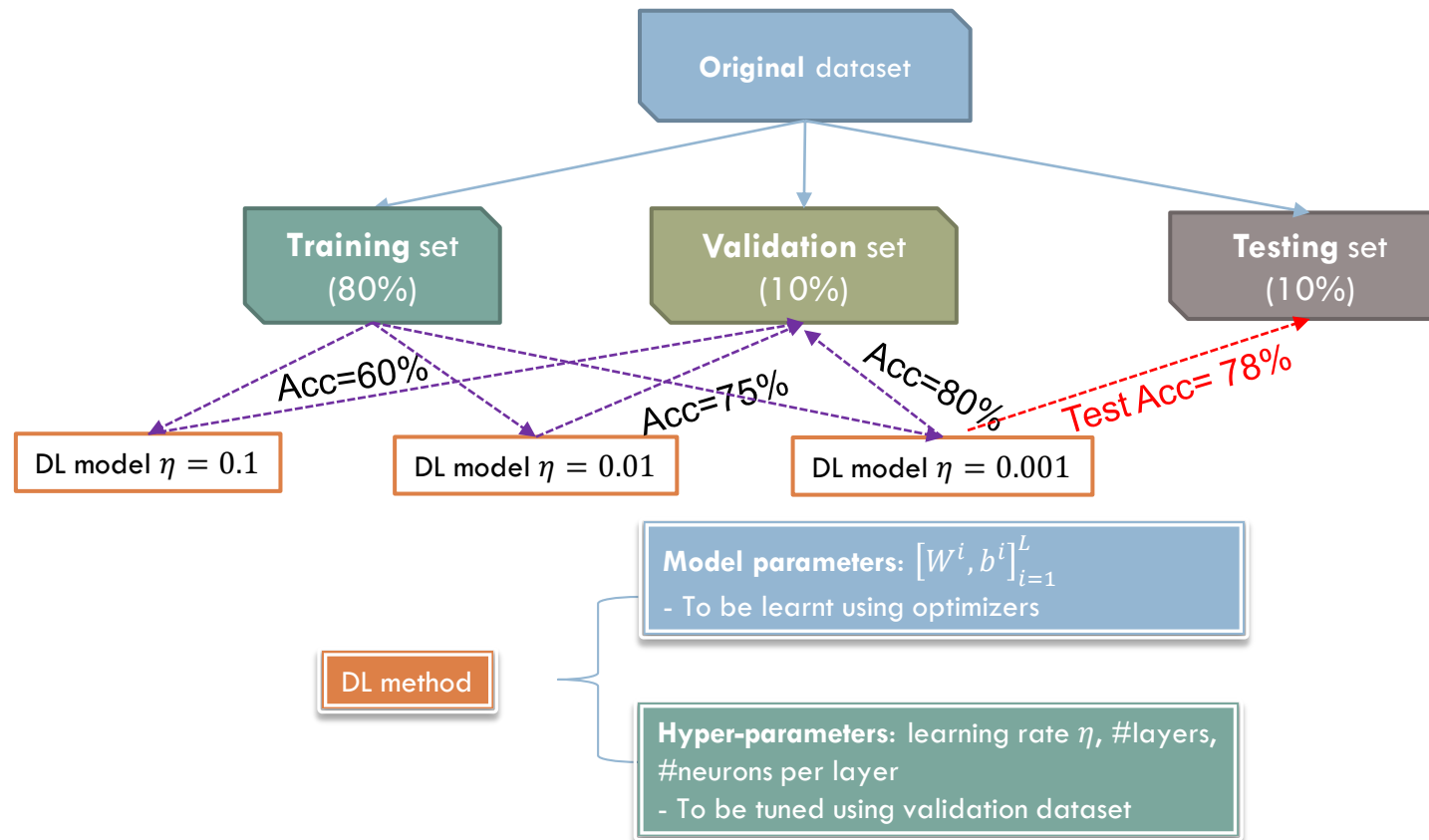


TPU (Source: Wikipedia)

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

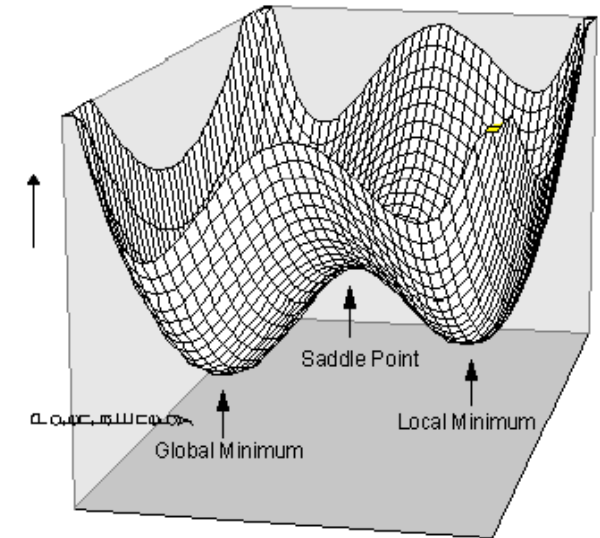
- Highly **non-linear** and **non-convex** function
- The **loss surface** is very **complex**
- Many local minima points, but the number of saddle points is even **exponentially much more**

□ 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 ϵ_k .

Require: Initial parameter θ

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 ϵ , momentum parameter α .

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

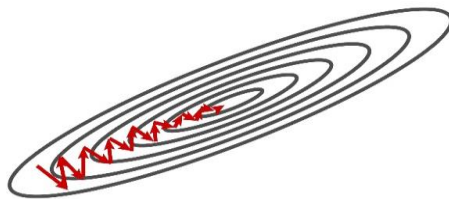
 Compute velocity update: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$

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

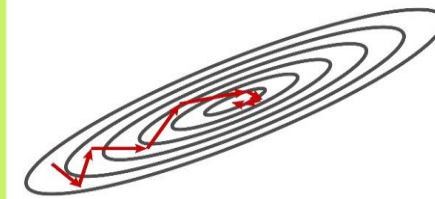
end while

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

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 ϵ , momentum parameter α .

Require: Initial parameter θ , 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): $g \leftarrow \frac{1}{m} \nabla_{\tilde{\theta}} \sum_i L(f(x^{(i)}; \tilde{\theta}), y^{(i)})$

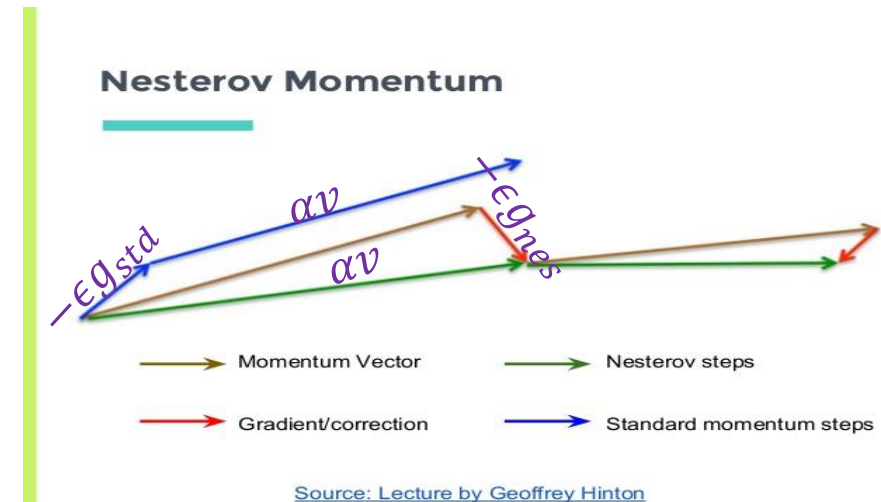
 Compute velocity update: $v \leftarrow \alpha v - \epsilon g$

 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 ϵ

Require: Initial parameter θ

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

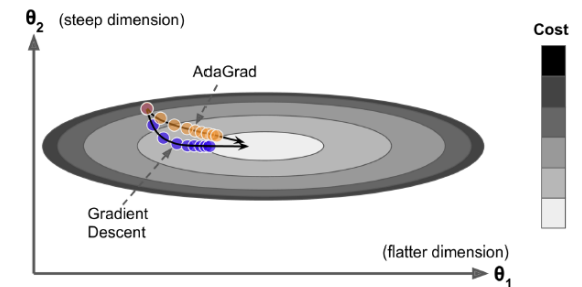
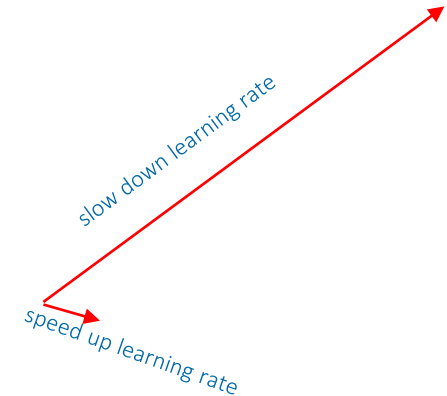
 Accumulate squared gradient: $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g} \odot \mathbf{g}$

 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 ϵ , decay rate ρ .

Require: Initial parameter θ

Require: Small constant δ , 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 ϵ (Suggested default: 0.001)

Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$.
(Suggested defaults: 0.9 and 0.999 respectively)

Require: Small constant δ used for numerical stabilization. (Suggested default: 10^{-8})

Require: Initial parameters θ

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: $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \rho_1^t}$

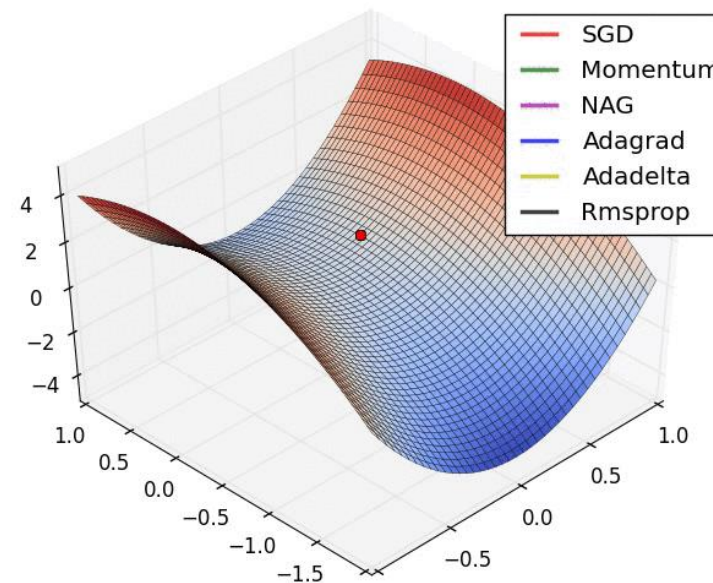
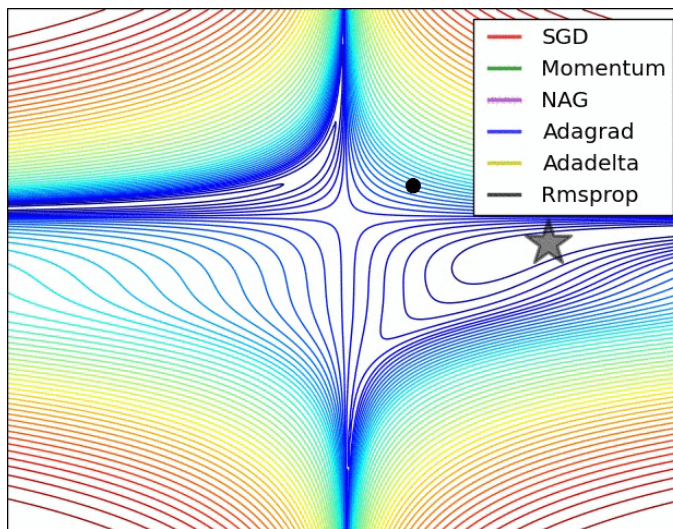
 Correct bias in second moment: $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1 - \rho_2^t}$

 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

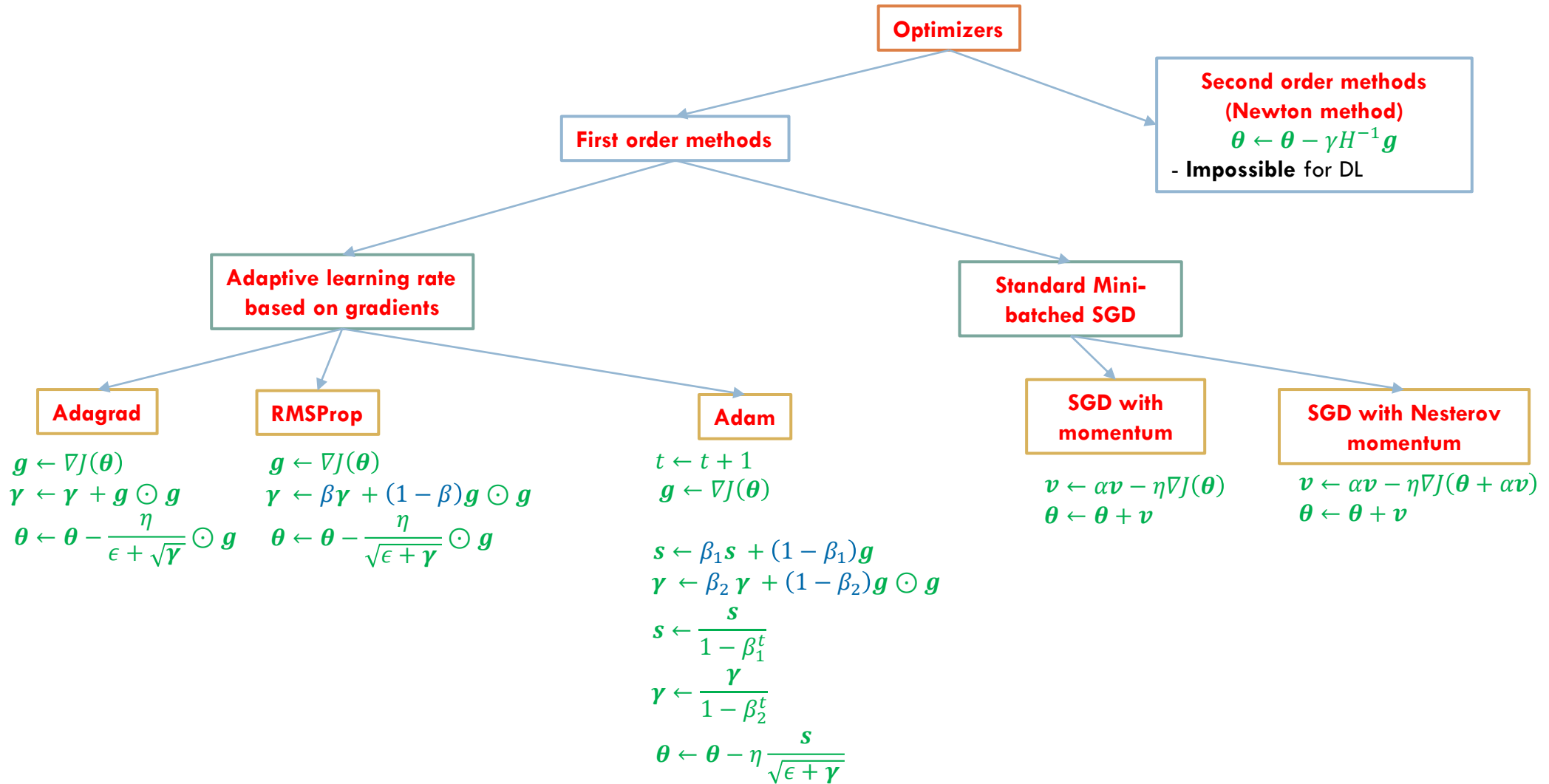
□ TensorFlow pre-implemented methods for TF 1.x:

- `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

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

