Tsinghua Deep Learning Summer School
2018/7/24

Multi-layer Perceptron and convolutional neural network

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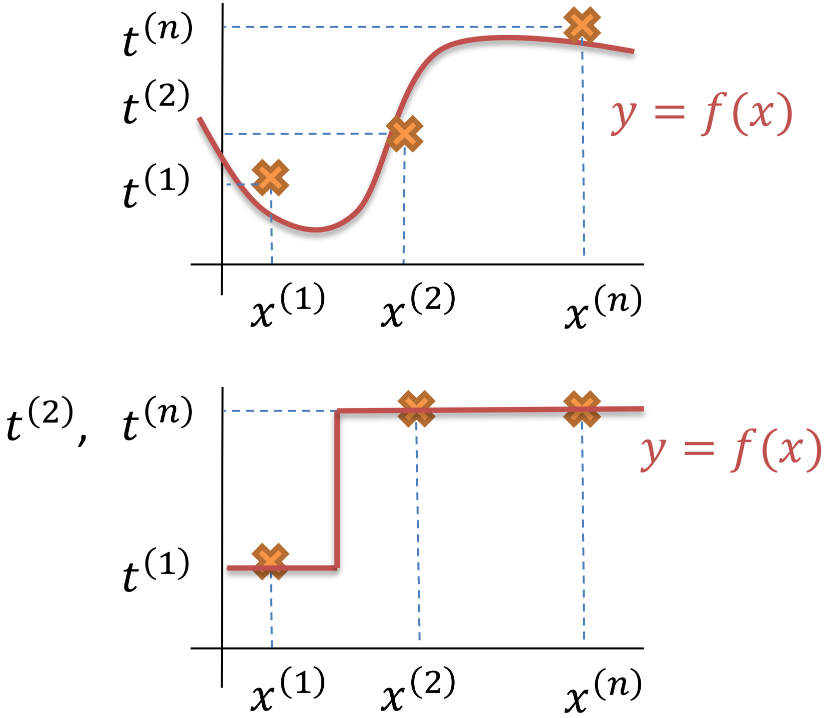
Outline

- Regression and classification
- Multi-layer perceptron
- Convolutional neural network
- Practical tricks

Regression and classification

Given a set of data points $x^{(n)} \in R^m$ and the corresponding labels $t^{(n)} \in \Omega$: $\{(x^{(1)}, t^{(1)}), (x^{(2)}, t^{(2)}), \dots, (x^{(N)}, t^{(N)})\}$, for a new data point x, predict its label

- The goal is to find a mapping
$$f: R^m \to \Omega$$
- If Ω is a continuous set, this is called regression
- If Ω is a discrete set, this is called classification



Linear regression

- $f(x)$ is linear

bias

$$f(x) = w^T x + b$$

where $w \in R^n, b \in R$.

- Choose he cost function as the mean squared error (MSE)

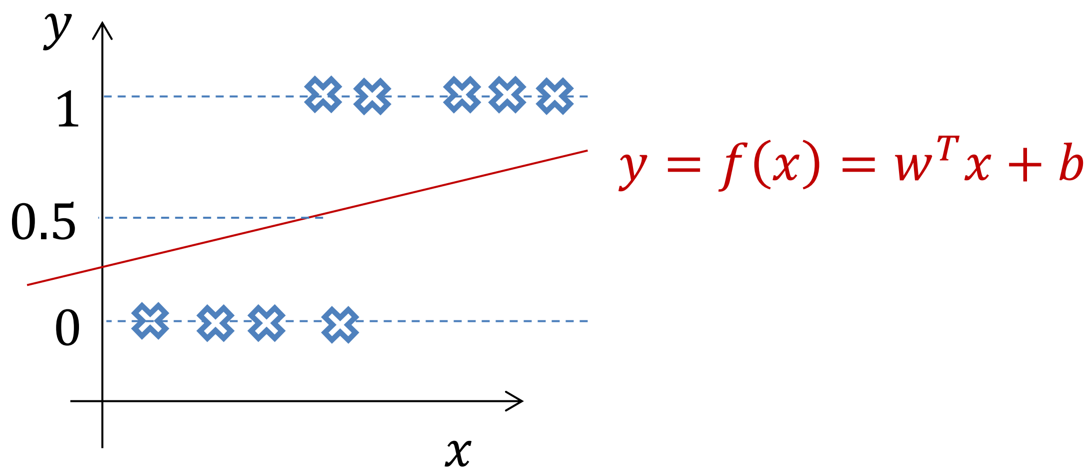
$$E = \sum_{n=1}^{N} \left(f\left(x^{(n)}\right) - t^{(n)}\right)^2 = \sum_{n=1}^{N} \left(w^T x^{(n)} + b - t^{(n)}\right)^2$$

- Find optimal w^* and b^* by minimizing the cost function

$$\left.\begin{aligned} \nabla_w E &= \sum_{n=1}^{N} \left(w^T x^{(n)} + b - t^{(n)}\right) x^{(n)} = 0 \\ \nabla_b E &= \sum_{n=1}^{N} \left(w^T x^{(n)} + b - t^{(n)}\right) = 0 \end{aligned}\right\} w^*, b^*$$

Linear regression as classification

- Suppose $t \in \{0,1\}$. Consider the 1D case



- Regression
  - Prediction $y = f(x)$ which is continuous
- Classification
  - Prediction $y = \begin{cases} 1, \text{if } f(x) \geq 0.5 \\ 0, \text{if } f(x) < 0.5 \end{cases}$

Representation of class labels

- For classification, given $\{(x^{(1)}, t^{(1)}), \ldots, (x^{(N)}, t^{(N)})\}$, the goal is to find a mapping from $x^{(n)}$ to $t^{(n)}$

$$f: R^m \to \Omega$$

where Ω is a discrete set

- $t^{(n)}$ can be a (discrete) scalar or vector

Suppose there are 5 classes in total

Seldom used

Scalar representation

$$t^{(1)} = 1$$
$$t^{(3)} = 3$$

Vector representation

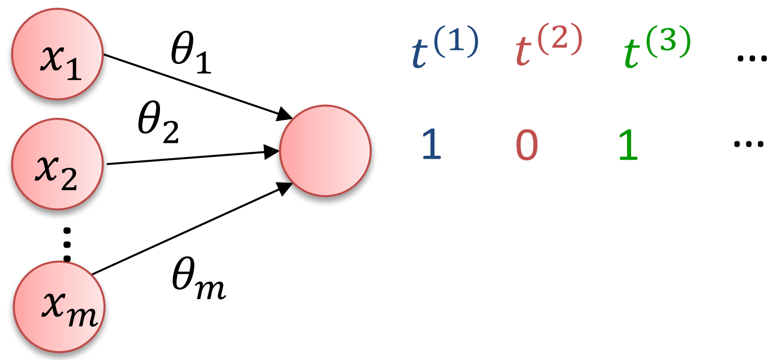
$$t^{(1)} = (1, 0, 0, 0, 0)^T$$
$$t^{(3)} = (0, 0, 1\ 0, 0)^T$$

Usually used

- 1-of-K representation
- Property: $t_k{}^{(n)} \in \{0,1\}$; $\sum_k t_k^{(n)} = 1$

2-class problems

- For 2-class problems, one 0-1 unit is enough for representing a label

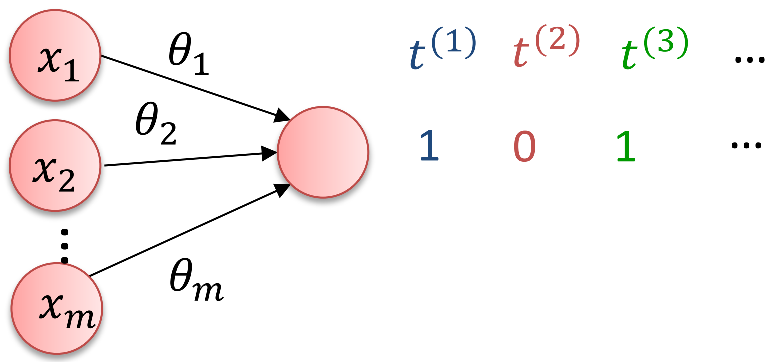


This representation has been used in linear classification by minimizing

$$\sum_{n=1}^{N}\left(f\left(x^{(n)}\right)-t^{(n)}\right)^2=\sum_{n=1}^{N}\left(w^{\mathrm{T}}x^{(n)}+b-t^{(n)}\right)^2$$

Logistic regression

- For 2-class problems, one 0-1 unit is enough for representing a label

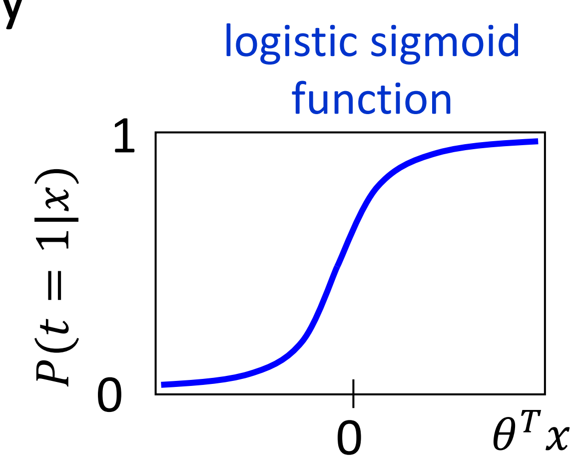


- We try to learn a conditional probability

$$P(t=1|x) = \frac{1}{1+\exp(-\theta^\top x)} \triangleq h(x)$$

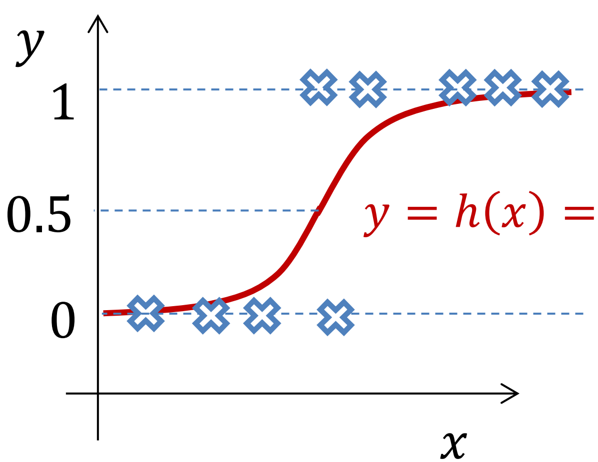
$$P(t=0|x) = 1 - P(t=1|x) = 1 - h(x)$$

where x is input and t is label



Logistic regression

- Our goal is to search for a value of θ so that the probability $P(t = 1|x) = h(x)$ is
  - large when x belongs to class 1 and
  - small when x belongs to class 0 (so that $P(t = 0|x)$ is large)
- As we're estimating a conditional probability (continuous), it's "regression"



$$y = h(x) = \frac{1}{1 + \exp(-\theta^{\mathrm{T}} x)}$$

Regression

Prediction $y = h(x)$

Classification

Prediction $y = \begin{cases} 1, \text{if } h(x) \geq 0.5 \\ 0, \text{if } h(x) < 0.5 \end{cases}$

Or equivalently

$$y = \begin{cases} 1, \text{if } \theta^T x \geq 0 \\ 0, \text{if } \theta^T x < 0 \end{cases}$$

Questions

$$y = h(x) = \frac{1}{1 + \exp(-\theta^{\mathrm{T}} x)}$$

- Why not use a linear function for $h(x)$
  - $P(t = 1|x) = h(x)$ should be a probability
- Why should $h(x)$ be a probability?
  - You'll see the reason soon
- Can we minimize the MSE between $h(x)$ and t?

$$E(\theta) = \frac{1}{N} \sum_{n=1}^{N} \left(h\left(x^{(n)}\right) - t^{(n)} \right)^2$$

  - Yes you can, but here we introduce another error function

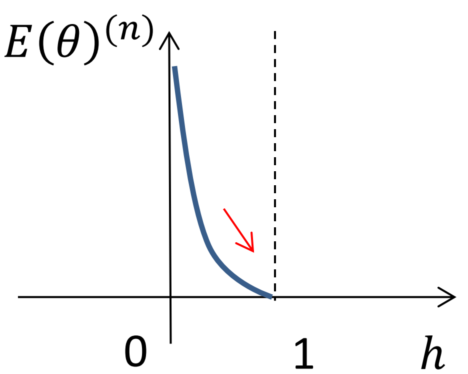
Cross-entropy error function

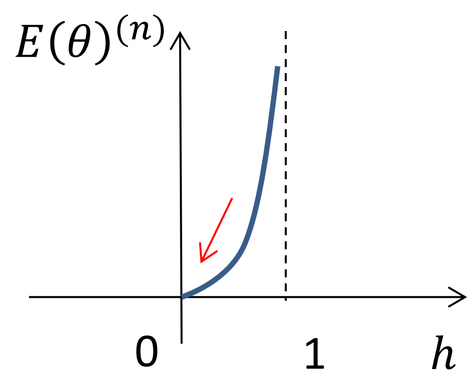
- For a set of training examples with binary labels $\{(x^{(n)}, t^{(n)}) : n = 1, \ldots, N\}$ define the *cross-entropy* error function

$$E(\theta) = -\frac{1}{N}\sum_{n=1}^{N}\left(t^{(n)}\ln(h(x^{(n)})) + (1 - t^{(n)})\ln(1 - h(x^{(n)}))\right)$$

$$E(\theta)^{(n)} = -t^{(n)}\ln(h(x^{(n)})) - (1 - t^{(n)})\ln(1 - h(x^{(n)}))$$

  - If $t^{(n)} = 1$, then
    $E(\theta)^{(n)} = -\ln(h)$
  - If $t^{(n)} = 0$, then
    $E(\theta)^{(n)} = -\ln(1 - h)$





Maximum likelihood formulation

- *Recall* the maximum conditional likelihood estimation:
  - 1. write down the conditional likelihood function
  - 2. take log and maximize
- Given a dataset $\{(x^{(1)}, t^{(1)}), \ldots, (x^{(N)}, t^{(N)})\}$ where $t^{(n)} \in \{0,1\}$
- View $t^{(n)}$ as a Bernoulli variable and $P(t^{(n)} = 1|x^{(n)}) = h(x^{(n)}; \theta)$. The conditional likelihood function

$$P(t^{(1)}, \ldots, t^{(N)}|X; \theta) = \Pi_{n=1}^{N} h(x^{(n)})^{t^{(n)}} (1 - h(x^{(n)}))^{1-t^{(n)}}$$

- Maximizing the likelihood is equivalent to minimizing

$$\begin{aligned} E(\theta) &= -\frac{1}{N} \ln P(t^{(1)}, \ldots, t^{(N)}) \\ &= -\frac{1}{N} \sum_{n=1}^{N} \left(t^{(n)} \ln h(x^{(n)}) + (1 - t^{(n)}) \ln(1 - h(x^{(n)})) \right) \end{aligned}$$

Training and testing

$$E(\theta) = -\frac{1}{N}\sum_{n=1}^{N}\left(t^{(n)}\ln h(x^{(n)}) + (1-t^{(n)})\ln(1-h(x^{(n)}))\right)$$

$$h(x) = \frac{1}{1+\exp(-\theta^{\mathrm{T}}x)}$$

$$\frac{\partial h}{\partial \theta} = h(1-h)$$

- Calculate the gradient (exercise)

$$\nabla E(\theta) = \frac{1}{N}\sum_{n} x^{(n)}\left(h(x^{(n)}) - t^{(n)}\right)$$

- Some regularization term can be incorporated into the cost function

$$J(\theta) = E(\theta) + \lambda\left|\left|\theta\right|\right|^2/2$$

- Training: learn θ to minimize the cost function

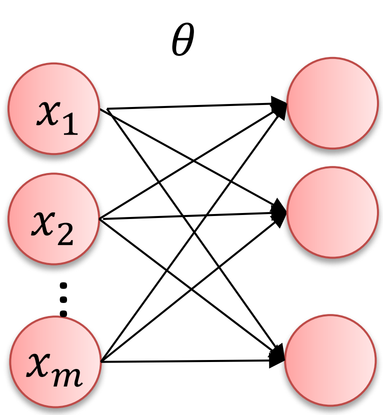
$$\theta \leftarrow \theta - \alpha\nabla J(\theta)$$

where α is the learning rate

- Testing: for a new input x, if $P(t=1|x) > P(t=0|x)$ then we predict the input as class 1, and 0 otherwise

More than two classes

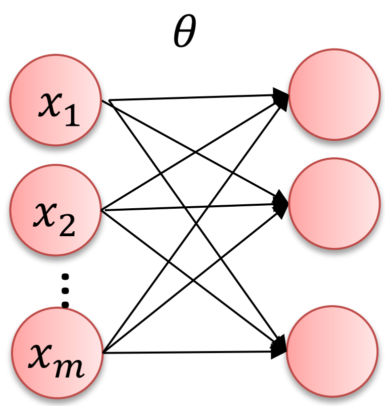
- For K-class problems ($K > 2$),
  - One unit is enough for representing a label if it can take discrete values, e.g., $0, 1, 2, \dots, K$ ← scalar representation
  - K 0-1 units can be also used to represent a label ← vector representation



$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	…
0	0	0	
1	0	1	…
0	1	0	…

More than two classes

- For K-class problems ($K > 2$), K 0-1 units is used to represent a label



$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	…
0	0	0	
1	0	1	…
0	1	0	

Note that $\sum_k t_k^{(n)} = 1$

- We try to learn a hypothesis $h(x)$ of the form

$$h(x) \triangleq \begin{bmatrix} P(t_1 = 1|x;\theta) \\ P(t_2 = 1|x;\theta) \\ \vdots \\ P(t_K = 1|x;\theta) \end{bmatrix} = \frac{1}{\sum_{j=1}^{K} \exp(\theta^{(j)\top} x)} \begin{bmatrix} \exp(\theta^{(1)\top} x) \\ \exp(\theta^{(2)\top} x) \\ \vdots \\ \exp(\theta^{(K)\top} x) \end{bmatrix}$$

More than two classes

Then $$h_k(x) = P(t_k = 1|x) = \frac{\exp(\theta^{(k)\top}x)}{\sum_{j=1}^{K}\exp(\theta^{(j)\top}x)}$$

- Given a test input x, estimate $P(t_k = 1|x)$ for each value of $k = 1, \ldots, K$.
- Goal: search for a value of θ so that the probability $P(t_k = 1|x)$ is
  - large when x belongs to the k-th class and
  - small when x belongs to other classes

where $$\theta = \left[\begin{array}{cccc} | & | & | & | \\ \theta^{(1)} & \theta^{(2)} & \cdots & \theta^{(K)} \\ | & | & | & | \end{array}\right].$$

- Since $h_k(x)$ is a (continuous) probability, we need to transform it into discrete values for classification ←How?

Softmax function

$$h_k(x) = P(t_k = 1|x) = \frac{\exp(\theta^{(k)\top} x)}{\sum_{j=1}^{K} \exp(\theta^{(j)\top} x)}$$

- The following function is called *softmax* function

$$\psi(z_i) = \frac{\exp(z_i)}{\sum_j \exp(z_j)} = \frac{\exp(z_i)}{\exp(z_i) + \sum_{j \neq i} \exp(z_j)} \in (0, 1)$$

- If $z_i > z_j$ for all $j \neq i$
  - Then $\psi(z_i) > \psi(z_j)$ for all $j \neq i$ but it is smaller than 1
- If $z_i \gg z_j$ for all $j \neq i$,
  - then $\psi(z_i) \to 1$ and $\psi(z_j) \to 0$ for $j \neq i$.

Error function

- The MSE function

vector

$$E = \frac{1}{N}\sum_{n=1}^{N} E^{(n)} \qquad \text{where} \qquad E^{(n)} = \frac{1}{2}\|h(x^{(n)}) - t^{(n)}\|^2$$

- The cross-entropy error function

$$E(\theta) = \frac{1}{N}\sum_{n=1}^{N} E^{(n)}(\theta), \quad \text{where} \quad E^{(n)}(\theta) = -\sum_{i=1}^{K} t_i^{(n)} \ln h_i^{(n)}$$

- In practice, the cross-entropy error function works better

Conditional maximum likelihood

- *Recap of categorical distribution :* It is defined over a single discrete variable x with K diff states where K is finite
$$P(\mathrm{x}=k|\boldsymbol{p})=p_k$$
where $\boldsymbol{p}\in[0,1]^K$ and $\sum_{k=1}^{K}p_k=1$
- Now we represent the category variable x using the one-hot vector $\boldsymbol{t}=(0,\dots,0,1,0,\dots,0)^\top$, then
$$P(\boldsymbol{t}|\boldsymbol{p})=\Pi_{k=1}^{K}p_k^{t_k}=\Pi_{k=1}^{K}P(t_k=1)^{t_k}$$
- Given a dataset $\left\{\left(\boldsymbol{x}^{(1)},\boldsymbol{t}^{(1)}\right),\dots,\ \left(\boldsymbol{x}^{(N)},\boldsymbol{t}^{(N)}\right)\right\}$. Maximize the conditional likelihood function (iid assumption):
$$P\left(\boldsymbol{t}^{(1)},\dots,\boldsymbol{t}^{(N)}\middle|\boldsymbol{X}\right)=\Pi_{n=1}^{N}\Pi_{k=1}^{K}P(\boldsymbol{t}_k^{(n)}=1|\boldsymbol{x}^{(n)})^{t_k^{(n)}}$$

In what follows, we will not use boldface for vectors

Cross-entropy error function

- The conditional data likelihood function

$$P(t^{(1)},\ldots,t^{(N)}|X;\theta) = \Pi_{n=1}^{N}\Pi_{k=1}^{K}P(t_k^{(n)}=1|x^{(n)})^{t_k^{(n)}}$$

- The cross-entropy error function is

Take log and negative, then minimize

$$E(\theta) = -\frac{1}{N}\ln P(t^{(1)},\ldots,t^{(N)})$$

$$= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}t_k^{(n)}\ln\frac{\exp(\theta^{(k)\top}x^{(n)})}{\sum_{j=1}^{K}\exp(\theta^{(j)\top}x^{(n)})}$$

$$E(\theta) = \frac{1}{N}\sum_{n=1}^{N}E^{(n)}(\theta), \quad E^{(n)}(\theta) = -\sum_{i=1}^{K}t_i^{(n)}\ln h_i^{(n)}$$

where $h_i^{(n)} = P(t_i^{(n)}=1|x^{(n)}) = \frac{\exp(u_i^{(n)})}{\sum_{j=1}^{K}\exp(u_j^{(n)})}, \quad u_k^{(n)} = \theta^{(k)\top}x^{(n)}$

Calculate the gradient

- By defining the local sensitivity

$$\delta_k^{(n)} \triangleq \frac{\partial E^{(n)}}{\partial u_k^{(n)}} = -\left(t_k^{(n)} - h_k^{(n)}\right) \quad \text{where } u_k^{(n)} = \theta^{(k)\top} x^{(n)}$$

- It can be shown that (the derivation is not covered in this lecture)

$$\frac{\partial E^{(n)}}{\partial \theta^{(k)}} = \delta_k^{(n)} x^{(n)}$$

- The overall gradient

$$\nabla_{\theta^{(k)}} E(\theta) = \frac{1}{N} \sum_{n=1}^{N} \frac{\partial E^{(n)}}{\partial \theta^{(k)}} = -\frac{1}{N} \sum_{n=1}^{N} \left(t_k^{(n)} - h_k^{(n)})\right) x^{(n)}$$

$$= -\frac{1}{N} \sum_{n=1}^{N} \left(t_k^{(n)} - P(t_k^{(n)} = 1 | x^{(n)})\right) x^{(n)}$$

Training and testing

- Calculate the gradient of the cross-entropy error function

$$\nabla_{\theta^{(k)}} E(\theta) = -\frac{1}{N} \sum_{n=1}^{N} \left(t_k^{(n)} - h_k^{(n)} \right) x^{(n)}$$

- As before, some regularization term can be incorporated into the cost function

$$J(\theta) = E(\theta) + \lambda \left| |\theta| \right|^2 / 2$$

- Training: minimize the cost function with gradient $\nabla J(\theta)$

$$\theta \leftarrow \theta - \alpha \nabla J(\theta)$$

where α is the learning rate

- Testing: find the maximum $P(t_k = 1|x)$ among k for a new input x

$$P(t_k = 1|x) = \frac{\exp(\theta^{(k)\top} x)}{\sum_{j=1}^{K} \exp(\theta^{(j)\top} x)}$$

Stochastic gradient descent

- Batch gradient descent algorithm updates the parameters θ of the objective $J(\theta)$ as,
$$\theta = \theta - \alpha \nabla_\theta J(\theta)$$
where $J(\theta)$ denotes the cost over the full training set
- SGD updates and computes the gradient using only a single or a few training examples
$$\theta = \theta - \alpha \nabla_\theta J\left(\theta; x^{(i)}, t^{(i)}\right)$$
with a pair $(x^{(i)}, t^{(i)})$ from the training set.
- Often a minibatch is used (e.g., size 256) instead of a single example
  – Reduces the variance in the parameter update
  – Take advantage of highly optimized matrix operations

Introducing bias

- So far we have assumed

$$h_k(x) = P(t_k = 1|x) = \frac{\exp(u_k^{(n)})}{\sum_{j=1}^{K} \exp(u_j^{(n)})} \qquad u_k^{(n)} = \theta^{(k)\top} x^{(n)}$$

- Sometimes a bias is introduced into $u_k^{(n)}$ and the parameters become $\{W, b\}$

$$u_k^{(n)} = W^{(k)\top} x^{(n)} + b^{(k)}$$

- It's easy to show that

$$\nabla_{W^{(k)}} E(\theta) = -\frac{1}{N} \sum_{n=1}^{N} \left(t_k^{(n)} - h_k(x^{(n)}) \right) x^{(n)}$$

$$\nabla_{b^{(k)}} E(\theta) = -\frac{1}{N} \sum_{n=1}^{N} \left(t_k^{(n)} - h_k(x^{(n)}) \right)$$

- Regularization is often applied on W only

$$J(W, b) = E(W, b) + \lambda \left|\left|W\right|\right|^2 / 2$$

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- Convolutional neural network
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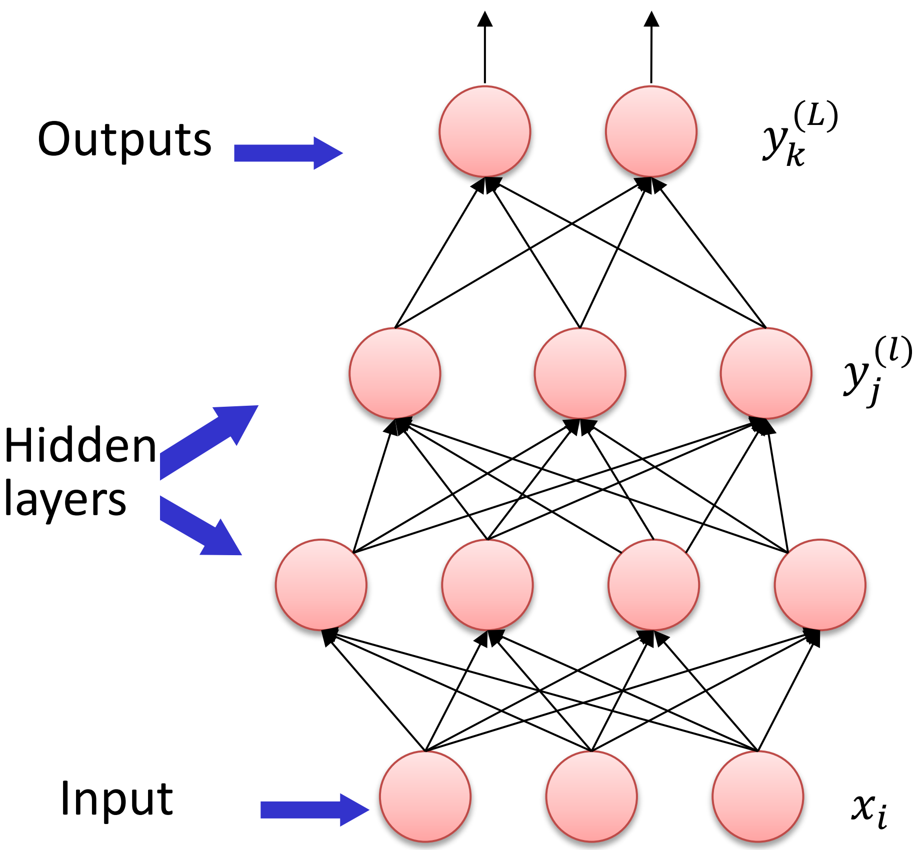
Multi-layer Perceptron (MLP)



- There are a total of L layers except the input
- Connections:
  - Full connections between layers
  - No feedback connections between layers
  - No lateral connections in the same layer
- Every neuron receives input from previous layer and fire according to an activation function

Activation functions

- Logistic function

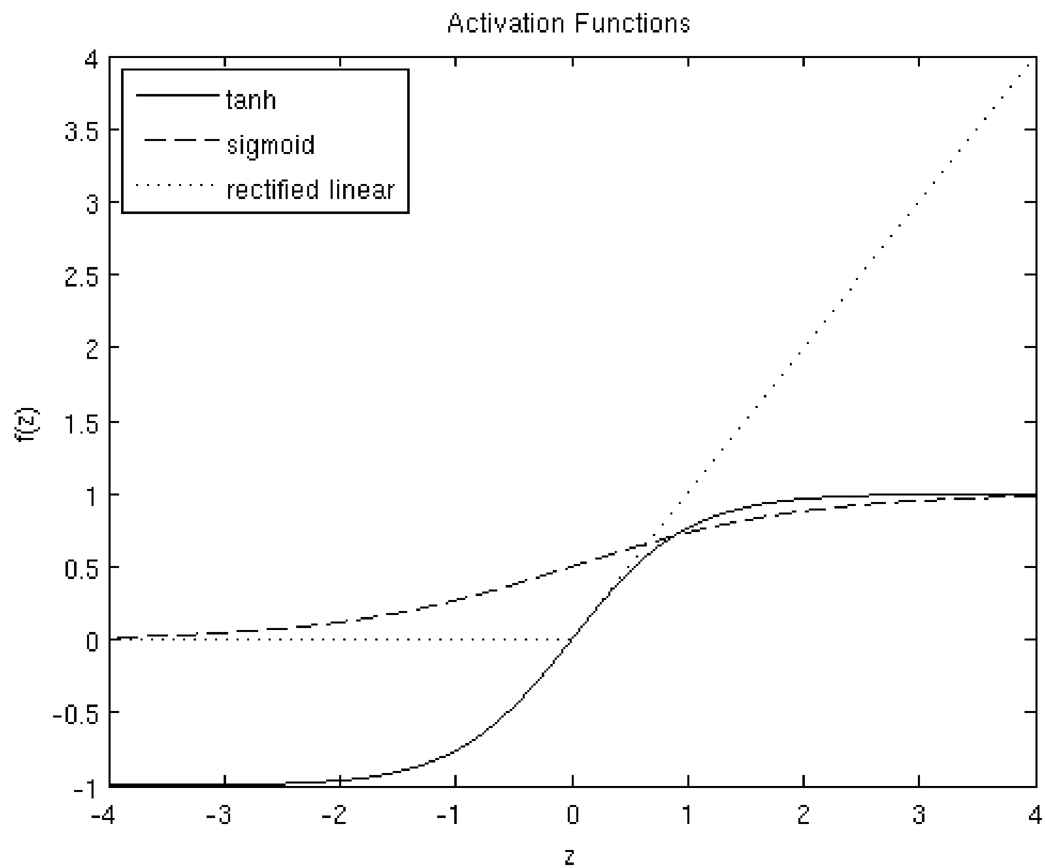
$$f(z) = \frac{1}{1 + \exp(-z)}$$

- Hyperbolic tangent function

$$f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

- Rectified linear activation function (ReLU)

$$f(z) = \max(0, z)$$



Activation functions

- Logistic function

$$f(z) = \frac{1}{1 + \exp(-z)} \xrightarrow{\text{gradient}} f'(z) = f(z)(1 - f(z))$$

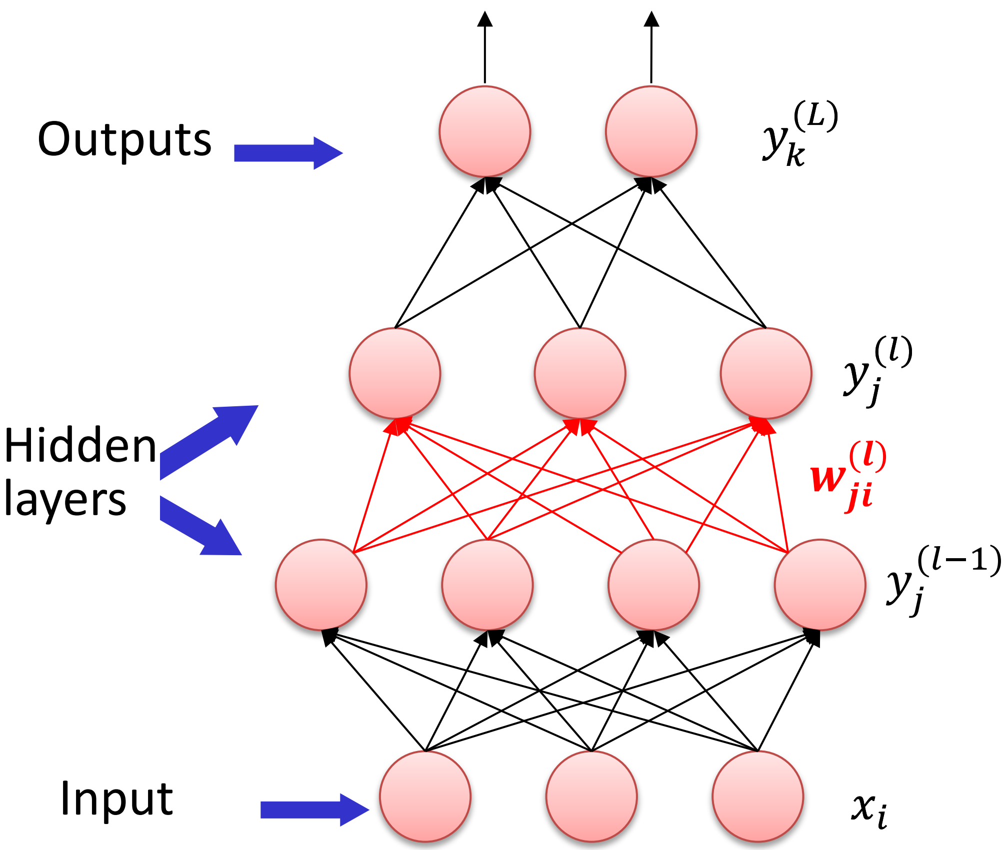
- Hyperbolic tangent function

$$f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \xrightarrow{\text{gradient}} f'(z) = 1 - f(z)^2$$

- Rectified linear activation function (ReLU)

$$f(z) = \max(0, z) \xrightarrow{\text{gradient}} f'(z) = \begin{cases} 1, & \text{if } z \geq 0, \\ 0, & \text{else} \end{cases}$$

Forward pass



For $l = 1, \dots, L-1$ calculate the input to neuron j in the l-th layer

$$u_j^{(l)} = \sum_i w_{ji}^{(l)} y_i^{(l-1)} + b_j^{(l)}$$

and its output

$$y_j^{(l)} = f(u_j^{(l)})$$

where $f(\cdot)$ is activation function

- Note $y^{(0)} = x$
- There are desired outputs t for each input sample
- For $l = L$, $f(\cdot)$ can be an activation function or the softmax function

Error functions for BP

- Error function $$E = \frac{1}{N}\sum_{n=1}^{N} E^{(n)}$$

where $E^{(n)}$ is the error function for each input sample n

- Squared error, or Euclidean loss

$$E^{(n)} = \frac{1}{2}\sum_{k=1}^{K}(t_k - y_k^{(L)})^2,\ y_k^{(L)} = \frac{1}{1+\exp(-w_k^{(L)\top} y^{(L-1)} - b_k^{(L)})}$$

Is ReLU applicable?

- Cross-entropy error

$$E^{(n)} = -\sum_{k=1}^{K} t_k \ln y_k^{(L)},\quad y_k^{(L)} = \frac{\exp(w_k^{(L)\top} y^{(L-1)} + b_k^{(L)})}{\sum_{j=1}^{K}\exp(w_j^{(L)\top} y^{(L-1)} + b_j^{(L)})}$$

where t is target of the form $(0, 0, \ldots, 1, 0, 0)^T$

In what follows, except $E^{(n)}$, for clarity, we will omit the superscript (n) on x, t, u, y etc. for each input sample.

Weight adjustment

- Weight adjustment

Learning rate

$$w_{ji}^{(l)} = w_{ji}^{(l)} - \alpha \frac{\partial E}{\partial w_{ji}^{(l)}} \qquad b_j^{(l)} = b_j^{(l)} - \alpha \frac{\partial E}{\partial b_j^{(l)}}$$

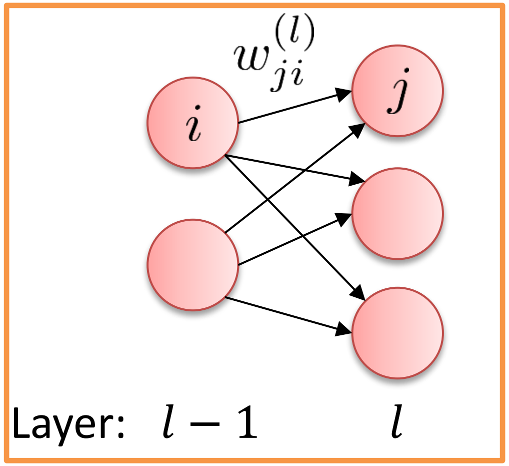
- Weight decay is often used on ${w_{ji}}^{(l)}$ (not necessary on ${b_j}^{(l)}$) which amounts to adding an additional term on the cost function

$$J = E + \frac{\lambda}{2} \sum_{i,j,l} (w_{ji}^{(l)})^2$$

- Weight adjustment on w is changed to

$$w_{ji}^{(l)} = w_{ji}^{(l)} - \alpha \frac{\partial J}{\partial w_{ji}^{(l)}} = w_{ji}^{(l)} - \alpha \frac{\partial E}{\partial w_{ji}^{(l)}} - \alpha \lambda w_{ji}^{(l)}$$

Gradient and local sensitivity



- Define local sensitivity $\delta_i^{(l)} = \frac{\partial E^{(n)}}{\partial u_i^{(l)}}$
- Then for $1 \leq l \leq L$

$$\frac{\partial E^{(n)}}{\partial w_{ji}^{(l)}} = \delta_j^{(l)} \frac{\partial u_j^{(l)}}{\partial w_{ji}^{(l)}} = \delta_j^{(l)} f(u_i^{(l-1)})$$

$$\frac{\partial E^{(n)}}{\partial b_j^{(l)}} = \delta_j^{(l)},$$

since ${u_j}^{(l)} = \sum_i w_{ji}^{(l)} f(u_i^{(l-1)}) + b_j^{(l)}$, where f is the activation function and $f(u_i^{(0)}) = x$.

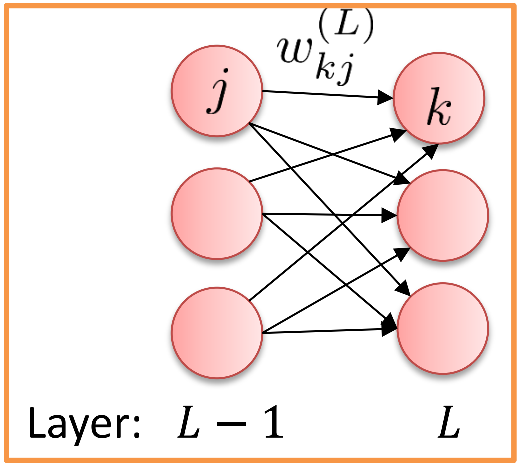
Computing the gradients amounts to computing the local sensitivity in each layer!

Local sensitivity for MSE layer

- If the squared error is used then the output of the last layer units of MLP are

$$y_k^{(L)} = f(u_k^{(L)}) = f(w_k^{(L)\top} \boxed{y^{(L-1)}} + b_k^{(L)})$$

Output of the units on the (L-1)-th layer



where the activation function f can be

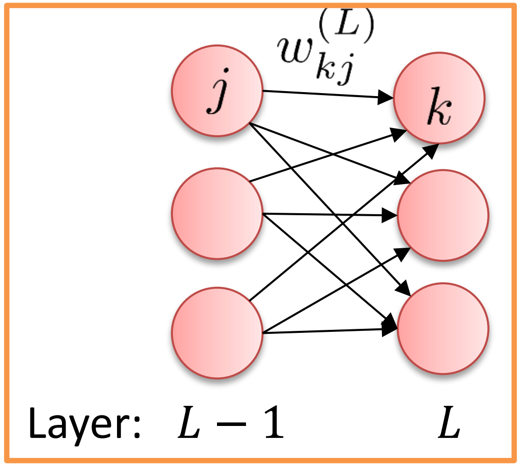
✓ logistic sigmoid ✓ tanh ✓ ReLU

- Recall the error for each sample $E^{(n)} = \frac{1}{2}\sum_{k=1}^{K}(t_k - y_k^{(L)})^2,$
- Local sensitivity

$$\delta_k^{(L)} \triangleq \frac{\partial E^{(n)}}{\partial u_k^{(L)}} = \left(y_k^{(L)} - t_k\right) f'(u_k^{(L)})$$

Recall local sensitivity for softmax layer

- If the softmax regression is used in the last layer of an MLP, then θ is replaced with $w^{(L-1)}$ and $b^{(L-1)}$ and the probabilistic function becomes



Output of the units on the (L-1)-th layer

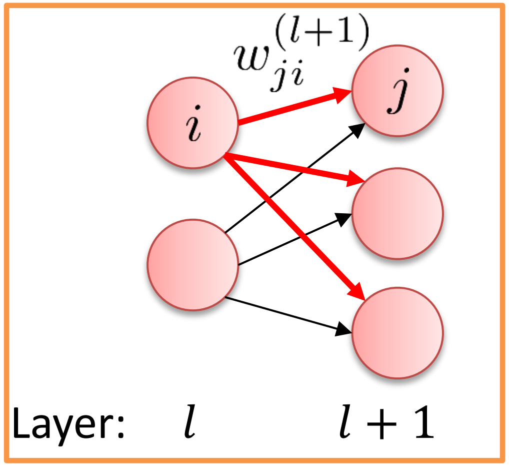
$$y_k^{(L)} \triangleq P(t_k = 1 | \boxed{y^{(L-1)}}) = \frac{\exp(w_k^{(L)\top} y^{(L-1)} + b_k^{(L)})}{\sum_{j=1}^{K} \exp(w_j^{(L)\top} y^{(L-1)} + b_j^{(L)})}$$

- Local sensitivity

$$\delta_k^{(L)} \triangleq \frac{\partial E^{(n)}}{\partial u_k^{(L)}} = y_k^{(L)} - t_k$$

Local sensitivity for other layers

- Define local sensitivity $\delta_i^{(l)} = \dfrac{\partial E^{(n)}}{\partial u_i^{(l)}}$
- If $1 \le l < L$, i.e., neuron i is a hidden neuron, it has an effect on all neurons in the next layer, therefore its local sensitivity is



$$\delta_i^{(l)} = \frac{\partial E^{(n)}}{\partial u_i^{(l)}} = \sum_j \frac{\partial E^{(n)}}{\partial u_j^{(l+1)}} \frac{\partial u_j^{(l+1)}}{\partial y_i^{(l)}} \frac{\partial y_i^{(l)}}{\partial u_i^{(l)}} = \sum_j \delta_j^{(l+1)} w_{ji}^{(l+1)} f'(u_i^{(l)})$$

$$u_j^{(l+1)} = \sum_i w_{ji}^{(l+1)} y_i^{(l)} + b_j^{(l+1)} \qquad y_i^{(l)} = f(u_i^{(l)})$$

where f can be any activation function

Therefore we compute ${\delta_i}^{(l)}$ backward, from $l = L, L-1, \dots, 1$, and in the sequel $\partial E / \partial W^{(l)}$ and $\partial E / \partial b^{(l)}$ backward

Backpropagation in vector-matrix form

- Local sensitivity $$\delta^{(l)} = \left(\frac{\partial E^{(n)}}{\partial u_1^{(l)}}, \frac{\partial E^{(n)}}{\partial u_2^{(l)}}, \dots \right)^T$$
- For the output layer L

$$\delta^{(L)} = (y - t) \odot f'(u^{(L)}) \quad \text{or} \quad \delta^{(L)} = (y - t)$$

where $\odot$ denotes element-wise multiplication

- For the hidden layer $1 \leq l < L$

$$\delta^{(l)} = (W^{(l+1)})^\top \delta^{(l+1)} \odot f'(u^{(l)})$$

- Calculate the gradients $0 \leq l < L$

$$\frac{\partial E^{(n)}}{\partial w^{(l)}} = \delta^{(l)} (f(u^{(l-1)}))^\top, \quad \frac{\partial E^{(n)}}{\partial b^{(l)}} = \delta^{(l)}$$

for each sample n

- Update weights

sum over n

$$W^{(l)} = W^{(l)} - \frac{\alpha}{N} \sum_n \frac{\partial E^{(n)}}{\partial W^{(l)}} - \alpha \lambda W^{(l)}, \quad b^{(l)} = b^{(l)} - \frac{\alpha}{N} \sum_n \frac{\partial E^{(n)}}{\partial b^{(l)}}$$

Implementation

- Run forward process
  - Calculate $f\left(u^l\right)$ and $f'\left(u^l\right)$ for $l = 1,2, \dots, L$
- Run backward process
  - Calculate $\delta^{(l)}$ and $\partial E / \partial W^{(l)}$,$\partial E / \partial b^{(l)}$ for $l = L, L-1, \dots, 1$
- Update $W^{(l)}$ and $b^{(l)}$ for $l = 1,2, \dots, L$
- Modular programming $\longleftarrow$ Basic idea of tensorflow, Caffe, etc.
  - Implement the layer as a class and provide functions for forward calculation and backward calculation, respectively
  - The forward functions and backward functions differ according to the type of the layer, e.g., input layer, hidden layer, softmax output layer, sigmoid output layer, etc.
  - Then you can design different structures of MLP by specifying the layer modules in a main file

More flexible setting

- The input layer or hidden layer

$$y_j{}^{(l)} = f\left(\sum_i w_{ji}^{(l)} y_i^{(l-1)} + b_j^{(l)}\right)$$

  can be decomposed into two layers
  - Fully connected layer: $u_j{}^{(l)} = \sum_i w_{ji}^{(l)} y_i^{(l-1)} + b_j^{(l)}$
  - Activation layer: $y_j^{(l)} = f(u_j{}^{(l)})$
- The squared error layer $E^{(n)} = \frac{1}{2}\left\|f\left(u^{(L)}\right) - t\right\|^2$

  can be decomposed into two layers
  - Activation layer: $y_k^{(L)} = f(u_k{}^{(L)})$, where f can be any function
  - Loss layer: $E^{(n)} = \frac{1}{2}\left\|y^{(L)} - t\right\|^2$

Question

- Consider the squared error function

$$E^{(n)} = \frac{1}{2}\left|\left|f\left(W^{(L)}y^{(L-1)} + b^{(L)}\right) - t\right|\right|^2$$

How many layers can be designed?

Fc layer + activation layer + Euclidean loss layer

More flexible setting

- The cross-entropy error layer $E^{(n)} = -\sum_{k=1}^{K} t_k \ln f\left(u_k^{(L)}\right)$ can be decomposed into two layers
  - Softmax layer: $y_k^{(L)} = f(u_k{}^{(L)})$, where f is the softmax function
  - Loss layer: $E^{(n)} = -\sum_{k=1}^{K} t_k \ln y_k^{(L)}$
  - But this is unnecessary! Why?
- Consider this error

$$E^{(n)} = -\sum_{k=1}^{K} t_k \ln f\left(\sum_i w_{ki}^{(l)} y_i^{(l-1)} + b_k^{(l)}\right)$$

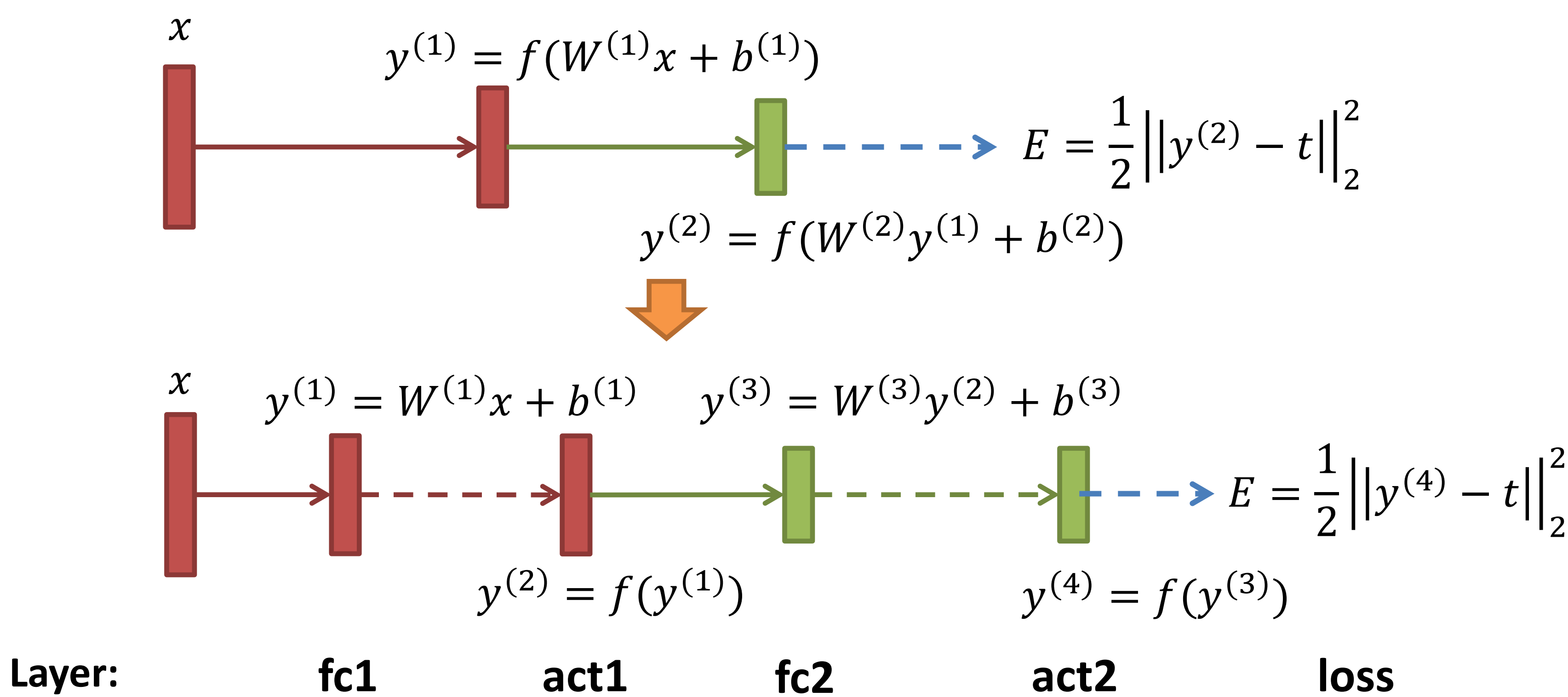
How many layers can be designed?

Fc layer + softmax crossentropy layer

Example

- An MLP with one hidden layer using the squared error function

Solid arrow: w/ param.
Dashed arrow: w/o param.



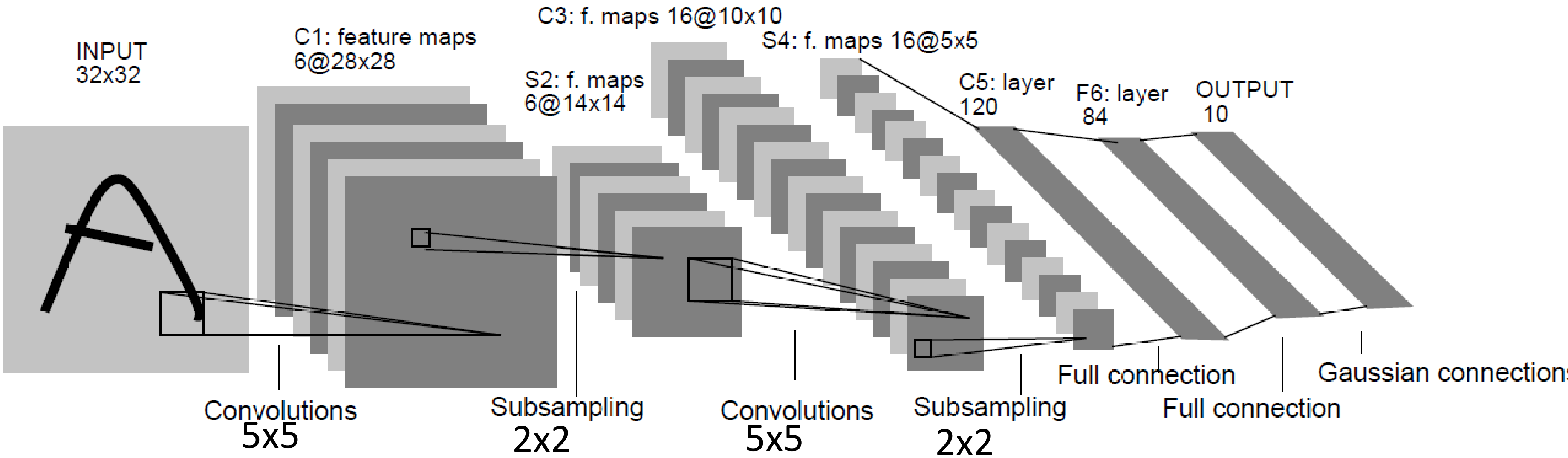
Problem 1

- Derive the local sensitivity δ and gradient $\partial E/\partial w$ and $\partial E/\partial b$ where applicable for
  - fully connected layer
  - sigmoid layer
  - ReLU layer
  - Euclidean loss layer
- These layers are shown in the previous slide

Outline

- Regression and classification
- Multi-layer perceptron
- Convolutional neural network
- Practical tricks

A typical example



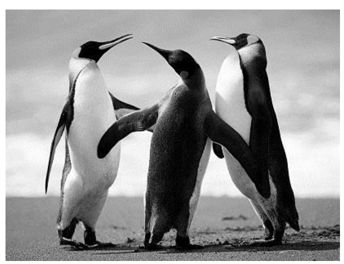
- Local connections and weight sharing
- C layers: convolution
  - Output $y_i = f(\sum_{\Omega} w_j x_j + b)$ where Ω is the patch size, $f(\cdot)$ is the sigmoid function, w and b are parameters
- S layers: subsampling (avg pooling)
  - Output $y_i = f\left(\frac{1}{|\Omega|}\sum_{\Omega} x_j\right)$ where Ω is the pooling size

Two new layers

- Define two additional layers with forward computation and backward computation
  – Convolution layer and pooling layer

input kernel feature map

Convolution



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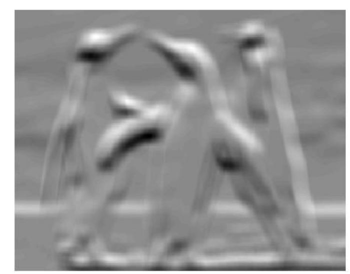
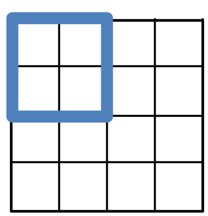
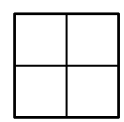


Pooling



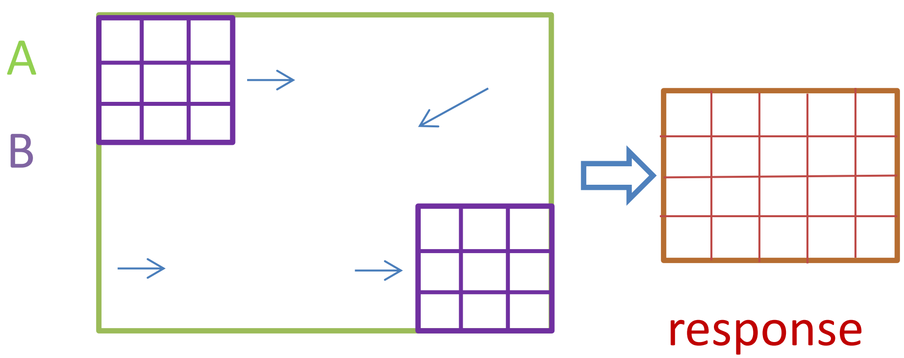
average or max



poolingsize=2x2

Motivation for convolution

- Suppose there are two 2D images A and B where the size of B is smaller than that of A
- Compute the similarity between B and each part of A
- Naively, we could slide B on A and calculate the similarity one by one



Cosine similarity between two matrices x and y:

$$s = \sum_{i,j} x_{ij} y_{ij}$$

if the two matrices have unit Frobenius norm

But this process can be very slow! We have other choices…

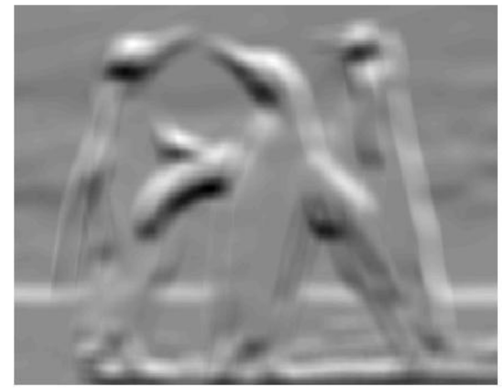
Example

figure

kernel

*

feature map

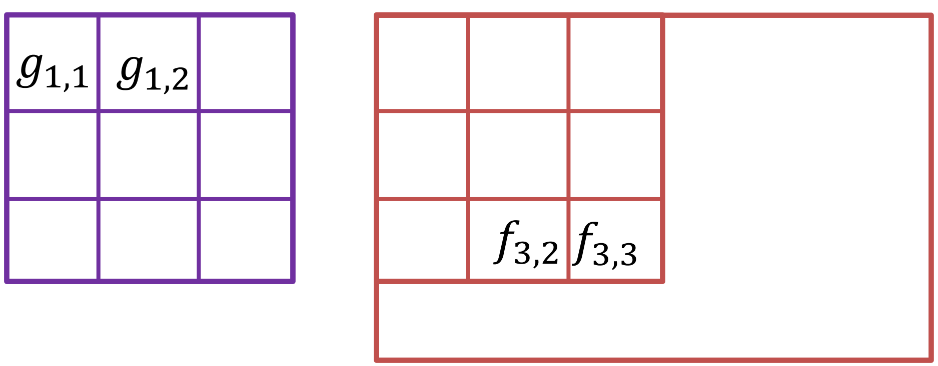


The higher a pixel value (brighter) in the feature map, the more similar between the filter and the corresponding patch in the figure

2D convolution

- Suppose there are two matrices f and g with sizes $M \times N$ and $K_1 \times K_2$, respectively, where $M \geq K_1, N \geq K_2$
- Discrete convolution of the two matrices

$$h[m,n] = (f * g)[m,n] \triangleq \sum_{k_1=1}^{K_1} \sum_{k_2=1}^{K_2} f[m-k_1, n-k_2]g[k_1,k_2]$$



When $m = 4, n = 4$

$$(f * g)_{m,n} = f_{3,3}g_{1,1} + f_{3,2}g_{1,2} + f_{3,1}g_{1,3} + f_{2,3}g_{2,1} + \cdots$$

- valid shape: the size of h is $(M - K_1 + 1) \times (N - K_2 + 1)$
- full shape: the size of h is $(M + K_1 - 1) \times (N + K_2 - 1)$
- same shape: the size of h is $M \times N$

Matlab example

```
>> A = round(3*rand(4))

A =

     0     0     1     2
     2     2     0     0
     2     1     2     2
     3     0     1     1

>> B = round(2*rand(3))-1

B =

     0     0    -1
     1    -1     1
    -1     1     1
```

```
>> C = conv2(A,B,'full')

C =

     0     0     0     0    -1    -2
     0     0    -1    -1    -1     2
     2     0    -3     0     1     0
     0    -1     4     3    -1     1
     1    -2     5     1     4     3
    -3     3     2     0     2     1

>> D = conv2(A,B,'valid')

D =

    -3     0
     4     3
```

Matlab example

```
>> A = round(3*rand(4))

A =

     0     0     1     2
     2     2     0     0
     2     1     2     2
     3     0     1     1

>> B = round(2*rand(3))-1

B =

     0     0    -1
     1    -1     1
    -1     1     1
```

```
>> C = conv2(A,B,'full')

C =

     0     0     0     0    -1    -2
     0     0    -1    -1    -1     2
     2     0    -3     0     1     0
     0    -1     4     3    -1     1
     1    -2     5     1     4     3
    -3     3     2     0     2     1

>> D = conv2(A,B,‘same')
D =
     0    -1    -1    -1
     0    -3     0     1
    -1     4     3    -1
    -2     5     1     4
```

Python example

```
import numpy
from scipy import signal
A = numpy.array([[0,0,1,2],[2,2,0,0],[2,1,2,2],[3,0,1,1]])
B = numpy.array([[0,0,-1],[1,-1,1],[-1,1,1]])
C = signal.convolve2d(A,B,mode='full')
print(C)
C = signal.convolve2d(A,B,mode='valid')
print(C)
C = signal.convolve2d(A,B,mode=‘same')
print(C)
```

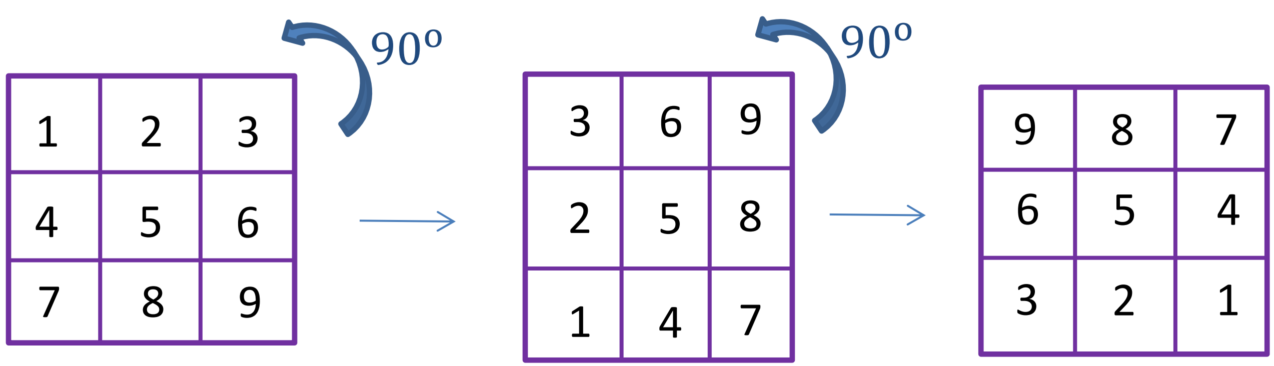
You would obtain the same results as before

Relationship between similarity and convolution

- Calculating the the similarity between matrix g and each part of matrix f is equivalent to calculating $f * \tilde{g}$ where

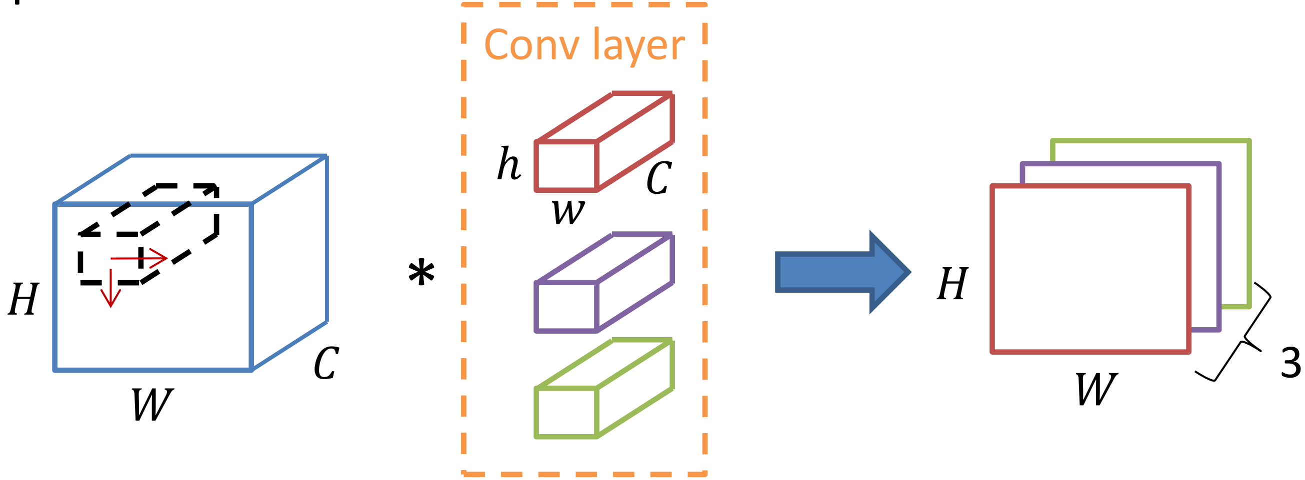
$$\tilde{g}_{1,1} = g_{M,N}, \tilde{g}_{1,2} = g_{M,N-1}, \dots, \tilde{g}_{1,N} = g_{M,1}$$
$$\tilde{g}_{2,1} = g_{M-1,N}, \tilde{g}_{2,2} = g_{M-1,N-1}, \dots, \tilde{g}_{2,N} = g_{M-1,1}$$
$$\vdots \qquad\qquad \vdots$$
$$\tilde{g}_{M,1} = g_{1,N}, \tilde{g}_{M,2} = g_{1,N-1}, \dots, \tilde{g}_{M,N} = g_{1,1}$$

- In Matlab, the above flip operation can be realized by applying the command rot90() twice [or rot180()]



3D convolution

- Why 3D convolution?
  - The input might be 3D, e.g., RGB channels
- In general we assume the number of channels in the input is the same as that in the kernel (filter)
- Convolve a 2D feature map in the 3D input with the *corresponding* 2D section in the 3D kernel, then sum over all sections to yield one feature map

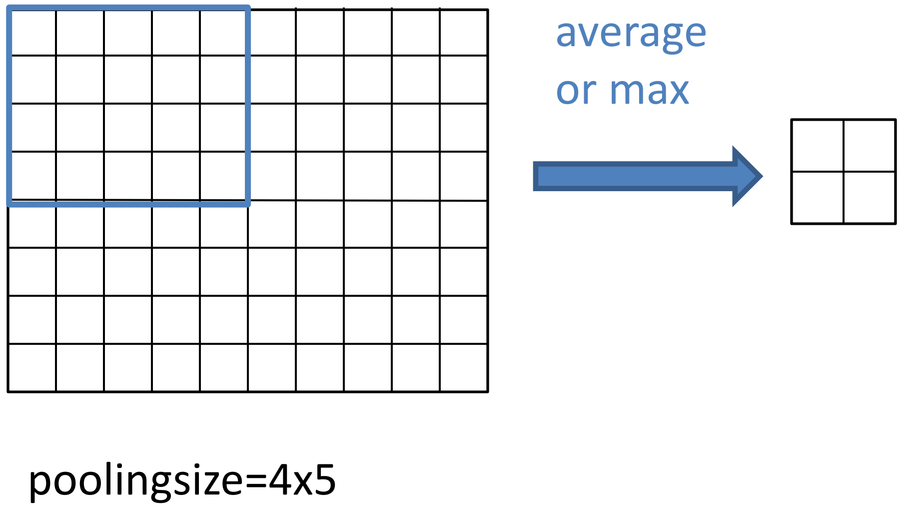


The number of parameters in this layer is $h \times w \times C \times 3$

Why do we use convolution?

- Convolution has fast algorithms, e.g., Fast Fourier Transform (FFT)
- It does not slide one signal on the other signal!
- However, when GPU is used, FFT may not be needed as GPU can compute matrix multiplication in parallel
  – Can we transform the similarity calculation to matrix multiplication form?

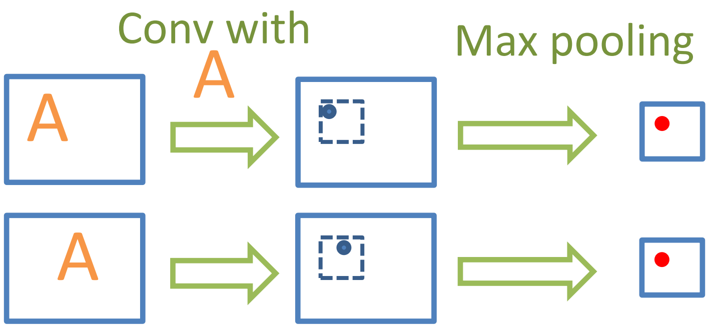
Pooling in local regions



- Divide the convolved features into *disjoint* $m \times n$ regions, and take the mean (or maximum) feature activation over these regions to obtain the pooled features
- How about 3D input?
  - Channel-wise pooling: if the input has C channels, then the output also has C channels

Why do we need pooling

- Reduce the number of features for final classification
  - Consider images of 96×96 pixels. Suppose we have learned 400 features over 8×8 inputs. This results in an output of size $(96 - 8 + 1)^2 \times 400 = 3{,}168{,}400$ features per example
- Enlarge the effective region of features in the next layer
  - A feature learned in the pooled maps will have larger effective regions in the pixel space
- Realize invariance
  - After pooling, features tend to be translation invariant in local regions



This is similar to the receptive fields of visual neurons, whose sizes increase along the visual hierarchy

Backward computation

- We have discussed the forward computation of the convolutional layer and pooling layer
- For BP
  - in the convolutional layer, you need to calculate the local sensitivity and parameter gradient
  - in the pooling layer, you need to calculate the local sensitivity
- But this is a little bit complicated
  - Fortunately, we have toolboxes

Deep learning tools

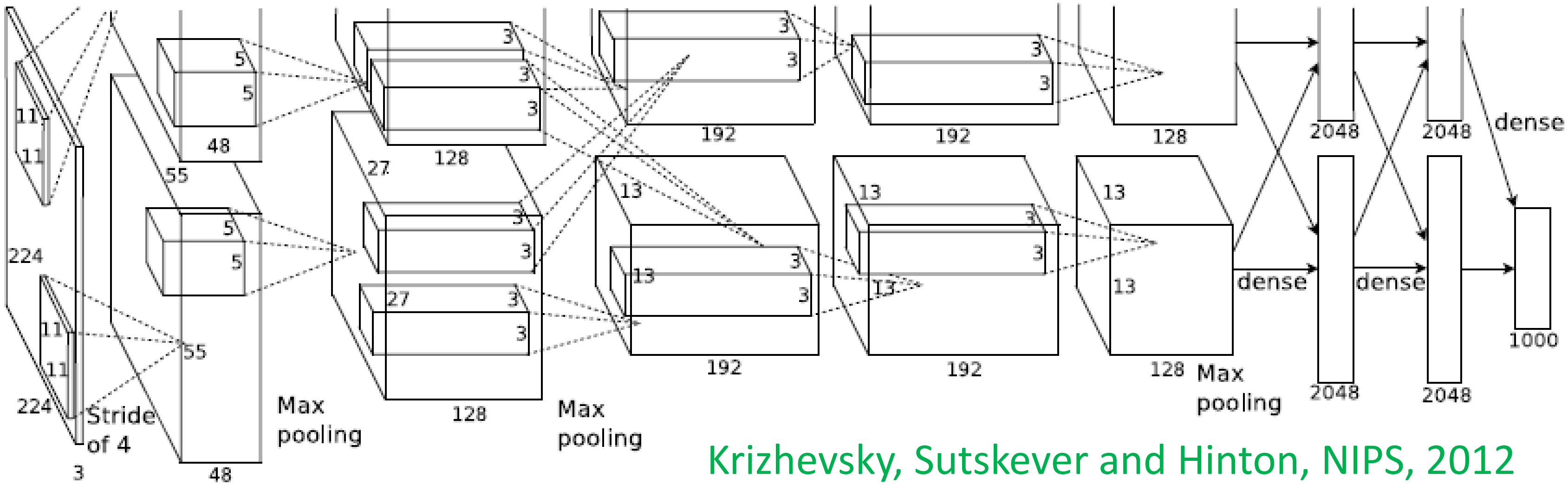
- Theano @ University of Montreal
- Caffe @ UC Berkley
- TensorFlow @ Google
- Torch andy PyTorch @ Facebook

Construction of CNN

- The convolutional layers and pooling layers can be combined freely with other layers that we have discussed
  - Fully connected layer
  - Sigmoid layer
  - ReLU layer
  - Euclidean loss layer
  - Cross-entropy loss layer

  as well as other layers that we haven't discussed, e.g.,
  - Local response normalization layer (Krizhevsky et al. 2012)
  - Dropout layer (Srivastava et al., 2014)
  - PReLU layer (He et al., 2015)
  - Batch normalization layer (Ioffe and Szegedy, 2015)

CNN for image classification



Krizhevsky, Sutskever and Hinton, NIPS, 2012

- Network dimension: 150,528(input)-253,440–186,624–64,896–64,896–43,264–4096–4096–1000(output)
- In total: 60 million parameters
- Task: classify 1.2 million high-resolution images in the ImageNet LSVRC-2010 contest into the 1000 different classes
- Results: state-of-the-art accuracy on ImageNet

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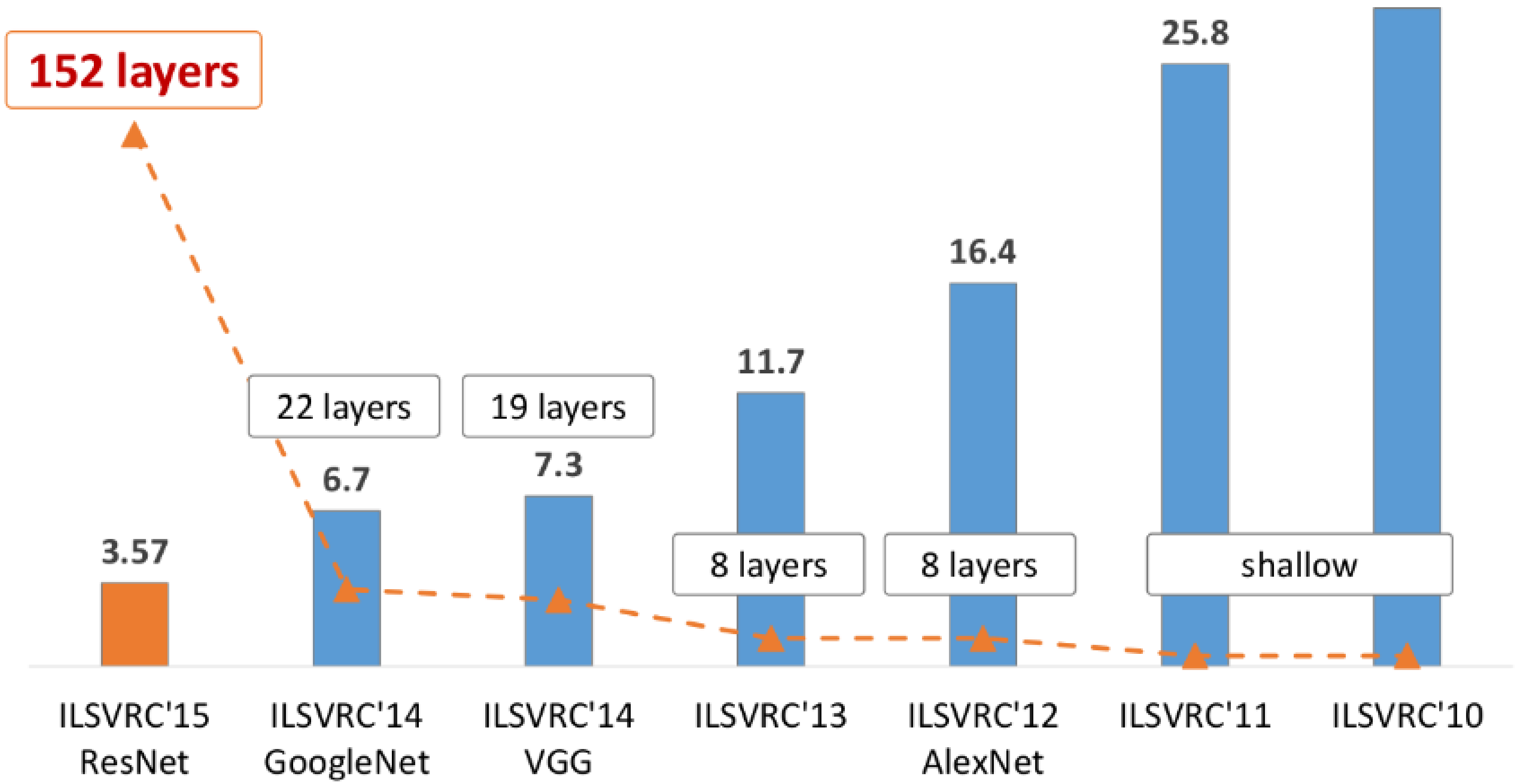
The deeper, the better

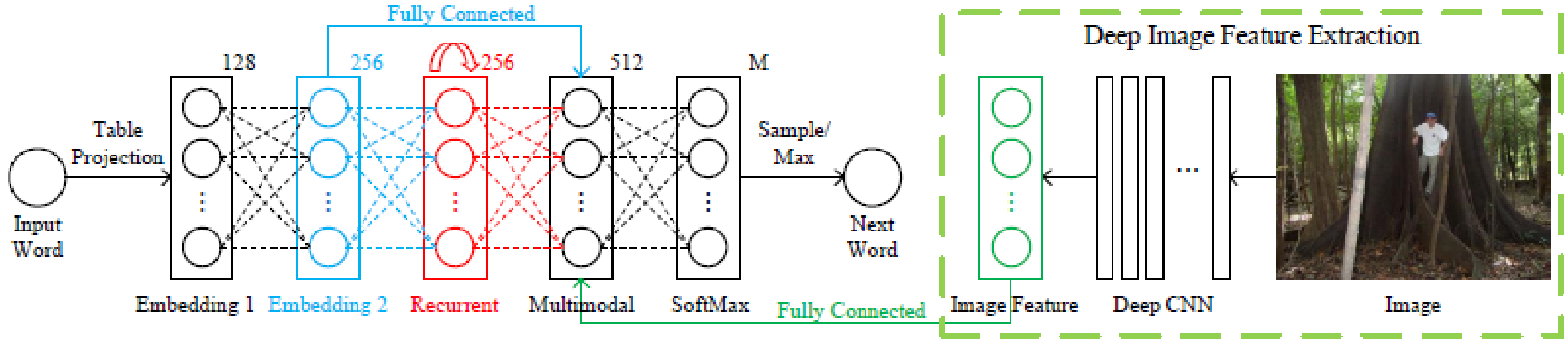


He, 2015

A Neural Algorithm of Artistic Style

Gatys et al., 2015

CNN + Recurrent neural network

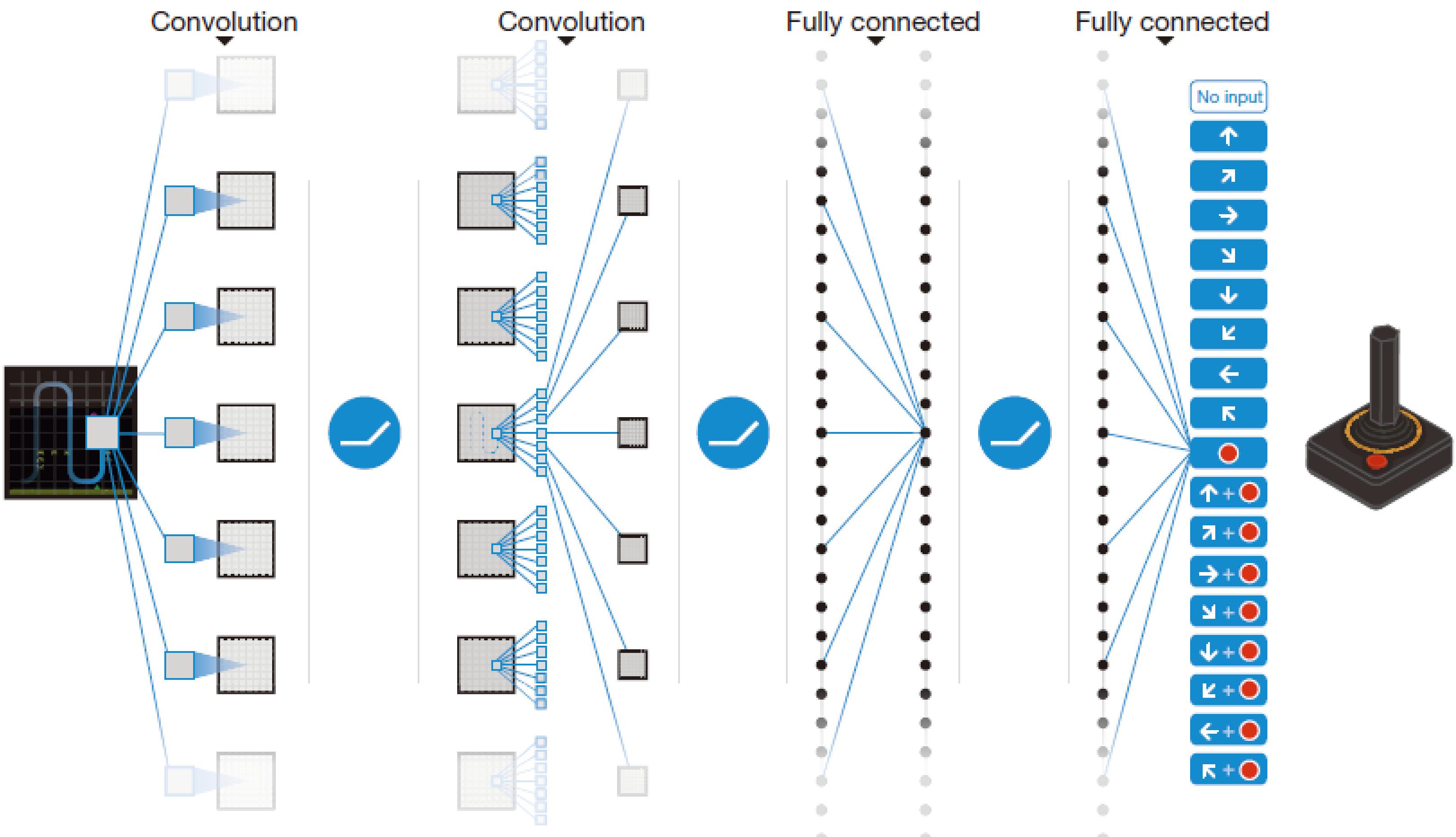


Mao et al., 2014

CNN + reinforcement learning

- Atari 2600 platform offers 49 games
- Google's deep Q-network (DQN) performs the same as or better than the human expert in 29 games
- The same network, same learning algorithms

DQN



Mnih et al., 2015

Outline

- Regression and classification
- Multi-layer perceptron
- Convolutional neural network
- Practical tricks

Weight initialization

W inputting to a neuron is drawn from a distribution:

- Gaussian
  - a Gaussian distribution with zero mean and fixed std, e.g., 0.01
- Xavier
  - a distribution with zero mean and a specific std $1/\sqrt{n_{\mathrm{in}}}$ where n_{in} is the number of neurons feeding into the neuron
  - Gaussian distribution or uniform distribution is often used
- MSRA
  - a Gaussian distribution with zero mean and a specific std $2/\sqrt{n_{\mathrm{in}}}$

Learning rate

- In SGD the learning rate α is typically much smaller than a corresponding learning rate in batch gradient descent because there is much more variance in the update.
- Choosing the proper schedule
  - One standard method is to use a small enough constant learning rate that gives stable convergence in the initial epoch (full pass through the training set) or two of training and then halve the value of the learning rate as convergence slows down.
  - An even better approach is to evaluate a held out set after each epoch and anneal the learning rate when the change in objective between epochs is below a small threshold.
  - Another commonly used schedule is to anneal the learning rate at each iteration t as $\frac{a}{b+t}$ where a and b dictate the initial learning rate and when the annealing begins respectively.

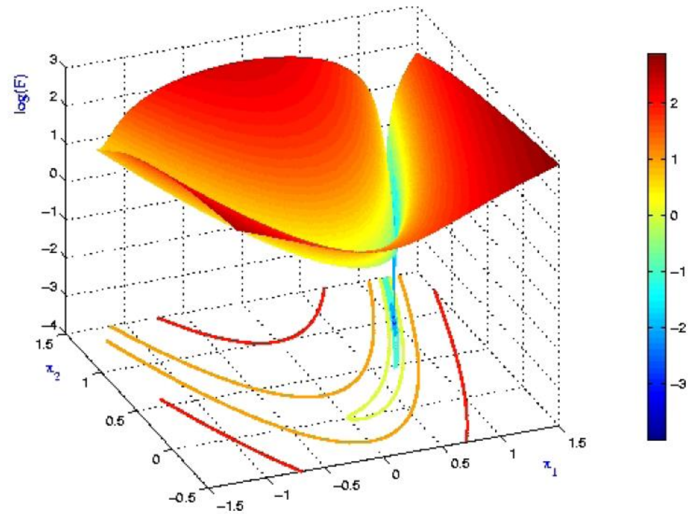
Order of training samples

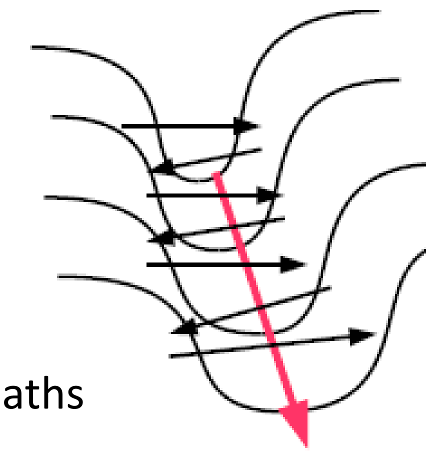
- If the data is given in some meaningful order, this can bias the gradient and lead to poor convergence
- Generally a good method to avoid this is to randomly shuffle the data prior to each epoch of training.

Pathological curvature

- The objective has the form of a long shallow ravine leading to the optimum and steep walls on the sides
    - as seen in the well-known Rosenbrock function
- The objectives of deep architectures have this form near local optima and thus standard SGD tends to oscillate across the narrow ravine

$$f(x,y) = (1-x)^2 + 100(y-x^2)^2$$





Black arrows: gradient descent paths

Momentum

- Momentum is one method for pushing the objective more quickly along the shallow ravine
- The momentum update is given by,

$$v = \gamma v - \alpha \nabla_\theta J\left(\theta; x^{(i)}, t^{(i)}\right)$$
$$\theta = \theta + v$$

  - v is the current velocity vector
  - $\gamma \in (0,1]$ determines for how many iterations the previous gradients are incorporated into the current update.
  - One strategy: γ is set to 0.5 until the initial learning stabilizes and then is increased to 0.9 or higher

Problem 2

- Implement MLPs using python for classifying MNIST handwritten digits
  ① Construct an MLP with one hidden layer of 256 units using sigmoid activation function and crossentropy loss
  ② Redo ① using ReLU activation function and compare the performance
- A code framework is provided including a softmax_cross_entropy layer class and SGD
- Your task:
  - Add momentum to SGD with $\gamma = 0.9$
  - Implement a FcLayer class in a fc_layer.py file, a SigmoidLayer class in sigmoid_layer.py, and a ReluLayer class in a relu_layer.py file

Summary

- Regression and classification
  - Linear regression
  - Logistic regression
  - Softmax regression
- Multi-layer perceptron
  - FC layer, sigmoid layer, ReLU layer, loss layer
  - backpropagation
- Convolutional neural network
  - Convolutional layer and pooling layer
- Practical tricks
  - Weight initialization, learning rate, order of training samples, momentum