LASSONDE SCHOOL OF ENGINEERING | YORK UNIVERSITÉ UNIVERSITY

No. 6

Artificial Neural Networks

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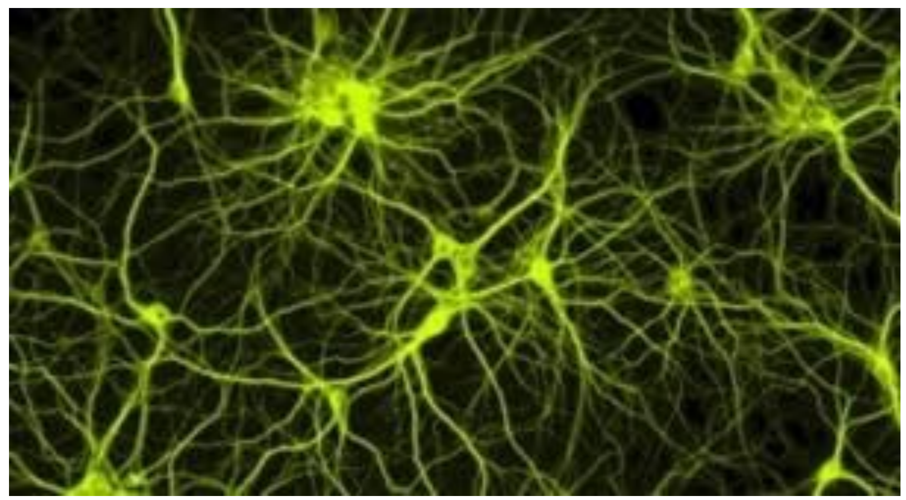
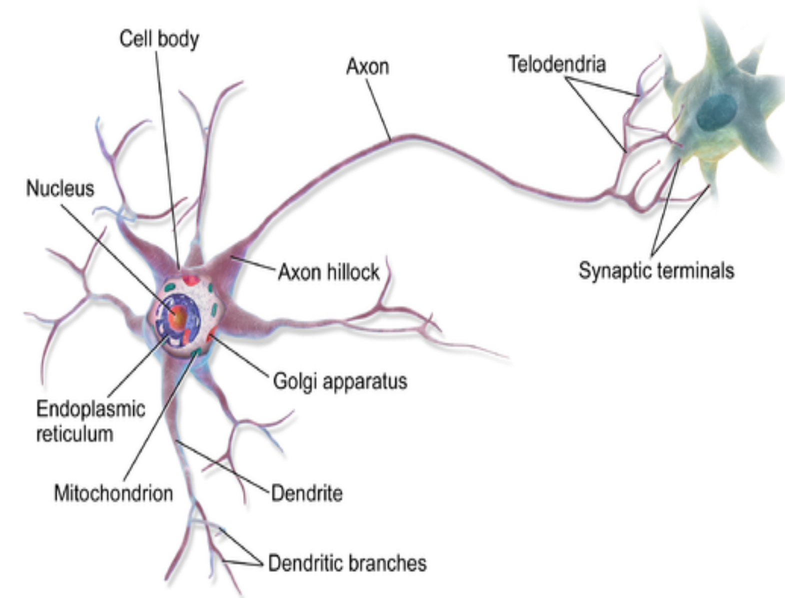
Outline

- **Neural Networks: background**
- **Network Structure**
- **Learning Criterion**
- **Optimization (SGD + Back-propagation)**
- **Fine-tuning tricks**
- **Advanced Topics on Deep Learning**
  - **Other Network Structures (CNNs, RNNs/LSTMs)**
  - **Sequence to Sequence Learning**
  - **Unsupervised Learning (RBMs, auto-encoders, …)**

Brain: biological neuronal networks

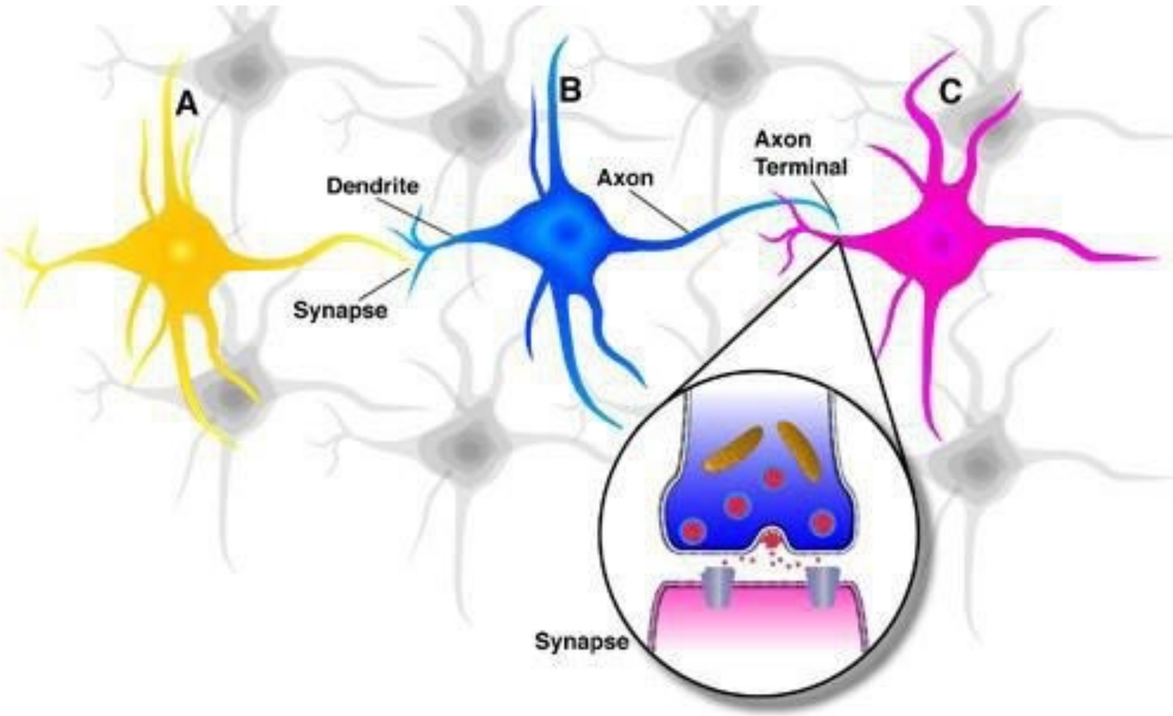
brain	biological Neuronal nets	neuron

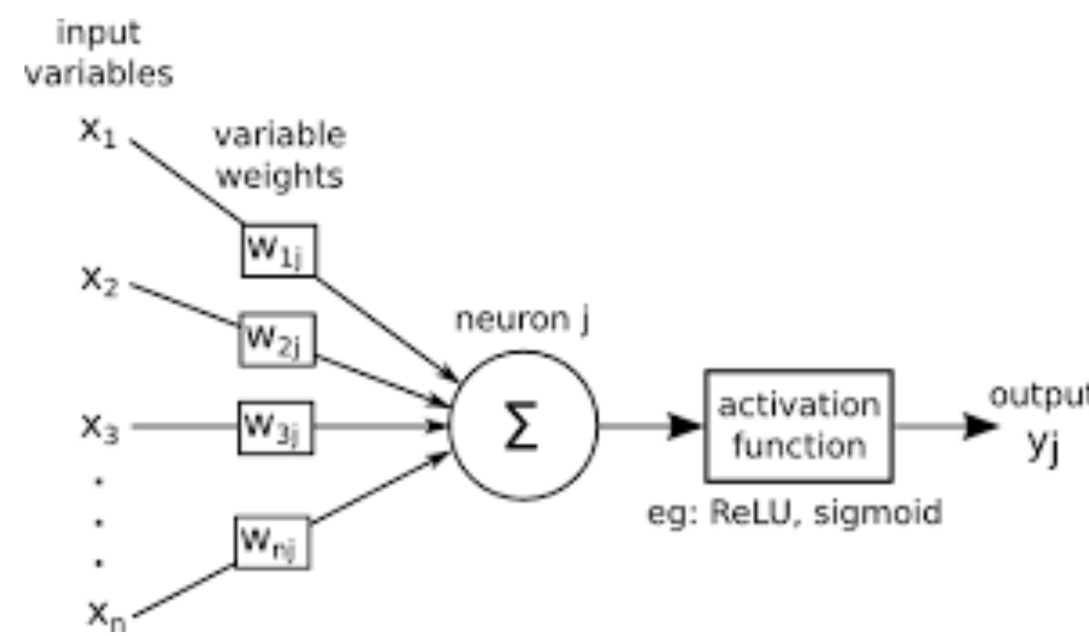




- 100 billion (10^{12}) neurons; 100 trillion (10^{15}) connections.
- Neuron itself is simple.
- Connections and weights are more important in neuronal networks.
- Connections and weights are all learnable.

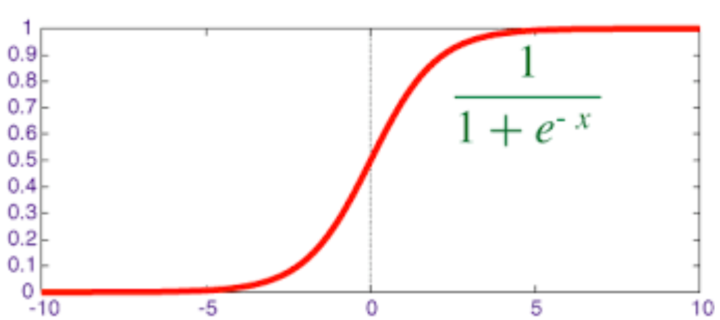
Artificial Neuron: a math model



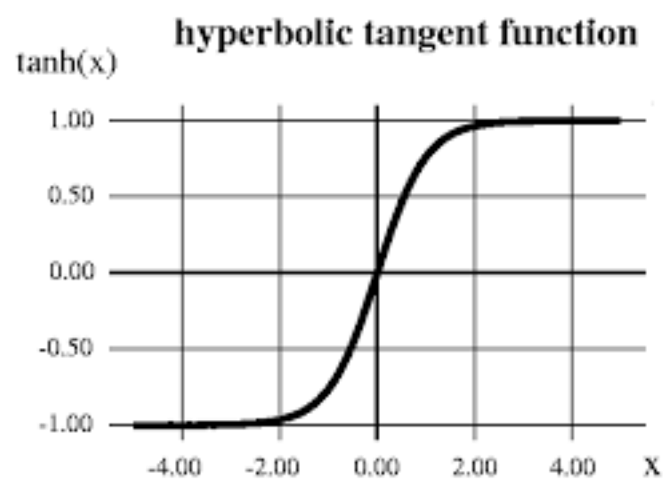


- **Linear combination + a nonlinear activation function**

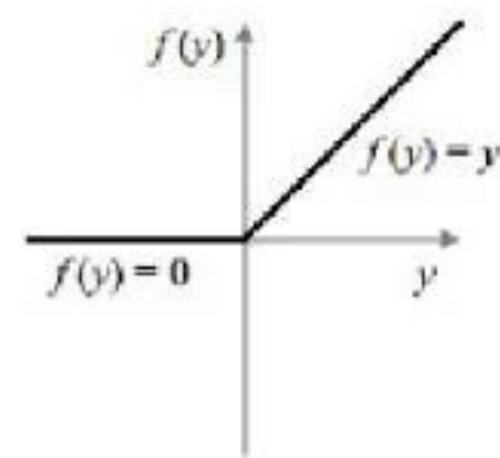
sigmoid



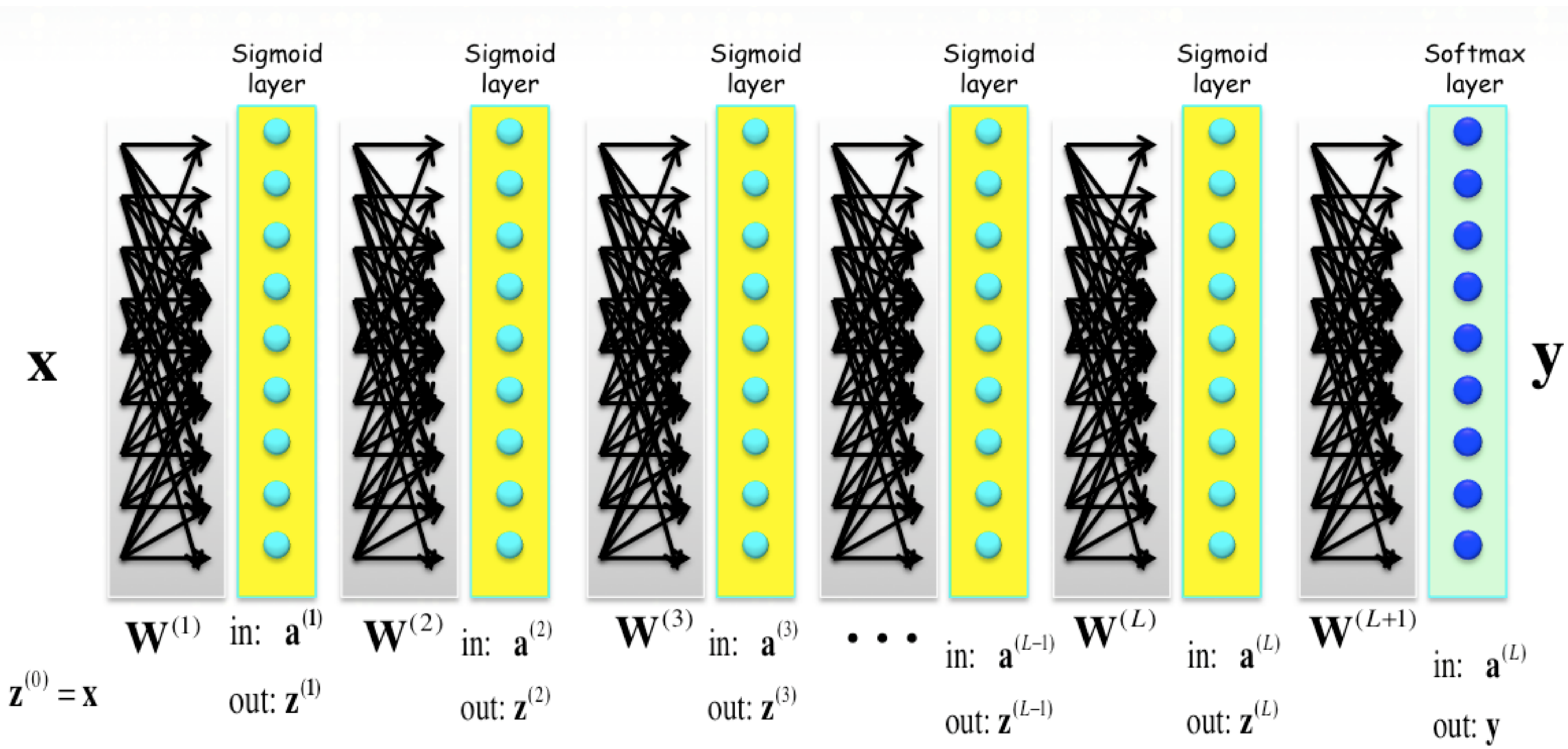
tanh



rectified linear (ReLU)



(Deep) (Artificial) Neural Networks



Sigmoid layer:

$$\mathbf{a}^{(l)} = W^{(l)}\mathbf{z}^{(l-1)} \qquad l = 1, 2, \cdots, L$$

$$\mathbf{z}^{(l)} = \sigma(\mathbf{a}^{(l)}) \Rightarrow z_k^{(l)} = \frac{1}{1+e^{-a_k^{(l)}}} \qquad l = 1, 2, \cdots, L$$

Softmax layer:

$$\mathbf{a}^{(L+1)} = W^{(L+1)}\mathbf{z}^{(L)}$$

$$\mathbf{y} = \text{softmax}(\mathbf{a}^{(L+1)}) \Rightarrow \mathbf{y}_i = \frac{e^{\mathbf{a}_i^{(L+1)}}}{\sum_{j=1}^{N} e^{\mathbf{a}_j^{(L+1)}}}$$

multi-layer feedforward structure → **deep neural networks**

Neural Networks: (a bit) theory

- ***Universal Approximator Theory, established around 1989-90***

  - ***G. Cybenko (1989); K. Hornik (1991)***

Let $\varphi(\cdot)$ be a nonconstant, bounded, and monotonically-increasing continuous function. Let I_m denote the m-dimensional unit hypercube $[0,1]^m$. The space of continuous functions on I_m is denoted by $C(I_m)$. Then, given any function $f \in C(I_m)$ and $\varepsilon > 0$, there exists an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$, where $i = 1, \cdots, N$, such that we may define:

$$F(x) = \sum_{i=1}^{N} v_i \varphi\left(w_i^T x + b_i\right)$$

as an approximate realization of the function f where f is independent of φ; that is,

$$|F(x) - f(x)| < \varepsilon$$

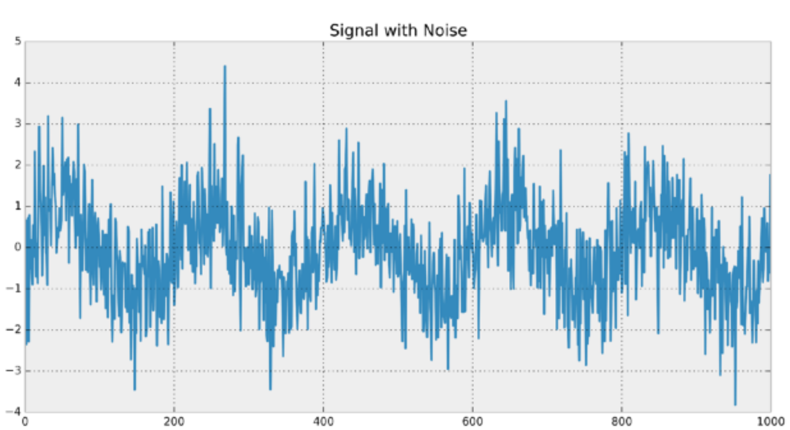
for all $x \in I_m$. In other words, functions of the form $F(x)$ are dense in $C(I_m)$.

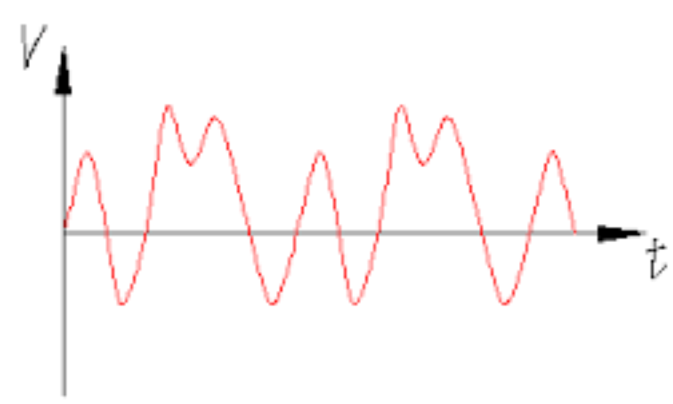
- **One hidden layer is theoretically sufficient, but it may becomes extremely large.**

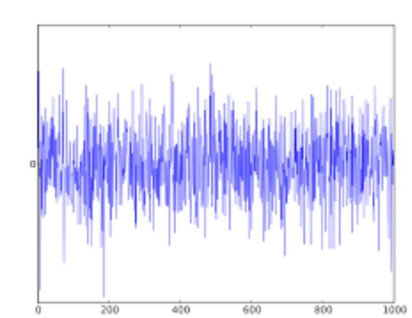
Neural Networks: (a bit) theory

- ***Universal Approximator Theory*** **is a double-edged sword:**
  - **Model is powerful**
  - **Overfitting**

data = signal + noise







Learning Neural Networks is an optimization problem

- **Given *training data: (x_1,t_1), (x_2,t_2), …***
- **Given a network to be learnt: y = f (x I W)**
- **The error function (the objective function)**
  - **Mean square error (MSE):**

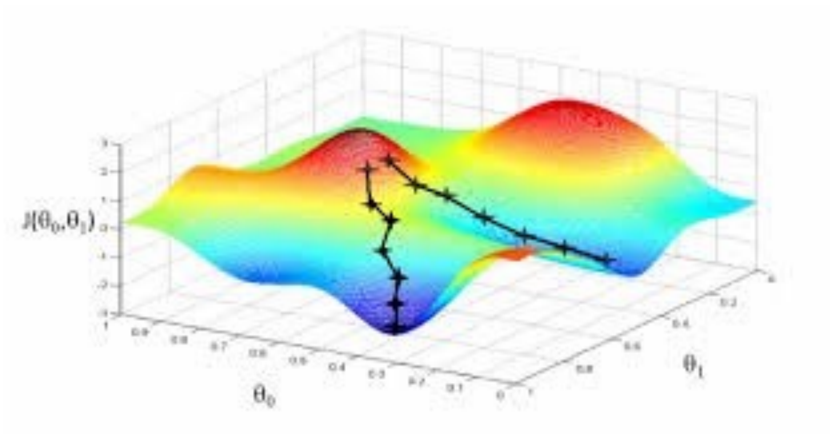
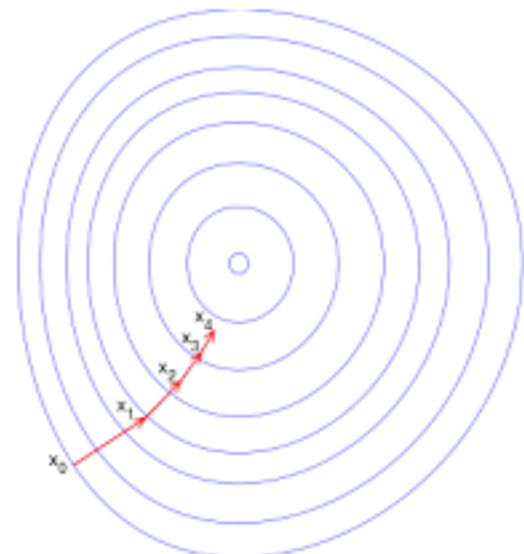
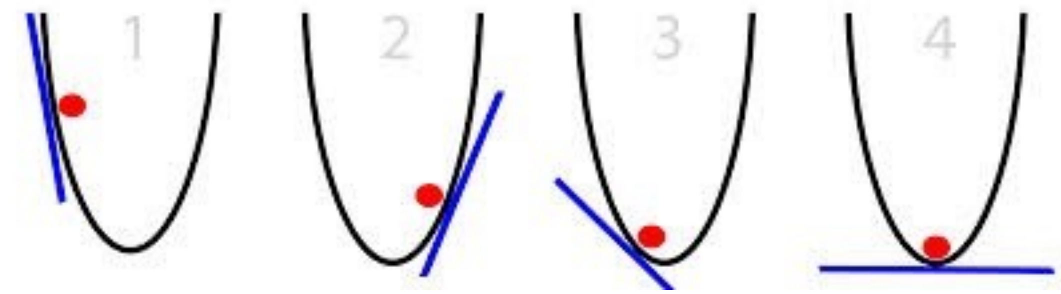
$$Q(\mathbf{W}) = \sum_i \Big(f(\mathbf{x}_i|\mathbf{W}) - t_i \Big)^2$$

  - **Cross entropy error (CE):**

$$Q(\mathbf{W}) = \sum_i \mathrm{KL}\Big(\{t_i\} \,||\, \{f(\mathbf{x}_i|\mathbf{W})\} \Big) = -\sum_{t=1}^{N} \{\ln f(\mathbf{x}_t|\mathbf{W})\}_{l_i}$$

Gradient Descent

- **Gradient Descent: hill-climbing**

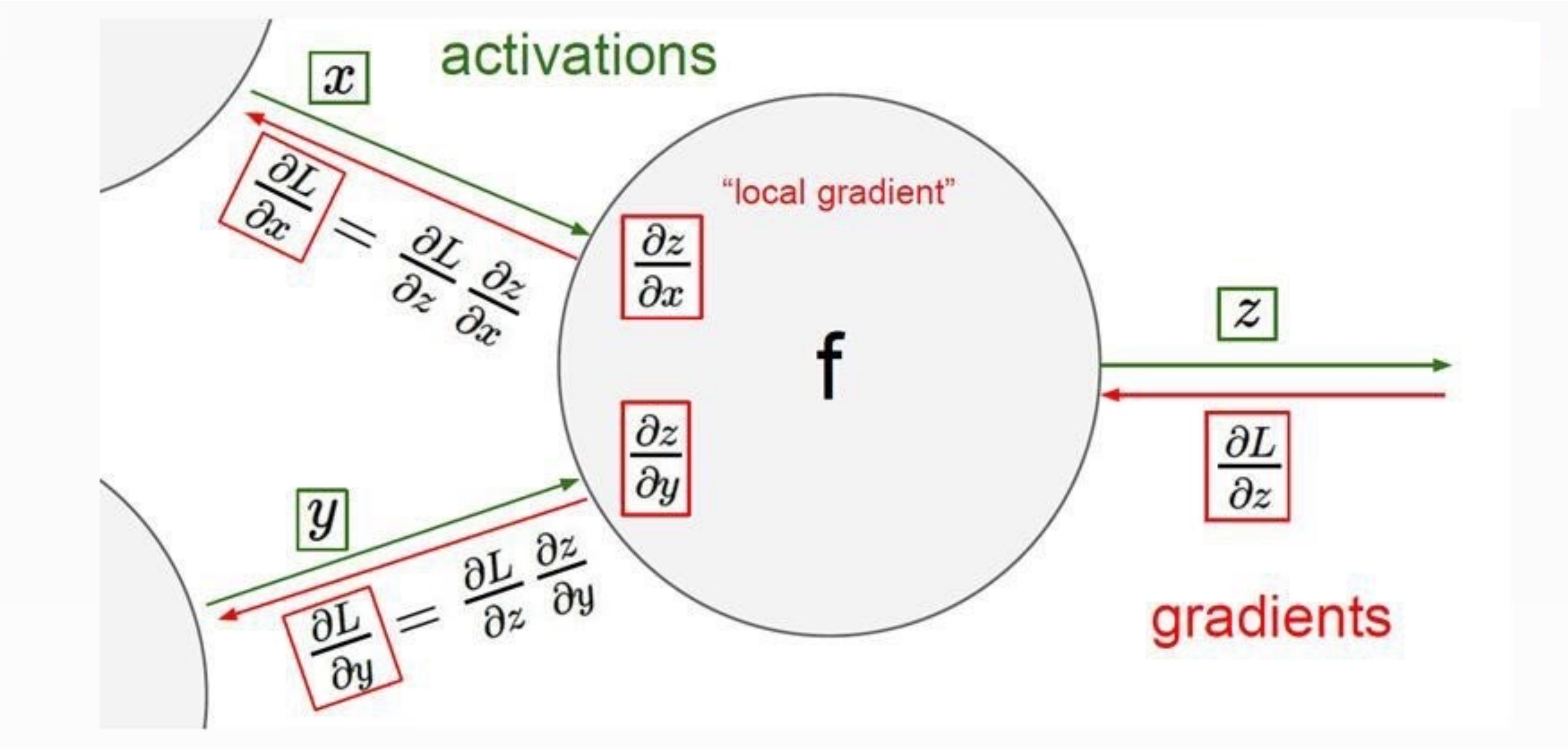




- **Iteratively update network based on the gradient**

$$\mathbf{W}^{(l+1)} = \mathbf{W}^{(l)} - \epsilon \cdot \frac{\partial Q(\mathbf{W})}{\partial \mathbf{W}}\bigg|_{\mathbf{W}=\mathbf{W}^{(l)}}$$

Error Back-propagation (BP)

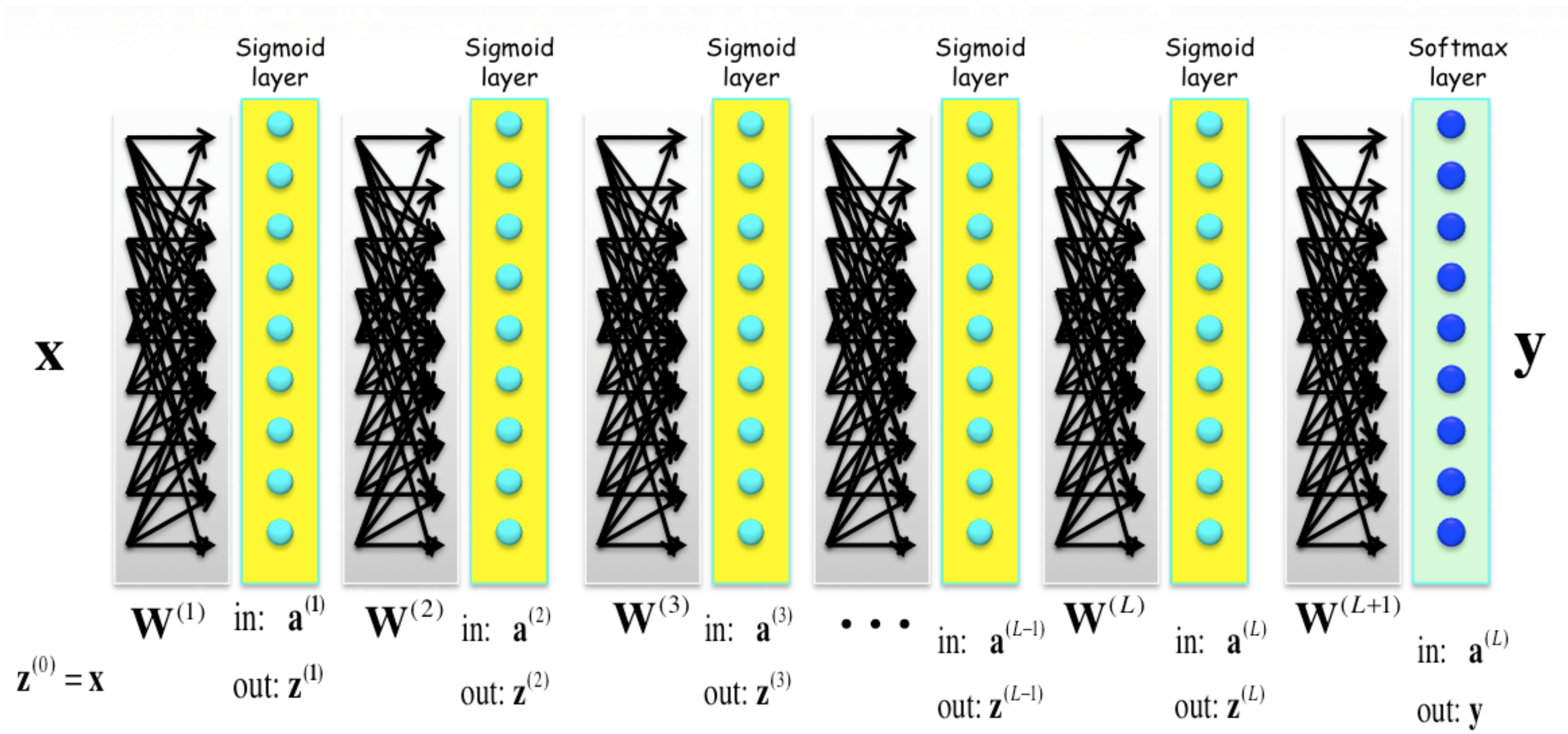
- **The key problem: how to computer gradients in the most efficient way?**
  - **The Error Back-Propagation (BP) Algorithm**
- **A local perspective on how BP works …**
- **Based on the well-known chain rule in Calculus …**



Mini-batch Stochastic Gradient Descent

- **Given all *training data: (x_1,t_1), (x_2,t_2), …***
- **Randomly select a mini-batch (10-1000 samples) of data**
  - **For every sample in the mini-batch *(x_i,t_i)***
  - ***Forward pass: use NN to compute x_i —> y_i***
  - ***Accumulate error for the mini-batch Q_i***
  - ***Backward pass*: back-propagate error *Q_i to compute gradients***
  - **Update network weights:** $$\mathbf{W}^{(l+1)} = \mathbf{W}^{(l)} - \epsilon \cdot \frac{\partial Q(\mathbf{W})}{\partial \mathbf{W}}\bigg|_{\mathbf{W}=\mathbf{W}^{(l)}}$$

Neural Networks: how to compute gradients



- **Define error signals in each layer:** $\mathrm{e}^{(l)} = \frac{\partial}{\partial \mathbf{a}^{(l)}} Q(\mathbf{W})$

$$\frac{\partial}{\partial \mathbf{W}^{(l)}} Q(\mathbf{W}) = \frac{\partial Q(\mathbf{W})}{\partial \mathbf{a}^{(l)}} \frac{\partial \mathbf{a}^{(l)}}{\partial \mathbf{W}^{(l)}} = \mathbf{e}^{(l)} (\mathbf{z}^{l-1})^{\mathsf{T}}$$

- **Backward pass: back-propagate error signals through the whole network**

Error Back-propagation (BP)

- **Multi-layer feedforward structure; sigmoid activations; cross-entropy errors**

Given a training set $\mathbf{X} = \{\mathbf{x}_t, l_t \mid t = 1, 2, \cdots, N\}$

$$Q(\mathbf{W}) = -\sum_{t=1}^{N} \{\ln f(\mathbf{x}_t | \mathbf{W})\}_{l_t}$$

Compute the error signals for each layer:

Softmax layer l=L+1

$$e_{tk}^{(L+1)} = \frac{1}{y_{l_t}(\mathbf{x}_t, \mathbf{W})} \frac{\partial y_{l_t}(\mathbf{x}_t, \mathbf{W})}{\partial a_k^{(L+1)}} = \delta(l_t - k) - y_{l_t}$$

Sigmoid layer l=1,2,...,L

$$e_{tk}^{(l)} = \frac{\partial Q_t(W)}{\partial a_k^{(l)}} = \sum_{j=1}^{N} \frac{\partial Q_t(W)}{\partial a_j^{(l+1)}} \frac{\partial a_j^{(l+1)}}{\partial a_k^{(l)}} = \sum_{j=1}^{N} e_{tj}^{(l+1)} \frac{\partial a_j^{(l+1)}}{\partial a_k^{(l)}} = \sum_{j=1}^{N} e_{tj}^{(l+1)} \cdot z_k^{(l)} \cdot (1 - z_k^{(l)}) \cdot W_{kj}^{(l+1)}$$

$$= z_k^{(l)} \cdot (1 - z_k^{(l)}) \cdot \sum_{j=1}^{N} e_{tj}^{(l+1)} W_{jk}^{(l+1)}$$

Neural Networks Learning in practice

- **Open source toolkits:** ***Tensorflow*, *Torch,* CNTK, MXNet etc …**
- **Computationally intensive (GPUs)**
- **Many tuning tricks:**
  - **Mini-batch size**
  - **Epoch**
  - **Learning rates (annealing schedule)**
  - **Network initialization**
  - **Weight Decay (L2 norm regularization)**
  - **Momentum**
  - **Dropout**
  - **Batch Normalization**
  - **…**

Neural Networks Initialization

- **NNs initialization is critical for a good convergence.**
- **Random Initialization is sufficient.**
  - **Uniform distribution**
  - **Norm distribution**
- **Controlling the dynamic range (variance) is the key.**
- **A widely used trick from Glorot and Bengio (2010):**

$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}, \frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}\right]$$

Weight Decay

- **Weight decaying is equivalent to L_2 norm regularization.**

$$Q(\mathbf{W}) + \lambda \cdot ||\mathbf{W}||_2$$

- **Updating formula with weight decay:**

$$\mathbf{W}^{(l+1)} = \mathbf{W}^{(l)} - \epsilon \cdot \frac{\partial Q(\mathbf{W})}{\partial \mathbf{W}}\bigg|_{\mathbf{W}=\mathbf{W}^{(l)}} - \lambda \cdot \mathbf{W}^{(l)}$$

Momentum

- **Momentum is a simple technique to accelerate convergence in slow but relevant directions, dampen oscillation in really steep directions.**

- **Averaging the velocity at each updating step:**

$$\Delta \mathbf{W}^{(l+1)} = \left.\frac{\partial Q(\mathbf{W})}{\partial \mathbf{W}}\right|_{\mathbf{W}=\mathbf{W}^{(l)}} + \eta \cdot \Delta \mathbf{W}^{(l)}$$

$$\mathbf{W}^{(l+1)} = \mathbf{W}^{(l)} - \epsilon \cdot \Delta \mathbf{W}^{(l+1)}$$

Image 2: SGD without momentum

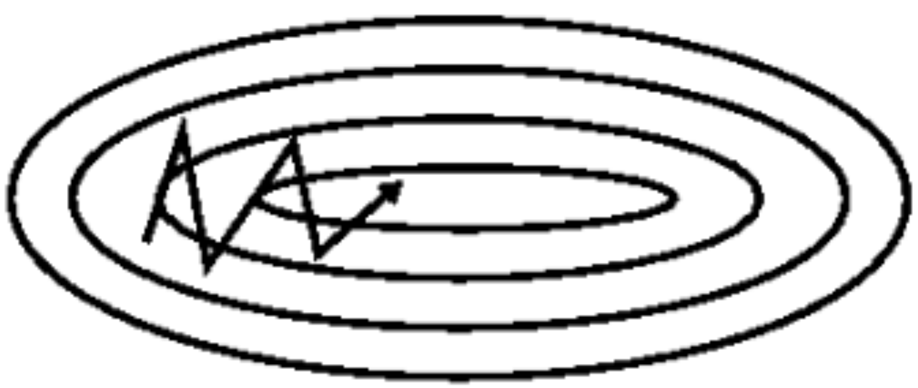
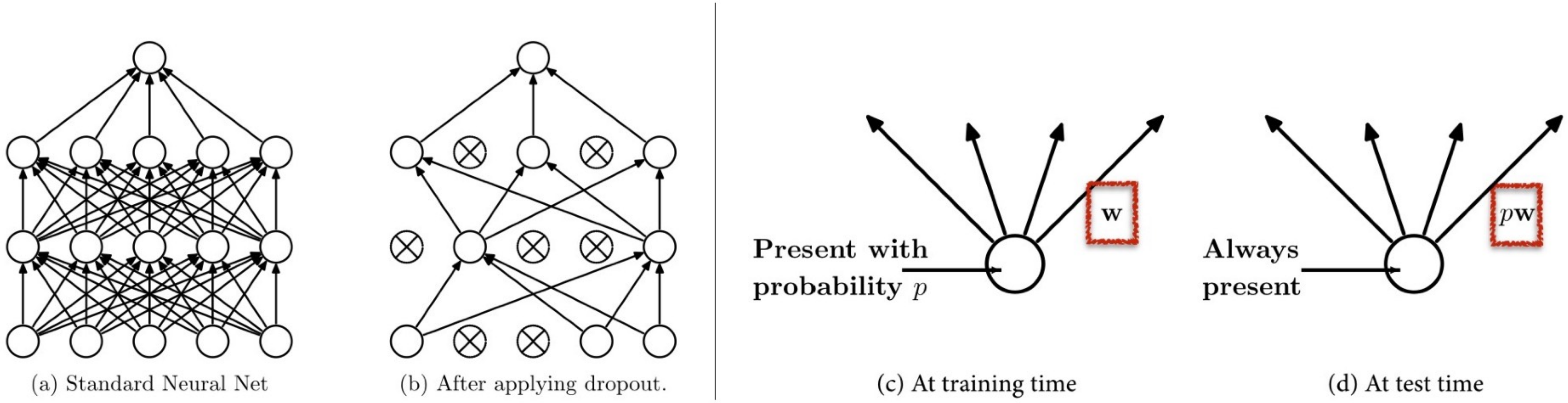


Image 3: SGD with momentum

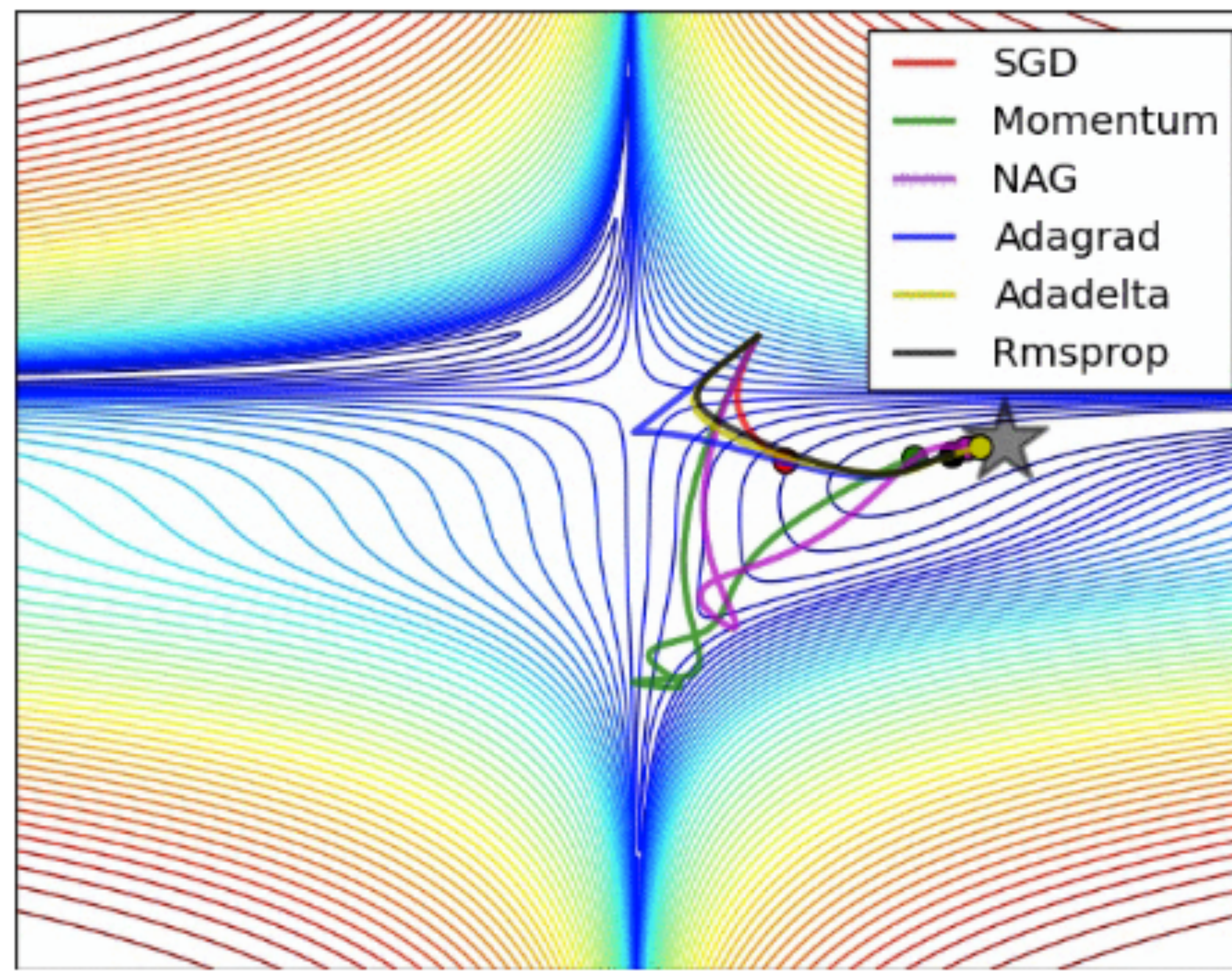
Dropout

- **Dropbox is a simple regularization technique.**
- **Randomly drop-out some nodes in training.**
- **Equivalent to adding noises in training**
- **A relevant technique: *data augmentation***

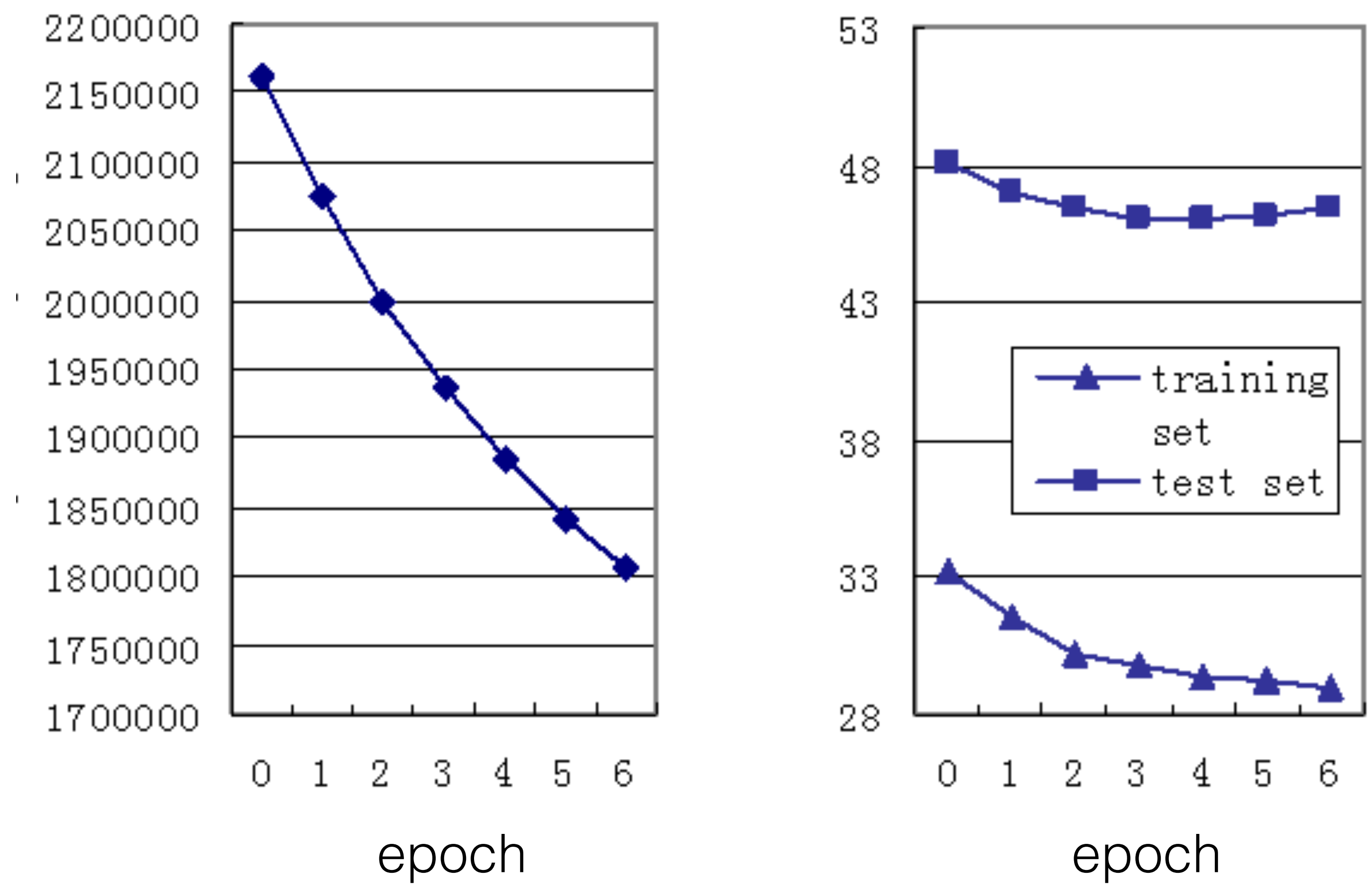


Other Optimization Algorithms

- In addition to SGD, many other optimization algorithms may be used:
  - Nesterov accelerated gradient descent
  - Adagrad
  - Adadelta
  - RMSprop
  - Adam
  - Hessian-free



Monitoring Three Learning Curves



- **How does your learning go?**
  - **The objective function**
  - **The error rates in the training set**
  - **The error rates in a development set**

Insights from Figures

- **Monitoring learning curves tells you a lot about the learning process …**

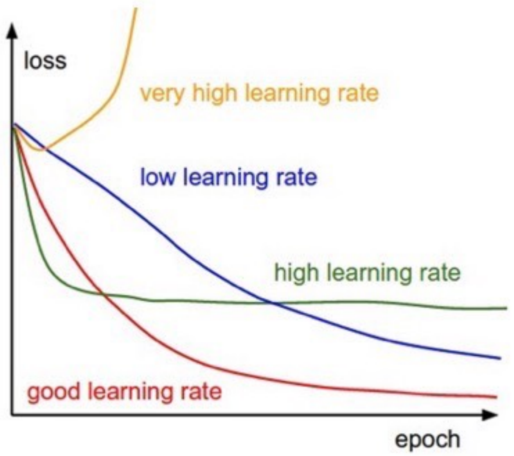


Figure 1

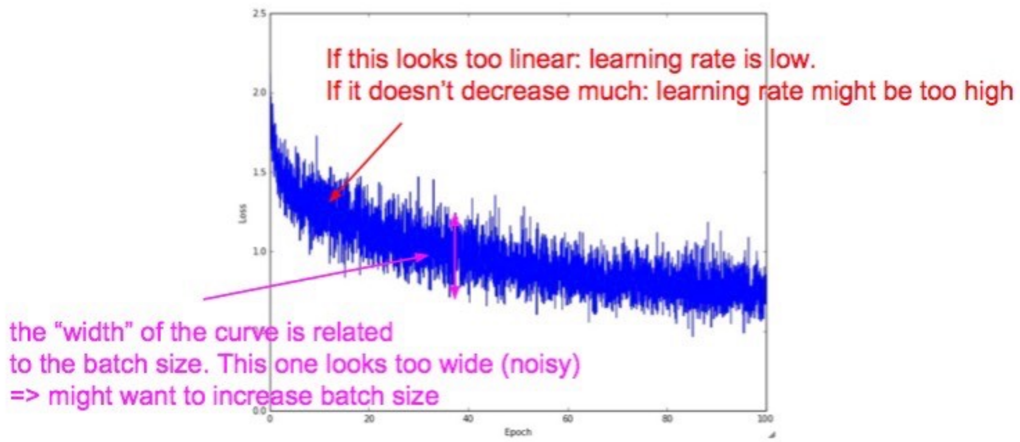


Figure 2

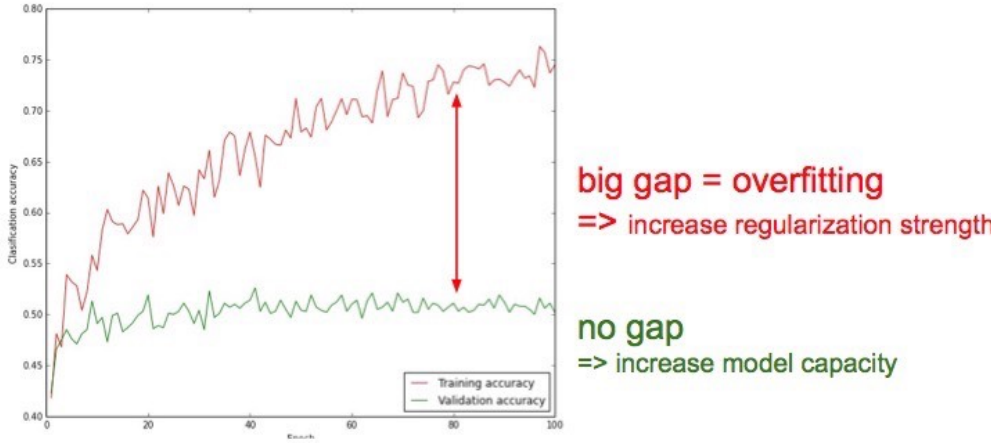
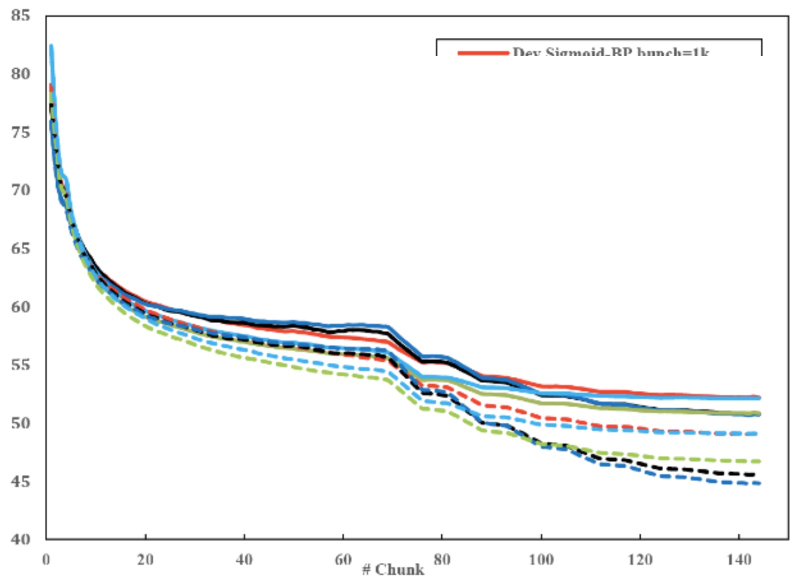


Figure 3

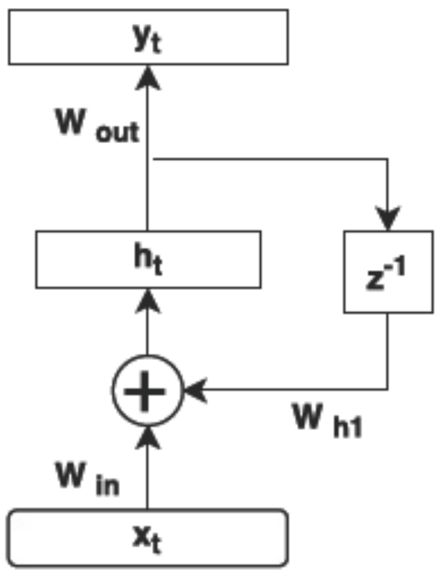


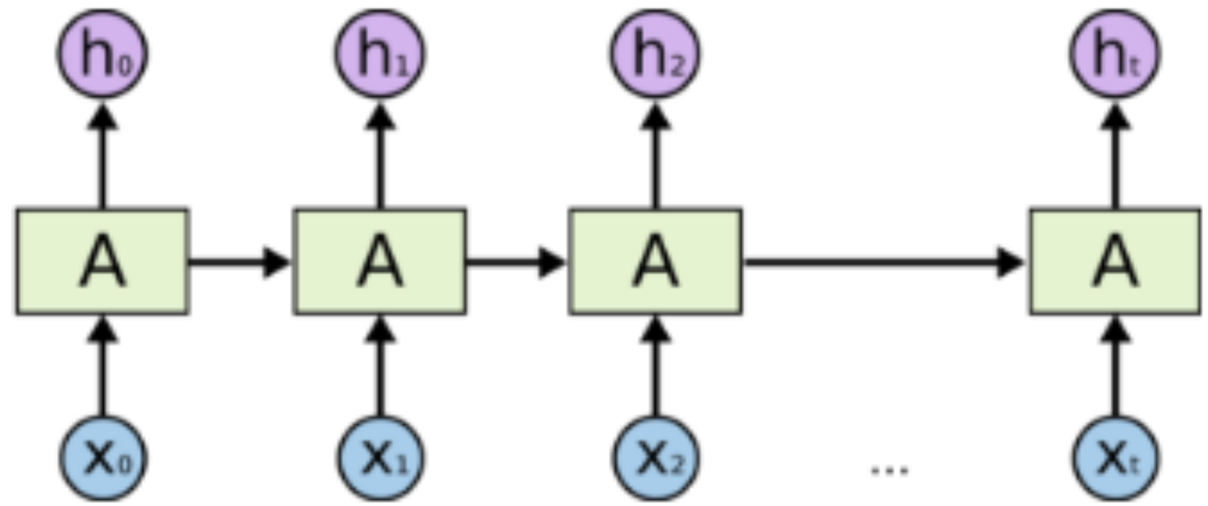
Neural Networks Structures

- Feedforward multi-layer DNNs
  - Fixed-size input —> fixed-size output
  - Memoryless
  - Fully-connected —> input location sensitive
- Recurrent Neural networks (RNNs)
- Convolutional Neural Networks (CNNs)

RNNs

- **Plain RNNs**

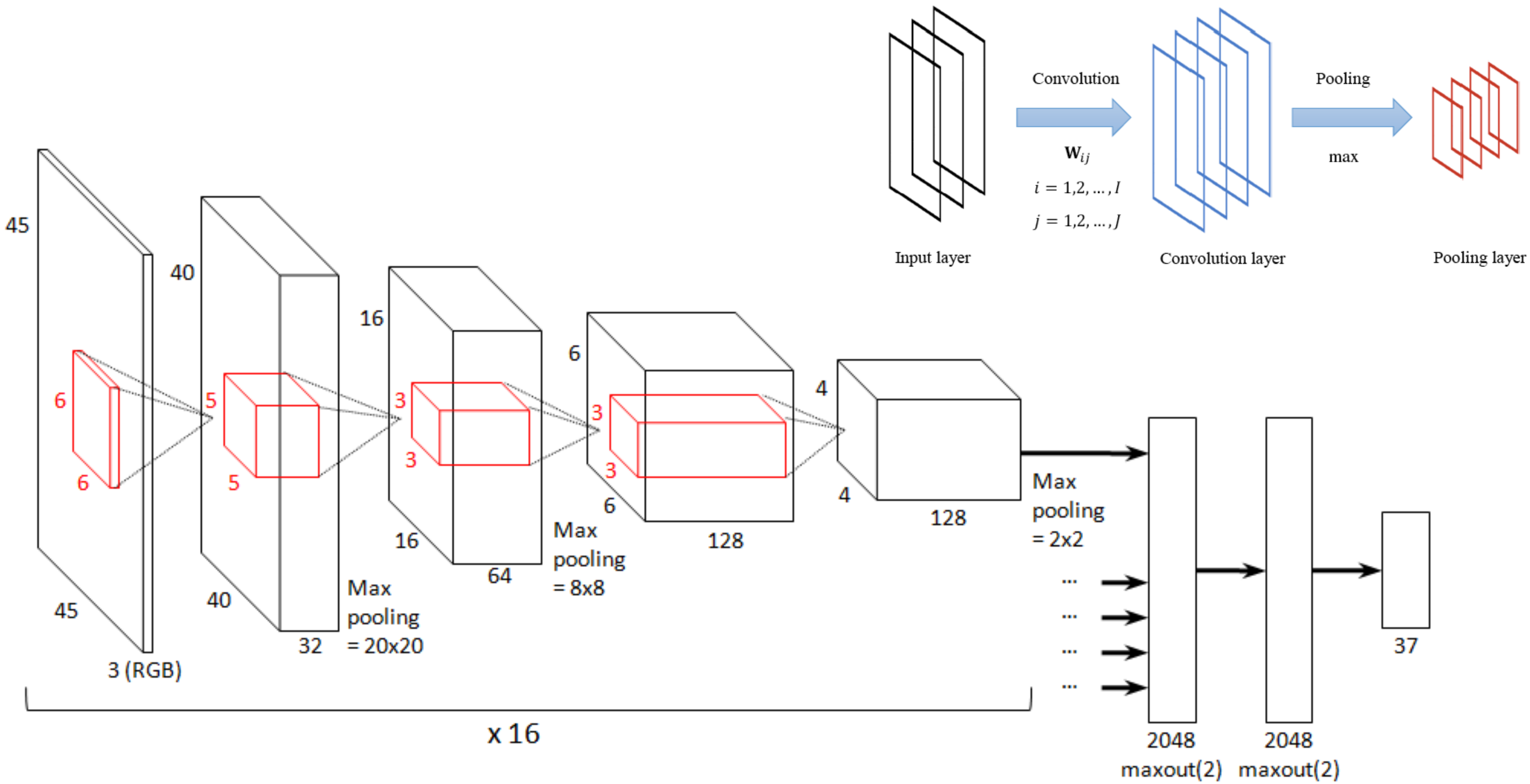




- **RNNs are notoriously hard to learn**
  - **Computationally expensive**
  - **Gradient vanishing or exploding**
- **Long Short-Term Memory (LSTM)**

CNNs

- **Each CNN layer: a convolution layer + a pooling layer**
- **Insensitive to input locations; suitable for image recognition**



Neural Networks Learning in practice

- **Open Source Toolkits:**
  - **Google's *Tensorflow* (https://www.tensorflow.org/)**
  - ***Facebook's Torch and pyTorch* (http://torch.ch/)**
  - ***Microsoft's* CNTK (https://github.com/Microsoft/CNTK/wiki)**
  - **MXNet (http://mxnet.io/)**
  - **more**

Advanced Topics in Deep Learning

- Convolutional Neural Networks (CNNs)
- Recurrent Neural Networks (RNNs) and LSTMs
- Sequence to Sequence Learning
- Bottleneck Features
- Unsupervised Learning:
  - Restricted Boltzmann Machine (RBM)
  - (De-noising) Auto-Encoder
  - Generative Adversarial Networks