

## Week 2: Optimization and Frameworks

Instructor: Ruixuan Wang  
wangruix5@mail.sysu.edu.cn

School of Data and Computer Science  
Sun Yat-Sen University

7 March, 2019

## 1 Backpropagation

## 2 Stochastic optimization

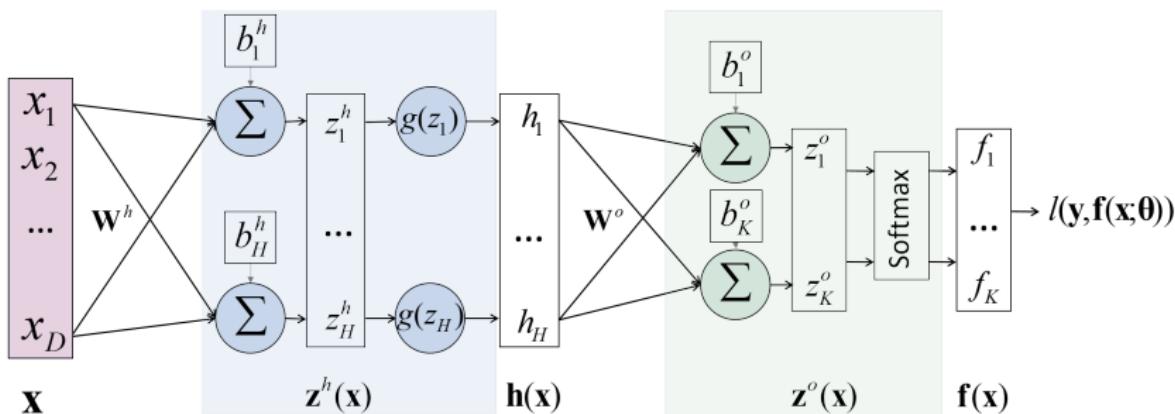
## 3 Hyper-parameter tuning

## 4 Deep learning frameworks

# Derivatives: basic

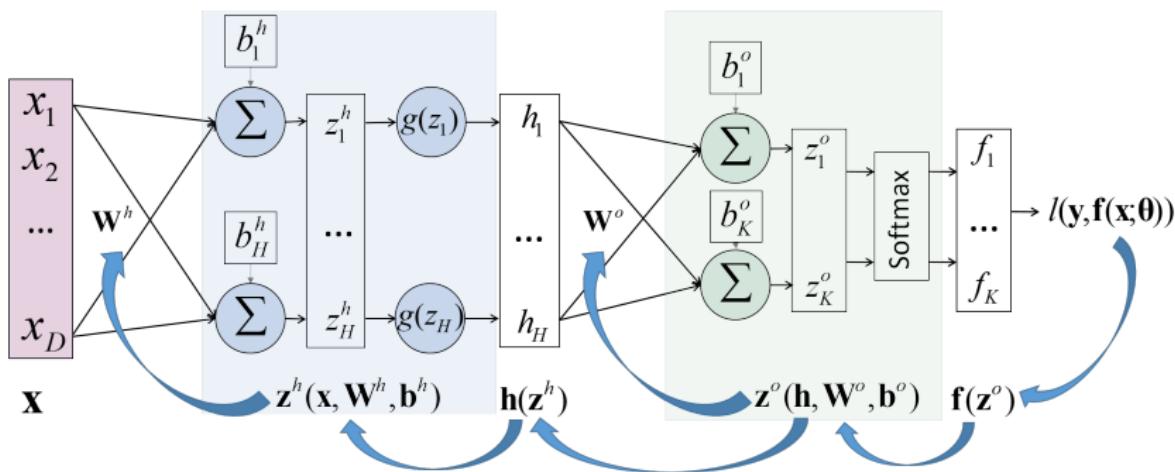
- $L(\theta) = a$        $\frac{dL}{d\theta} = 0$
- $L(\theta) = a\theta$        $\frac{dL}{d\theta} = a$
- $L(\theta) = au(\theta)$        $\frac{dL}{d\theta} = a \frac{du}{d\theta}$
- $L(\theta) = u(\theta) + v(\theta) - w(\theta)$        $\frac{dL}{d\theta} = \frac{du}{d\theta} + \frac{dv}{d\theta} - \frac{dw}{d\theta}$
- $L(\theta) = \frac{u(\theta)}{v(\theta)}$        $\frac{dL}{d\theta} = \frac{1}{v} \frac{du}{d\theta} - \frac{u}{v^2} \frac{dv}{d\theta}$
- $L(\theta) = u^n(\theta)$        $\frac{dL}{d\theta} = nu^{n-1} \frac{du}{d\theta}$
- $L(\theta) = \frac{1}{u(\theta)}$        $\frac{dL}{d\theta} = -\frac{1}{u^2} \frac{du}{d\theta}$
- $L(\theta) = \ln u(\theta)$        $\frac{dL}{d\theta} = \frac{1}{u(\theta)} \frac{du}{d\theta}$
- $L(\theta) = e^{u(\theta)}$        $\frac{dL}{d\theta} = e^{u(\theta)} \frac{du}{d\theta}$
- $L(\theta) = f(u(\theta))$        $\frac{dL}{d\theta} = \frac{df}{du} \frac{du}{d\theta}$

## Training a two-layer network classifier



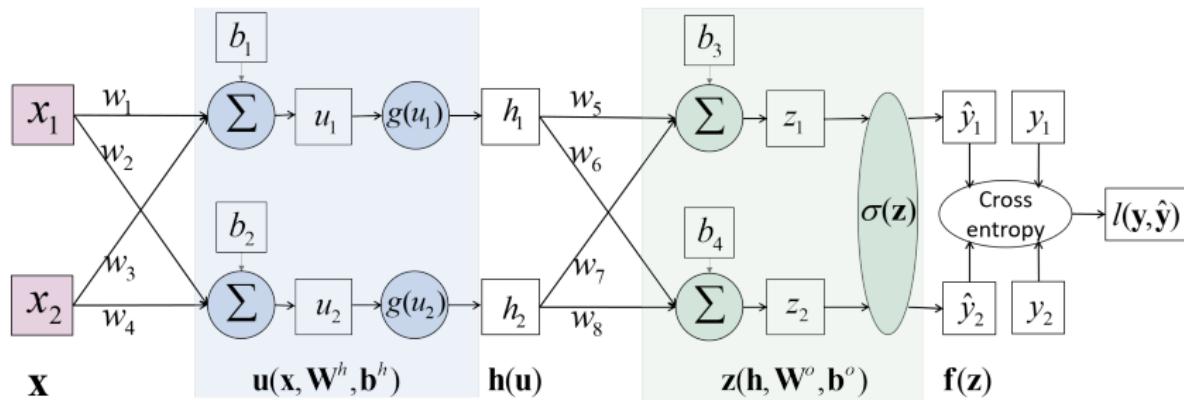
- Loss function  $l(\mathbf{y}, \mathbf{f}(\mathbf{x}; \boldsymbol{\theta}))$  measures difference between prediction  $\mathbf{f}(\mathbf{x}; \boldsymbol{\theta})$  and ideal output  $\mathbf{y}$ .
  - Model parameters  $\boldsymbol{\theta} = \{\mathbf{W}^h, \mathbf{b}^h, \mathbf{W}^o, \mathbf{b}^o\}$
  - Training network: minimize loss with gradient descent to find best  $\boldsymbol{\theta}^*$

## Backpropagation: computation of gradient with chain rule



- Gradient of loss function over model parameters can be computed with chain rule.

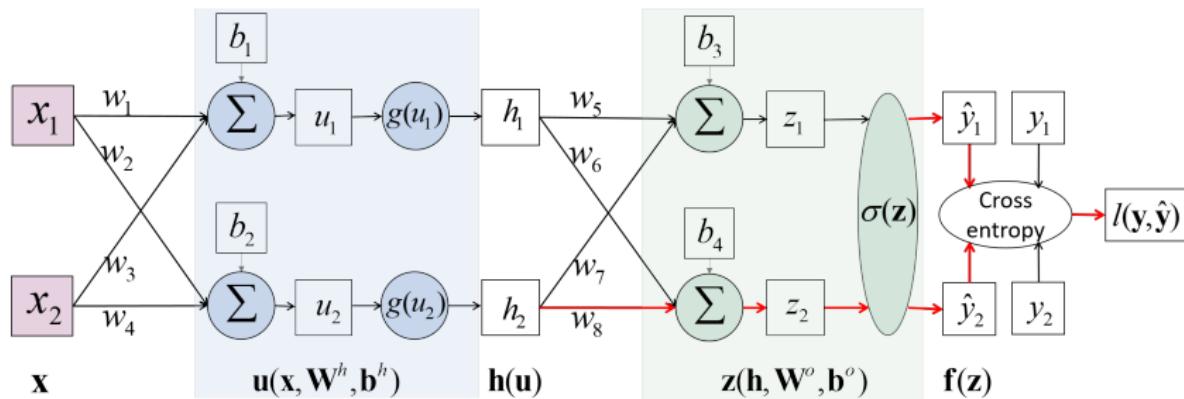
# A simpler 2-layer network



- ReLU  $g(u_i) = \max(0, u_i)$ , Softmax  $\sigma(\mathbf{z})$
- Cross entropy loss  $l(\mathbf{y}, \hat{\mathbf{y}})$
- Model parameters  $\theta = [w_1, \dots, w_8, b_1, \dots, b_4]^T$

$$\mathbf{W}^h = \begin{bmatrix} w_1 & w_3 \\ w_2 & w_4 \end{bmatrix}, \mathbf{b}^h = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \mathbf{W}^o = \begin{bmatrix} w_5 & w_7 \\ w_6 & w_8 \end{bmatrix}, \mathbf{b}^o = \begin{bmatrix} b_3 \\ b_4 \end{bmatrix}$$

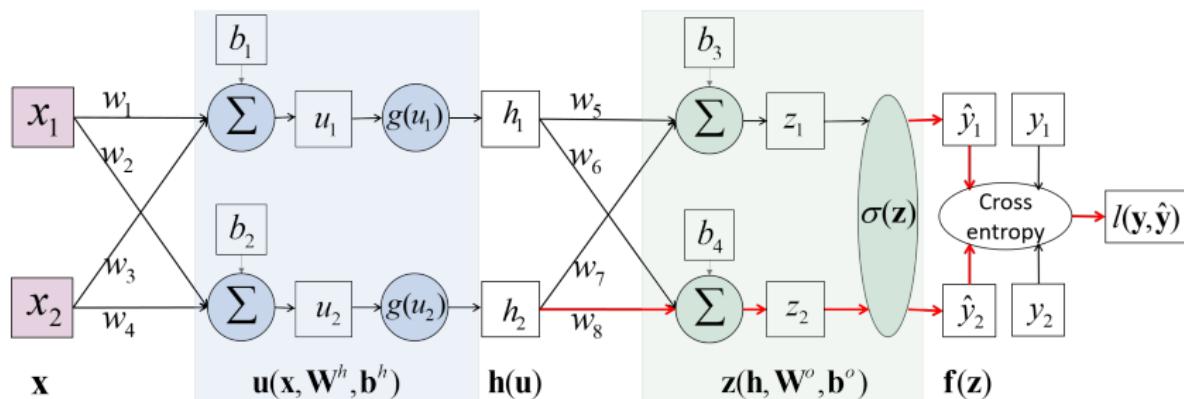
# Backpropagation: one derivative example



- Backpropagation: computation of gradient with chain rule
- an example:

$$\frac{\partial l}{\partial w_8} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial w_8}$$

# Backpropagation: one derivative example (cont')



- Pre-softmax function  $z_2 = h_1 w_6 + h_2 w_8 + b_4$ , therefore

$$\frac{\partial z_2}{\partial w_8} = h_2$$

- To compute  $\frac{\partial l}{\partial z_2}$ , need to compute derivative of softmax  $\frac{\partial \hat{y}_j}{\partial z_2}$

# Derivative of softmax function

## Softmax function

$$\hat{y}_j = \sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \quad \text{for } j = 1, \dots, K.$$

$$\begin{aligned}\frac{\partial \hat{y}_j}{\partial z_i} &= \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \frac{dz_j}{dz_i} - \frac{e^{z_j}}{(\sum_{k=1}^K e^{z_k})^2} e^{z_i} \\ &= \hat{y}_j \frac{dz_j}{dz_i} - \hat{y}_j \hat{y}_i \\ &= \begin{cases} \hat{y}_i(1 - \hat{y}_i), & \text{if } i = j \\ -\hat{y}_i \hat{y}_j, & \text{if } i \neq j \end{cases}\end{aligned}$$

# Derivative of softmax function

Softmax function

$$\hat{y}_j = \sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \quad \text{for } j = 1, \dots, K.$$

$$\begin{aligned}\frac{\partial \hat{y}_j}{\partial z_i} &= \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \frac{dz_j}{dz_i} - \frac{e^{z_j}}{(\sum_{k=1}^K e^{z_k})^2} e^{z_i} \\ &= \hat{y}_j \frac{dz_j}{dz_i} - \hat{y}_j \hat{y}_i \\ &= \begin{cases} \hat{y}_i(1 - \hat{y}_i), & \text{if } i = j \\ -\hat{y}_i \hat{y}_j, & \text{if } i \neq j \end{cases}\end{aligned}$$

# Derivative of softmax function

## Softmax function

$$\hat{y}_j = \sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \quad \text{for } j = 1, \dots, K.$$

$$\begin{aligned}\frac{\partial \hat{y}_j}{\partial z_i} &= \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \frac{dz_j}{dz_i} - \frac{e^{z_j}}{(\sum_{k=1}^K e^{z_k})^2} e^{z_i} \\ &= \hat{y}_j \frac{dz_j}{dz_i} - \hat{y}_j \hat{y}_i \\ &= \begin{cases} \hat{y}_i(1 - \hat{y}_i), & \text{if } i = j \\ -\hat{y}_i \hat{y}_j, & \text{if } i \neq j \end{cases}\end{aligned}$$

# Derivative of loss function over pre-softmax

- Network output  $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x}; \boldsymbol{\theta}) = (\hat{y}_1, \hat{y}_2, \dots, \hat{y}_K)$
- Ideal output  $\mathbf{y} = (y_1, \dots, y_K) = (0, \dots, 1, \dots, 0)$
- Cross entropy loss

$$l(\mathbf{y}, \hat{\mathbf{y}}) = - \sum_{k=1}^K y_k \log \hat{y}_k$$

- Derivative of  $l$  over  $z_i$ , with chain rule

$$\begin{aligned} \frac{\partial l}{\partial z_i} &= - \sum_{k=1}^K y_k \frac{\partial \log \hat{y}_k}{\partial z_i} = - \sum_{k=1}^K y_k \frac{1}{\hat{y}_k} \frac{\partial \hat{y}_k}{\partial z_i} \\ &= -y_i \frac{1}{\hat{y}_i} \hat{y}_i (1 - \hat{y}_i) - \sum_{k \neq i} y_k \frac{1}{\hat{y}_k} (-\hat{y}_k \hat{y}_i) \\ &= \hat{y}_i \left( \sum_{k=1}^K y_k \right) - y_i = \hat{y}_i - y_i \end{aligned}$$

# Derivative of loss function over pre-softmax

- Network output  $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x}; \boldsymbol{\theta}) = (\hat{y}_1, \hat{y}_2, \dots, \hat{y}_K)$
- Ideal output  $\mathbf{y} = (y_1, \dots, y_K) = (0, \dots, 1, \dots, 0)$
- Cross entropy loss

$$l(\mathbf{y}, \hat{\mathbf{y}}) = - \sum_{k=1}^K y_k \log \hat{y}_k$$

- Derivative of  $l$  over  $z_i$ , with chain rule

$$\begin{aligned} \frac{\partial l}{\partial z_i} &= - \sum_{k=1}^K y_k \frac{\partial \log \hat{y}_k}{\partial z_i} = - \sum_{k=1}^K y_k \frac{1}{\hat{y}_k} \frac{\partial \hat{y}_k}{\partial z_i} \\ &= -y_i \frac{1}{\hat{y}_i} \hat{y}_i (1 - \hat{y}_i) - \sum_{k \neq i} y_k \frac{1}{\hat{y}_k} (-\hat{y}_k \hat{y}_i) \\ &= \hat{y}_i \left( \sum_{k=1}^K y_k \right) - y_i = \hat{y}_i - y_i \end{aligned}$$

# Derivative of loss function over pre-softmax

- Network output  $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x}; \boldsymbol{\theta}) = (\hat{y}_1, \hat{y}_2, \dots, \hat{y}_K)$
- Ideal output  $\mathbf{y} = (y_1, \dots, y_K) = (0, \dots, 1, \dots, 0)$
- Cross entropy loss

$$l(\mathbf{y}, \hat{\mathbf{y}}) = - \sum_{k=1}^K y_k \log \hat{y}_k$$

- Derivative of  $l$  over  $z_i$ , with chain rule

$$\begin{aligned} \frac{\partial l}{\partial z_i} &= - \sum_{k=1}^K y_k \frac{\partial \log \hat{y}_k}{\partial z_i} = - \sum_{k=1}^K y_k \frac{1}{\hat{y}_k} \frac{\partial \hat{y}_k}{\partial z_i} \\ &= -y_i \frac{1}{\hat{y}_i} \hat{y}_i (1 - \hat{y}_i) - \sum_{k \neq i} y_k \frac{1}{\hat{y}_k} (-\hat{y}_k \hat{y}_i) \\ &= \hat{y}_i \left( \sum_{k=1}^K y_k \right) - y_i = \hat{y}_i - y_i \end{aligned}$$

# Derivative of loss function over pre-softmax

- Network output  $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x}; \boldsymbol{\theta}) = (\hat{y}_1, \hat{y}_2, \dots, \hat{y}_K)$
- Ideal output  $\mathbf{y} = (y_1, \dots, y_K) = (0, \dots, 1, \dots, 0)$
- Cross entropy loss

$$l(\mathbf{y}, \hat{\mathbf{y}}) = - \sum_{k=1}^K y_k \log \hat{y}_k$$

- Derivative of  $l$  over  $z_i$ , with chain rule

$$\begin{aligned} \frac{\partial l}{\partial z_i} &= - \sum_{k=1}^K y_k \frac{\partial \log \hat{y}_k}{\partial z_i} = - \sum_{k=1}^K y_k \frac{1}{\hat{y}_k} \frac{\partial \hat{y}_k}{\partial z_i} \\ &= -y_i \frac{1}{\hat{y}_i} \hat{y}_i (1 - \hat{y}_i) - \sum_{k \neq i} y_k \frac{1}{\hat{y}_k} (-\hat{y}_k \hat{y}_i) \\ &= \hat{y}_i \left( \sum_{k=1}^K y_k \right) - y_i = \hat{y}_i - y_i \end{aligned}$$

# Derivative of loss function over weight parameters

From  $\frac{\partial z_2}{\partial w_8} = h_2$  and  $\frac{\partial l}{\partial z_i} = \hat{y}_i - y_i$

$$\frac{\partial l}{\partial w_8} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial w_8} = h_2(\hat{y}_2 - y_2)$$

Similarly,

$$\frac{\partial l}{\partial w_7} = \frac{\partial l}{\partial z_1} \frac{\partial z_1}{\partial w_7} = h_2(\hat{y}_1 - y_1)$$

$$\frac{\partial l}{\partial b_4} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial b_4} = \hat{y}_2 - y_2$$

Why called backpropagation?

- Propagation of prediction errors  $\hat{y}_i - y_i$  in gradient!

# Derivative of loss function over weight parameters

From  $\frac{\partial z_2}{\partial w_8} = h_2$  and  $\frac{\partial l}{\partial z_i} = \hat{y}_i - y_i$

$$\frac{\partial l}{\partial w_8} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial w_8} = h_2(\hat{y}_2 - y_2)$$

Similarly,

$$\frac{\partial l}{\partial w_7} = \frac{\partial l}{\partial z_1} \frac{\partial z_1}{\partial w_7} = h_2(\hat{y}_1 - y_1)$$

$$\frac{\partial l}{\partial b_4} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial b_4} = \hat{y}_2 - y_2$$

Why called backpropagation?

- Propagation of prediction errors  $\hat{y}_i - y_i$  in gradient!

# Derivative of loss function over weight parameters

From  $\frac{\partial z_2}{\partial w_8} = h_2$  and  $\frac{\partial l}{\partial z_i} = \hat{y}_i - y_i$

$$\frac{\partial l}{\partial w_8} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial w_8} = h_2(\hat{y}_2 - y_2)$$

Similarly,

$$\frac{\partial l}{\partial w_7} = \frac{\partial l}{\partial z_1} \frac{\partial z_1}{\partial w_7} = h_2(\hat{y}_1 - y_1)$$

$$\frac{\partial l}{\partial b_4} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial b_4} = \hat{y}_2 - y_2$$

Why called backpropagation?

- Propagation of prediction errors  $\hat{y}_i - y_i$  in gradient!

# Derivative of loss function over weight parameters

From  $\frac{\partial z_2}{\partial w_8} = h_2$  and  $\frac{\partial l}{\partial z_i} = \hat{y}_i - y_i$

$$\frac{\partial l}{\partial w_8} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial w_8} = h_2(\hat{y}_2 - y_2)$$

Similarly,

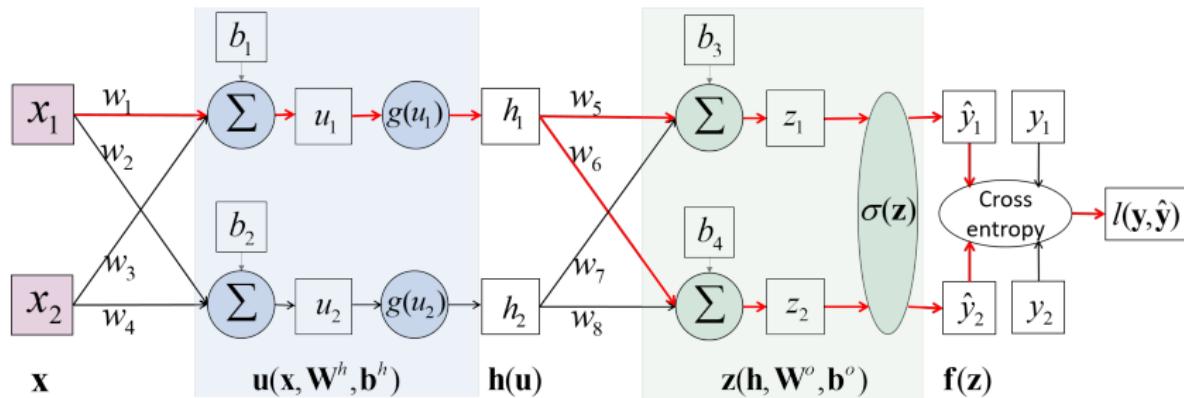
$$\frac{\partial l}{\partial w_7} = \frac{\partial l}{\partial z_1} \frac{\partial z_1}{\partial w_7} = h_2(\hat{y}_1 - y_1)$$

$$\frac{\partial l}{\partial b_4} = \frac{\partial l}{\partial z_2} \frac{\partial z_2}{\partial b_4} = \hat{y}_2 - y_2$$

Why called backpropagation?

- Propagation of prediction errors  $\hat{y}_i - y_i$  in gradient!

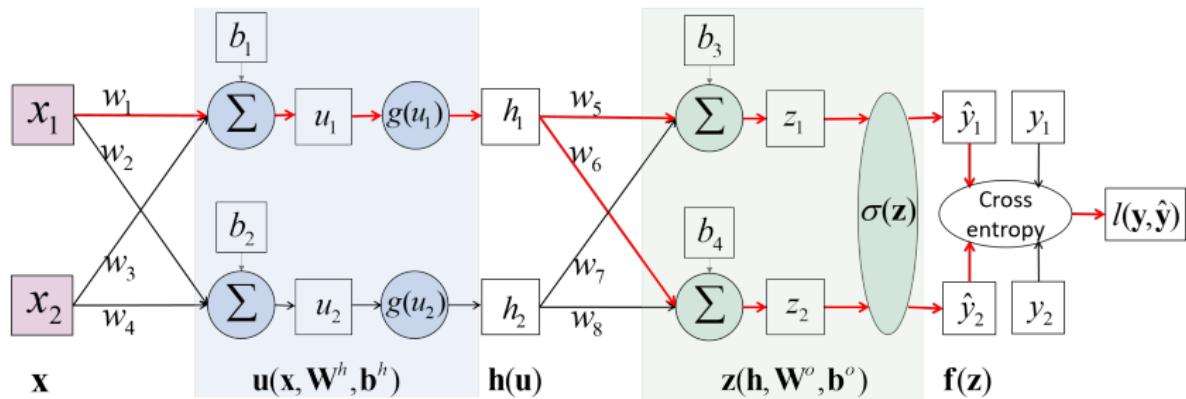
# Backpropagation: another derivative



- another example:

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial h_1} \frac{\partial h_1}{\partial w_1} = \left( \sum_i \frac{\partial l}{\partial z_i} \cdot \frac{\partial z_i}{\partial h_1} \right) \cdot \left( \frac{dh_1}{du_1} \cdot \frac{\partial u_1}{\partial w_1} \right)$$

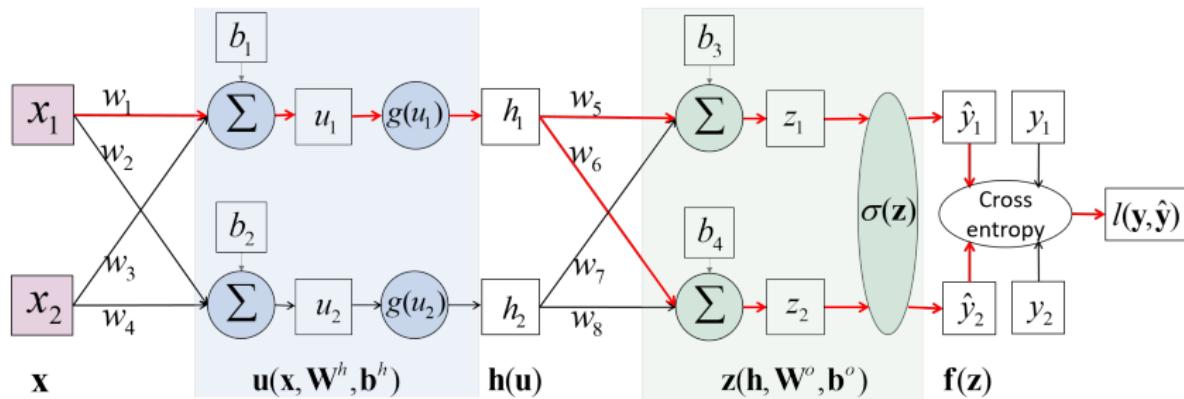
# Backpropagation: another derivative (cont')



$$\frac{\partial u_1}{\partial w_1} = \frac{\partial}{\partial w_1}(x_1 w_1 + x_2 w_2 + b_1) = x_1$$

$$\frac{dh_1}{du_1} = \frac{d}{du_1}(\max(0, u_1)) = 1_{u_1 > 0}$$

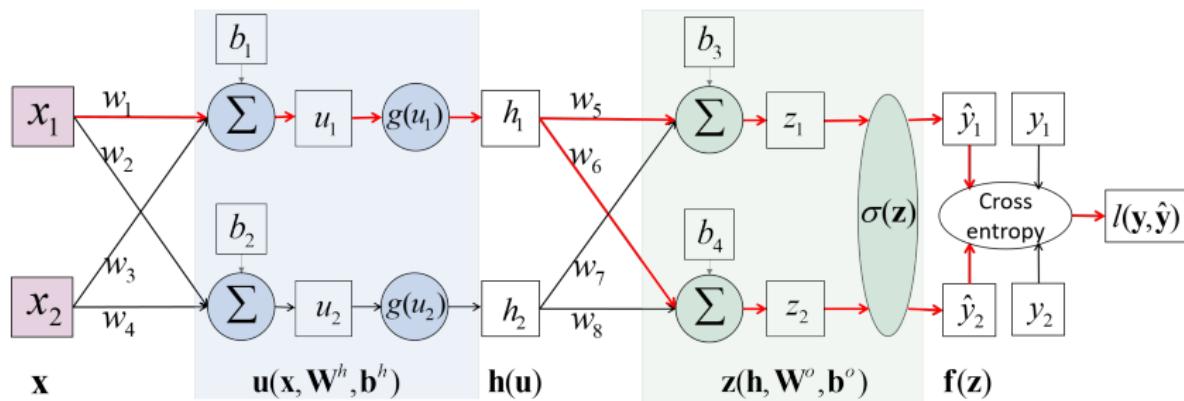
# Backpropagation: another derivative (cont')



$$\frac{\partial z_1}{\partial h_1} = \frac{\partial}{\partial h_1}(h_1 w_5 + h_2 w_7 + b_3) = w_5$$

$$\frac{\partial z_2}{\partial h_1} = \frac{\partial}{\partial h_1}(h_1 w_6 + h_2 w_8 + b_4) = w_6$$

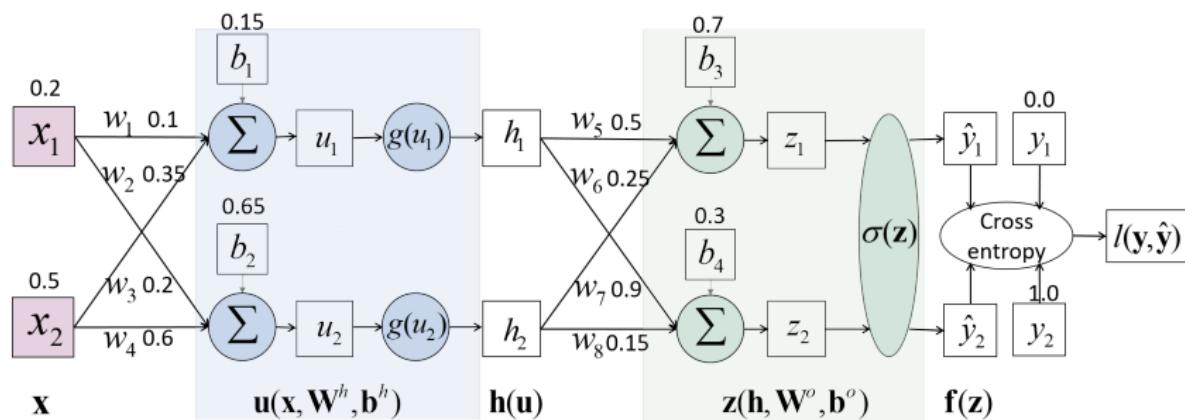
# Backpropagation: another derivative (cont')



$$\begin{aligned}
 \frac{\partial l}{\partial w_1} &= \left( \sum_i \frac{\partial l}{\partial z_i} \cdot \frac{\partial z_i}{\partial h_1} \right) \cdot \left( \frac{dh_1}{du_1} \cdot \frac{\partial u_1}{\partial w_1} \right) \\
 &= \begin{cases} x_1 \{w_5(\hat{y}_1 - y_1) + w_6(\hat{y}_2 - y_2)\}, & \text{if } u_1 > 0 \\ 0, & \text{if } u_1 \leq 0 \end{cases}
 \end{aligned}$$

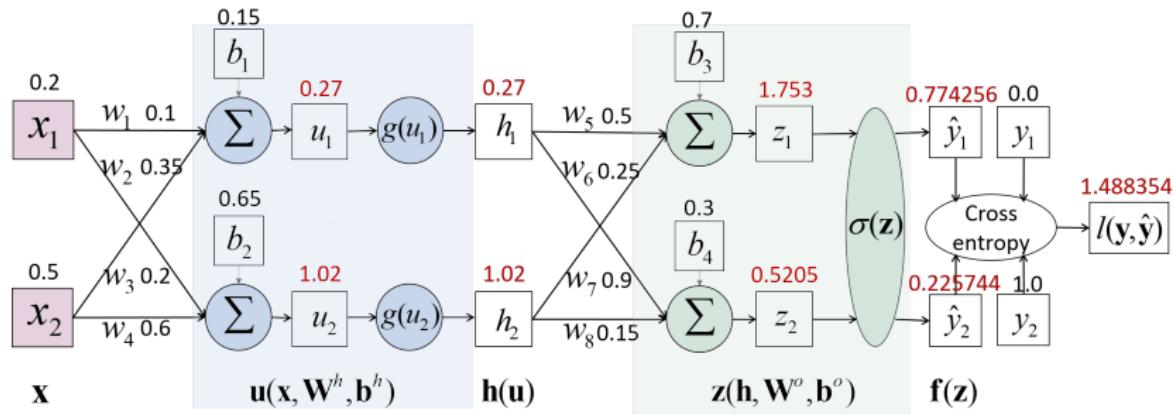
# Backpropagation: computation example

- Suppose we have a single input  $\mathbf{x} = [0.2, 0.5]^T$
- Ideal (expected) output  $\mathbf{y} = [0, 1]^T$
- Model parameters  $\theta$  was initialized as follows



# Backpropagation: computation example (cont')

- Forward computation first, with results in red



- Suppose learning rate  $\eta = 0.5$ , update with gradient descent,

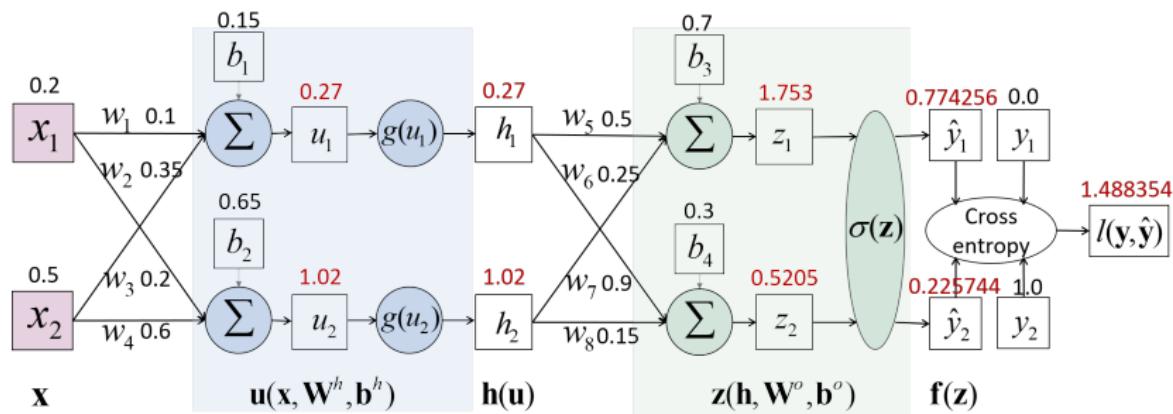
$$\theta_{t+1} = \theta_t - \eta \nabla L(\theta_t)$$

$$\frac{\partial l}{\partial w_8} = h_2(\hat{y}_2 - y_2) = 1.02 * (0.225744 - 1) = -0.789741$$

$$w_8 = 0.15 - 0.5 * (-0.789741) = 0.544871$$

# Backpropagation: computation example (cont')

- Forward computation first, with results in red



- Suppose learning rate  $\eta = 0.5$ , update with gradient descent,

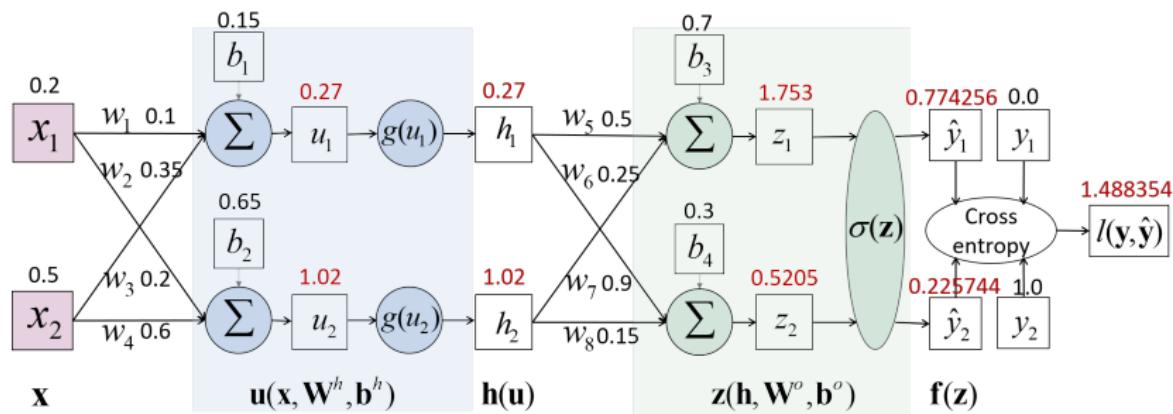
$$\theta_{t+1} = \theta_t - \eta \nabla L(\theta_t)$$

$$\frac{\partial l}{\partial w_8} = h_2(\hat{y}_2 - y_2) = 1.02 * (0.225744 - 1) = -0.789741$$

$$w_8 = 0.15 - 0.5 * (-0.789741) = 0.544871$$

# Backpropagation: computation example (cont')

- Forward computation first, with results in red



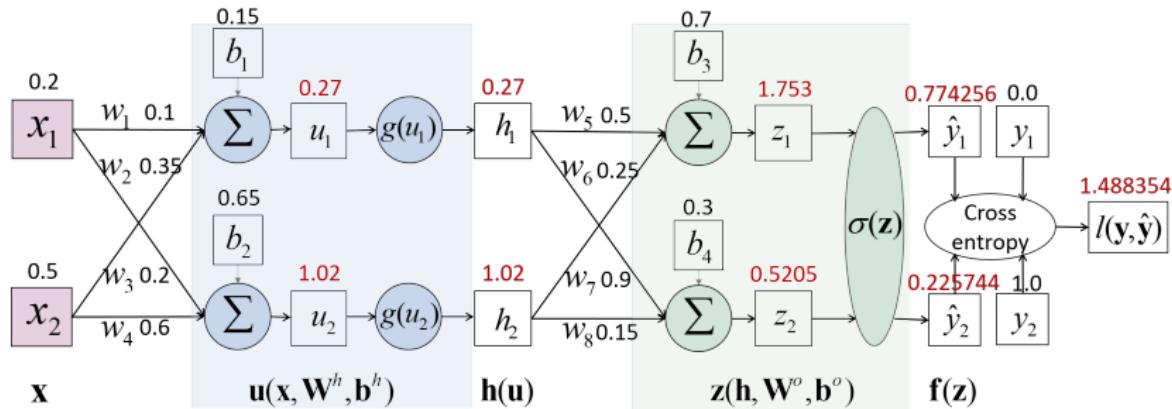
- Suppose learning rate  $\eta = 0.5$ , update with gradient descent,

$$\theta_{t+1} = \theta_t - \eta \nabla L(\theta_t)$$

$$\frac{\partial l}{\partial w_8} = h_2(\hat{y}_2 - y_2) = 1.02 * (0.225744 - 1) = -0.789741$$

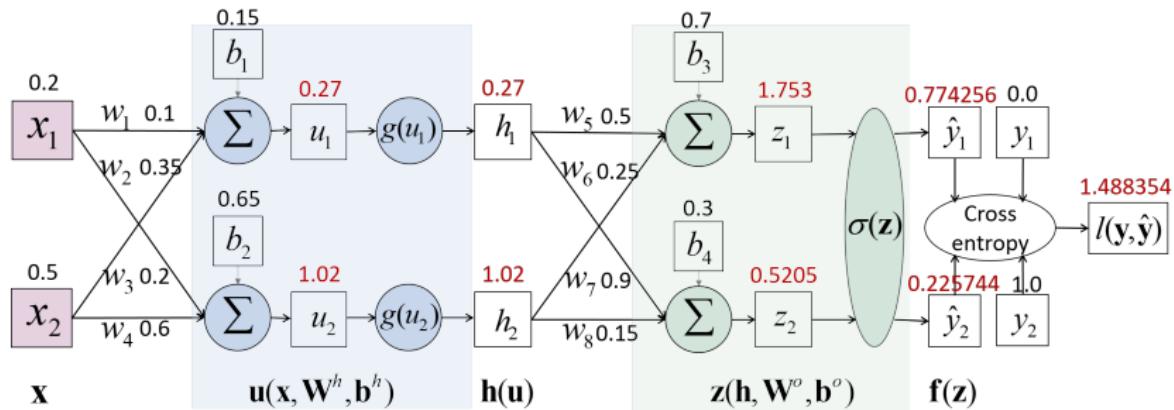
$$w_8 = 0.15 - 0.5 * (-0.789741) = 0.544871$$

# Backpropagation: computation example (cont')



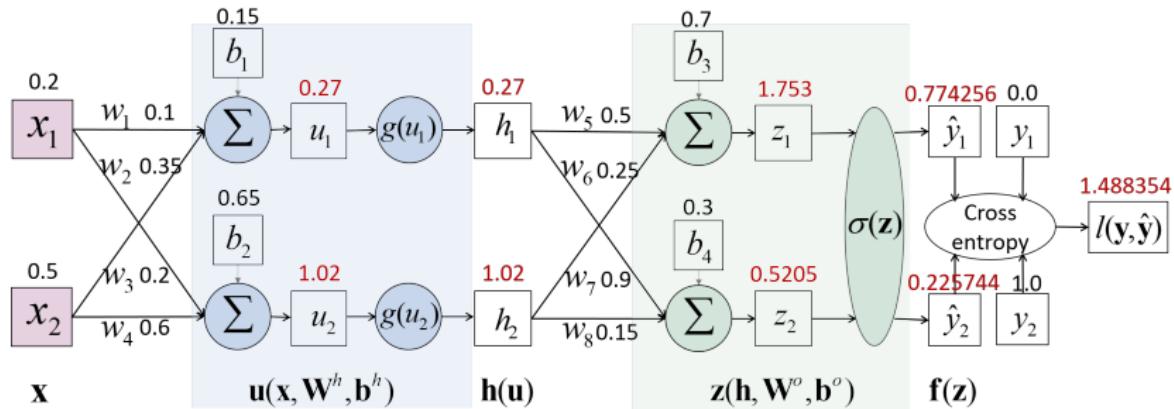
$$\begin{aligned}
 \frac{\partial l}{\partial w_1} &= x_1 \{w_5(\hat{y}_1 - y_1) + w_6(\hat{y}_2 - y_2)\} \\
 &= 0.2 * \{0.5 * (0.774256 - 0) + 0.25 * (0.225744 - 1.0)\} \\
 &= 0.038713 \\
 w_1 &= 0.1 - 0.5 * 0.038713 = 0.080644
 \end{aligned}$$

# Backpropagation: computation example (cont')



$$\begin{aligned}
 \frac{\partial l}{\partial w_1} &= x_1 \{w_5(\hat{y}_1 - y_1) + w_6(\hat{y}_2 - y_2)\} \\
 &= 0.2 * \{0.5 * (0.774256 - 0) + 0.25 * (0.225744 - 1.0)\} \\
 &= 0.038713 \\
 w_1 &= 0.1 - 0.5 * 0.038713 = 0.080644
 \end{aligned}$$

# Backpropagation: computation example (cont')



$$\begin{aligned}
 \frac{\partial l}{\partial w_1} &= x_1 \{w_5(\hat{y}_1 - y_1) + w_6(\hat{y}_2 - y_2)\} \\
 &= 0.2 * \{0.5 * (0.774256 - 0) + 0.25 * (0.225744 - 1.0)\} \\
 &= 0.038713 \\
 w_1 &= 0.1 - 0.5 * 0.038713 = 0.080644
 \end{aligned}$$

Above example used *single* data to update model parameters.

How to update parameters if we have lots of (training) data?

- Training dataset  $D = \{(\mathbf{x}_n, \mathbf{y}_n) | n = 1, \dots, N\}$
- Loss function

$$L(\boldsymbol{\theta}) = \frac{1}{N} \sum_{n=1}^N l(\mathbf{y}_n, \mathbf{f}(\mathbf{x}_n; \boldsymbol{\theta}))$$

Above example used *single* data to update model parameters.

How to update parameters if we have lots of (training) data?

- Training dataset  $D = \{(\mathbf{x}_n, \mathbf{y}_n) | n = 1, \dots, N\}$
- Loss function

$$L(\boldsymbol{\theta}) = \frac{1}{N} \sum_{n=1}^N l(\mathbf{y}_n, \mathbf{f}(\mathbf{x}_n; \boldsymbol{\theta}))$$

# Batch gradient descent

- Update model parameters using all data with gradient descent

$$\begin{aligned}\boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta \nabla L(\boldsymbol{\theta}_t) \\ &= \boldsymbol{\theta}_t - \frac{\eta}{N} \sum_{n=1}^N \nabla l(\mathbf{y}_n, \mathbf{f}(\mathbf{x}_n; \boldsymbol{\theta}_t))\end{aligned}$$

where  $\eta$  is learning rate,  $\nabla L(\boldsymbol{\theta}_t)$  is gradient of loss function  $L$  over current model parameters  $\boldsymbol{\theta}_t$ .

- Very slow, and intractable for big data to fit in memory
- Guarantee to find minimum of loss function

```
for iter in range(nb_epochs):
    params_grad = eval_grad(loss_func, dataset, params)
    params = params - learning_rate * params_grad
```

# Batch gradient descent

- Update model parameters using all data with gradient descent

$$\begin{aligned}\boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta \nabla L(\boldsymbol{\theta}_t) \\ &= \boldsymbol{\theta}_t - \frac{\eta}{N} \sum_{n=1}^N \nabla l(\mathbf{y}_n, \mathbf{f}(\mathbf{x}_n; \boldsymbol{\theta}_t))\end{aligned}$$

where  $\eta$  is learning rate,  $\nabla L(\boldsymbol{\theta}_t)$  is gradient of loss function  $L$  over current model parameters  $\boldsymbol{\theta}_t$ .

- Very slow, and intractable for big data to fit in memory
- Guarantee to find minimum of loss function

```
for iter in range(nb_epochs):
    params_grad = eval_grad(loss_func, dataset, params)
    params = params - learning_rate * params_grad
```

# Stochastic gradient descent

- Update model parameters using each single data  $(\mathbf{x}_n, \mathbf{y}_n)$

$$\begin{aligned}\boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta \nabla L(\boldsymbol{\theta}_t) \\ &= \boldsymbol{\theta}_t - \eta \nabla l(\mathbf{y}_n, \mathbf{f}(\mathbf{x}_n; \boldsymbol{\theta}_t))\end{aligned}$$

- Very fast update, tractable for big data
- May jump to better local minimum
- Converge almost certainly to local minimum
- Convergence fluctuates

```
for i in range(nb_epochs):
    np.random.shuffle(dataset)
    for example in dataset:
        params_grad = eval_grad(loss_func, example, params)
        params = params - learning_rate * params_grad
```

# Stochastic gradient descent

- Update model parameters using each single data  $(\mathbf{x}_n, \mathbf{y}_n)$

$$\begin{aligned}\boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta \nabla L(\boldsymbol{\theta}_t) \\ &= \boldsymbol{\theta}_t - \eta \nabla l(\mathbf{y}_n, \mathbf{f}(\mathbf{x}_n; \boldsymbol{\theta}_t))\end{aligned}$$

- Very fast update, tractable for big data
- May jump to better local minimum
- Converge almost certainly to local minimum
- Convergence fluctuates

```
for i in range(nb_epochs):
    np.random.shuffle(dataset)
    for example in dataset:
        params_grad = eval_grad(loss_func, example, params)
        params = params - learning_rate * params_grad
```

# Mini-batch gradient descent

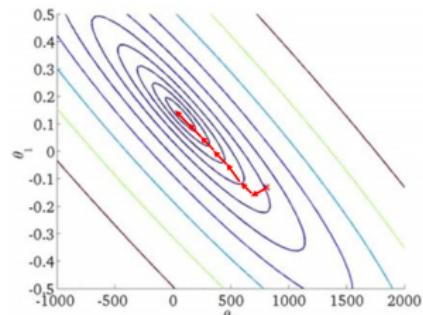
- Update model parameters using a mini-batch of data  $S \subset D$

$$\begin{aligned}\boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta \nabla L(\boldsymbol{\theta}_t) \\ &= \boldsymbol{\theta}_t - \frac{\eta}{|S|} \sum_{(\mathbf{x}_n, \mathbf{y}_n) \in S} \nabla l(\mathbf{y}_n, \mathbf{f}(\mathbf{x}_n; \boldsymbol{\theta}_t))\end{aligned}$$

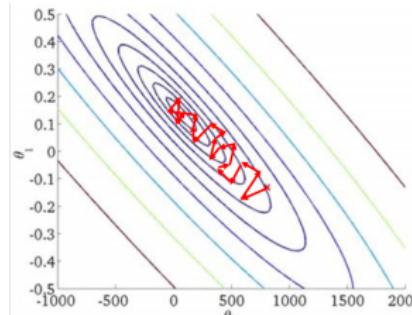
- In general  $|S|$  ranges between tens and two/three hundreds
- Take the best of batch and stochastic gradient descents

```
for i in range(nb_epochs):
    np.random.shuffle(dataset)
    for batch in get_batches(dataset, batch_size=64):
        params_grad = eval_grad(loss_func, batch, params)
        params = params - learning_rate * params_grad
```

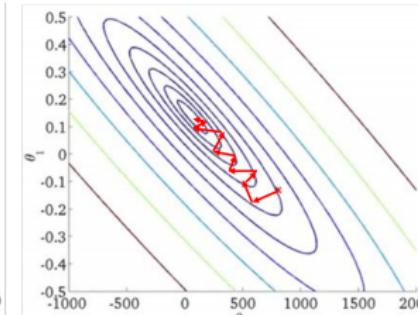
# Mini-batch gradient descent (cont')



Batch gradient descent



Stochastic gradient descent

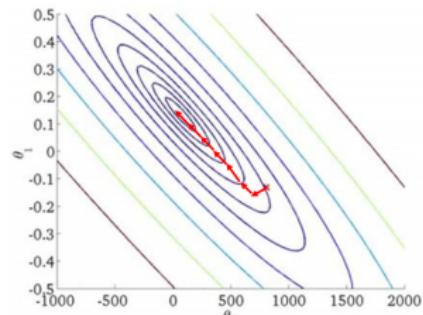


Mini-batch gradient descent

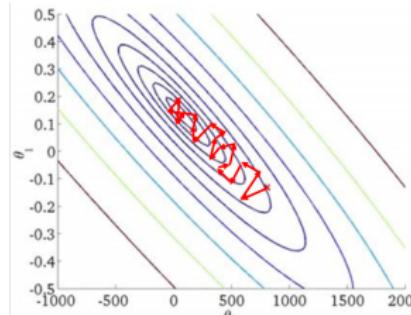
## Challenges of mini-batch stochastic gradient

- adjust learning rate
- well approximate true gradient with mini-batch data

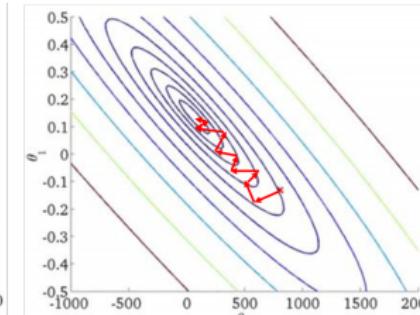
# Mini-batch gradient descent (cont')



Batch gradient descent



Stochastic gradient descent



Mini-batch gradient descent

## Challenges of mini-batch stochastic gradient

- adjust learning rate
- well approximate true gradient with mini-batch data

# Momentum

- consider downhill directions from previous steps

$$\mathbf{v}_{t+1} = \gamma \mathbf{v}_t + \eta \nabla L(\boldsymbol{\theta}_t)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_{t+1}$$

- $\gamma = 0.9$  or similar value
- $\mathbf{v}_{t+1} = \eta \{ \nabla L(\boldsymbol{\theta}_t) + \gamma \nabla L(\boldsymbol{\theta}_{t-1}) + \gamma^2 \nabla L(\boldsymbol{\theta}_{t-2}) + \dots \}$
- reduce oscillations in stochastic/mini-batch gradient descent

# Momentum

- consider downhill directions from previous steps

$$\mathbf{v}_{t+1} = \gamma \mathbf{v}_t + \eta \nabla L(\boldsymbol{\theta}_t)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_{t+1}$$

- $\gamma = 0.9$  or similar value
- $\mathbf{v}_{t+1} = \eta \{ \nabla L(\boldsymbol{\theta}_t) + \gamma \nabla L(\boldsymbol{\theta}_{t-1}) + \gamma^2 \nabla L(\boldsymbol{\theta}_{t-2}) + \dots \}$
- reduce oscillations in stochastic/mini-batch gradient descent



(a) SGD without momentum



(b) SGD with momentum

# Momentum (cont')

- Momentum may cause ball roll down too fast (red arrow)!
- Need a smarter ball knowing when to slow down before the hill slopes up again (blue arrow).



# Nesterov accelerated gradient (NAG)

- Look ahead, i.e., consider downhill direction at future's approximate position  $\theta_t - \gamma v_t$

$$\begin{aligned}v_{t+1} &= \gamma v_t + \eta \nabla L(\theta_t - \gamma v_t) \\ \theta_{t+1} &= \theta_t - v_{t+1}\end{aligned}$$

- Avoid ball going down too fast with accumulated momentum

# Nesterov accelerated gradient (NAG)

- Look ahead, i.e., consider downhill direction at future's approximate position  $\theta_t - \gamma v_t$

$$v_{t+1} = \gamma v_t + \eta \nabla L(\theta_t - \gamma v_t)$$

$$\theta_{t+1} = \theta_t - v_{t+1}$$

- Avoid ball going down too fast with accumulated momentum

# Nesterov accelerated gradient (NAG)

- Look ahead, i.e., consider downhill direction at future's approximate position  $\theta_t - \gamma v_t$

$$v_{t+1} = \gamma v_t + \eta \nabla L(\theta_t - \gamma v_t)$$

$$\theta_{t+1} = \theta_t - v_{t+1}$$

- Avoid ball going down too fast with accumulated momentum

Momentum and NAG update gradient.  
Can we update learning rate over iterations?

# Adagrad

- Adaptively update learning rate for each parameter, with square root of sum of squares of its historical derivatives

$$g_{t+1,i} = g_{t,i} + \left( \frac{\partial L(\theta_t)}{\partial \theta_i} \right)^2$$

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{g_{t+1,i}} + \epsilon} \frac{\partial L(\theta_t)}{\partial \theta_i}$$

- Larger update in history for  $\theta_i$  will cause smaller learning rate  $\eta / (\sqrt{g_{t+1,i}} + \epsilon)$  in updating  $\theta_i$ .
- No need to manually tune learning rate.
- $g_{t+1,i}$  becomes larger over iterations, causing very small learning rate ultimately for each  $\theta_i$ .

# Adagrad

- Adaptively update learning rate for each parameter, with square root of sum of squares of its historical derivatives

$$g_{t+1,i} = g_{t,i} + \left( \frac{\partial L(\theta_t)}{\partial \theta_i} \right)^2$$

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{g_{t+1,i}} + \epsilon} \frac{\partial L(\theta_t)}{\partial \theta_i}$$

- Larger update in history for  $\theta_i$  will cause smaller learning rate  $\eta / (\sqrt{g_{t+1,i}} + \epsilon)$  in updating  $\theta_i$ .
- No need to manually tune learning rate.
- $g_{t+1,i}$  becomes larger over iterations, causing very small learning rate ultimately for each  $\theta_i$ .

# RMSprop (Root Mean Square propagation)

- Solve monotonically decreasing learning rate issue in Adagrad

$$\begin{aligned} g_{t+1,i} &= \gamma g_{t,i} + (1 - \gamma) \left( \frac{\partial L(\theta_t)}{\partial \theta_i} \right)^2 \\ \theta_{t+1,i} &= \theta_{t,i} - \frac{\eta}{\sqrt{g_{t+1,i}} + \epsilon} \frac{\partial L(\theta_t)}{\partial \theta_i} \end{aligned}$$

- $\gamma = 0.9$  or similar value
- $g_{t+1,i}$  is exponential decaying average of squared derivatives
- No need to manually tune learning rate

# RMSprop (Root Mean Square propagation)

- Solve monotonically decreasing learning rate issue in Adagrad

$$\begin{aligned} g_{t+1,i} &= \gamma g_{t,i} + (1 - \gamma) \left( \frac{\partial L(\theta_t)}{\partial \theta_i} \right)^2 \\ \theta_{t+1,i} &= \theta_{t,i} - \frac{\eta}{\sqrt{g_{t+1,i}} + \epsilon} \frac{\partial L(\theta_t)}{\partial \theta_i} \end{aligned}$$

- $\gamma = 0.9$  or similar value
- $g_{t+1,i}$  is exponential decaying average of squared derivatives
- No need to manually tune learning rate

# Adam (Adaptive Moment Estimation)

- Adds momentum and bias to RMSprop

$$\begin{aligned}
 m_{t+1,i} &= \beta_1 m_{t,i} + (1 - \beta_1) \frac{\partial L(\theta_t)}{\partial \theta_i} \\
 g_{t+1,i} &= \beta_2 g_{t,i} + (1 - \beta_2) \left( \frac{\partial L(\theta_t)}{\partial \theta_i} \right)^2 \\
 \hat{m}_{t+1,i} &= \frac{m_{t+1,i}}{1 - \beta_1^{t+1}} \\
 \hat{g}_{t+1,i} &= \frac{g_{t+1,i}}{1 - \beta_2^{t+1}} \\
 \theta_{t+1,i} &= \theta_{t,i} - \frac{\eta}{\sqrt{\hat{g}_{t+1,i}} + \epsilon} \hat{m}_{t+1,i}
 \end{aligned}$$

- $m_{t+1,i}$  and  $g_{t+1,i}$  are first (mean) and second moment (uncentered variance) of derivative
- $m_{t+1,i}$  and  $g_{t+1,i}$  are biased toward zero, so  $\hat{m}_{t+1,i}$  and  $\hat{g}_{t+1,i}$

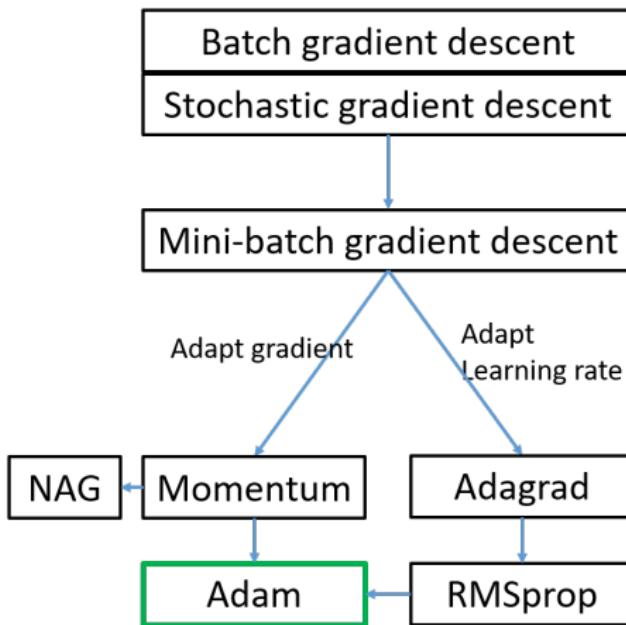
# Adam (Adaptive Moment Estimation)

- Adds momentum and bias to RMSprop

$$\begin{aligned}
 m_{t+1,i} &= \beta_1 m_{t,i} + (1 - \beta_1) \frac{\partial L(\theta_t)}{\partial \theta_i} \\
 g_{t+1,i} &= \beta_2 g_{t,i} + (1 - \beta_2) \left( \frac{\partial L(\theta_t)}{\partial \theta_i} \right)^2 \\
 \hat{m}_{t+1,i} &= \frac{m_{t+1,i}}{1 - \beta_1^{t+1}} \\
 \hat{g}_{t+1,i} &= \frac{g_{t+1,i}}{1 - \beta_2^{t+1}} \\
 \theta_{t+1,i} &= \theta_{t,i} - \frac{\eta}{\sqrt{\hat{g}_{t+1,i}} + \epsilon} \hat{m}_{t+1,i}
 \end{aligned}$$

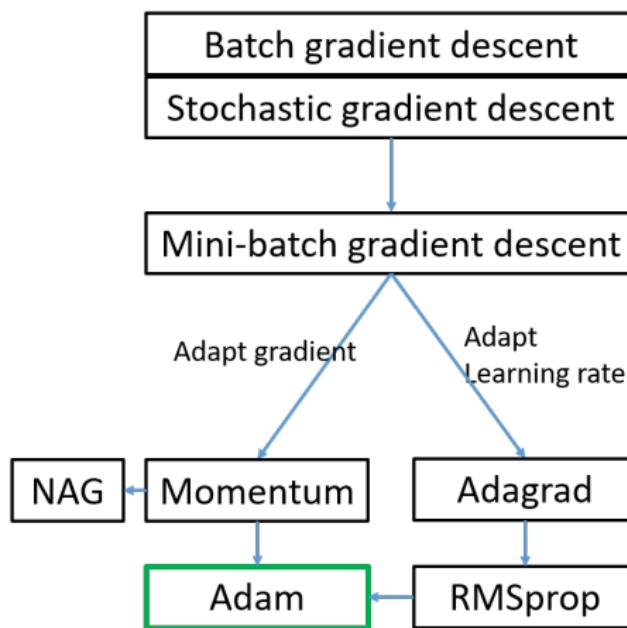
- $m_{t+1,i}$  and  $g_{t+1,i}$  are first (mean) and second moment (uncentered variance) of derivative
- $m_{t+1,i}$  and  $g_{t+1,i}$  are biased toward zero, so  $\hat{m}_{t+1,i}$  and  $\hat{g}_{t+1,i}$

# Gradient descent: summary



- However, actually vanilla SGD or mini-batch gradient with simple decreasing learning rate schedule works well!

# Gradient descent: summary



- However, actually vanilla SGD or mini-batch gradient with simple decreasing learning rate schedule works well!

# Hyper-parameter tuning

The above is about finding network's weight parameters.

We also need to determine

- parameters in gradient descent, e.g., learning rate
- number of network layers and number of neurons per layer

These are called *hyper-parameters!*

# Hyper-parameter tuning

The above is about finding network's weight parameters.

We also need to determine

- parameters in gradient descent, e.g., learning rate
- number of network layers and number of neurons per layer

These are called *hyper-parameters*!

# Hyper-parameter tuning (cont')

How to choose from multiple sets of hyper-parameter values?

- Rule: choose the set with which the trained network model has better *generalization* performance!

Generalization ability

How well does the trained model work for unseen data?

# Hyper-parameter tuning (cont')

How to choose from multiple sets of hyper-parameter values?

- Rule: choose the set with which the trained network model has better *generalization* performance!

## Generalization ability

How well does the trained model work for unseen data?

# Hyper-parameter tuning (cont')

How to choose from multiple sets of hyper-parameter values?

- Rule: choose the set with which the trained network model has better *generalization* performance!

Generalization ability

How well does the trained model work for unseen data?

举一反三

# Data set for hyper-parameter tuning

Whole data set divided:

- Training set (e.g., 60%): used to train model parameter
- Validation set (e.g., 20%): to find optimal hyper-parameters
- Test set (e.g., 20%): to evaluate final model's performance



Training set



Validation set



Test set

- Choose the set of hyper-parameters with which the trained model has the best performance on the validation set.

# Data set for hyper-parameter tuning

Whole data set divided:

- Training set (e.g., 60%): used to train model parameter
- Validation set (e.g., 20%): to find optimal hyper-parameters
- Test set (e.g., 20%): to evaluate final model's performance



Training set



Validation set



Test set

- Choose the set of hyper-parameters with which the trained model has the best performance on the validation set.

# Data set for hyper-parameter tuning (cont')

When whole set is small: K-fold cross validation

- for each run, use one unique subset as validation set, the other ( $K-1$ ) subsets as training set
- average performance over  $K$  runs



(training + validation) set split into k-folds



Test set

# Hyper-parameter tuning: grid search

Where are the multiple sets of hyper-parameters from?

## Grid search

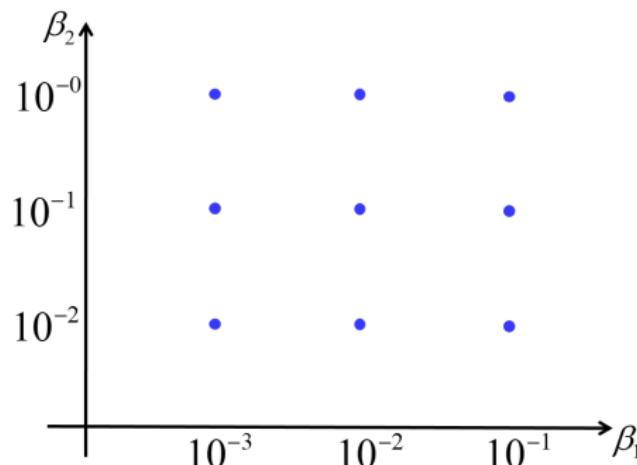
- exhaustive searching in hyper-parameter space
- often in log scale
- only for small number of hyper-parameters

# Hyper-parameter tuning: grid search

Where are the multiple sets of hyper-parameters from?

## Grid search

- exhaustive searching in hyper-parameter space
- often in log scale
- only for small number of hyper-parameters

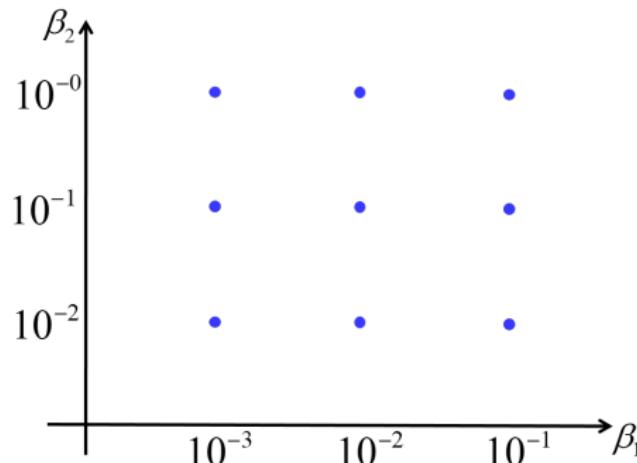


# Hyper-parameter tuning: grid search

Where are the multiple sets of hyper-parameters from?

Grid search

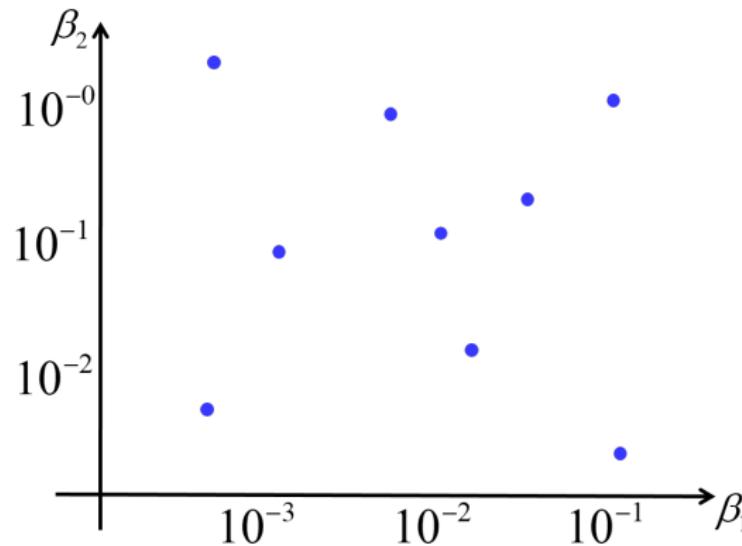
- exhaustive searching in hyper-parameter space
- often in log scale
- only for small number of hyper-parameters



# Hyper-parameter tuning: random search

## Random search

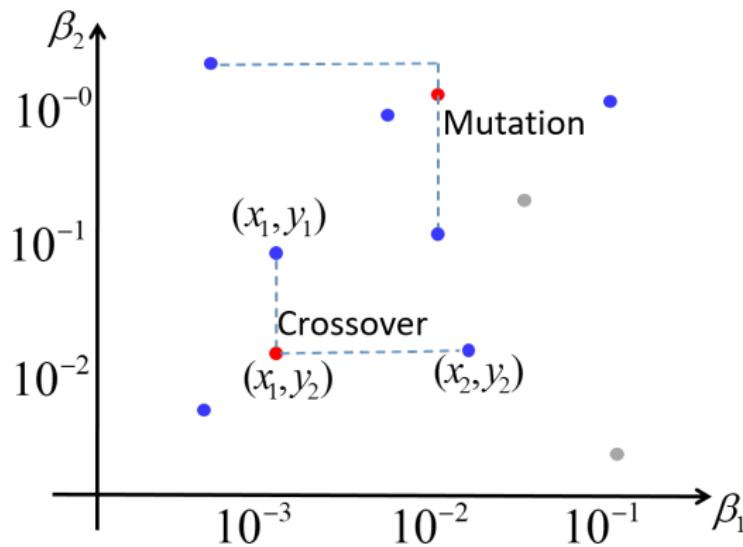
- randomly sample multiple times in hyper-parameter space
- better than grid method if hyper-parameter number is higher



# Hyper-parameter tuning: evolutionary method

## Evolutionary optimization

- repeat: replace worst-performing hyper-parameter sets (gray) with new sets (red) through crossover and mutation



Google used the method to find better network structures; see Jaderberg et al., 2017, "Population Based Training of Neural Networks"

# Deep learning frameworks/platforms

In practice, how do we get a real deep learning system?

- construct the structure of a neural network
- minimize the loss function with training dataset

# Deep learning frameworks/platforms

In practice, how do we get a real deep learning system?

- construct the structure of a neural network
- minimize the loss function with training dataset

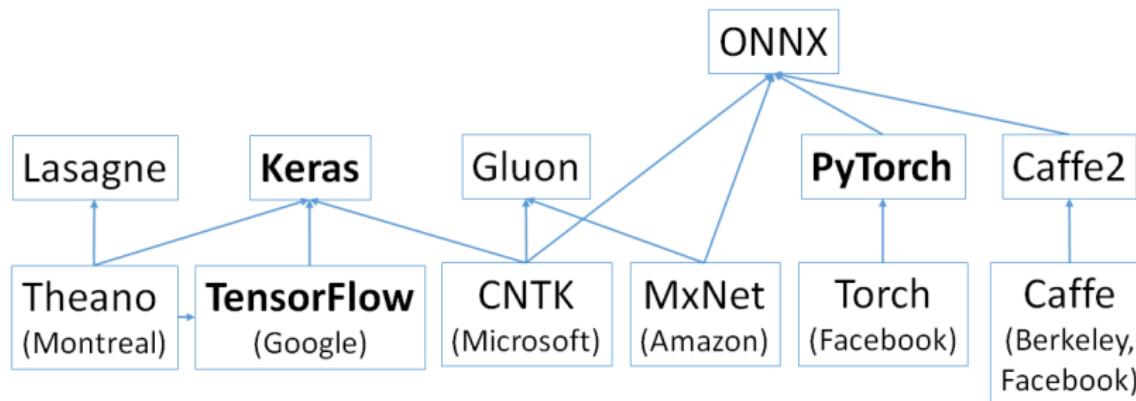
Such functions are provided by deep learning frameworks/platforms (including libraries, packages, toolkits)!

# Deep learning frameworks/platforms

In practice, how do we get a real deep learning system?

- construct the structure of a neural network
- minimize the loss function with training dataset

Such functions are provided by deep learning frameworks/platforms (including libraries, packages, toolkits)!



# It is simple to construct a network

Construct a two-layer network and run to get gradient

- PyTorch coding is more natural and easy to learn

TensorFlow

```
import numpy as np
np.random.seed(0)
import tensorflow as tf

N, D = 3, 4

with tf.device('/gpu:0'):
    x = tf.placeholder(tf.float32)
    y = tf.placeholder(tf.float32)
    z = tf.placeholder(tf.float32)

    a = x * y
    b = a + z
    c = tf.reduce_sum(b)

grad_x, grad_y, grad_z = tf.gradients(c, [x, y, z])

with tf.Session() as sess:
    values = {
        x: np.random.randn(N, D),
        y: np.random.randn(N, D),
        z: np.random.randn(N, D),
    }
    out = sess.run([c, grad_x, grad_y, grad_z],
                  feed_dict=values)
    c_val, grad_x_val, grad_y_val, grad_z_val = out
```

PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4

x = Variable(torch.randn(N, D).cuda(),
             requires_grad=True)
y = Variable(torch.randn(N, D).cuda(),
             requires_grad=True)
z = Variable(torch.randn(N, D).cuda(),
             requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()

print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
```

# It is simple to train a network

Construct a two-layer network and train it over 50 iterations

- Keras is as simple as PyTorch, but less flexible

## Keras

```
from keras.models import Sequential
from keras.layers.core import Dense, Activation
from keras.optimizers import SGD

N, D, H = 64, 1000, 100

model = Sequential()
model.add(Dense(input_dim=D, output_dim=H))
model.add(Activation('relu'))
model.add(Dense(input_dim=H, output_dim=D))

optimizer = SGD(lr=1e0)
model.compile(loss='mean_squared_error',
              optimizer=optimizer)

x = np.random.randn(N, D)
y = np.random.randn(N, D)
history = model.fit(x, y, nb_epoch=50,
                     batch_size=N, verbose=0)
```

## PyTorch

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)

learning_rate = 1e-4
for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    model.zero_grad()
    loss.backward()

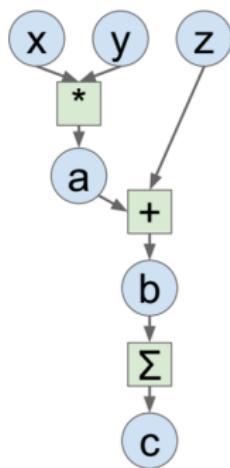
    for param in model.parameters():
        param.data -= learning_rate * param.grad.data
```

# Computational graph - TensorFlow

## Static computational graph

- define-then-run: define graph (function) once, then compute
- more efficient, e.g., save memory

## Computational Graphs



Create forward computational graph

## TensorFlow

```

# Basic computational graph
import numpy as np
np.random.seed(0)
import tensorflow as tf

N, D = 3, 4

x = tf.placeholder(tf.float32)
y = tf.placeholder(tf.float32)
z = tf.placeholder(tf.float32)

a = x * y
b = a + z
c = tf.reduce_sum(b)

grad_x, grad_y, grad_z = tf.gradients(c, [x, y, z])

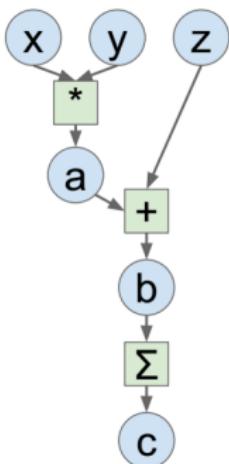
with tf.Session() as sess:
    values = {
        x: np.random.randn(N, D),
        y: np.random.randn(N, D),
        z: np.random.randn(N, D),
    }
    out = sess.run([c, grad_x, grad_y, grad_z],
                  feed_dict=values)
    c_val, grad_x_val, grad_y_val, grad_z_val = out
  
```

# Computational graph - PyTorch

## Dynamic computational graph

- define-by-run: construct graph (function) when computing
- more flexible, e.g., handle flexible inputs and outputs
- easier to construct complex graph and debug code!

## Computational Graphs



Forward pass  
looks just like  
numpy

## PyTorch

```

import torch
from torch.autograd import Variable

N, D = 3, 4

x = Variable(torch.randn(N, D),
             requires_grad=True)
y = Variable(torch.randn(N, D),
             requires_grad=True)
z = Variable(torch.randn(N, D),
             requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()

print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
  
```

# TensorFlow vs PyTorch: more

- Both provide gradient computation with auto-differentiation
- TensorFlow: easy product deployment; more online codes
- PyTorch: easy data loading, parallel processing
- For developing products: TensorFlow is winner!
- For doing research: PyTorch/Keras is winner

from <https://awni.github.io/pytorch-tensorflow/>

# TensorFlow vs PyTorch: more

- Both provide gradient computation with auto-differentiation
- TensorFlow: easy product deployment; more online codes
- PyTorch: easy data loading, parallel processing
- For developing products: TensorFlow is winner!
- For doing research: PyTorch/Keras is winner

from <https://awni.github.io/pytorch-tensorflow/>

# Summary

- Backpropagation: gradient descent with chain rule
- Mini-batch gradient descent and variants
- Hyper-parameter tuning: validation, searching
- deep learning frameworks: TensorFlow or PyTorch?

## Further reading:

- Sections 8.1, 8.3, 8.5, in textbook “Deep learning”,  
<http://www.deeplearningbook.org/>
- [http://cs231n.stanford.edu/slides/2017/cs231n\\_2017\\_lecture8.pdf](http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture8.pdf)
- Luo et al., Adaptive gradient methods with dynamic bound of learning rate. To appear in ICLR, 2019.

# About paper summary

Where to find good papers:

- <http://www.arxiv-sanity.com>
- International Conference on Machine Learning (ICML)
- Neural Information Processing Systems (NIPS)
- International Conference on Learning Representations (ICLR)
- Association for the Advancement of Artificial Intelligence (AAAI)
- International Conference on Computer Vision and Pattern Recognition (CVPR)
- International Conference on Computer Vision (ICCV)
- European Conference on Computer Vision (ECCV)

Suggestion:

- Team members discuss together what to write
- One/two to write, the other two/one to criticize

# About paper summary

Where to find good papers:

- <http://www.arxiv-sanity.com>
- International Conference on Machine Learning (ICML)
- Neural Information Processing Systems (NIPS)
- International Conference on Learning Representations (ICLR)
- Association for the Advancement of Artificial Intelligence (AAAI)
- International Conference on Computer Vision and Pattern Recognition (CVPR)
- International Conference on Computer Vision (ICCV)
- European Conference on Computer Vision (ECCV)

Suggestion:

- Team members discuss together what to write
- One/two to write, the other two/one to criticize

# About the course project

Contests/challenges can be from:

- <https://grand-challenge.org/challenges/> (those in 2018/2019)
- <http://cvpr2019.thecvf.com/program/workshops>
- <https://www.kaggle.com/competitions>
- <http://rrc.cvc.uab.es/>

Note:

- Choose those in 2018/2019
- Some deadlines are soon
- Need not choose active contests/challenges