CS 412 Intro. to Data Mining

Chapter 11. Deep Learning

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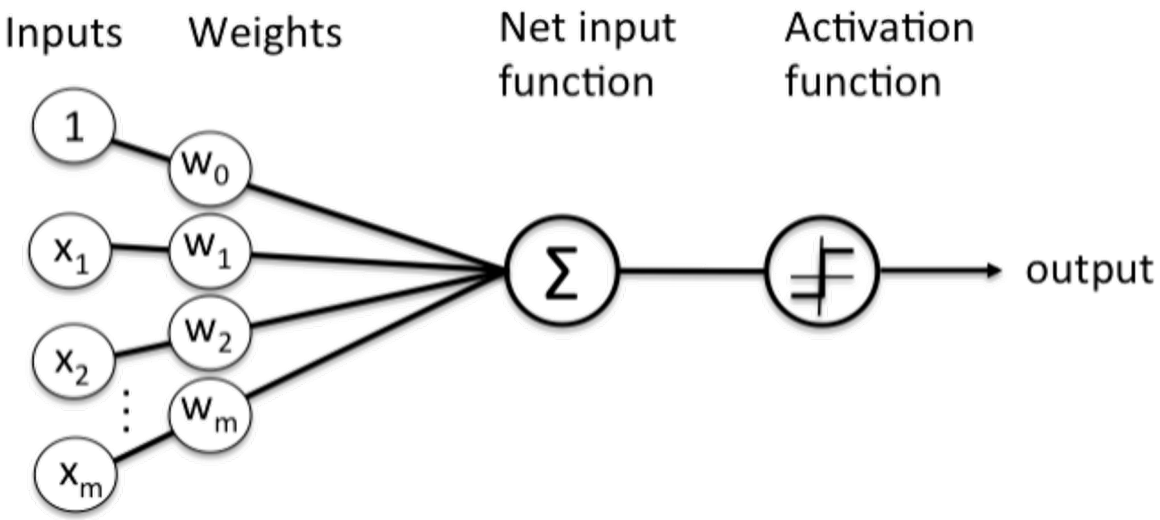
Chapter 11. Deep Learning

- Basic Techniques 
- Techniques to Improve Deep Learning Training
- Convolutional Neural Networks
- Recurrent Neural Networks
- Summary

Perceptron: Predecessor of a Neural Network



$$\hat{y} = f(\boldsymbol{W}^T \boldsymbol{x}) = f(\sum W_i x_i + b)$$

Activation Function
Adding non-linearity to the model

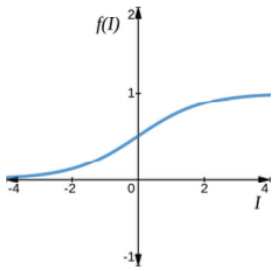
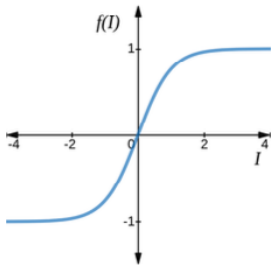
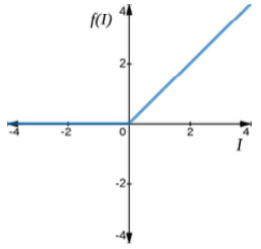
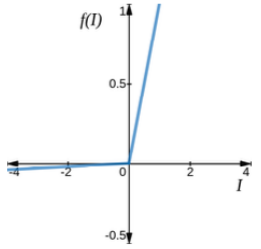
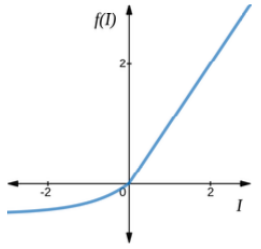
Weights

Bias
A measure of how easy it is to get the perceptron to output a 1

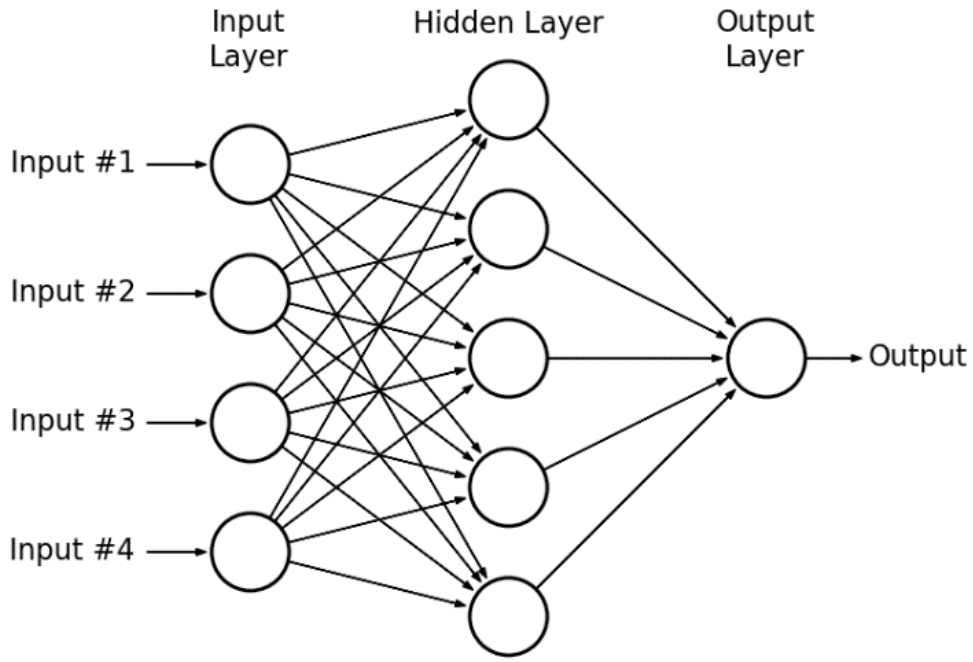
- Computes a weighted sum of inputs
- Invented in 1957 by Frank Rosenblatt. The original perceptron model does not have a non-linear activation function

Perceptron: Predecessor of a Neural Network

- Examples of activation functions

Sigmoid	$\frac{1}{1+e^{-I}}$	
Tanh	$\frac{e^{I}-e^{-I}}{e^{I}+e^{-I}}$	
ReLU	$\begin{cases} 0, I \leq 0 \\ I, I > 0 \end{cases}$	
Leaky ReLU	$\begin{cases} 0.01 \times I, I < 0 \\ I, I \geq 0 \end{cases}$	
ELU	$\begin{cases} \alpha(e^{I}-1), I \leq 0 \\ I, I > 0 \end{cases}$	

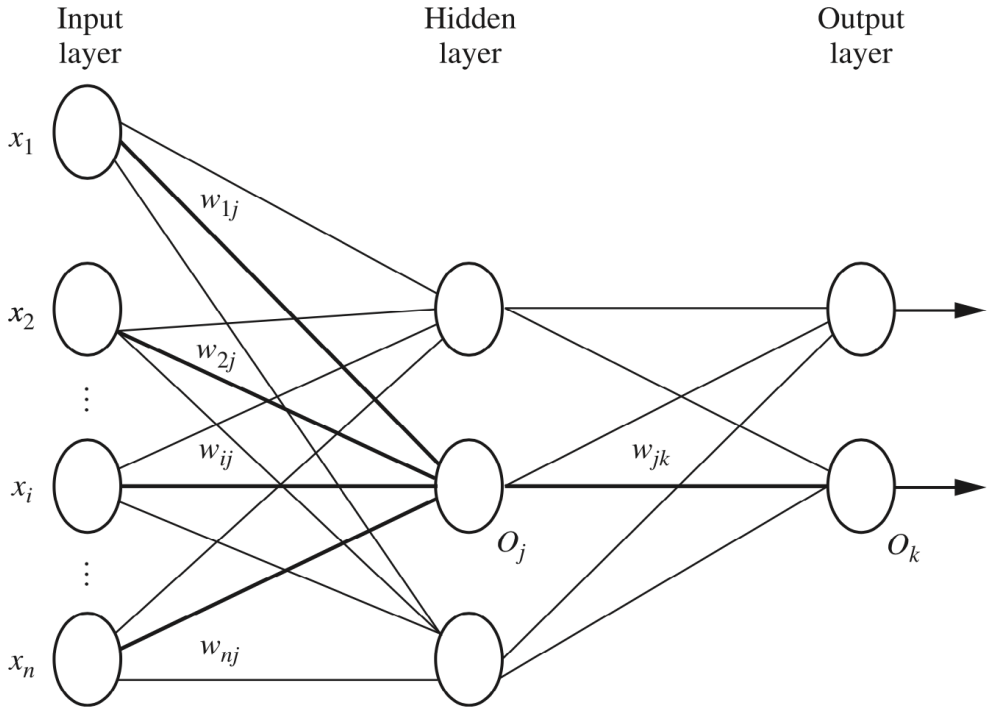
Multilayer Perceptron (MLP)

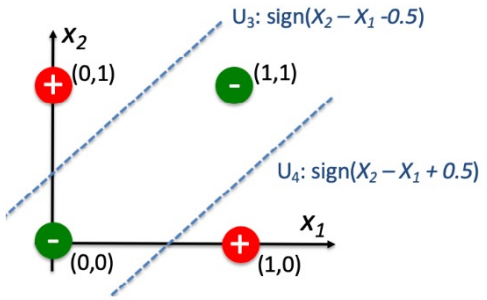


- Stacking multiple layers of perceptrons (adding hidden layers) makes a multilayer perceptron (MLP)
- MLP can engage in sophisticated decision making, where basic perceptrons fail
  - E.g. XOR problem

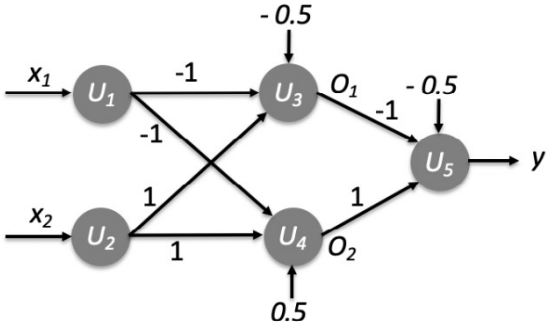
Feed-forward Neural Networks

- Why multiple layers
  - Automatic feature/representation learning
  - Learn complicate (nonlinear) mapping function

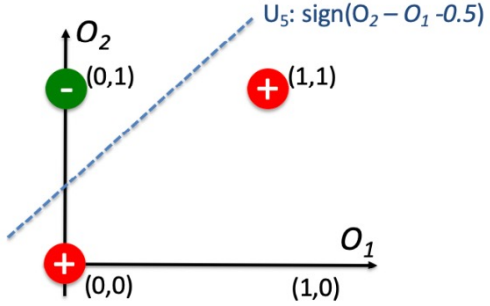




(a) Input 4 tuples

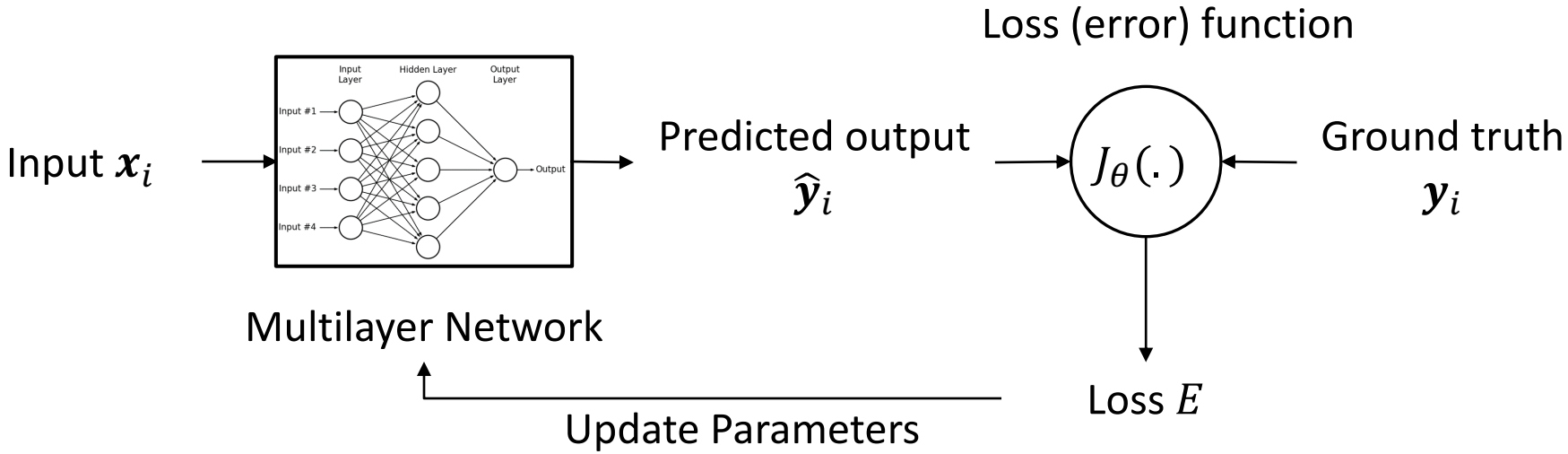


(b) MLP



(c) Outputs of two hidden units

Learning NN Parameters

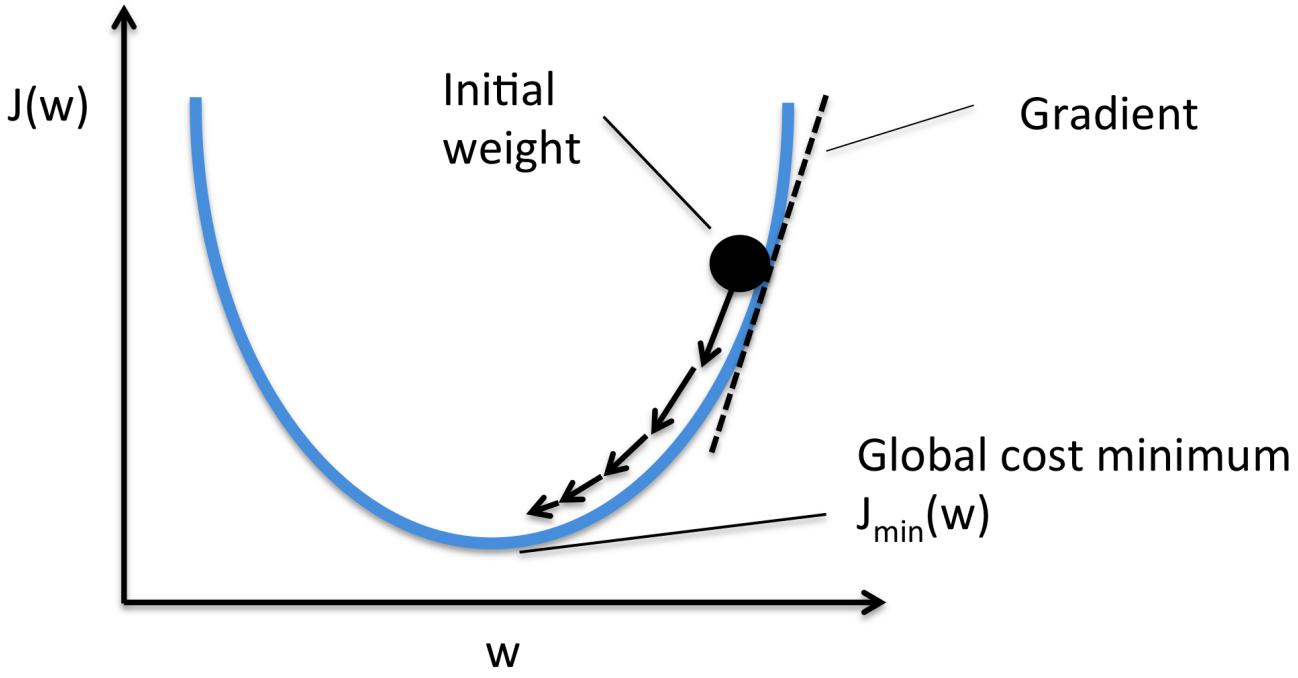


- **Gradient Descent Algorithm**
- **Input**: Training sample $\boldsymbol{x}_i$ and its label $\boldsymbol{y}_i$

1. **Feed Forward**: Get prediction $\hat{\boldsymbol{y}}_i = \mathrm{MLP}(x_i)$, and loss $E = J(\hat{\boldsymbol{y}}_i, \boldsymbol{y}_i)$
2. **Compute Gradient**: For each parameter θ_j (weights, bias), compute its gradient $\frac{\partial}{\partial \theta_j} J_\theta$
3. **Update Parameter**: $\theta_j = \theta_j - \eta \cdot \frac{\partial}{\partial \theta_j} J_\theta$

Explained later

Empirical Explanation of Gradient Descent

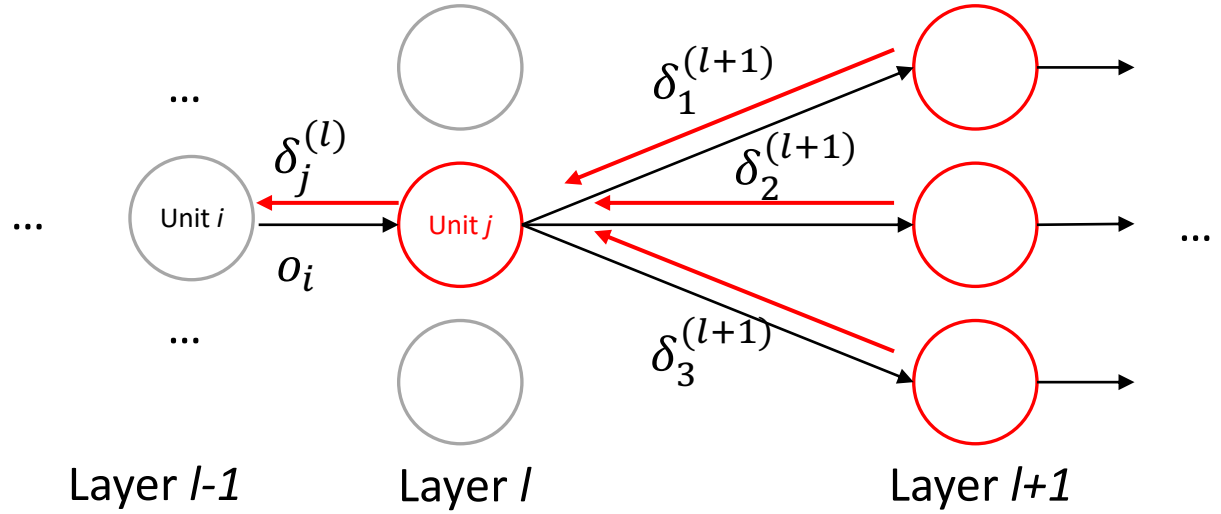


$$\theta_j = \theta_j - \eta \cdot \frac{\partial}{\partial \theta_j} J_\theta$$

η is the ***learning rate***, which controls the 'step size' of the optimization

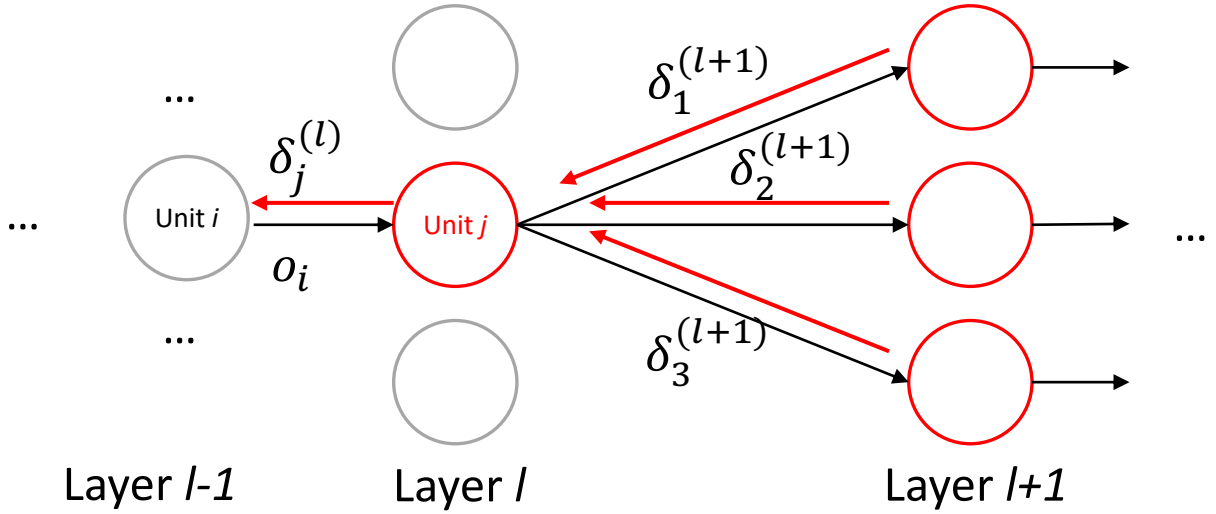
- Our objective is to minimize the loss function J, which is a function of the model parameters
- A gradient measures how much the output of a function changes if you change the inputs a little bit
- We update the parameters, based on their gradients, so that the loss function is going 'downhill'

Gradient Computation: Backpropagation



- The gradient of w_{ij} in the lth layer (corresponding to unit j in layer l, connected to unit i in layer l-1) is a function of
  - All 'error' terms from layer l+1 $\delta_k^{(l+1)}$ -- An auxiliary term for computation, not to be confused with gradients
  - Output from unit i in layer l-1 (input to unit j in layer l) -- Can be stored at the feed forward phase of computation

Gradient Computation: Backpropagation

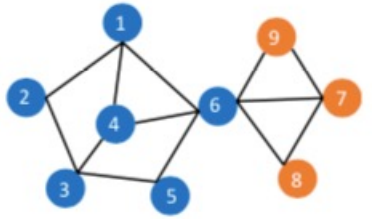
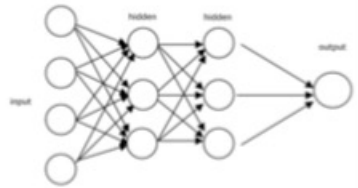
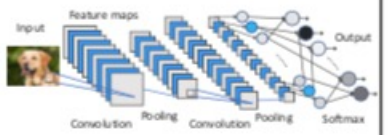
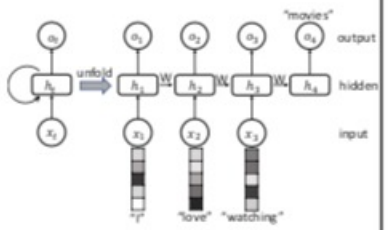
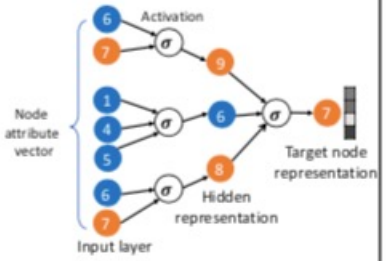


- The 'error' terms $\delta_j^{(l)}$ is a function of
  - All $\delta_k^{(l+1)}$ in the layer l+1, if layer l is a hidden layer
  - The overall loss function value, if layer l is the output layer
- We can compute the error at the output, and distribute backwards throughout the network's layers (backpropagation)

From Neural Networks to Deep Learning

- **Deep Learning** refers to training (deep) neural networks with many layers
  - More neurons, more layers
  - More complex ways to connect layers
- Deep Learning has some major advantages, making it popular
  - Tremendous improvement of performance in many tasks
    - Image recognition, natural language processing, AI game playing…
  - Requires no (or less) feature engineering, making end-to-end models possible
- Several factors lead to deep learning's success
  - Very large data sets
  - Massive amounts of computation power (GPU acceleration)
  - Advanced neural network structures and tricks
    - Convolutional neural networks, recurrent neural networks, graph convolution network …
    - Dropout, ReLU, residual connection, …

Overview of Typical Deep Learning Architectures

Data type	Multi-dimensional Features: credit rating, account balance $x = (4.5, 500, 3, 5)$ #deposits, #withdraws	Grid 	Sequence x = "I love watching movies."	Graph 
DL Architecture	Feed-forward Network 	CNN 	RNN 	GNN 

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Techniques to Improve Deep Learning Training

- Key Challenges for Training Deep Learning Models
- Responsive Activation Functions
- Adaptive Learning Rate
- Dropout
- Pretraining
- Cross Entropy

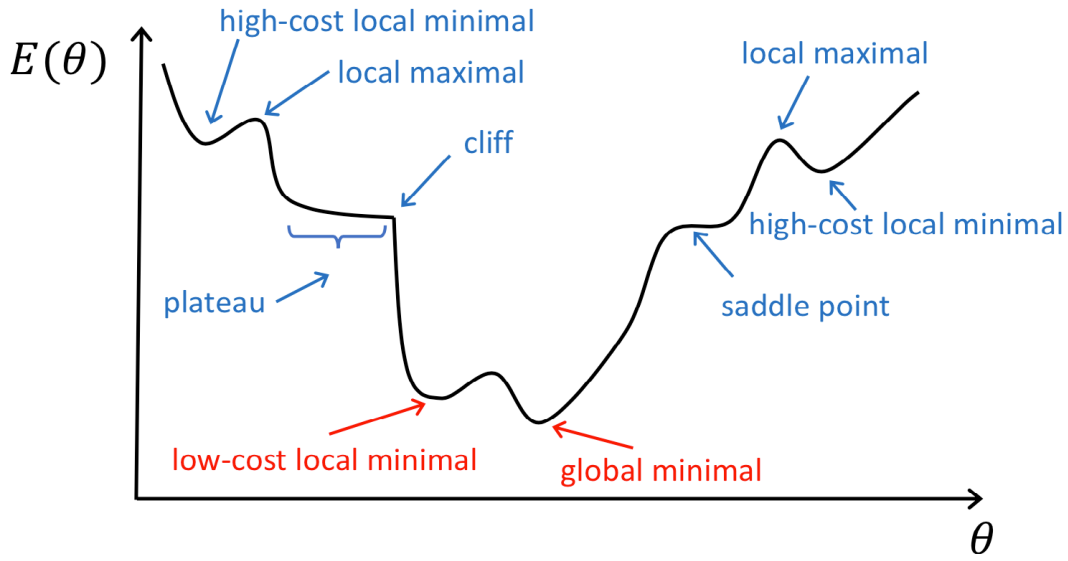
Key Challenges

- **Optimization Problem in Deep Learning**
  - Minimize the (approximated) training error *E*
  - (Stochastic) gradient descent to find the model parameter

$$E(\boldsymbol{\theta}) = \frac{1}{m}\sum_{l=1}^{m} \mathrm{Loss}(\hat{T}(X^l, \boldsymbol{\theta}), T^l)$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \boldsymbol{g}_t$$

- **Challenge 1: Optimization**
  - *E* is non-convex in general
  - How to find a high-quality local optima

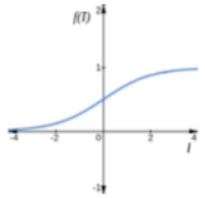
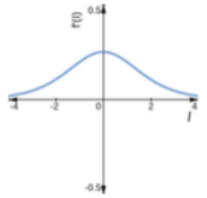
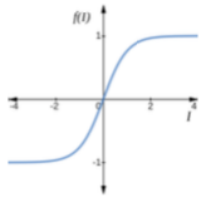
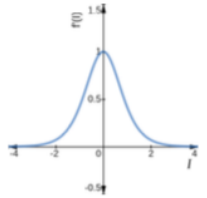
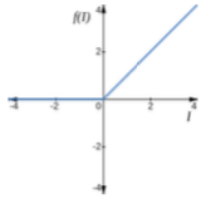
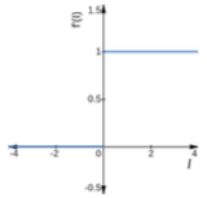
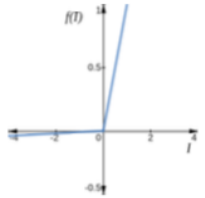
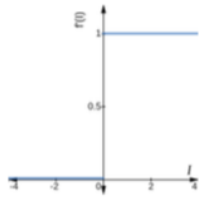
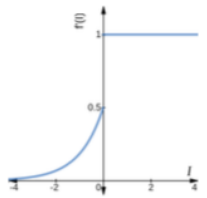


- **Challenge 2: Generalization**
  - What we do: minimize (approximated) training er
  - What we really want: minimize the generalization error
  - How to mitigate over-fitting

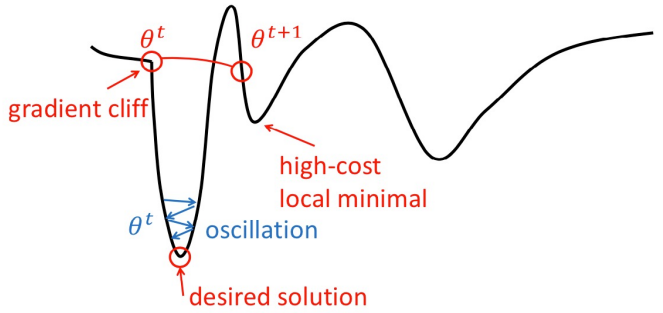
Responsive Activation Function

- **Saturation of Sigmoid Activation Function**
  - The output $O = \sigma(I) = \frac{1}{1+e^{-I}} \in (0,1)$
  - The derivative $\frac{\partial O}{\partial I} = O(1-O)$
  - The error of an output unit $\delta_j = O_j(1-O_j)(T_j - O_j)$ — $O_j(1-O_j)$ decaying
- **Saturation of Sigmoid Activation Function**
  - If $O_j \approx 1$ or $O_j \approx 0$, both derivative and error will be close to 0
  - Further exacerbated due to backpropagation → gradient vanishing → B.P. is stuck or takes long time to terminate
- **A More Responsive Activation Function: Rectified Linear Unit (RELU)**
  - The output *O=f(I) = I* if *I>0*, *O=0* otherwise
  - The gradient: $\frac{\partial O}{\partial I} = 1$ if $I > 0$ and $\frac{\partial O}{\partial I} = 0$
  - The error: 0 if the unit is inactive (*I<0*), otherwise, aggregate all error terms from the units in the next higher layer the unit is connected to, w/o decaying → avoid gradient vanishing

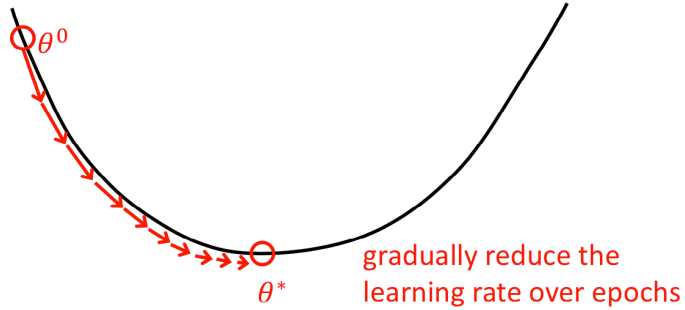
Activation Functions

Name	Definition ($f(I)$)	Plot	Derivative of $f(I)$	Plot
Sigmoid	$\frac{1}{1+e^{-I}}$		$f(I)(1-f(I))$	
Tanh	$\frac{e^{I}-e^{-I}}{e^{I}+e^{-I}}$		$1-f(I)^2$	
ReLU	$\begin{cases} 0, I \leq 0 \\ I, I > 0 \end{cases}$		$\begin{cases} 0, I \leq 0 \\ 1, I \geq 0 \end{cases}$	
Leaky ReLU	$\begin{cases} 0.01 \times I, I < 0 \\ I, I \geq 0 \end{cases}$		$\begin{cases} 0.01, I < 0 \\ 1, I \geq 0 \end{cases}$	
ELU	$\begin{cases} \alpha(e^{I}-1), I \leq 0 \\ I, I > 0 \end{cases}$		$\begin{cases} \alpha e^{I}, I \leq 0 \\ 1, I > 0 \end{cases}$	

Adaptive Learning Rate



- **Stochastic gradient descent to find a local optima**
  - Default choice for η: a fixed, small positive constant $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \boldsymbol{g}_t$
  - Problems: slow progress, or jump over 'gradient cliff', or oscillation
- **Adaptive learning rate: let η change over epoch**
  - Strategy #1: $\eta_t = \frac{1}{t}\eta_0$
  - Strategy #2: $\eta_t = (1 - \frac{t}{T})\eta_0 + \frac{t}{T}\eta_\infty$ if $t \leq T$ and $\eta_t = \eta_\infty$
    - Intuitions: smaller adjustment as algorithm progresses
    - $e.g.,\ \ \eta_0 = 0.9;\ \eta_\infty = 10^{-9}$
  - Strategy #3 (AdaGrad): $w_i^{(t+1)} \leftarrow w_i^{(t)} - \frac{\eta}{\sqrt{\sum_{\tau=1}^{t} g_{\tau,i}^2}} g_{t,i}$
    - Intuition: Magnitude of gradient g_t: used to slow down/speed up progress
  - Strategy #4 (Adam, RMSProp): decaying weighted sum of squared historical gradients



Adaptive Learning Rates: Adam

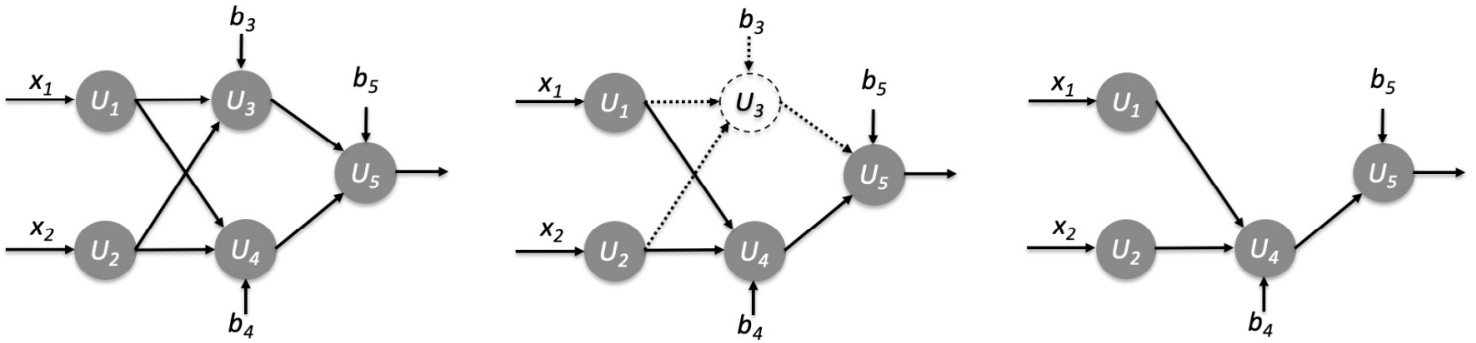
Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
$m_0 \leftarrow 0$ (Initialize 1st moment vector)
$v_0 \leftarrow 0$ (Initialize 2nd moment vector)
$t \leftarrow 0$ (Initialize timestep)
while θ_t not converged **do**
$t \leftarrow t + 1$
$g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
$m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
$v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
$\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
$\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
$\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
end while
return θ_t (Resulting parameters)

Dropout

- **The Purpose of Dropout: to Prevent Overfitting**
- **How does it works?**
  - At each epoch (ρ dropout rate, e.g., $\rho = 0.5$)
    - randomly dropout some non-output units
    - Perform B.P. on the dropout network
  - Scale the final model parameters

$$\boldsymbol{\theta}^* \leftarrow \rho \cdot \boldsymbol{\theta}^*$$

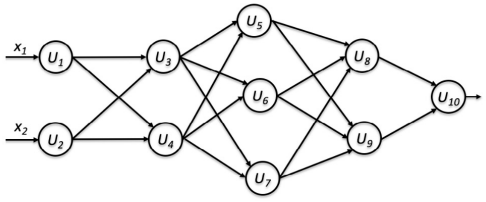


(a) Original network (b) Dropout U_3 (c) Dropout network

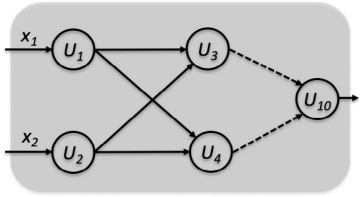
- **Why does Dropout Work?**
  - Dropout can be viewed as a regularization technique
    - Force the model to be more robust to noise, and to learn more generalizable features
  - Dropout vs. Bagging
    - Bagging: Each base model is trained *independently* on a bootstrap sample
    - Dropout: the model parameters of the current dropout network are updated based on that of the previous dropout network(s)

Pretraining

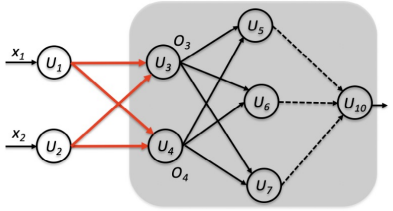
- **Pretraining:** the process of initializing the model in a suitable region
- **Greedy supervised pretraining**
  - pre-set the model parameters layer-by-layer in a greedy way
  - Start with simple model, add one additional layer at a time,
  - pretrain the parameters of the newly added layer, while fixing for other layers
  - Each time, equivalent to training a two-layered network
  - Followed up a fine—tuning process
- **Other Pretraining Strategies**
  - Unsupervised pretraining: based on auto-encoder
  - Hybrid strategy
- **Pretraining for transfer learning**



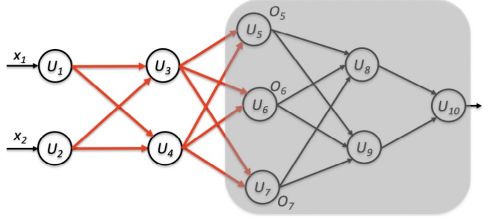
(a) original model to pretrain



(b) first iteration (1 hidden layer)



(c) second iteration (2 hidden layers)

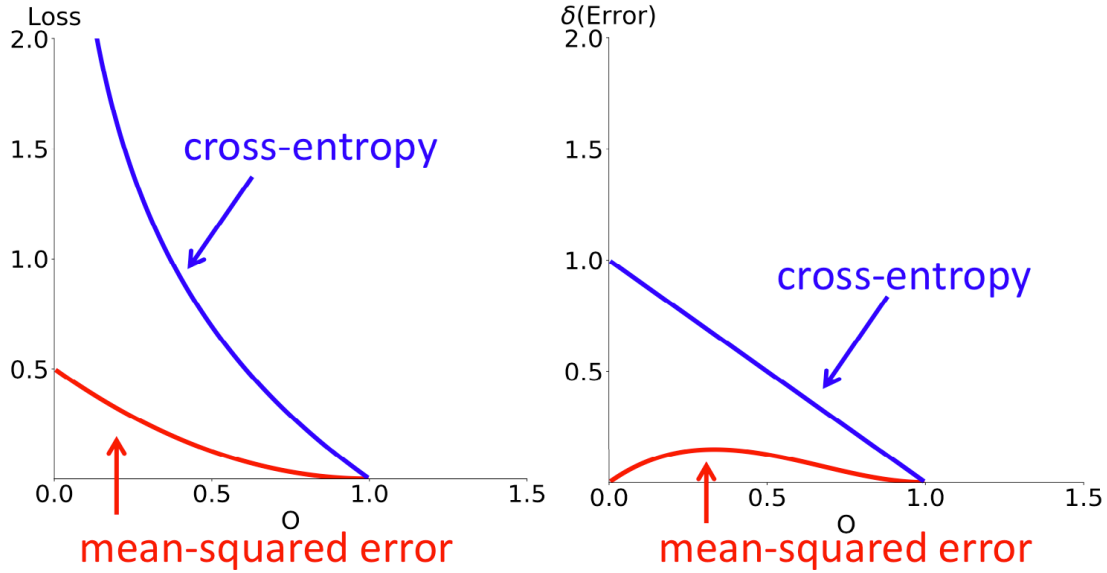


(d) third iteration (3 hidden layers)

Cross Entropy

- **Measure the disagreement between the actual (T) and predicted (O) target values**
  - For regression: mean-squared error
  - For (binary) classification: cross-entropy
- **Mean-squared error vs. Cross-entropy**

	Mean-squared error	Cross entropy
Loss	$\frac{1}{2}(T-O)^2$	$-T\log O-(1-T)\log(1-O)$
Error δ	$O(1-O)(T-O)$	$T-O$



Assuming T = 1 (positive tuple)

- **Cross-entropy for Multiclass Problem**
  - Actual target $T=(T_1,T_2,...,T_C)$
  - Predicted output $O=(O_1,O_2,...,O_C)$

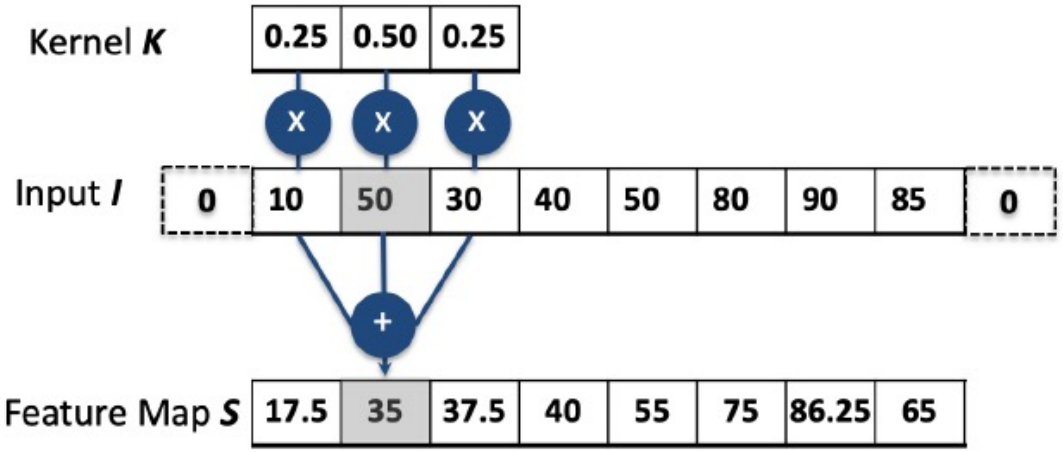
$$\text{Loss}(T,O)=-\sum_{j=1}^{C}T_j\log O_j$$

Chapter 11. Deep Learning

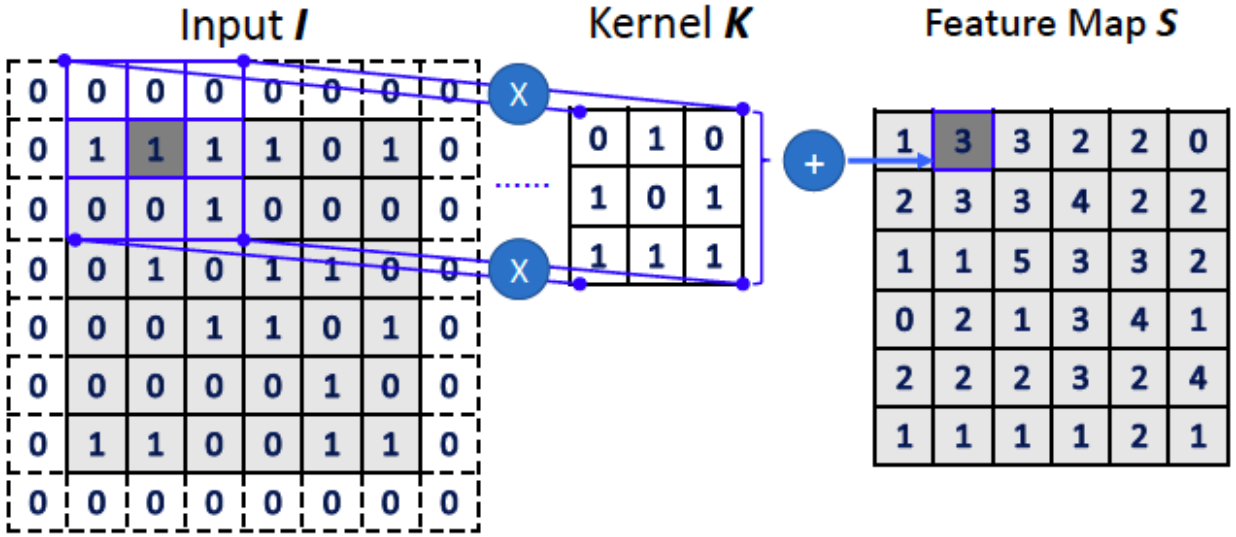
- Basic Techniques
- Techniques to Improve Deep Learning Training
- Convolutional Neural Networks 
- Recurrent Neural Networks
- Summary

Convolutional Neural Networks (CNN)

- What is convolution? $S = I * K$



1D Convolution



2D Convolution

$$S[i] = \sum_{p=-\frac{P-1}{2}}^{\frac{P-1}{2}} I[i+p]K[p], \quad (i = 1, ..., N)$$

$$S[i][j] = \sum_{q=-\frac{Q-1}{2}}^{\frac{Q-1}{2}} \sum_{p=-\frac{P-1}{2}}^{\frac{P-1}{2}} I[i+p][j+q]K[p][q]$$

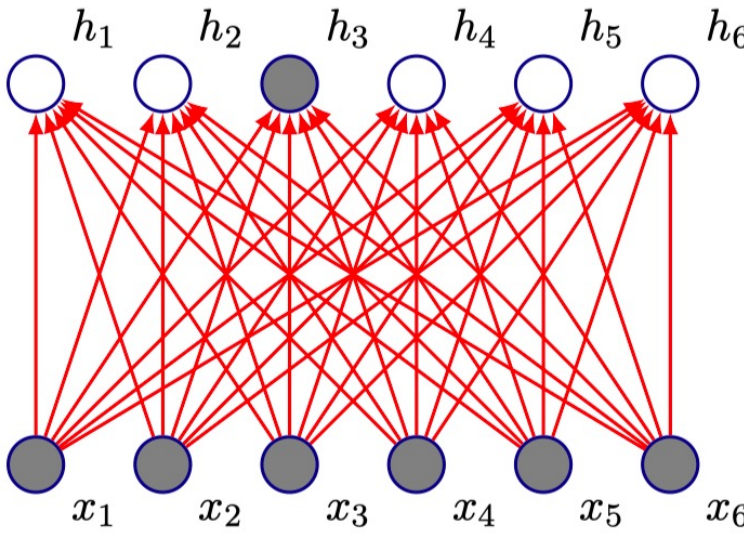
- The outputs are computed by sliding a **kernel** (of weights) on the inputs, and computing weighted sum locally

CNN Motivation

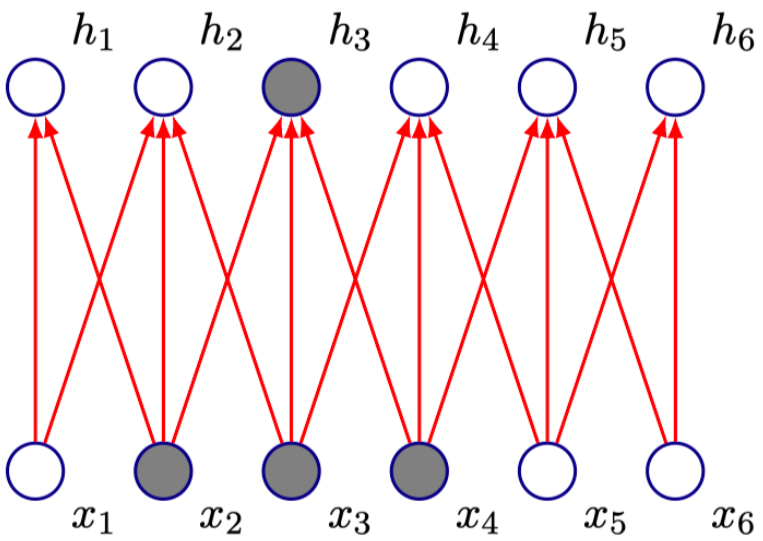
- Why not deep MLP (or feed-forward neural network)?
  - Deep multilayer perceptrons are **computationally expensive**, and **hard to train**.
    - Long training time, slow convergence, local minima
- Motivations of convolution
  - Sparse interactions
  - Parameter sharing
  - Translational equivalence
- The properties of CNNs are well aligned with properties of many forms of data (e.g. images, text), making them very successful

CNN Motivation

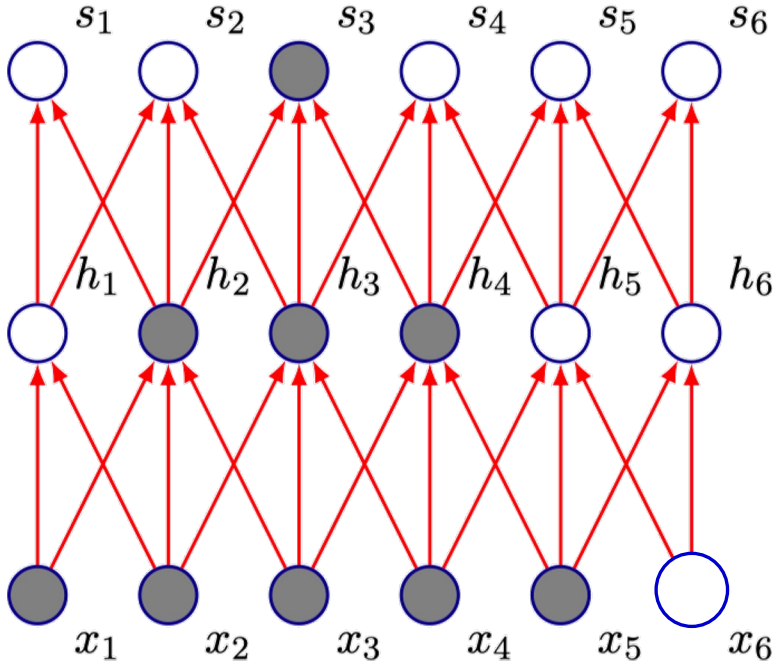
- Motivations of convolution
  - Sparse interactions
    - E.g. 1D convolution with kernel size 3
    - Units in deeper layers still connect to a wide range of inputs



MLP



CNN

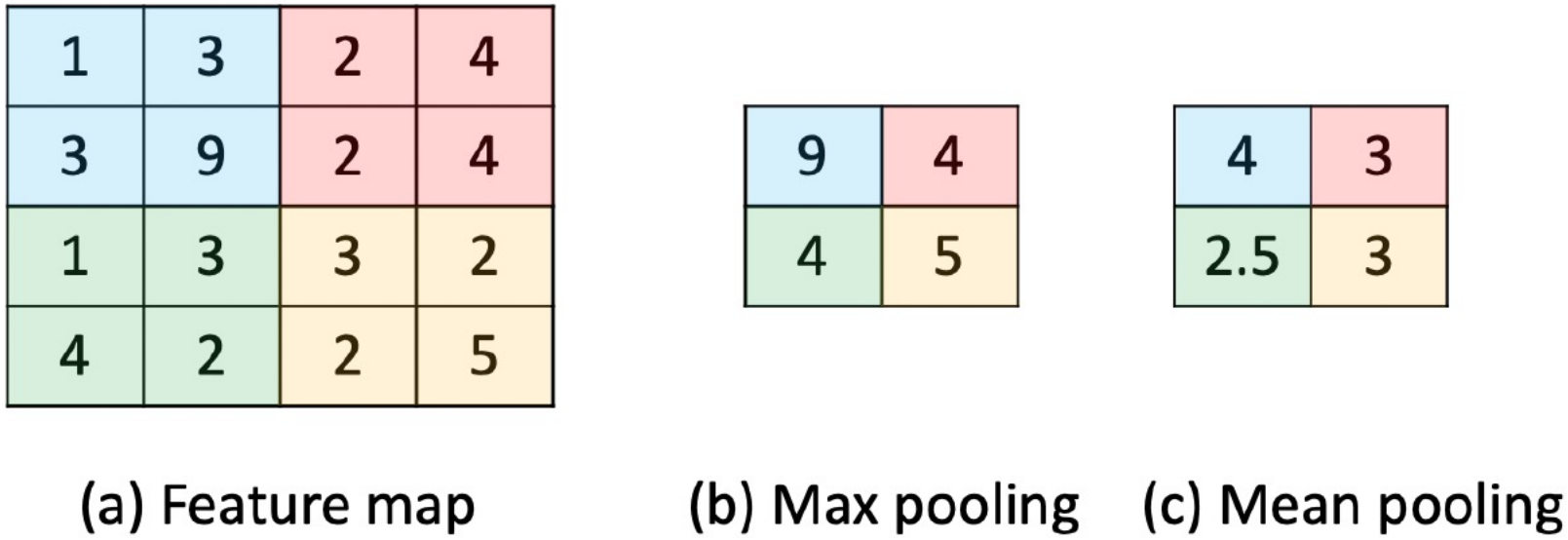


CNN Motivation

- Motivations of convolution
  - Parameter sharing
    - Each kernel is used on all locations of input
    - Reduce #parameters
  - Translational equivalence $f(g(x)) = g(f(x))$
    - Same input at different location gives same output
    - E.g. a cat at the upper right corner and at the lower left corner of an image, will produce the same outputs
    - E.g. “University of Illinois” at the start of the sentence and at the end of the sentence produce the same outputs

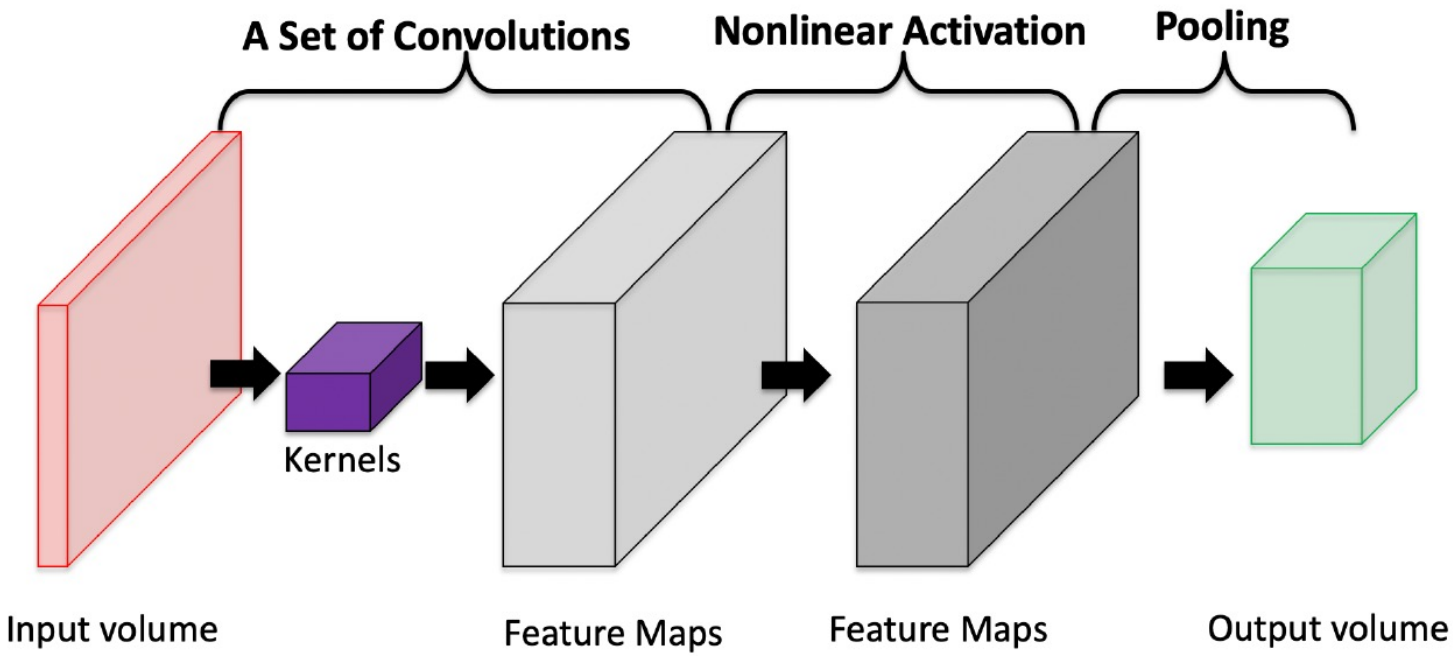
CNN: Pooling Layer

- Pooling (Subsampling)
  - Pool hidden units in the same neighborhood
    - Introduces invariance to local translations
    - Reduces the number of hidden units in hidden layer



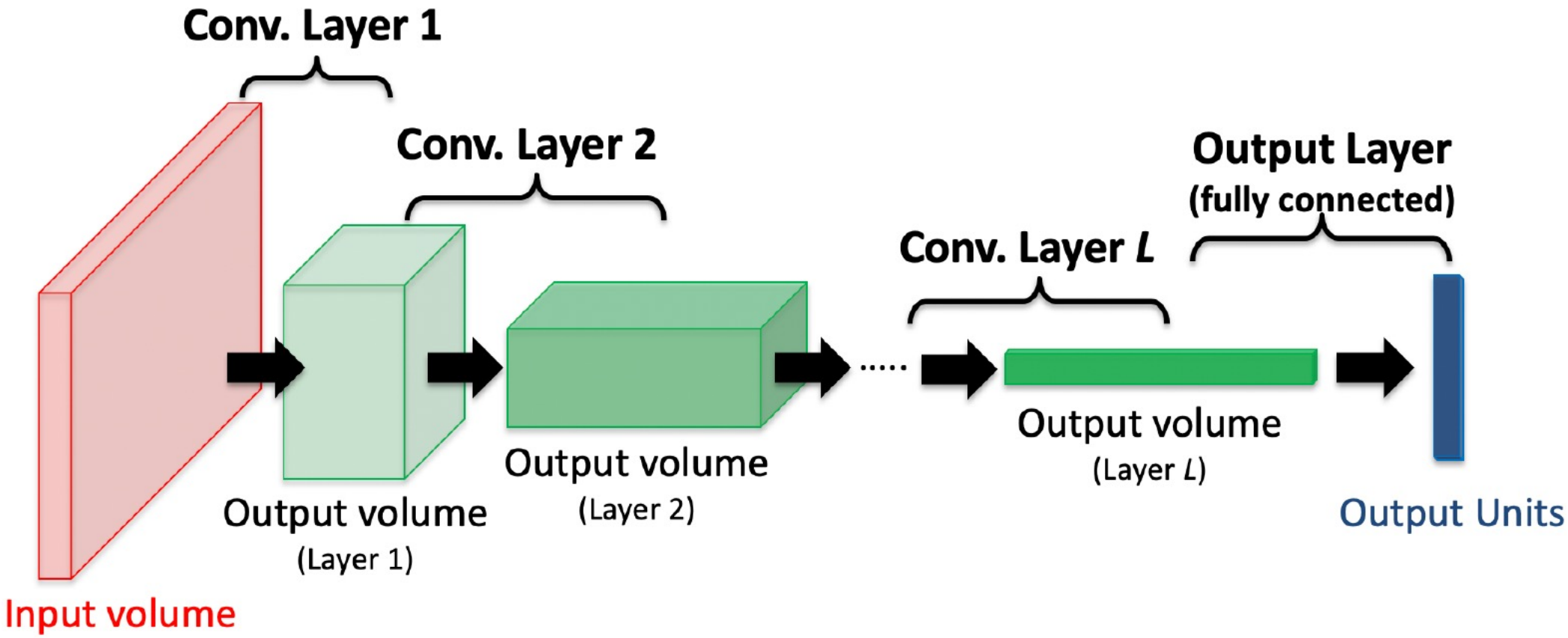
CNN: Convolutional Layer

- Multiple kernels (organized in a tensor)
  - Applied separately to the input volumn
  - Full in depth: producing a 2D feature map
  - Multiple feature maps are organized in a 3D tensor
- Followed by
  - nonlinear activation
  - pooling

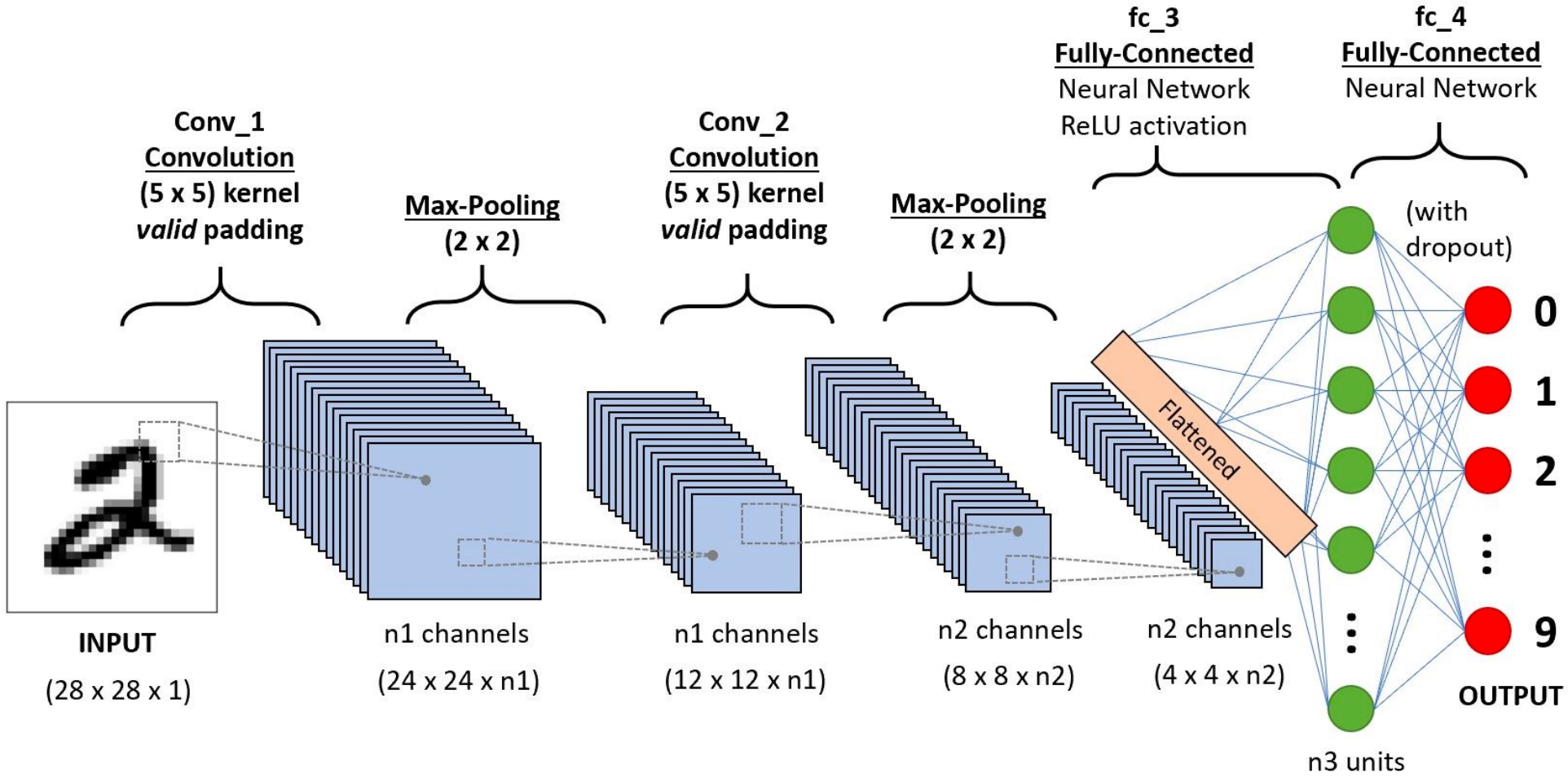


Convolutional Neural Networks

- CNN = NN has at least one convolutional layer
- Importance of # of layers



CovoluNN for Image Recognition: Example



An example CNN for hand written digit recognition

Chapter 11. Deep Learning

- Basic Techniques
- Techniques to Improve Deep Learning Training
- Convolutional Neural Networks
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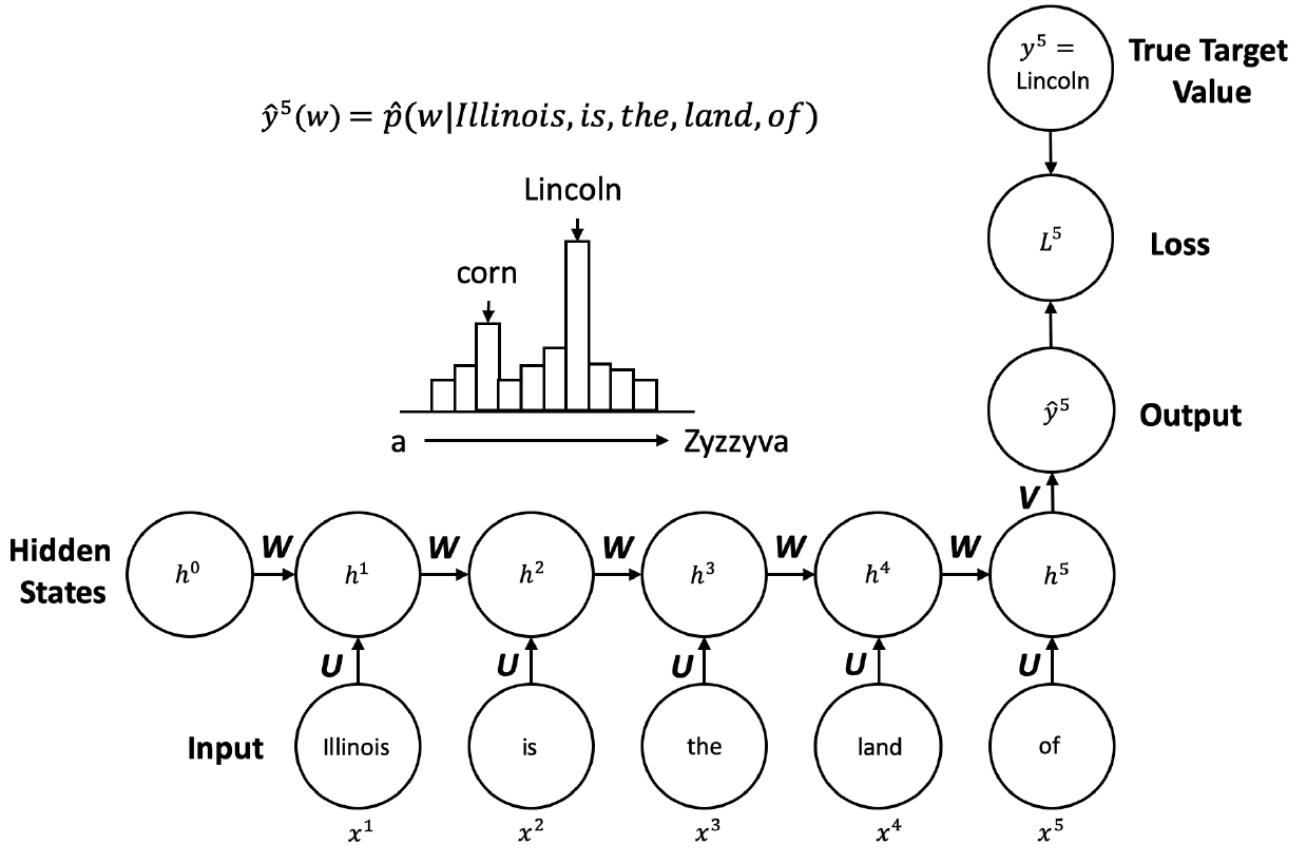
- Summary

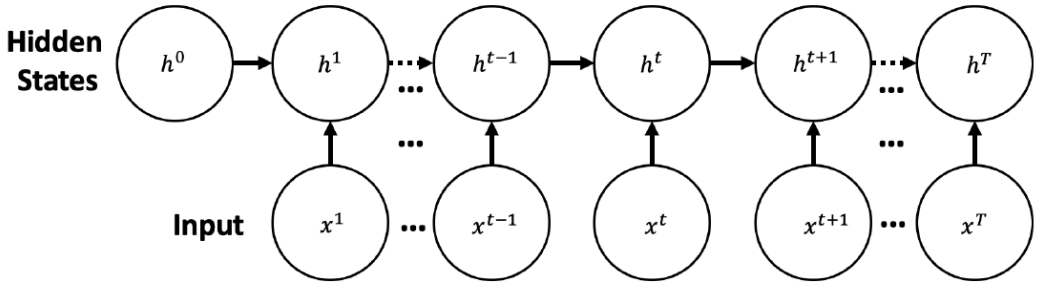
Recurrent Neural Networks

- Handling sequences with **Recurrent Neural Networks (RNN)**
  - At each time step, the input and the previous hidden state are fed into the network

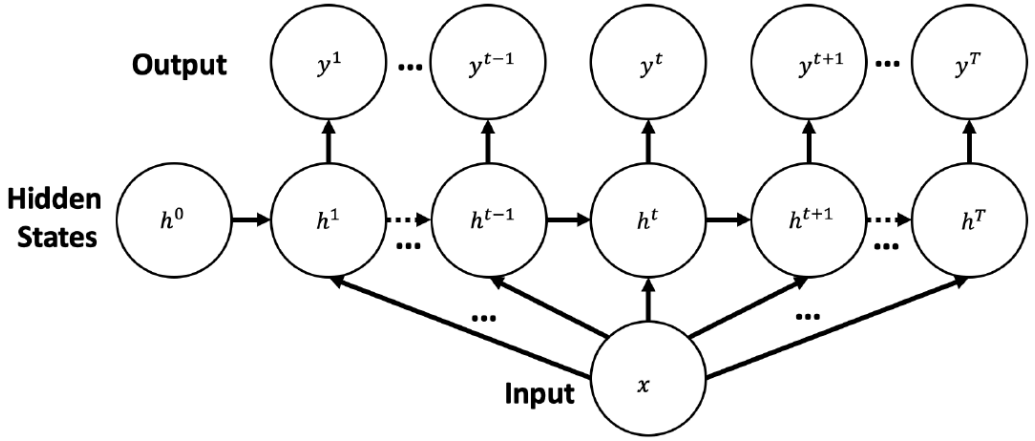
$$\boldsymbol{h}^t = f(\boldsymbol{U}\boldsymbol{x}^t + \boldsymbol{W}\boldsymbol{h}^{t-1} + \boldsymbol{a})$$
$$\hat{\boldsymbol{y}}^T = g(\boldsymbol{V}\boldsymbol{h}^T + \boldsymbol{b}).$$



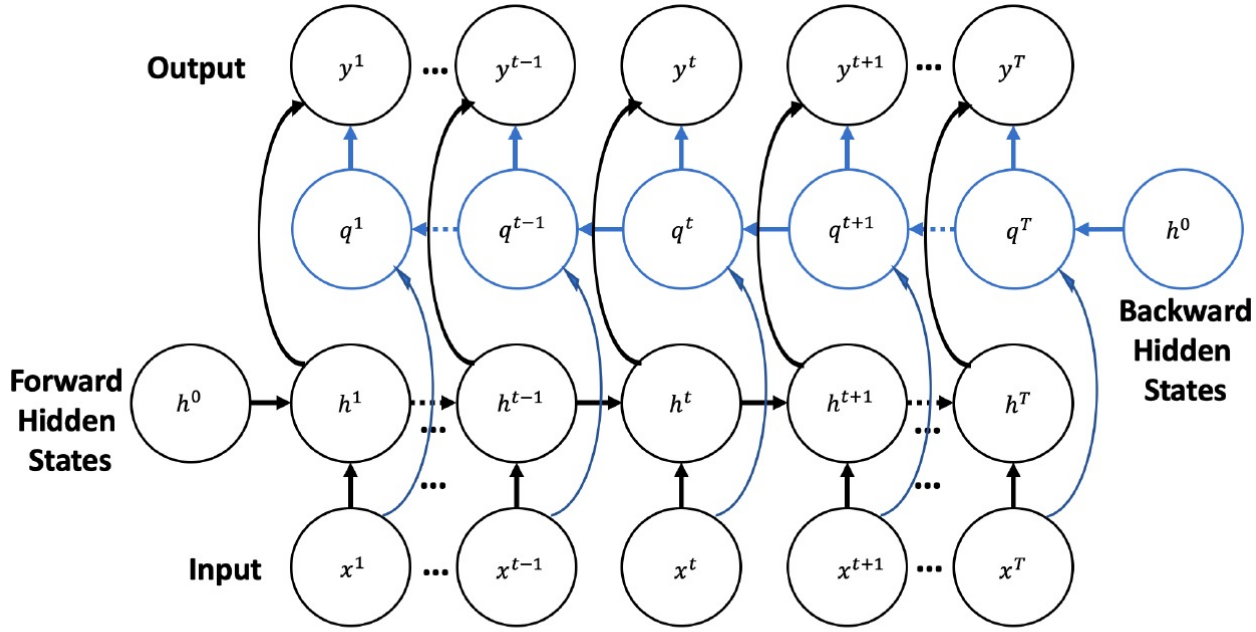
Different Types of RNNs



(a) RNN without output



(b) RNN with vector input



(c) bi-directional RNN

Recurrent Neural Networks: General Concepts

- Modeling the time dimension
  - Adding feedback loops connected to past decisions
  - Long-term dependencies: Use hidden states to preserve sequential information
- Training RNNs: Compute a gradient with BPTT (backpropagation through time)
- Major obstacles of RNN: Long-term dependence
  - An example: “The Urbana Sweetcorn Festival is held in every August .... There will be live music, food, beers ... . Enjoy the fresh **corn**.”
  - Long-term dependence calls for deep RNN, which make gradient vanishing and/or exploding problems even worse.
  - Solutions:
    - Gated RNNs (LSTM, GRU)
    - Attention mechanism (Transformer, BERT)

Summary

- Basic Concepts
  - Neuron, activation functions
  - MLP, feed-forward neural networks
  - Backpropagation algorithm
- Techniques to Improve Deep Learning Training
  - Key challenges: optimization vs. generalization
  - Responsive activation functions, adaptive learning rate, dropout, pretraining, cross-entropy
- Convolutional Neural Networks
  - Convolution, pooling, parameter sharing
- Recurrent Neural Networks
  - Sequence data, long term dependence

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