CS145: INTRODUCTION TO DATA MINING

6: Vector Data: Neural Network

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Methods to Learn: Last Lecture

	Vector Data	Set Data	Sequence Data	Text Data
Classification	**Logistic Regression; Decision Tree**; KNN **SVM**; NN			Naïve Bayes for Text
Clustering	K-means; hierarchical clustering; DBSCAN; Mixture Models			PLSA
Prediction	**Linear Regression** GLM*			
Frequent Pattern Mining		Apriori; FP growth	GSP; PrefixSpan	
Similarity Search			DTW	

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Neural Network

- Introduction
- Connection to Shallow Machine Learning Algorithms
- Multi-Layer Feed-Forward Neural Network
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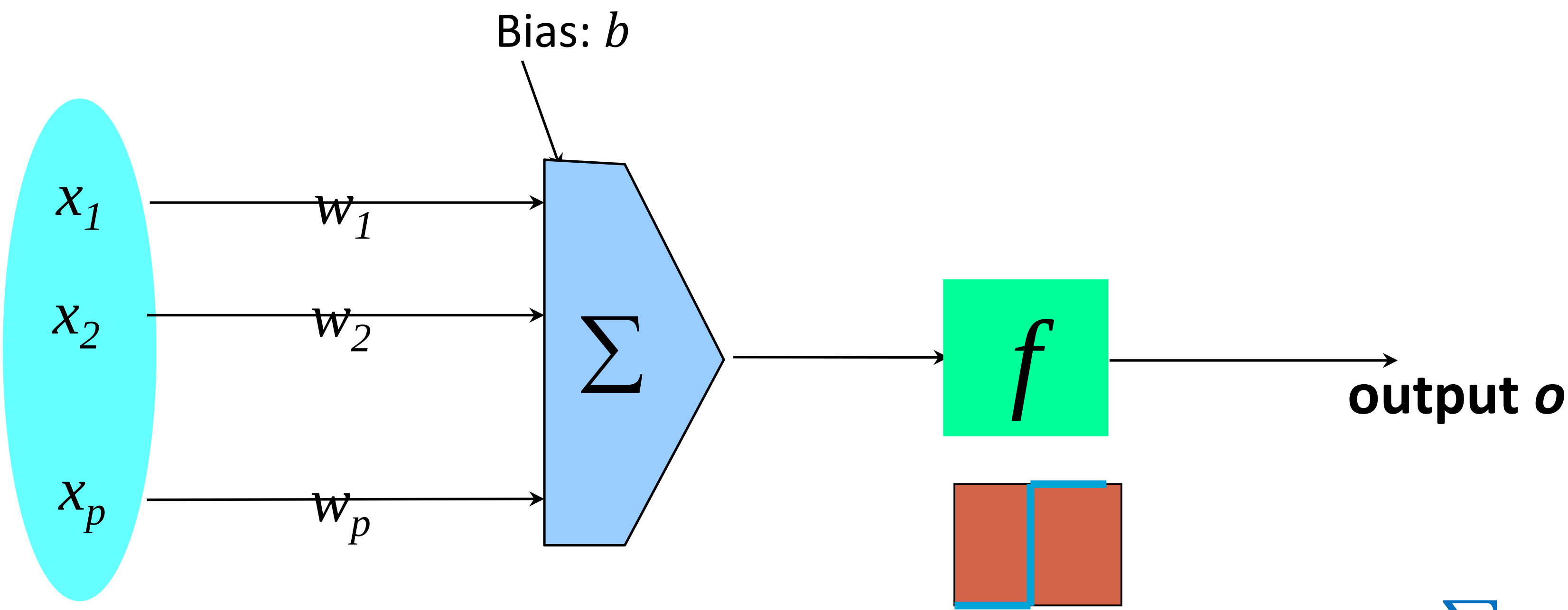
Artificial Neural Networks

- Consider humans:
  - Number of neurons ~10^{10}
  - Connections per neuron ~10^{4-5}
  - Neuron switching time ~.001 second
  - Scene recognition time ~.1 second
  - 100 inference steps doesn't seem like enough -> parallel computation
- Artificial neural networks
  - Many neuron-like threshold switching units
  - Many weighted interconnections among units
  - Highly parallel, distributed process
  - Emphasis on tuning weights automatically

Single Unit: Perceptron



Input vector x | **weight vector w** | **weighted sum** | **Activation function**

$$o = sign\left(\sum_j w_j x_j + b\right)$$

Important Concepts

- Architecture
- Activation function
- Loss function
- Optimization
- Regularization

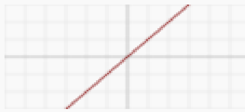
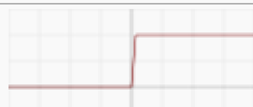
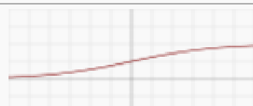
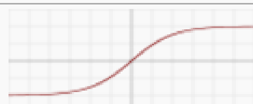
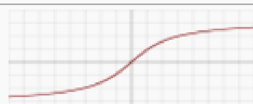
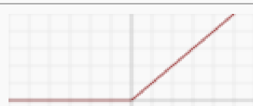
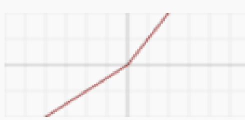
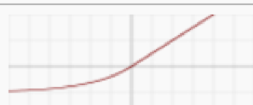
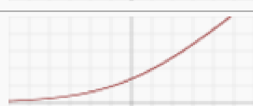
Architecture

- Decide the **network topology:**
  - Specify # of units in the *input layer*, # of *hidden layers* (if > 1), # of units in *each hidden layer*, the unit types, connection between layers, and # of units in the *output layer*
- Architecture specifies the function that maps input to output, which contains parameters to be learned

Activation function

- An activation function $f(\cdot)$ in the output layer can control the nature of the output (e.g., probability value in [0, 1])
- Activation functions bring nonlinearity into hidden layers, which increases the complexity of the model.
- Good activation functions should be differentiable for optimization purpose

Examples of Activation Functions

Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)(1 - f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU)[2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU)[3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$

Loss Functions

- How good are the outputs compared with the labels (target)?
  - Empirical risk
    - $\mathcal{L}(\boldsymbol{w}) = \frac{1}{n}\sum_i l\left(y^{(i)}, \hat{y}^{(i)}\right)$, where $\hat{y}^{(i)} = f\left(\boldsymbol{x}^{(i)}, \boldsymbol{w}\right)$
    - $\boldsymbol{w}$: parameters in the model
  - Loss function: difference between actual value and predicted value
    - $l(y, \hat{y})$

Example of Loss Functions

- Squared error
  - $l(y, \hat{y}) = (y - \hat{y})^2$
- (Binary) cross entropy loss
  - $l(y, \hat{y}) = -ylog\hat{y} - (1 - y)log(1 - \hat{y})$
  - $y \in \{0,1\}, \hat{y} \in [0,1]$
- Hinge loss
  - $l(y, \hat{y}) = \max(0,1 - y\hat{y})$
  - $y \in \{-1,1\}, \hat{y} \in (-\infty, +\infty)$

Optimization

- Given a training dataset, minimize the empirical risk
  - Find $\boldsymbol{w}$, such that $\mathcal{L}(\boldsymbol{w}) = \frac{1}{n}\sum_i l\left(y^{(i)}, \hat{y}^{(i)}\right)$ is minimized
- Solution:
  - Stochastic gradient descent + chain rule = backpropagation

Regularization

- Avoid overfitting
- Techniques
  - L2/L1 regularization
  - Dropout
  - Early stopping
  - …

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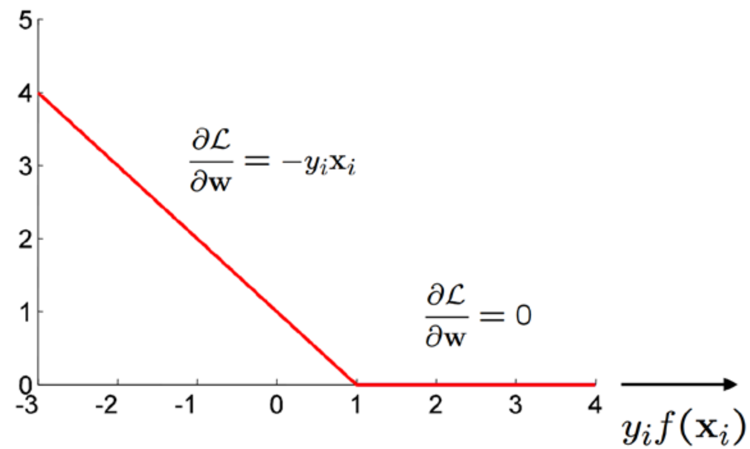
Perceptron

- Architecture:
  - A single neuron
- Activation function
  - Training: identity function
  - Inference: sign function/step function
- Loss function
  - $l(y, \hat{y}) = \max(0, -y\hat{y})$
- Optimization
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta y^{(i)} \boldsymbol{x}^{(i)}$, for a misclassified training data point $\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)$, i.e., $y^{(i)} w^T \boldsymbol{x}^{(i)} < 0$
  - η: learning rate

Linear SVM

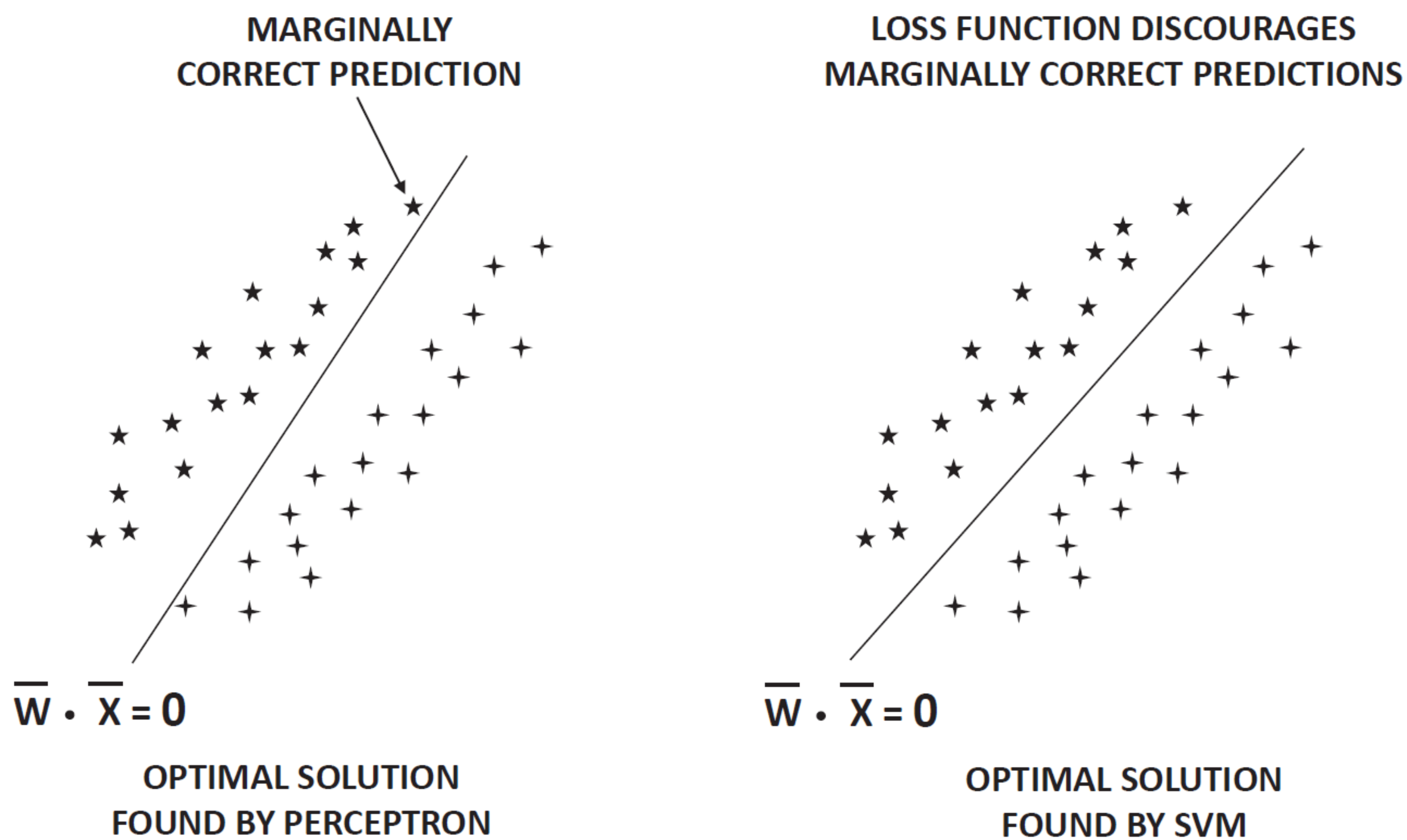
- Architecture:
  - A single neuron
- Activation function
  - Training: identity function
  - Inference: sign function/step function
- Loss function
  - $l(y, \hat{y}) = \max(0, 1 - y\hat{y})$
- Regularization
  - L2, i.e., $\frac{1}{2}\lambda||\boldsymbol{w}||^2$



- Optimization
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta(\lambda \boldsymbol{w} - y^{(i)}\boldsymbol{x}^{(i)})$, for a misclassified or barely correct training data point $\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)$, i.e., $y^{(i)}\boldsymbol{w}^T\boldsymbol{x}^{(i)} < 1$
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta\lambda\boldsymbol{w}$, for a confidently correct training data point
  - η: learning rate

Perceptron V.S. Linear SVM

- Source: http://www.charuaggarwal.net/neural.htm



Logistic Regression

- Architecture:
  - A single neuron
- Activation function
  - Sigmoid function
- Loss function
  - $l(y, \hat{y}) = -ylog\hat{y} - (1-y)log(1-\hat{y})$
  - Note $\hat{y}$ is the predicted probability of taking class 1
- Optimization
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta(y^{(i)} - \sigma(w^T \boldsymbol{x}^{(i)}))\boldsymbol{x}^{(i)}$, for a training data point $\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)$
  - η: learning rate

Question

- How about multivariate logistic regression?

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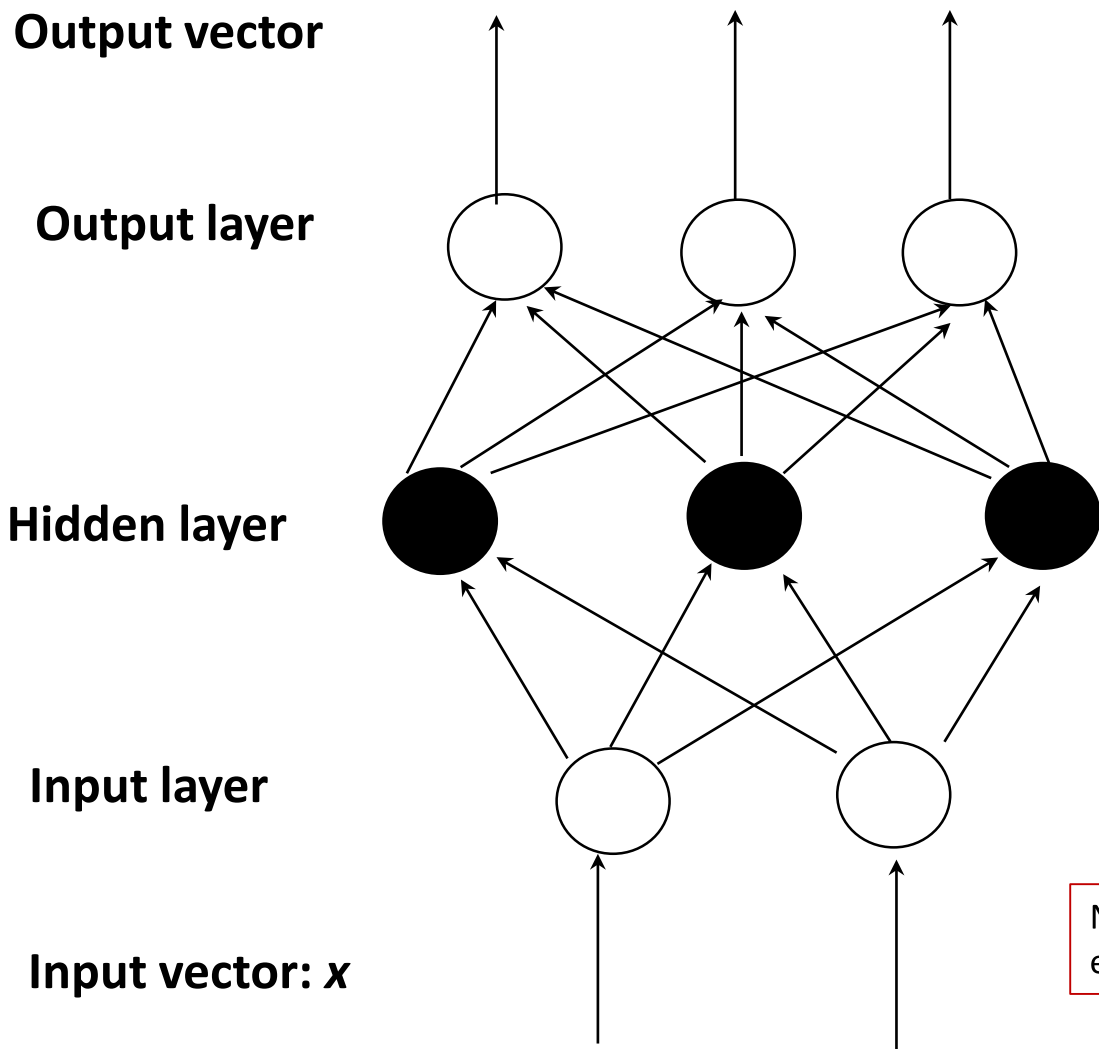
A Multi-Layer Feed-Forward Neural Network



A **two-layer** network

$$\boldsymbol{o} = g(W^{(2)}\boldsymbol{h} + b^{(2)})$$

$$\boldsymbol{h} = f(W^{(1)}\boldsymbol{x} + b^{(1)})$$

Bias term

Weight matrix

Nonlinear transformation,
e.g. sigmoid transformation

How A Multi-Layer Neural Network Works

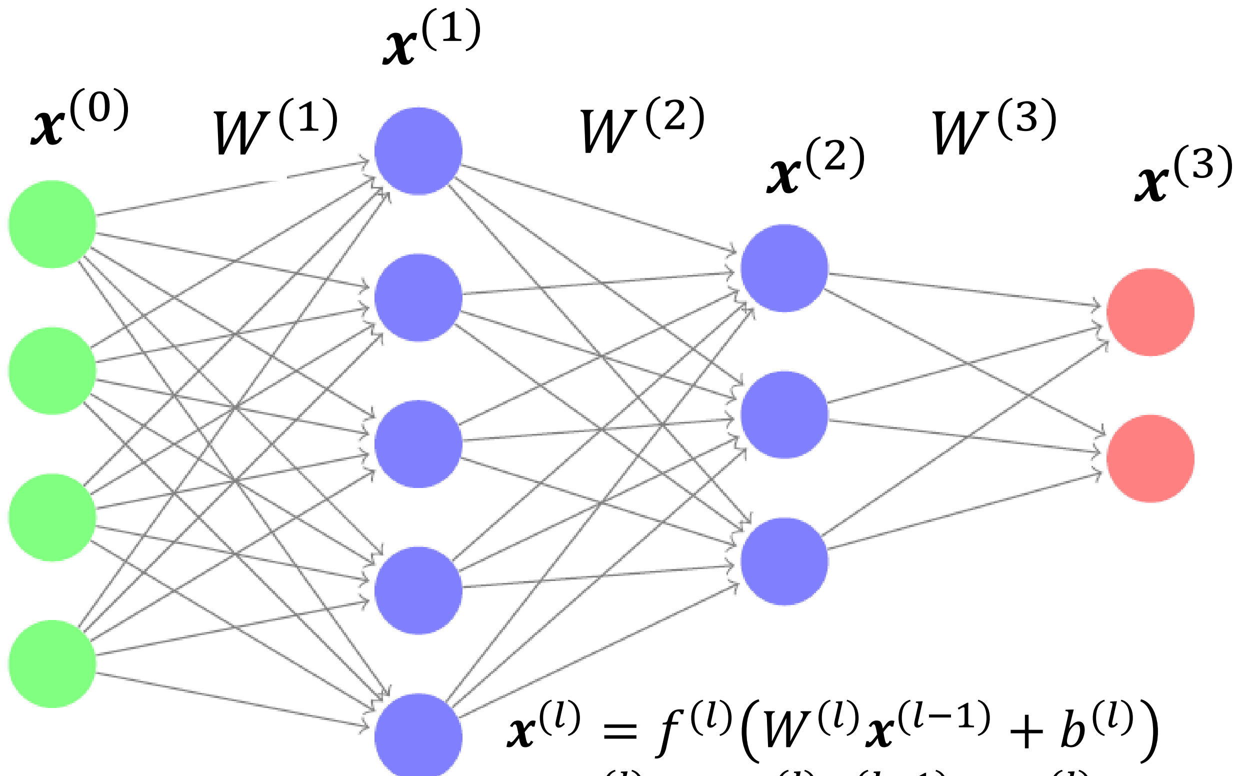
- The **inputs** to the network correspond to the attributes measured for each training tuple
- Inputs are fed simultaneously into the units making up the **input layer**
- They are then weighted and fed simultaneously to a **hidden layer**
  - The number of hidden layers is arbitrary
- The weighted outputs of the last hidden layer are input to units making up the **output layer**, which emits the network's prediction
- The network is **feed-forward**: None of the weights cycles back to an input unit or to an output unit of a previous layer
- From a math point of view, networks perform **nonlinear regression**: **Given enough hidden units and enough training samples, they can closely approximate any continuous function**

Learning by Backpropagation

- Iteratively process a set of training tuples & compare the network's prediction with the actual known target value
- For each training tuple, the weights are modified to **minimize the loss function** between the network's prediction and the actual target value, say **mean squared error**
  - Stochastic gradient descent + chain rule
- Modifications are made in the "**backwards**" direction: from the output layer, through each hidden layer down to the first hidden layer, hence "**backpropagation**"

Example

- Loss function: $E = \frac{1}{2}||\boldsymbol{y} - \widehat{\boldsymbol{y}}||^2$



$$\boldsymbol{x}^{(l)} = f^{(l)}\left(W^{(l)}\boldsymbol{x}^{(l-1)} + b^{(l)}\right)$$
$$z^{(l)} = W^{(l)}\boldsymbol{x}^{(l-1)} + b^{(l)}$$
$$E = \frac{1}{2}\left||y - \boldsymbol{x}^{(3)}\right||^2$$

Gradient for Layer 3 (Last Layer)

- Stochastic gradient for $W_{ij}^{(3)}$ and $b_i^{(3)}$
  - *Recall:*
    - $E = \frac{1}{2}\left\|y - \boldsymbol{x}^{(3)}\right\|^2 = \frac{1}{2}\sum_i \left(y_i - x_i^{(3)}\right)^2$
    - $x_i^{(3)} = f^{(3)}(z_i^{(3)})$
    - $z_i^{(3)} = \sum_j W_{ij}^{(3)} x_j^{(2)} + b_i^{(3)}$
  - $\frac{\partial E}{\partial W_{ij}^{(3)}} = \frac{\partial E}{\partial x_i^{(3)}} \frac{\partial x_i^{(3)}}{\partial z_i^{(3)}} \frac{\partial z_i^{(3)}}{\partial W_{ij}^{(3)}} = \underbrace{-(y_i - x_i^{(3)})\mathrm{f}'^{(3)}\left(\mathrm{z}_\mathrm{i}^{(3)}\right)}_{\boldsymbol{\delta}_i^{(3)}} \mathrm{x}_j^{(2)}$
  - $\frac{\partial E}{\partial b_i^{(3)}} = \frac{\partial E}{\partial x_i^{(3)}} \frac{\partial x_i^{(3)}}{\partial z_i^{(3)}} \frac{\partial z_i^{(3)}}{\partial b_i^{(3)}} = -(y_i - x_i^{(3)})\mathrm{f}'^{(3)}\left(\mathrm{z}_\mathrm{i}^{(3)}\right)$

Gradient for Layer 2

- Stochastic gradient for $W_{ij}^{(2)}$ and $b_i^{(2)}$
  - *Recall:*
    - $E = \frac{1}{2}\left\|y - \boldsymbol{x}^{(3)}\right\|^2 = \frac{1}{2}\sum_i \left(y_i - x_i^{(3)}\right)^2$; $x_i^{(3)} = f^{(3)}\left(z_i^{(3)}\right)$; $z_i^{(3)} = \sum_j W_{ij}^{(3)} x_j^{(2)} + b_i^{(3)}$
    - $x_j^{(2)} = f^{(2)}\left(z_j^{(2)}\right)$; $z_j^{(2)} = \sum_k W_{jk}^{(2)} x_k^{(1)} + b_j^{(2)}$
- $\frac{\partial E}{\partial W_{jk}^{(2)}} = \sum_i \frac{\partial E}{\partial x_i^{(3)}} \frac{\partial x_i^{(3)}}{\partial z_i^{(3)}} \frac{\partial z_i^{(3)}}{\partial x_j^{(2)}} \frac{\partial x_j^{(2)}}{\partial z_j^{(2)}} \frac{\partial z_j^{(2)}}{\partial W_{jk}^{(2)}}$

$$= \underbrace{\sum_i \underbrace{-(y_i - x_i^{(3)})\mathrm{f}'^{(3)}\left(\mathrm{z}_\mathrm{i}^{(3)}\right)}_{\delta_i^{(3)}} \mathrm{w}_{ij}^{(3)}\, \mathrm{f}'^{(2)}\left(\mathrm{z}_\mathrm{j}^{(2)}\right)}_{\delta_j^{(2)}} x_k^{(1)}$$

Gradient for Layer 1

- Stochastic gradient for $W_{ks}^{(1)}$
  - $\frac{\partial E}{\partial W_{ks}^{(1)}} = \sum_j \delta_j^{(2)} W_{jk}^{(2)} f'^{(1)}\left(z_k^{(1)}\right) x_s^{(0)}$

Question

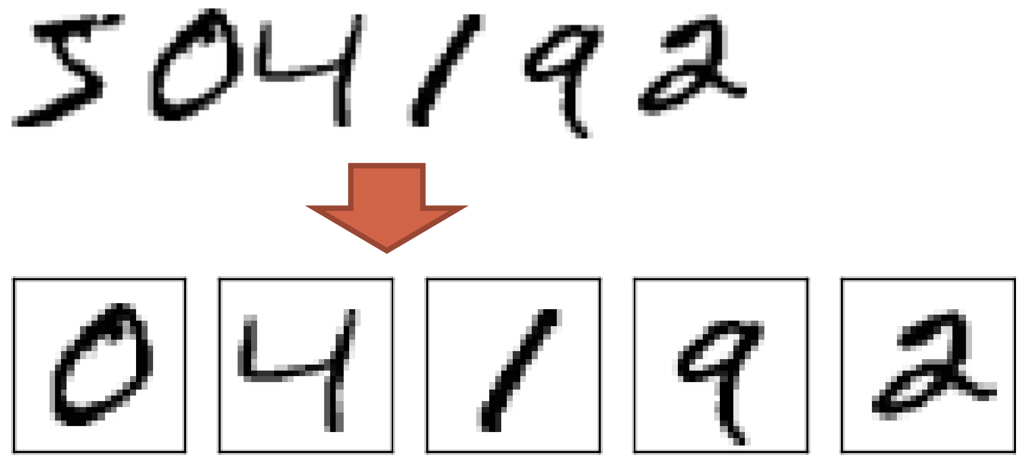
- What would be a general formula for $W_{kj}^{(l)}$?
  - $\mathrm{k} \rightarrow j \rightarrow i$
  - layer l-1 -> layer l -> layer l+1

Neural Network as a Classifier

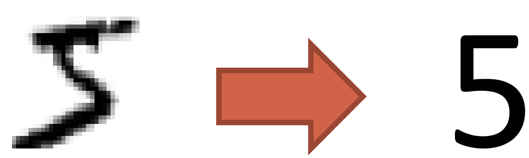
- Weakness
  - Long training time
  - Require a number of hyper-parameters typically best determined empirically, e.g., the network topology or "structure."
  - Poor interpretability: Difficult to interpret the symbolic meaning behind the learned weights and of "hidden units" in the network
- Strength
  - High tolerance to noisy data
  - Successful on an array of real-world data, e.g., hand-written letters
  - Algorithms are inherently parallel
  - Techniques have recently been developed for the extraction of rules from trained neural networks
  - Deep neural network is powerful

Digits Recognition Example

- Obtain sequence of digits by segmentation

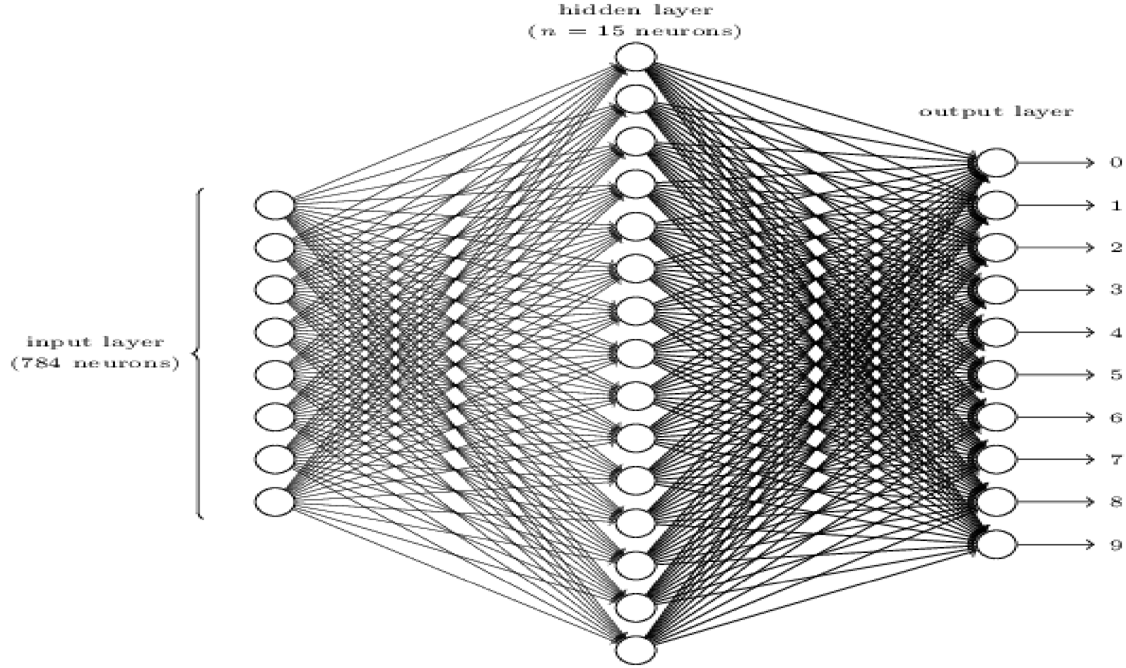


- Recognition (our focus)

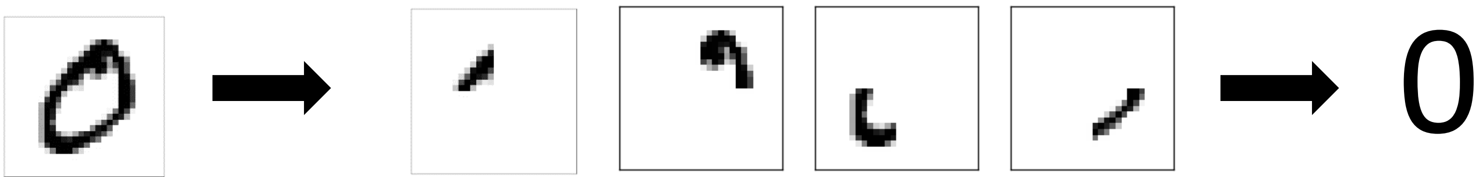


Digits Recognition Example

- The architecture of the used neural network



- What each neurons are doing?



Input image

Activated neurons detecting image parts

Predicted number

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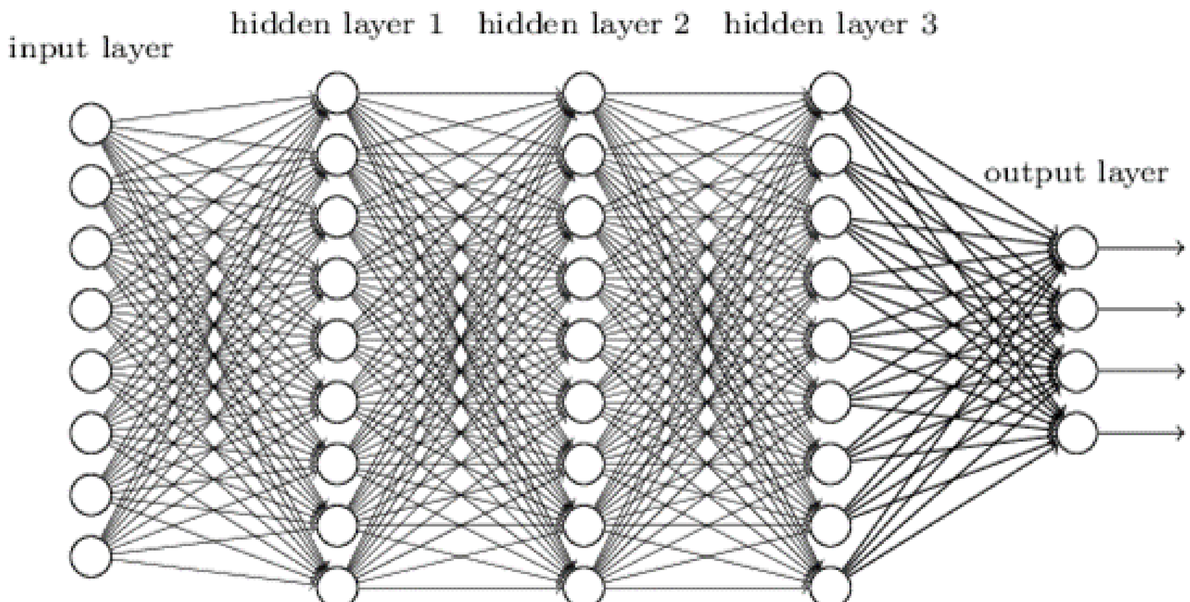
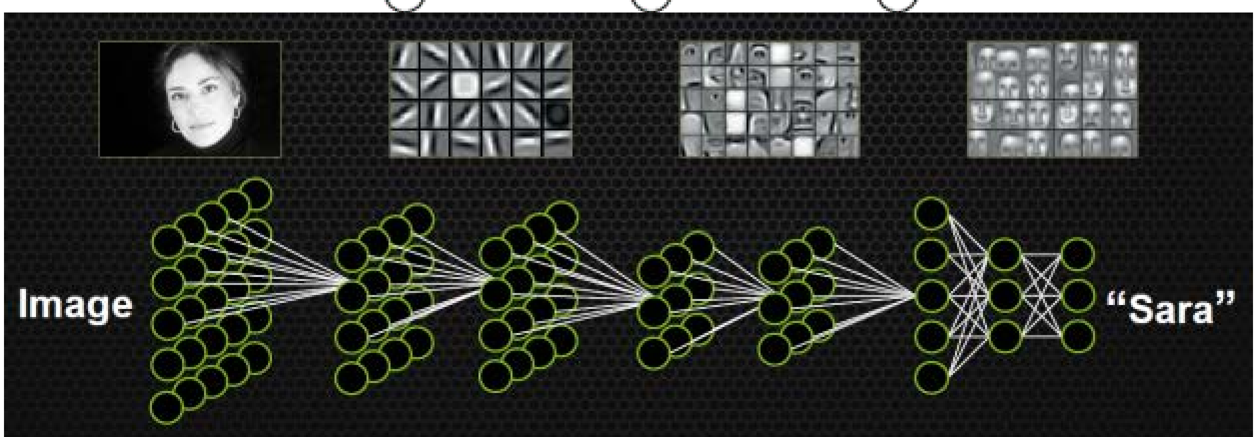
Towards Deep Learning

Deep neural network



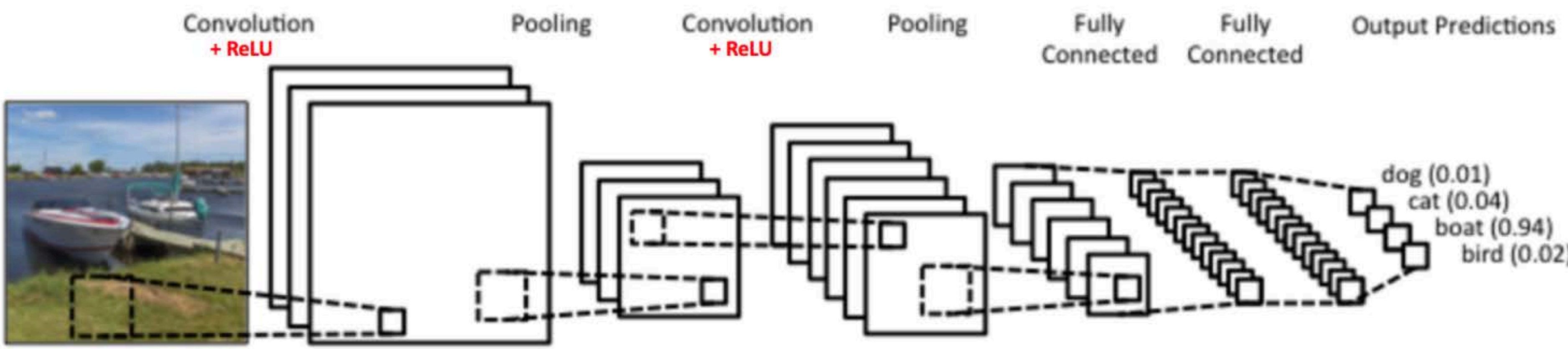


Popular Deep NNs

- Deep layers and parameter sharing
  - Convolutional Neural Network
    - Applications to: Images, NLP, Graph
  - Recurrent Neural Network
    - Applications to: Sequence data

Convolutional Neural Network

- The LeNet Architecture (By Yann LeCun et al.)



Source: https://ujjwalkarn.me/2016/08/11/intuitive-explanation-convnets/

Convolution

1	1	1	0	0
0	1	1	1	0
0	0	1	1	1
0	0	1	1	0
0	1	1	0	0

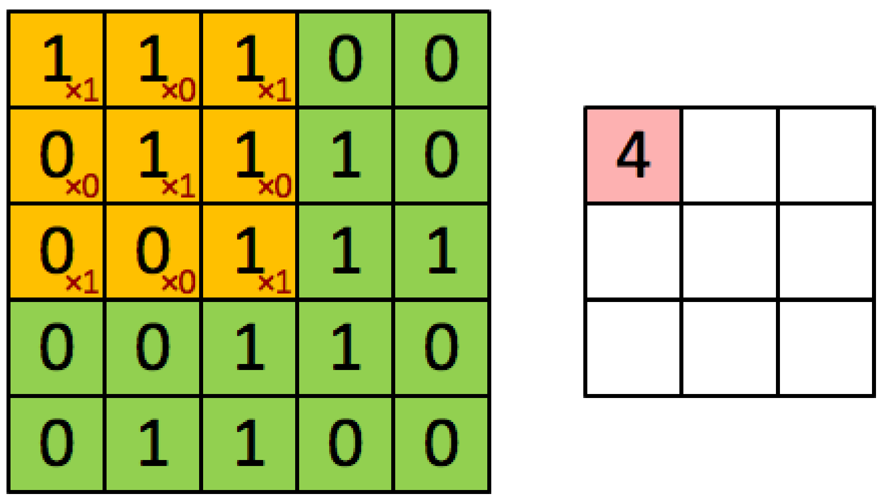
Input

*

1	0	1
0	1	0
1	0	1

Filter

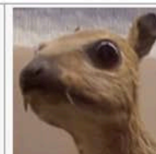
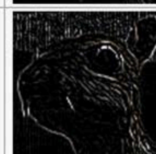
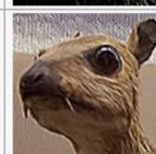
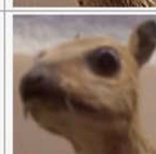
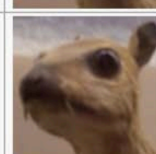
Convolution operator: weighted sum where weights are from filter matrix



Image

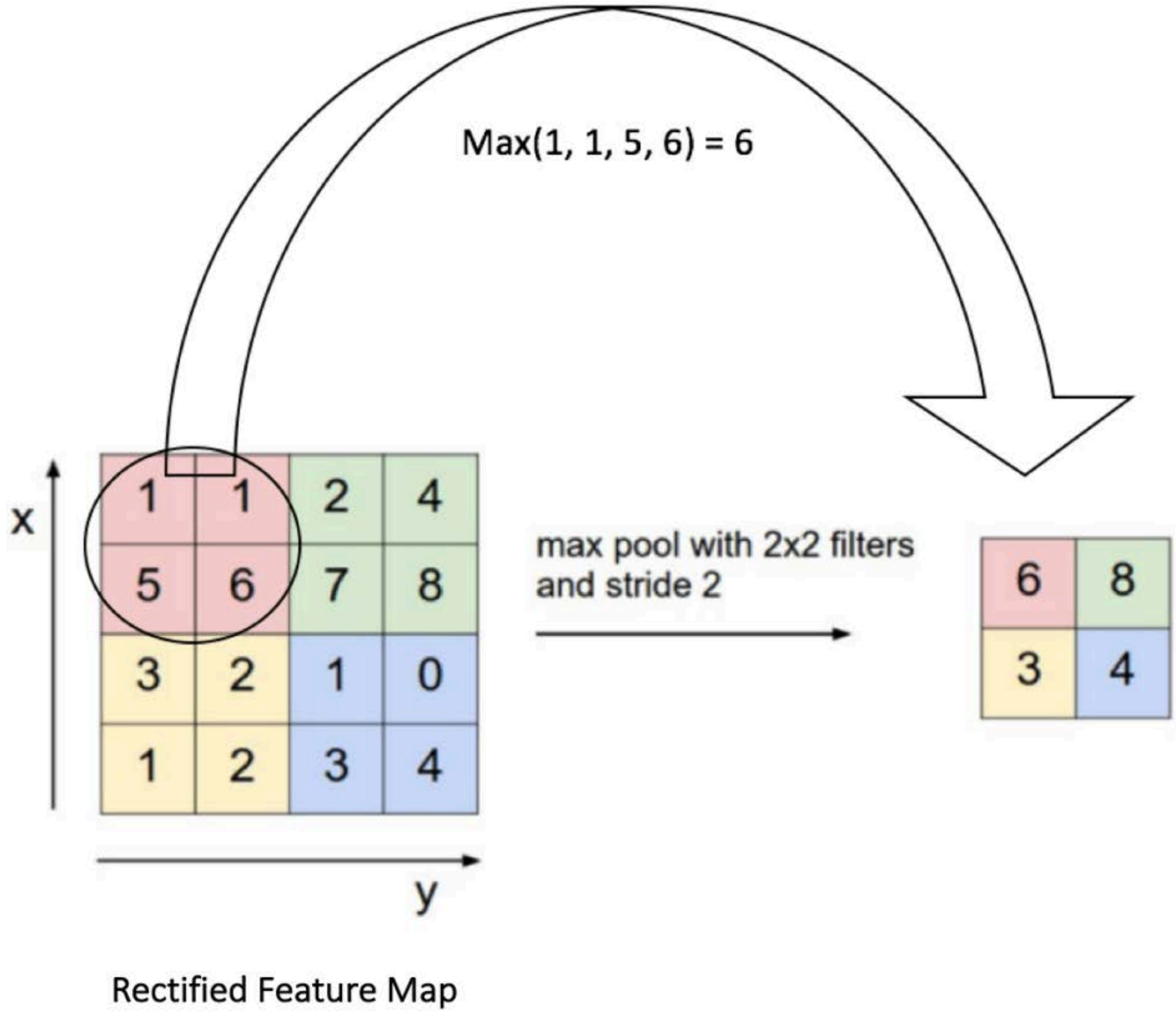
Convolved Feature

Effects of Different Filters

Operation	Filter	Convolved Image
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	
Edge detection	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Box blur (normalized)	$\frac{1}{9}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	
Gaussian blur (approximation)	$\frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	

Source: https://en.wikipedia.org/wiki/Kernel_(image_processing)

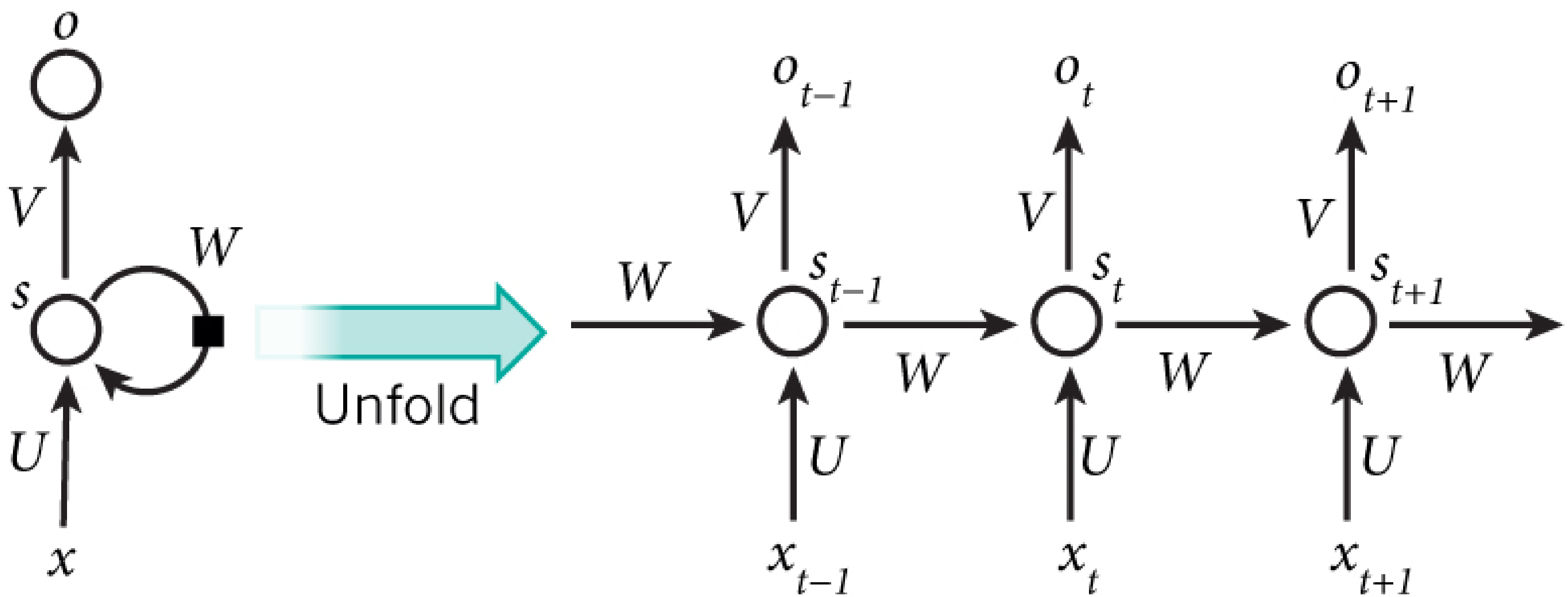
Pooling



Source: http://cs231n.github.io/convolutional-networks/

Recurrent Neural Network

- Model sequential information

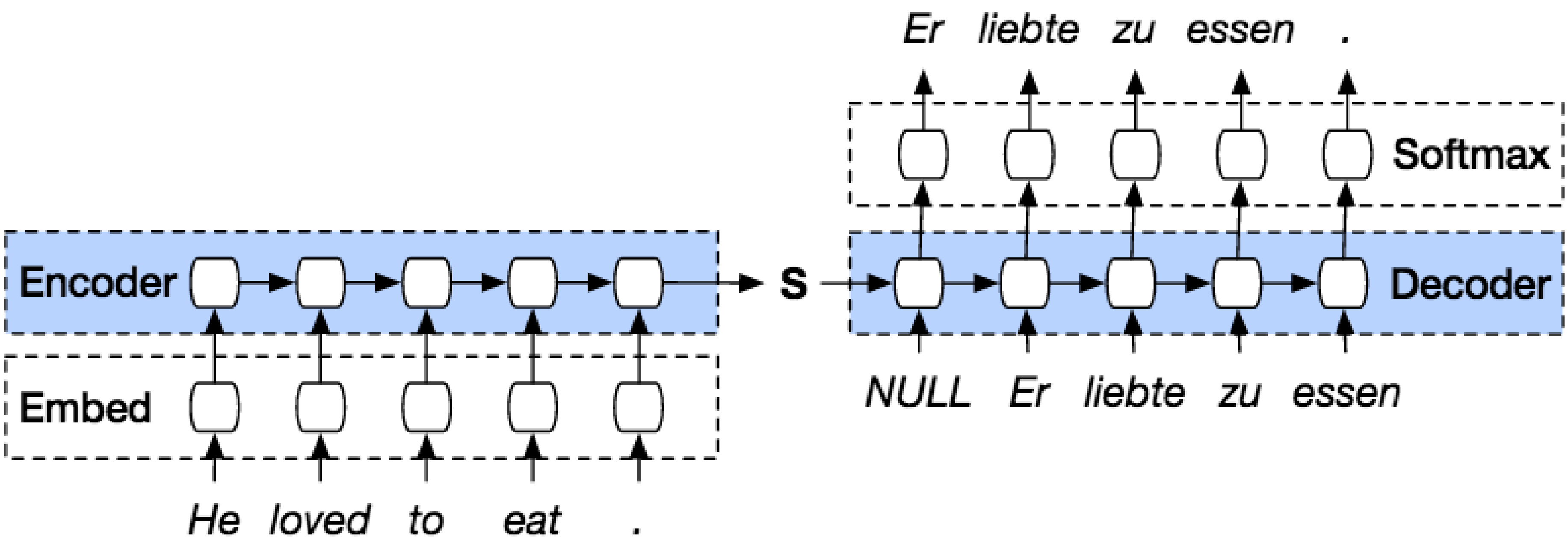


x_t: *input vector at time t*
s_t: *hidden state at time t*
o_t: *output vector at time t*

$$s_t = f(Ws_{t-1} + Ux_t)$$
$$o_t = g(Vs_t)$$

Application of Machine Translation

- Seq2Seq model



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Summary

- Neural Network
  - Architecture; activation function; loss function; backpropagation
- Existing shallow machine learning algorithms can be represented in NN
- Multilayer feedforward NN
- Deep learning

Further References

- 3Blue1Brown NN series: https://www.youtube.com/watch?v=aircAruvnKk&list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi
- Deep Learning
  - http://neuralnetworksanddeeplearning.com/
  - http://www.deeplearningbook.org/
  - http://www.charuaggarwal.net/neural.htm
  - http://d2l.ai/index.html