Introduction to Deep Learning

Neural Networks and Deep Learning

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Objective

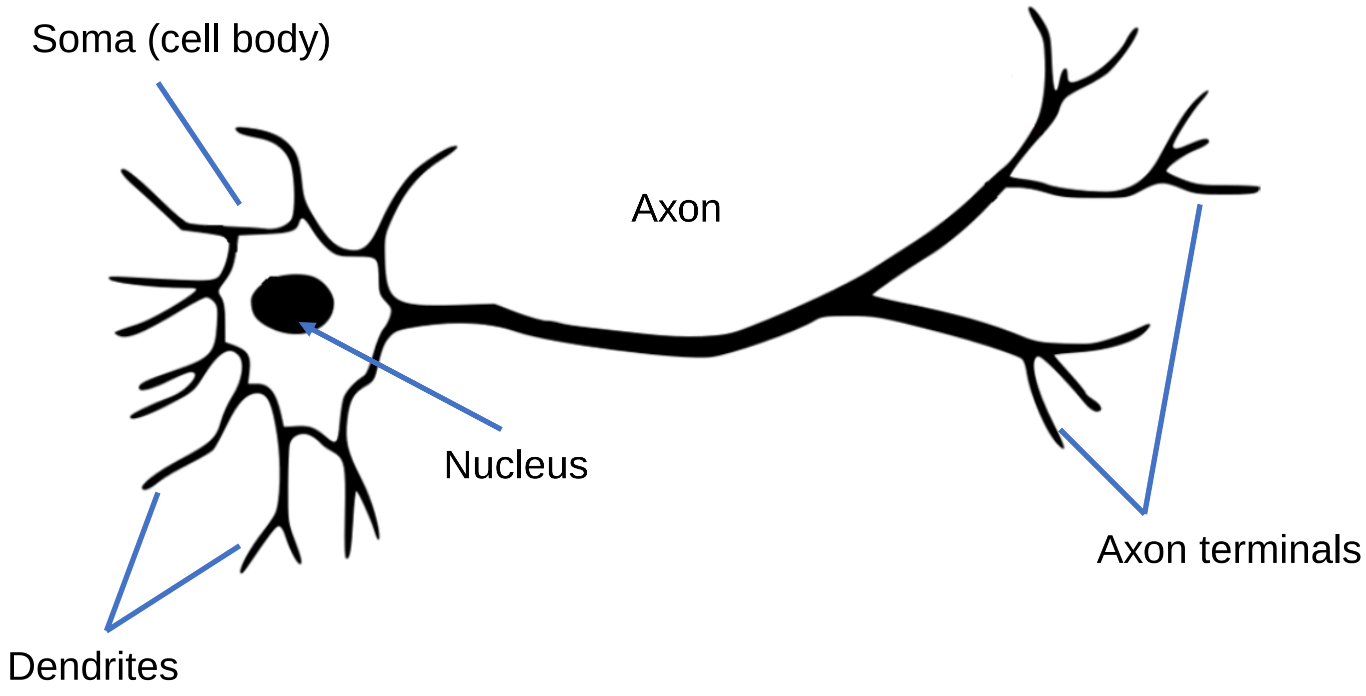
Objective

Describe the big-picture view of how neural networks work

Objective

Identify the basic building blocks and notations of deep neural networks

Illustrating A Biological Neuron



Neural Network

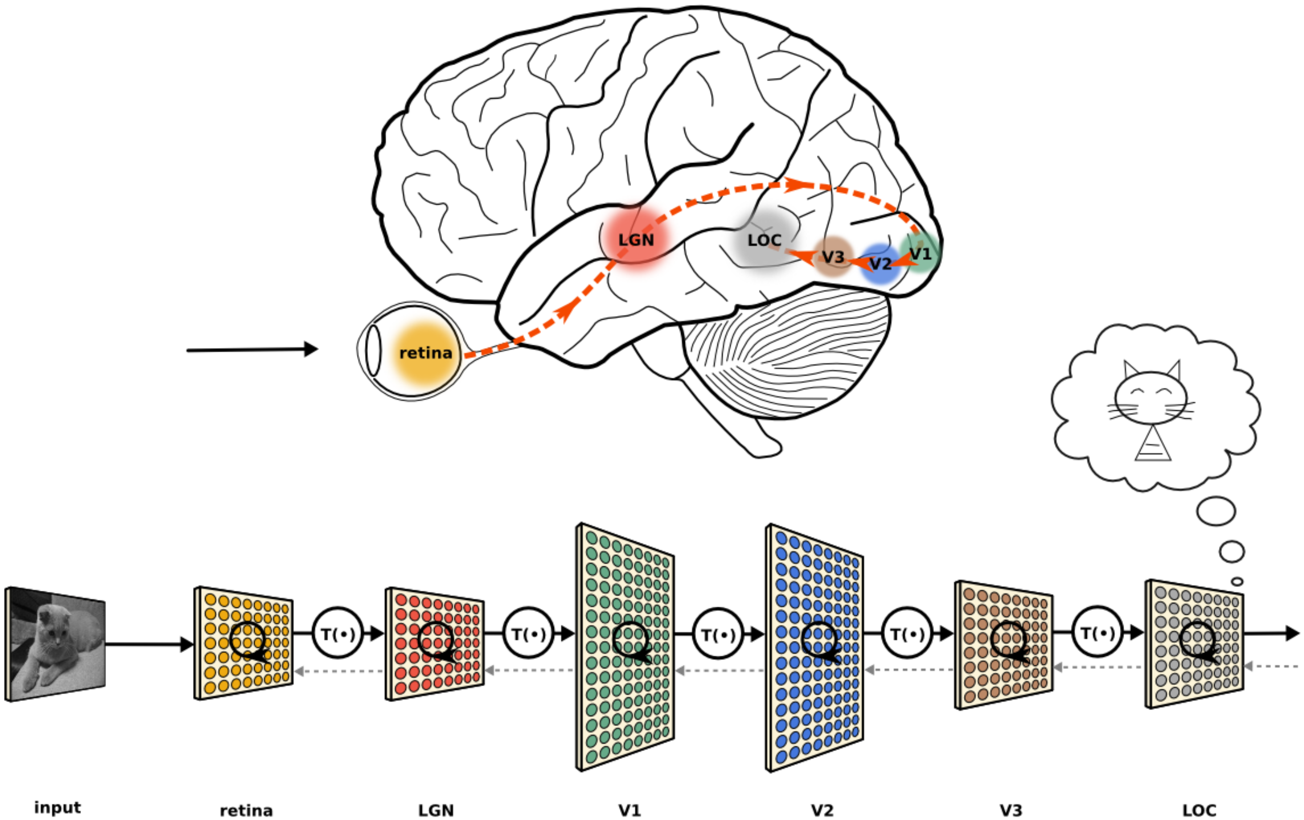
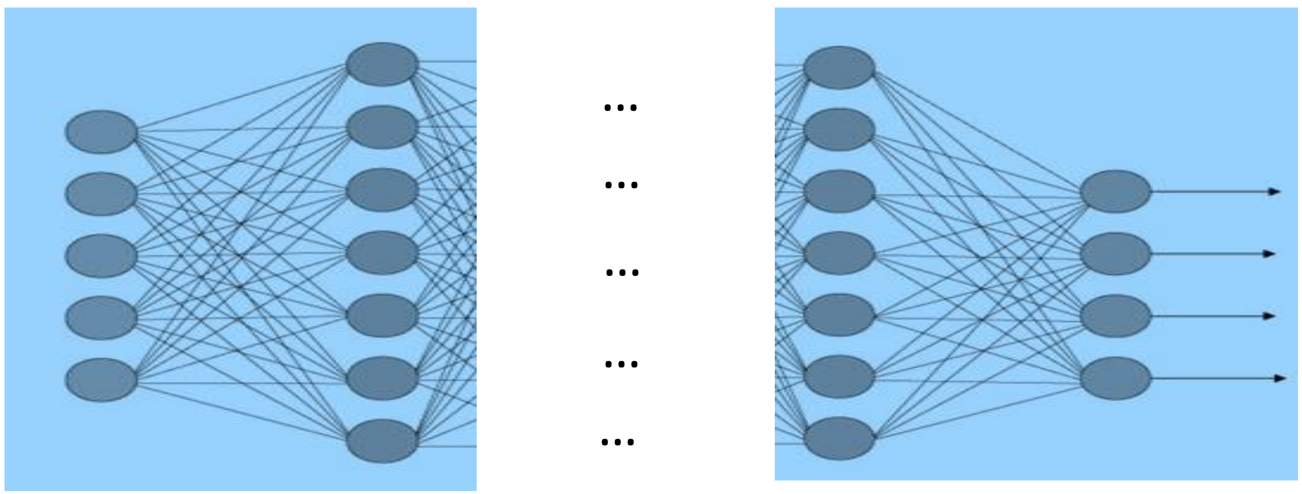
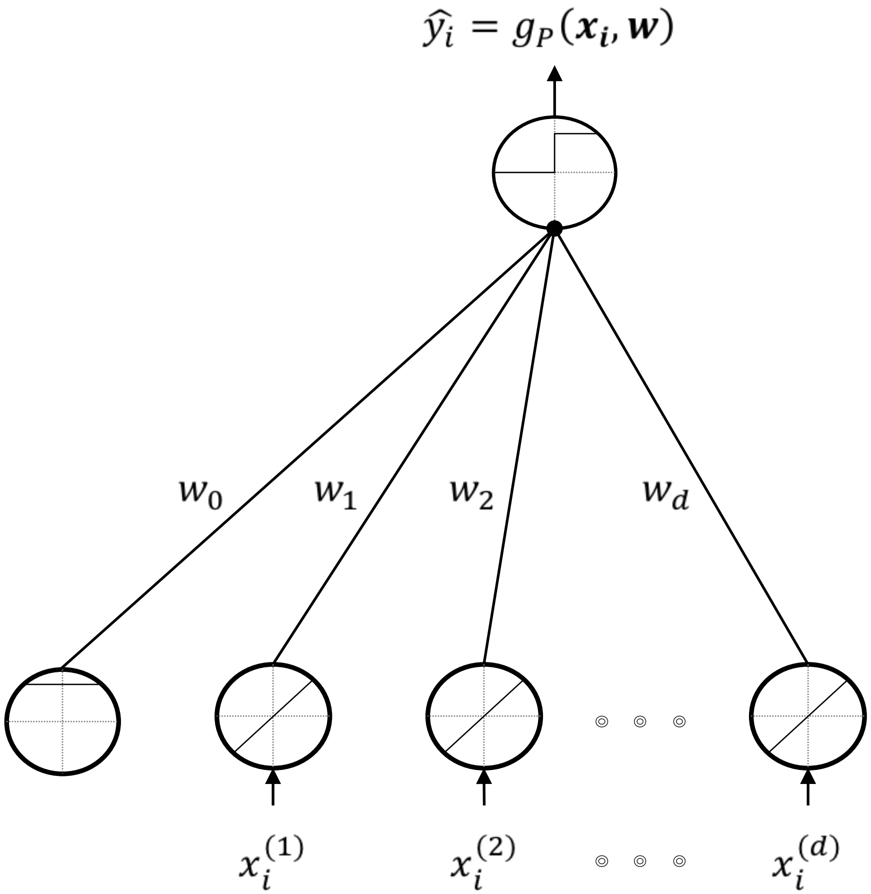


Figure source: https://neuwritesd.org/2015/10/22/deep-neural-networks-help-us-read-your-mind/

Artificial Neural Networks



Building Artificial Neural Networks



Output layer

Activation

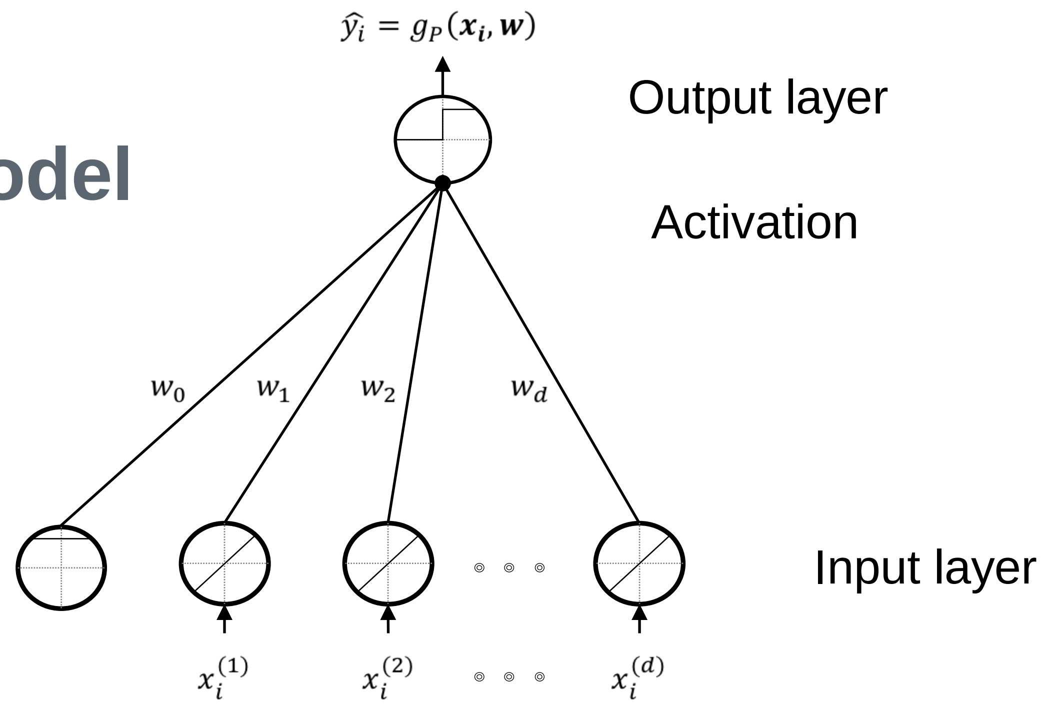
Input layer

Building Artificial Neural Networks (cont'd)

What does this "neuron" do?

$$g_P(\boldsymbol{x}_i, \boldsymbol{w}) = \begin{cases} 1, & \textit{if } \boldsymbol{w}^T\boldsymbol{x}_i > 0 \\ 0, & \text{otherwise} \end{cases}$$

The Perceptron model



Logistic Neuron

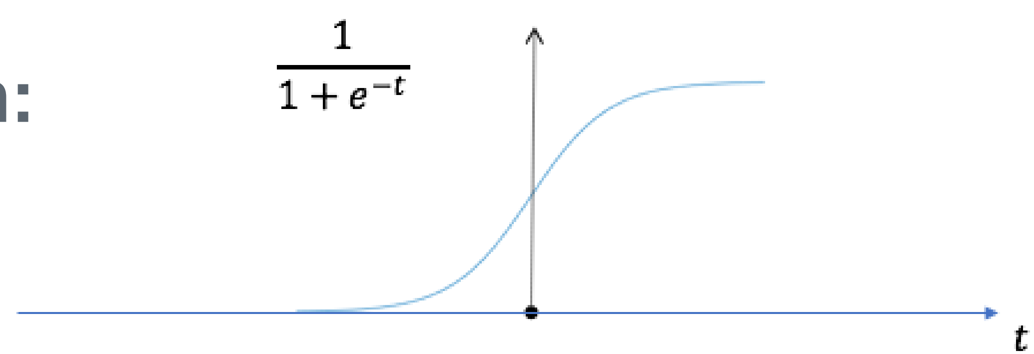
In Perceptron:

$$g_P(\boldsymbol{x_i}, \boldsymbol{w}) = \begin{cases} 1, & \text{if } \boldsymbol{w^T x_i} > 0 \\ 0, & \text{otherwise} \end{cases}$$

If we let:

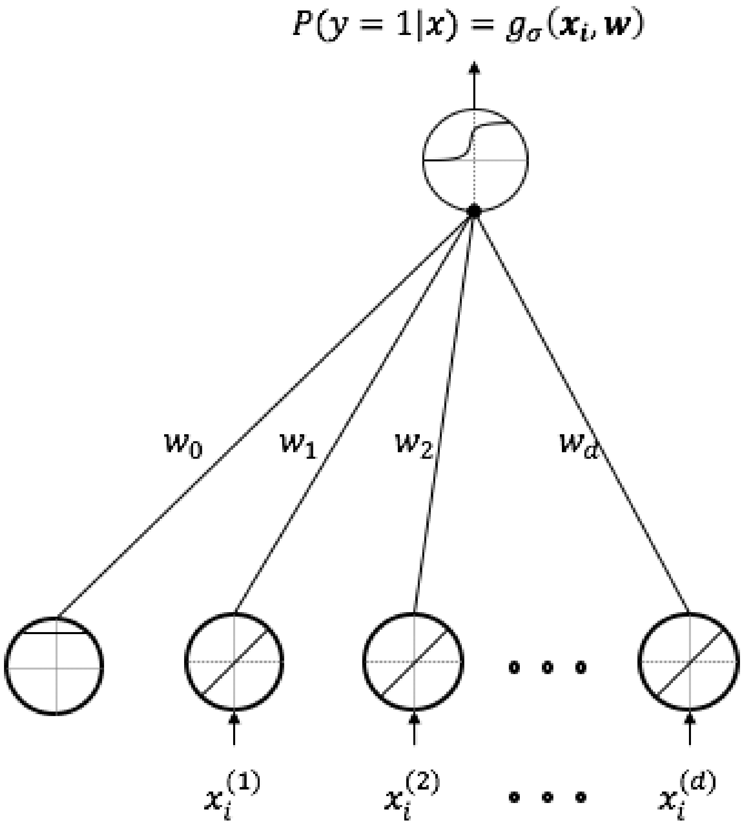
$$g_\sigma(\boldsymbol{x_i}, \boldsymbol{w}) = \frac{1}{1 + e^{-\boldsymbol{w}^T \boldsymbol{x}_i}}.$$

The logistic function:



Logistic Neuron (cont'd)

We have:



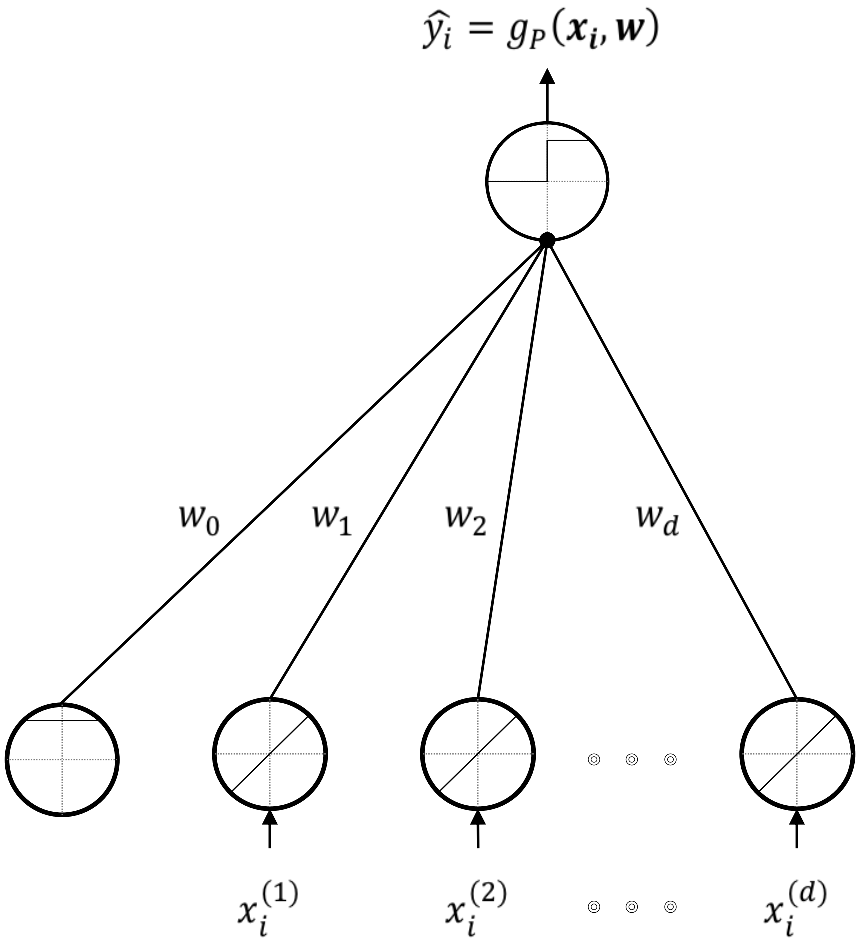
A probability prediction

Activation

Input layer

Learning in the Perceptron

- "Learning": how does the neuron adapt its weights in response to the inputs?



The Perceptron Learning Algorithm

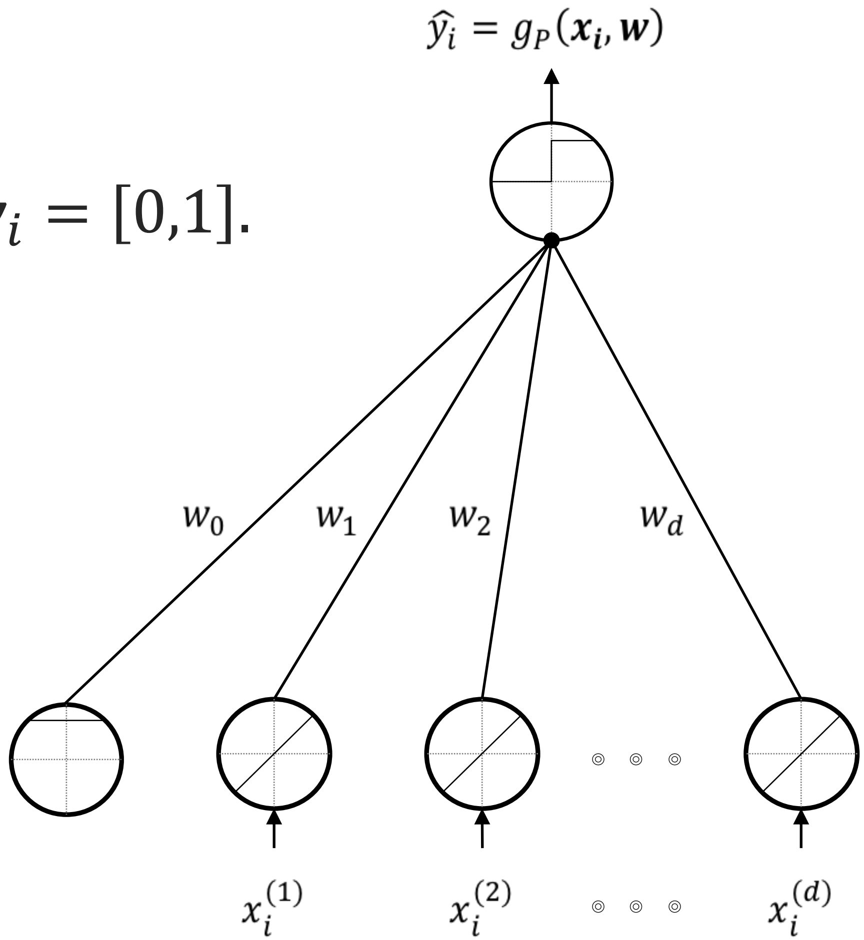
Input

- Training set

$D = \{(x_i, y_i), i \in [1,2, \dots n]\}. y_i = [0,1].$

Initialization

- Initialize the weights w(0) (and some thresholds)
- Weights may be set to 0 or small random values



The Perceptron Learning Algorithm (cont'd)

Iterate for t until a stop criterion is met

{

for each sample x_i with label y_i:

{

compute the output $\check{y}_i$ of the network

estimate the error of the network $e\big(w(t)\big) = \ y_i - \check{y}_i$

update the weight $w(t+1) = w(t) + e\big(w(t)\big)x_i$

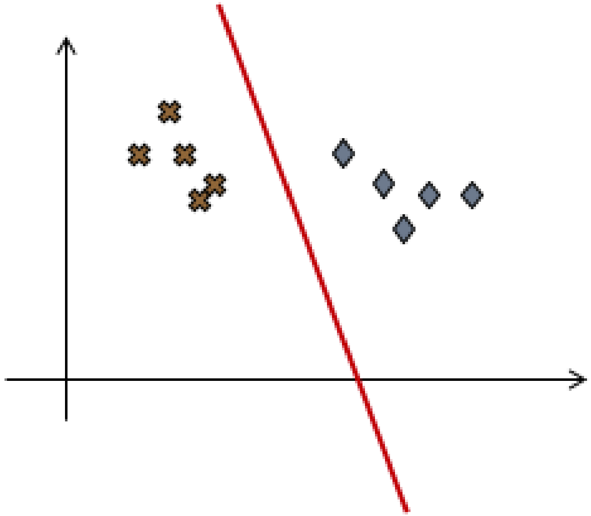
}

t++

}

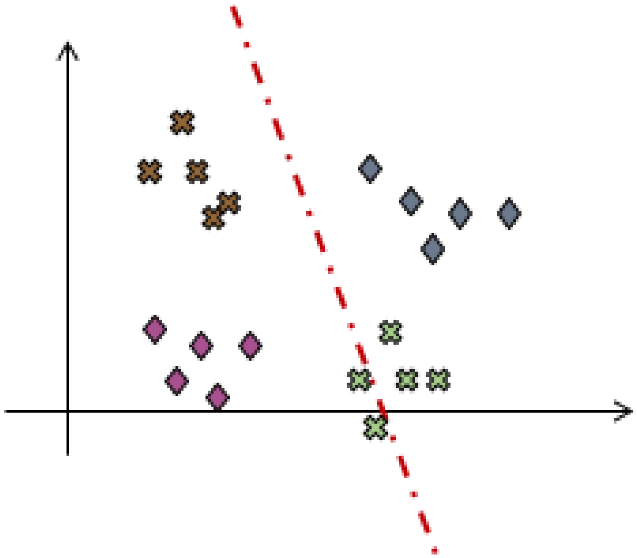
The Need for Multiple Layers

- This is easy and can be learned by the Perceptron Algorithm



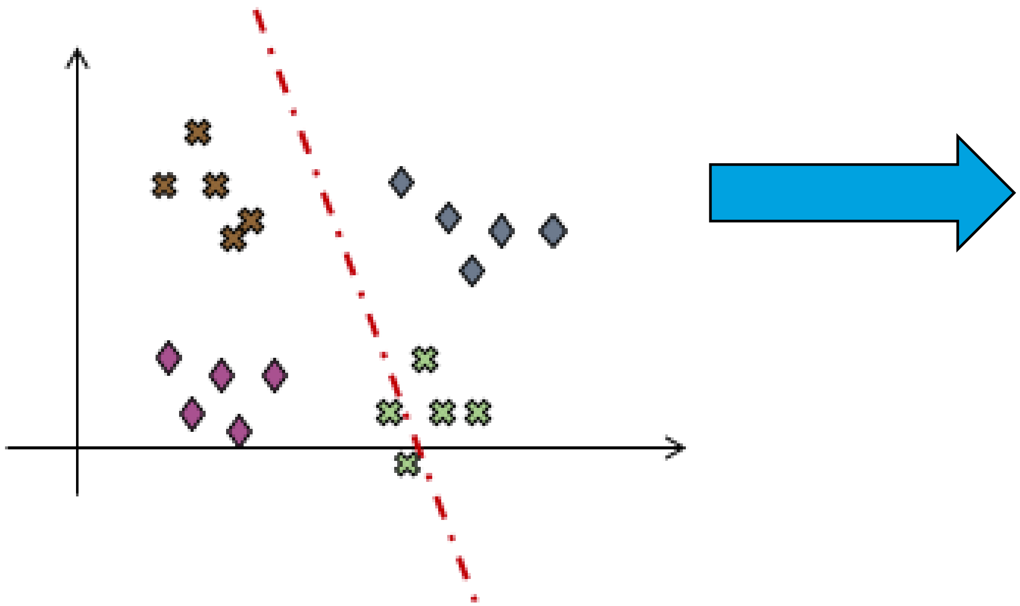
$$w_1x_1 + w_2x_2 + w_0 = 0$$

- But how about this?



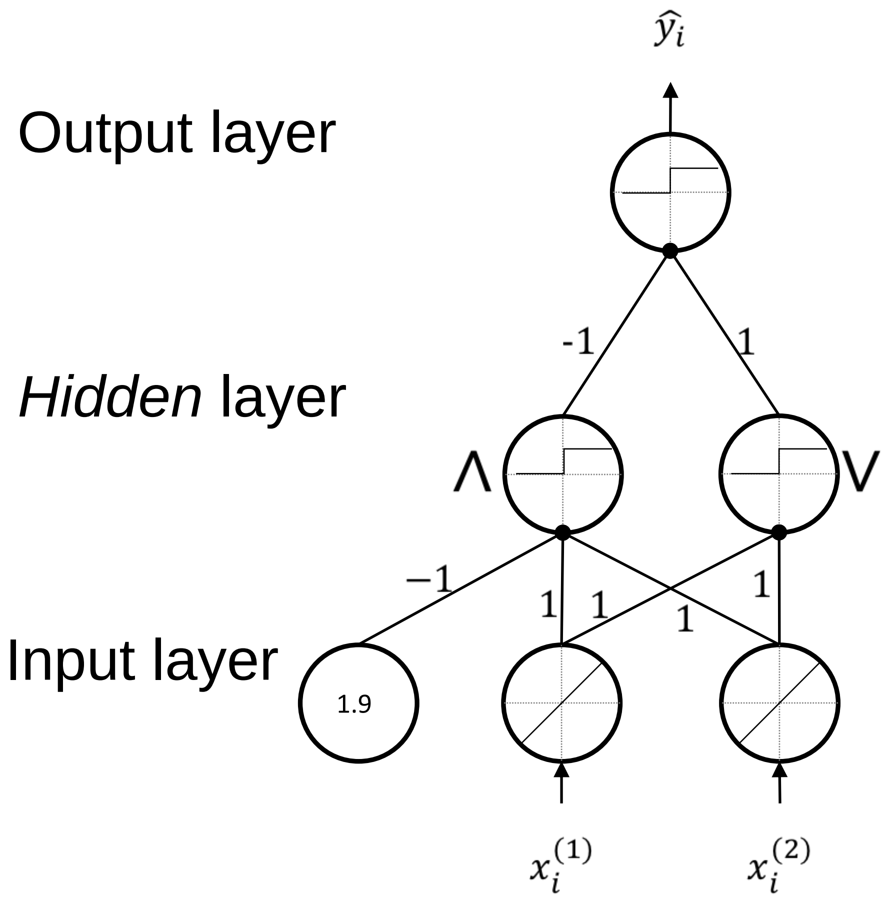
Extending to Multi-layer Neural Networks

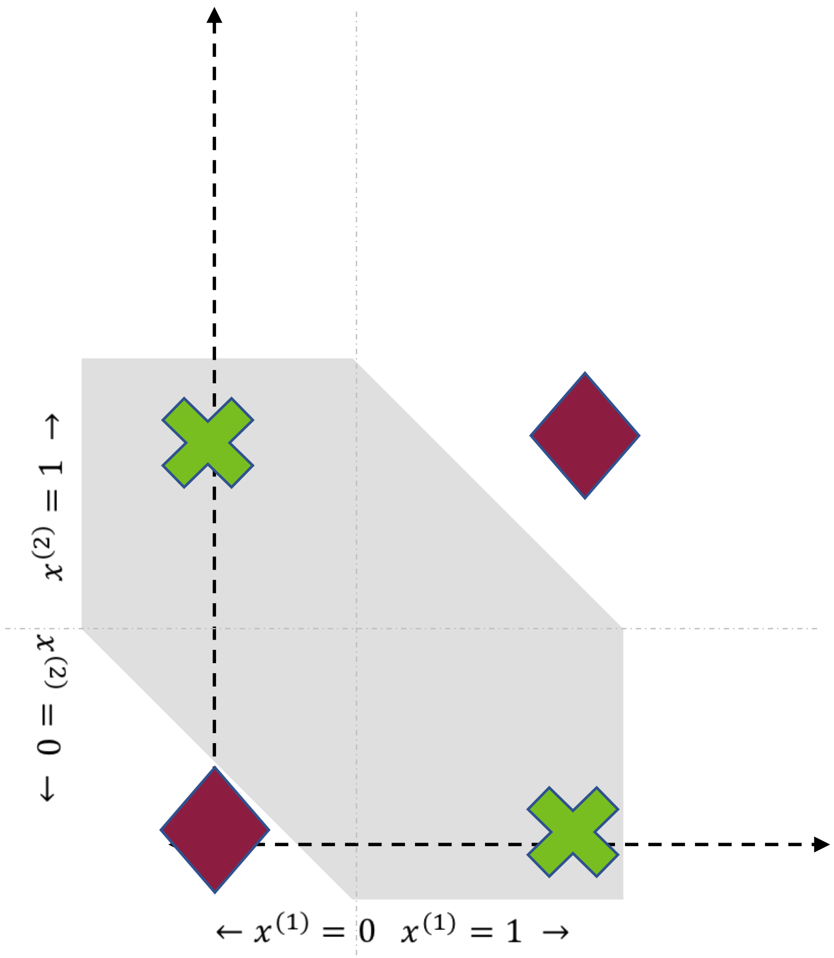
Question: Can a multi-layer version of the Perceptron (MLP) help solving the XOR problem?



The XOR Problem

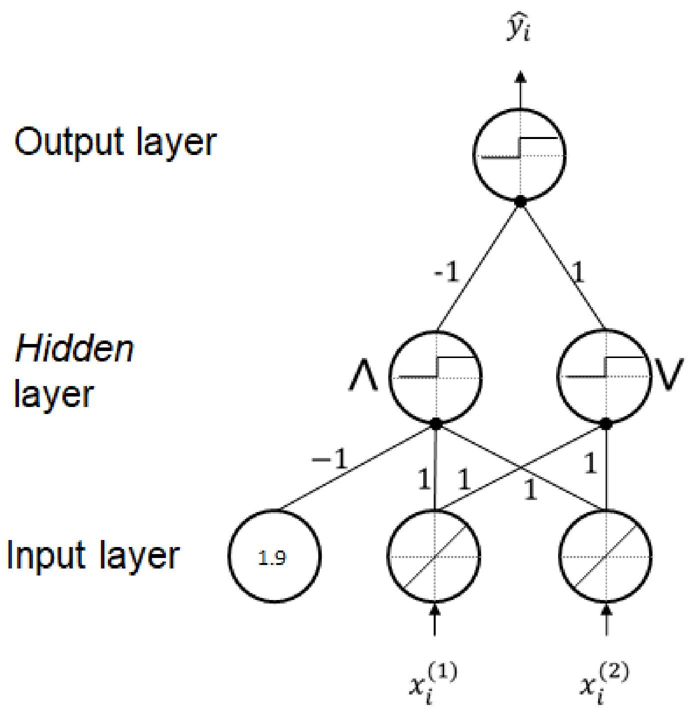
An MLP Solving the XOR Problem

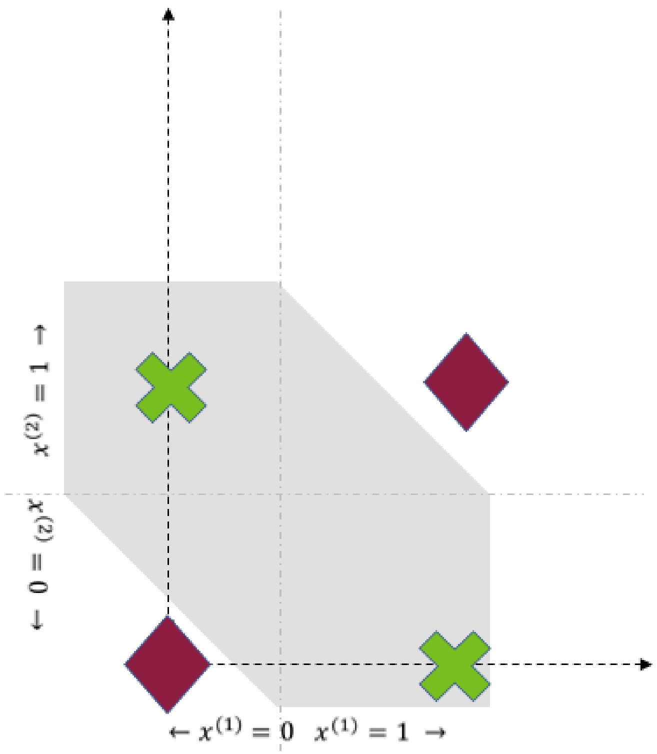




The Question of Learning

- **How can the network learn proper parameters from the given samples?**
  - Can the Perceptron algorithm be used?





Difficulty in Learning for MLP

Perceptron Learning Algorithm

- The weight update of the neuron is proportional to the “error” computed as $y_i - \hat{y}_i$.
  - This requires us to know the target output y_i.

Multi-layer Perceptron

- Except for the neurons on the output layer, other neurons (on the *hidden* layers) do not really have a target output given.

Back-propagation (BP) Learning for MLP

- **The key: Properly distribute error computed from output layer back to earlier layers to allow their weights to be updated in a way that reduce the error**
  - The basic philosophy of the BP algorithm

- **Differentiable activation functions**
  - We can use – e.g.,
    - the logistic neurons
    - neurons with sigmoid activation
    - or its variants

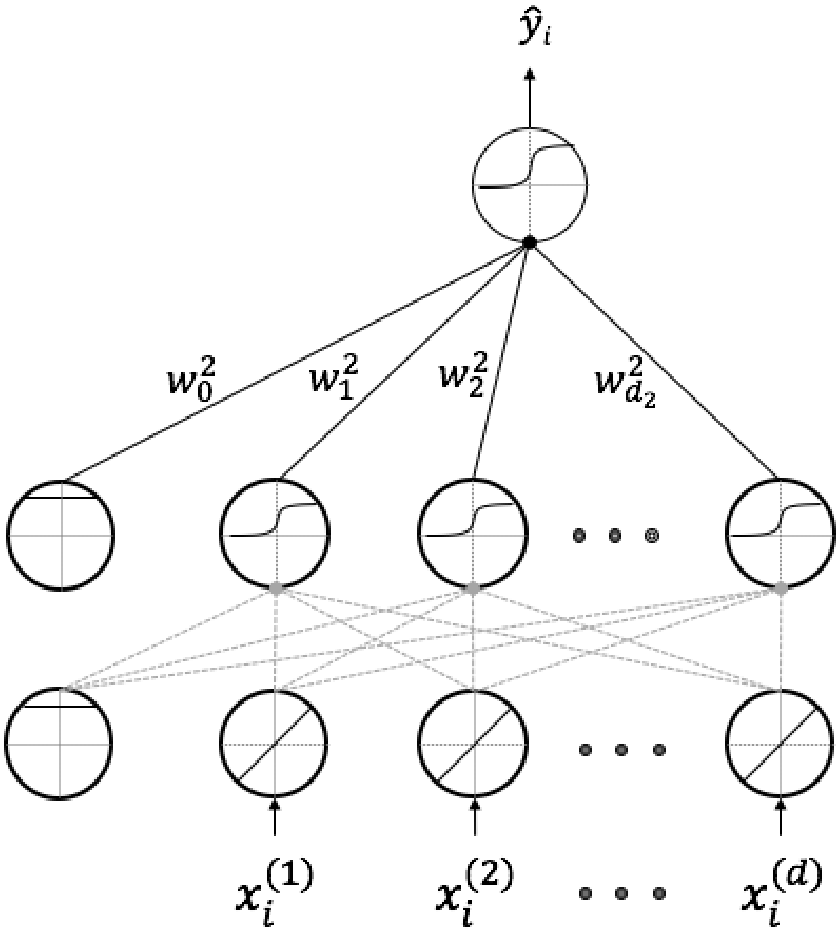
A Multi-Layer Neural Network

Using Logistic Neurons

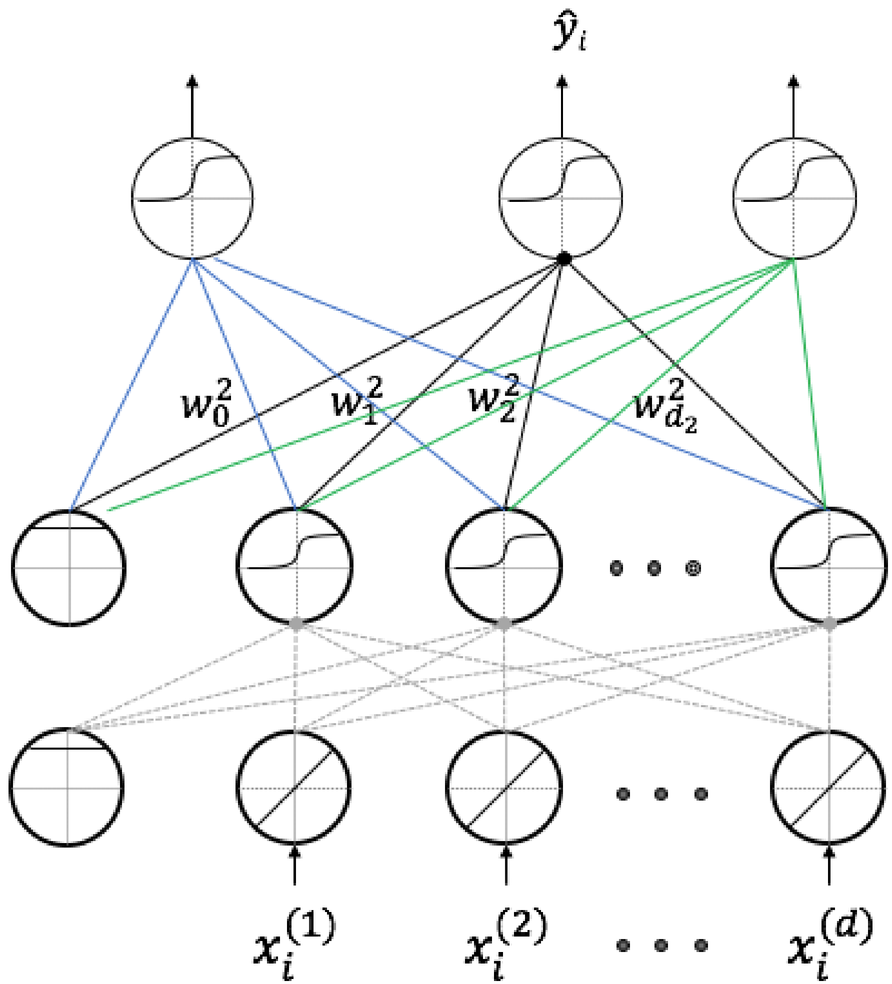
Output layer

Hidden layer

Input layer

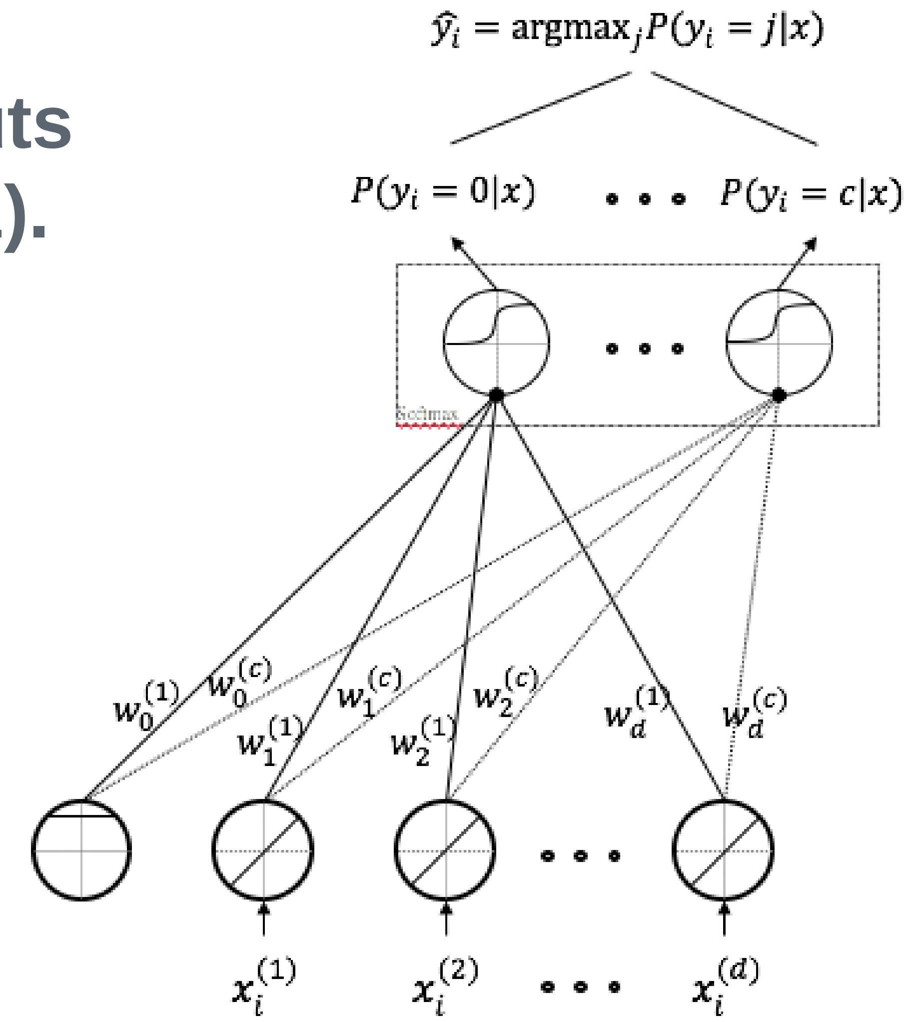


Handling Multiple (>2) Classes



Softmax for Handling Multiple Classes

- **Using *softmax* to normalize the outputs (so they add up to 1).**



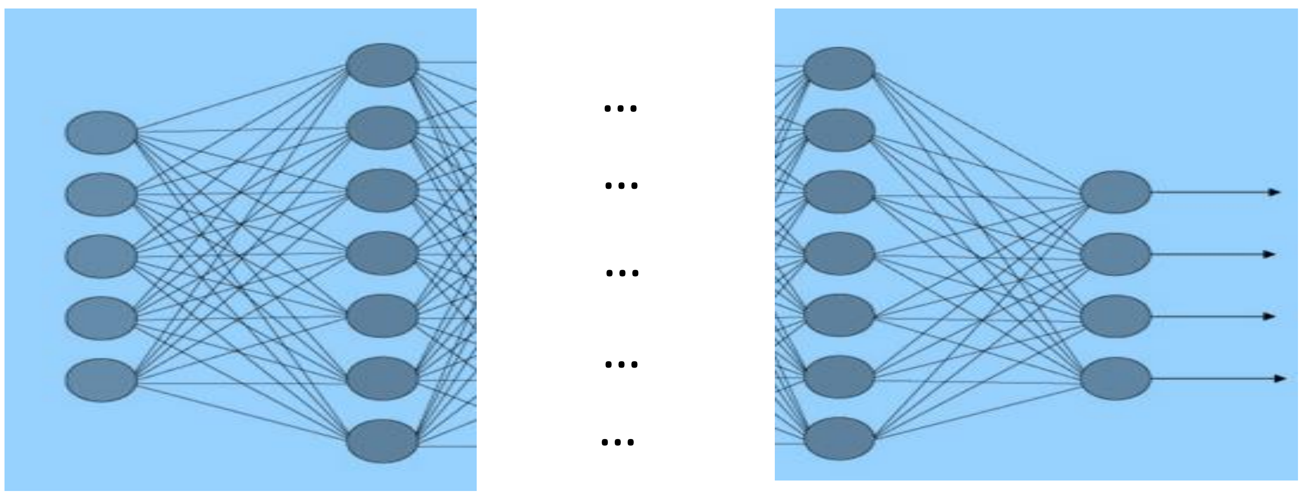
How to Compute “errors” in this Case?

Consider the cross-entropy as a loss function:

$$l(\boldsymbol{W}) = \sum_{i=1}^{n} \sum_{j=1}^{c} \mathbb{I}_j(y_i) \log P(y_i = j | x_i) \ ,$$

$$\mathbb{I}_j(y_i) = \begin{cases} 1, & if\ y_i = j \\ 0, & otherwise \end{cases}$$

Neural Networks and Deep Learning



Introduction to Deep Learning

Key Techniques Enabling Deep Learning

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Objective

Objective

Explain how, in principle, learning is achieved in a deep network

Objective

Explain key techniques that enable efficient learning in deep networks

Overview

- Back-propagation algorithm
- Design of activation functions
- Regularization for improving performance

* Technological advancement in computing hardware is certainly another enabling factor but our discussion will focus on basic, algorithmic techniques.

Back Propagation (BP) Algorithm

- **Simple Perceptron algorithm illustrates a path to learning by iterative optimization**
  - Updating weights based on network errors under current weights, and optimal weights are obtained when errors become 0 (or small enough)
- **Gradient descent is a general approach to iterative optimization**
  - Define a loss function J
  - Iteratively update the weights W according to the gradient of J with respect to W.

$\mathbf{W} \leftarrow \mathbf{W} - \eta \triangledown J(\mathbf{W})$ W is the parameter of the network; J is the objective function.

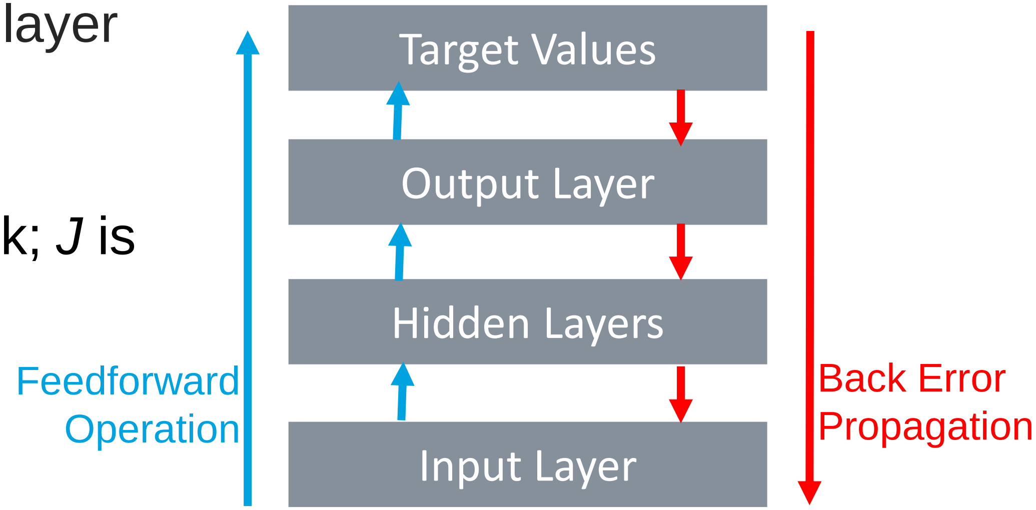
Back Propagation (BP) Algorithm (cont'd)

Generalizes/Implements the idea for multi-layer networks

- Gradient descent for updating weights in optimizing a loss function
- Propagating gradients back through layers
  - hidden layer weights are linked to loss gradient at output layer

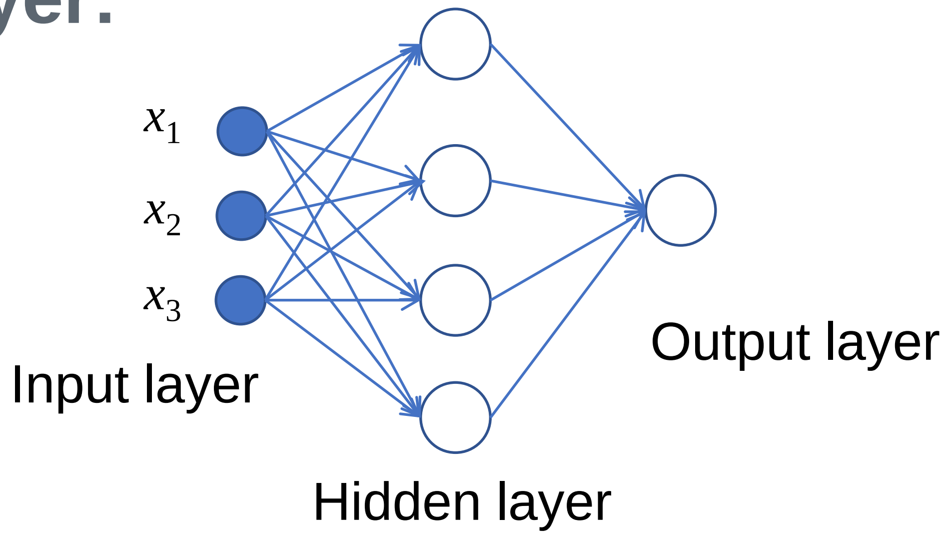
$$\mathbf{W} \leftarrow \mathbf{W} - \eta \bigtriangledown J(\mathbf{W})$$

W is the parameter of the network; *J* is the objective function.



Illustrating the BP Algorithm 1/6

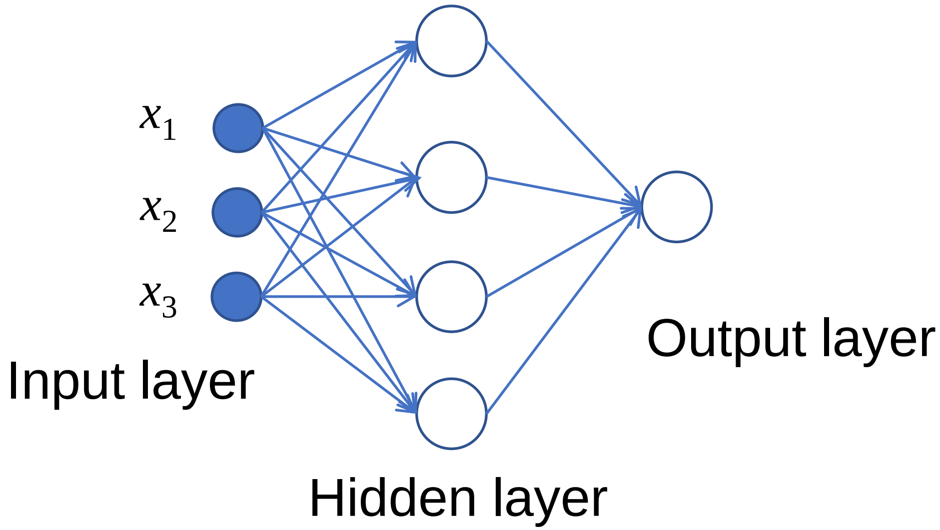
- **Let's consider a simple neural network with a single hidden layer. (We will only outline the key steps.)**
  - Let's write the net input and activation for a hidden node:
- **Let's write the net input and activation for the hidden layer:**



Illustrating the BP Algorithm 2/6

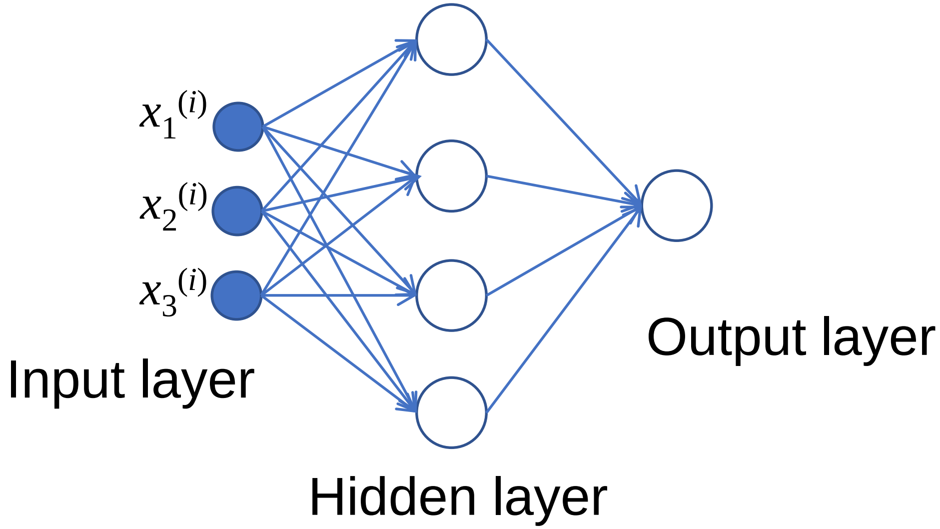
- Using matrix/vector notations, for the hidden layer:

- Similarly, for the output layer → Homework.



Illustrating the BP Algorithm 3/6

- Now consider m samples as input.
- Output layer is similarly done.



Illustrating the BP Algorithm 4/6

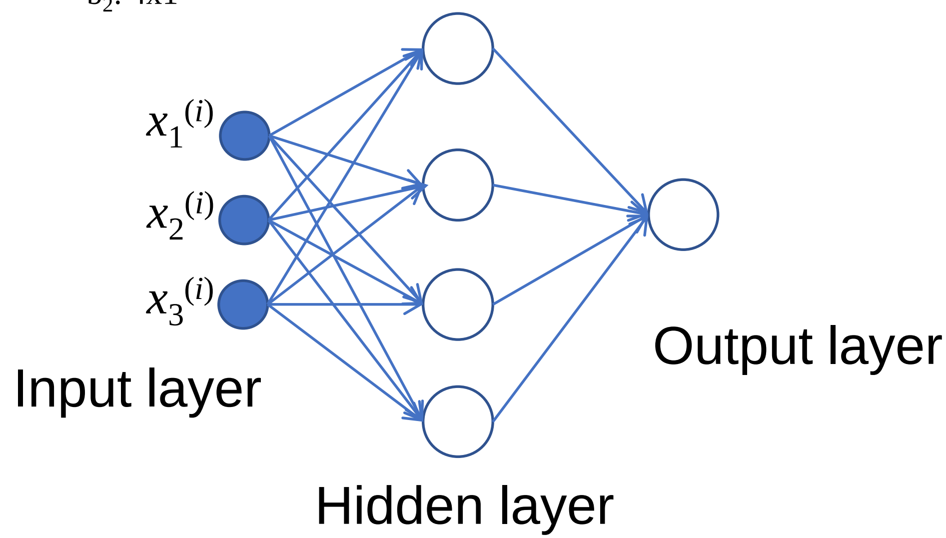
- Overall we have this flow of *feedforward* processing (note the notation change for simplicity: subscripts are for layers):

$$\xrightarrow[3\mathrm{xm}]{A_0=X} \boxed{Z_1=W_1A_0+b_1} \xrightarrow[4\mathrm{xm}]{Z_1} \boxed{A_1=f(Z_1)} \xrightarrow[4\mathrm{xm}]{A_1} \boxed{Z_2=W_2A_1+b_2} \xrightarrow[1\mathrm{xm}]{Z_2} \boxed{A_2=f(Z_2)} \xrightarrow[1\mathrm{xm}]{A_2} \boxed{L(A_2,Y)}$$

W_1: 4x3
b_1: 4x1

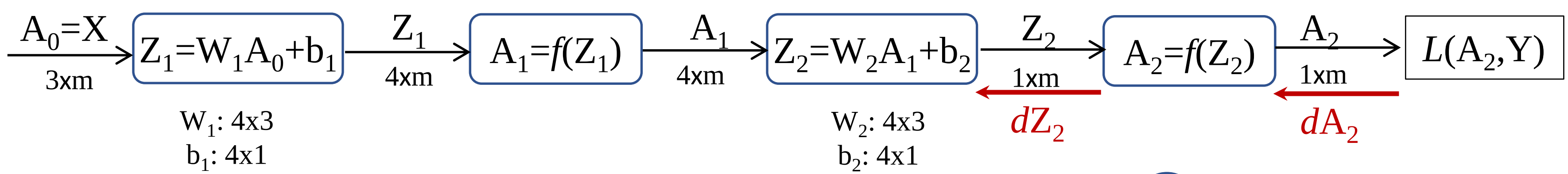
W_2: 4x3
b_2: 4x1

- **Consider** $\mathbf{dW_2} \triangleq \dfrac{\partial L}{\partial W_2}$

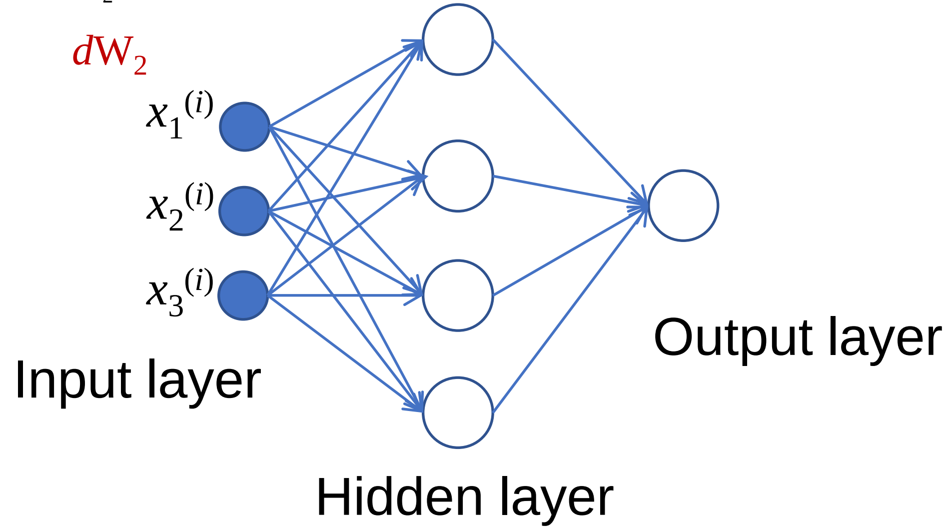


Illustrating the BP Algorithm 5/6

Back-propagation

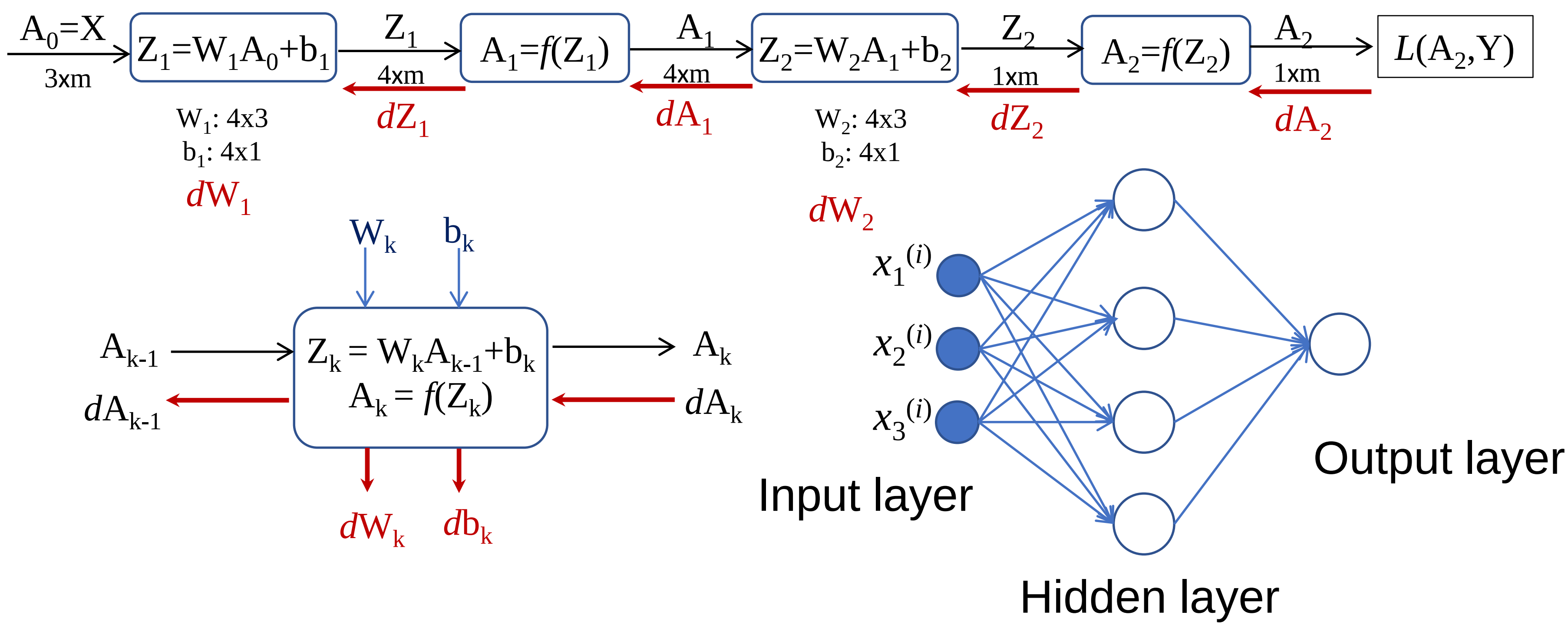


Consider $dW_1 \triangleq \frac{\partial L}{\partial W_1}$



Illustrating the BP Algorithm 6/6

A modular view of the layers



BP Algorithm Recap

- **The feedforward process: ultimately produce $A^{[K]}$ that leads to the prediction for Y.**
- **The backpropagation process:**
  - First compute the loss
  - Then compute the gradients via back-propagation through layers
  - Key: use the chain rule of differentiation
- **Essential to deep networks**
- **Suffers from several practical limitations**
  - gradient exploding
  - gradient vanishing
  - etc.
- **Many techniques were instrumental to enabling learning with BP algorithm for deep neural networks**

Activation Functions: Importance

- Provides non-linearity
- Functional unit of input-output mapping
- Its form impacts on gradients in BP algorithm

Activation Functions: Choices

Older Types

- Thresholding
- Logistic function
- tanh

Newer Types

- Rectifier $f(x) = \max(0, x)$ and its variants
- Rectified Linear Unit (ReLU)

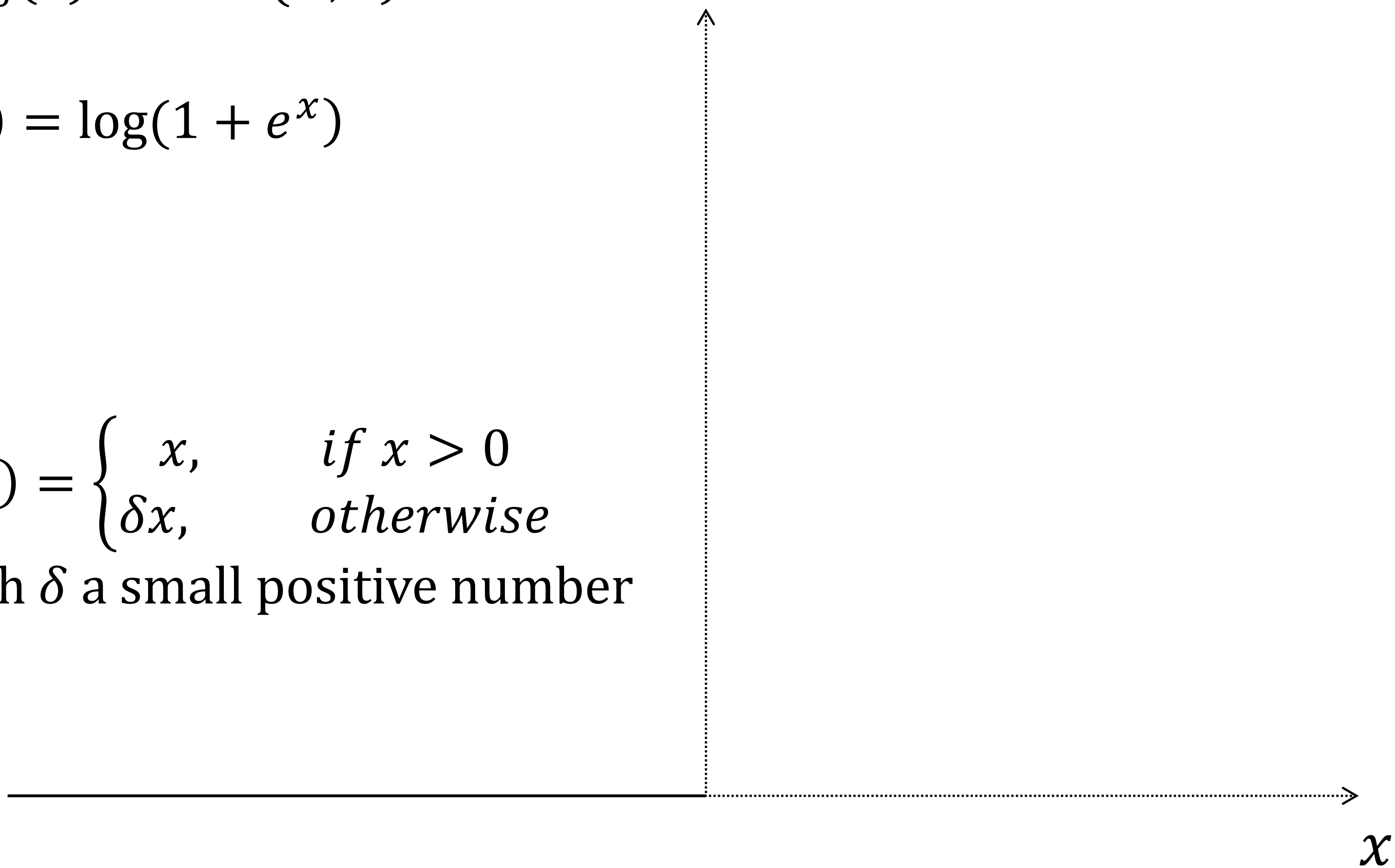
ReLU and Some Variants

$$a_{\mathrm{ReLU}}(x) = \max(0, x)$$

$$a_{\mathrm{s}}(x) = \log(1 + e^{x})$$

$$a_{\mathrm{L}}(x) = \begin{cases} x, & if\ x > 0 \\ \delta x, & otherwise \end{cases}$$

with δ a small positive number



The Importance of Regularization

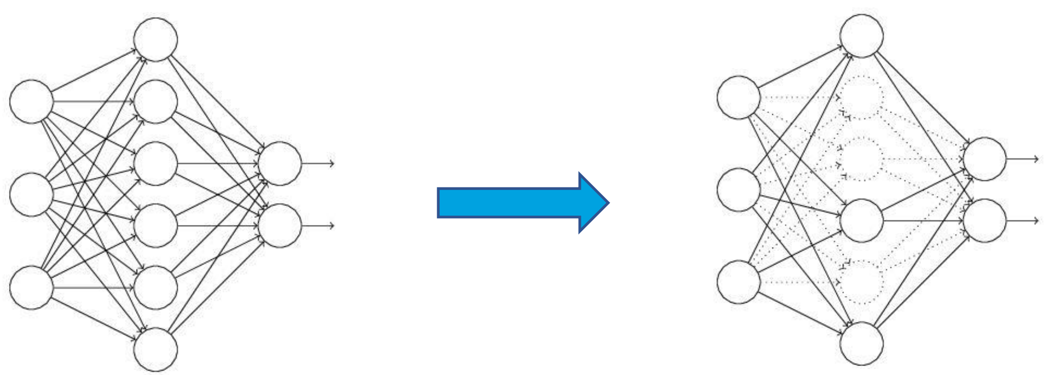
- **The parameter space is huge, if there is no constraint in search for a solution, the algorithm may converge to poor solutions.**
- **Overfitting is a typical problem**
  - Converging to local minimum good only for the training data

Some Ideas for Regularization

- **Favoring a network with small weights**
  - achieved by adding a term of L2-norm of the weights to original loss function
- **Preventing neurons from "co-adaptation" ➔ Drop-out**
- **Making the network less sensitive to initialization/learning rate etc.**
  - Batch normalization
- **Such regularization techniques have been found to be not only helpful but sometimes critical to learning in deep networks**

Drop-out

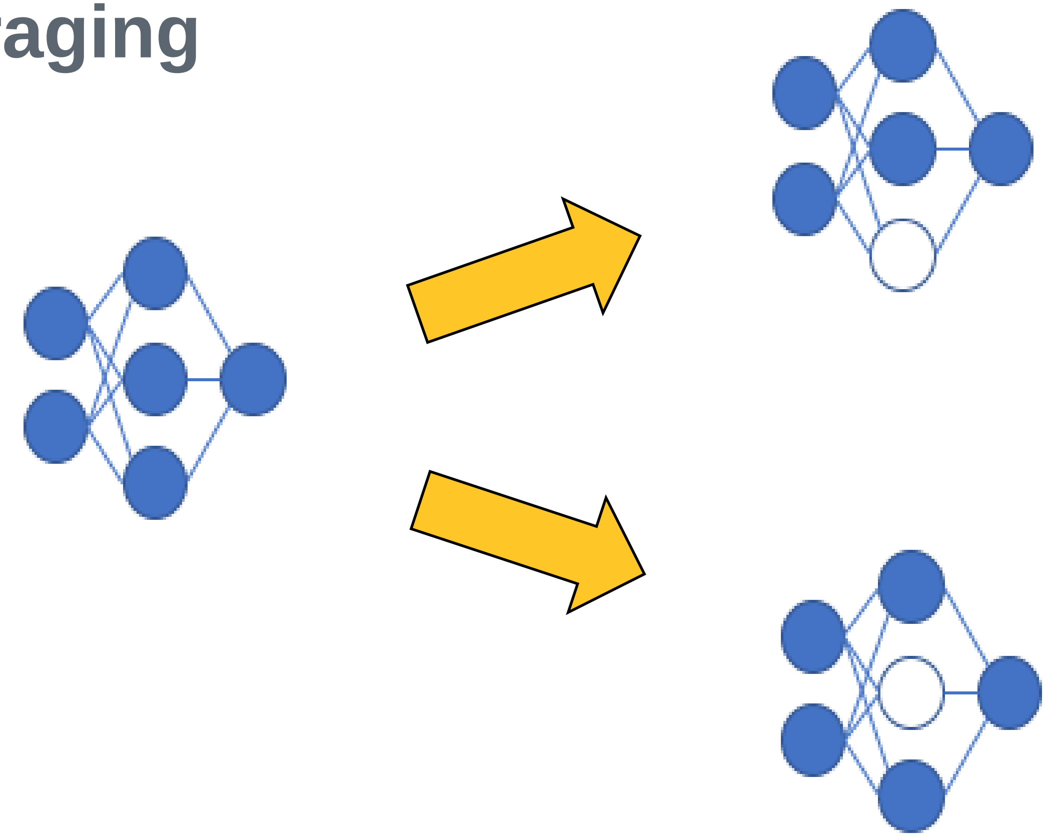
- Obtain (b) by randomly deactivate some hidden nodes in (a)
- For input x, calculate output y by using the activated nodes ONLY
- Use BP to update weights (which connect to the activated nodes) of network
- Activate all nodes
- Go back to first step



(a) (b)

Why Drop-out?

- Reducing co-adaptation of neuron
- Model averaging



Batch Normalization (BN)

- **Inputs to network layers are of varying distributions, the so-called internal covariate shift [Ioffe and Szegedy, 2015]**
  - Careful parameter initialization and low learning rate are required
- **BN was developed to solve this problem by normalizing layer inputs of a batch**

The Simple Math of BN

For a mini-batch with size = m, first calculate

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$$

Up to this point, $\widehat{x}$ has mean = 0 and standard deviation = 1

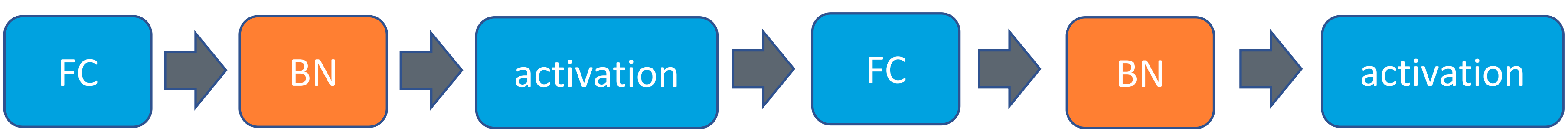
How is BN Used in Learning?

- Define two parameters and so that the output of the BN layer can be calculated as:

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)$$

- Parameters β and γ can be learned by minimizing the lost function via gradient descent

- Usually used right before the activation functions



Other Regularization Techniques

- **Weight sharing**
- **Training data conditioning**
- **Sparsity constraints**
- **Ensemble methods (committee of networks)**

➔ Some of these will be discussed in later examples of networks.

Introduction to Deep Learning

Some Basic Deep Architecture

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Arizona State University

Objective

Objective

Appraise the detailed architecture of a basic convolutional neural network

Objective

Explain the basic concepts and corresponding architecture for auto-encoders and recurrent neural networks

Overview

- **Convolutional Neural Network (CNN)**
  - will be given the most attention, for its wide range of application
- **Auto-encoder**
- **Recurrent Neural Networks (RNN)**

Convolutional Neural Network (CNN)

- Most useful for input data defined on grid-like structures, like images or audio
- Built upon concept of “convolution” for signal/image filtering
- Invokes other concepts like pooling, weight-sharing, and (visual) receptive field, etc.

Image Filtering via Convolution 1/5

Kernel coefficients

$$\frac{1}{12}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

Kernel or mask

image

255	128	128	240	1	128	24	255
255	128	245	240	1	128	24	255
245	128	245	240	1	128	128	128
24	24	24	255	255	0	0	0
0	0	0	0	0	0	0	0
245	245	128	128	128	128	245	245
245	245	245	240	240	240	255	240
255	240	128	240	240	128	240	255

Image Filtering via Convolution 2/5

New pixel value =
(1*255+
1*128+
1*128+
1*255+
4*128+
1*245+
1*245+
1*128+
1*245)/12=
2141/12
=178

255 1	128 1	128 1	240	1	128	24	255
255 1	128 4	245 1	240	1	128	24	255
245 1	128 1	245 1	240	1	128	128	128
24	24	24	255	255	0	0	0
0	0	0	0	0	0	0	0
245	245	128	128	128	128	245	245
245	245	245	240	240	240	255	240
255	240	128	240	240	128	240	255

Image Filtering via Convolution 3/5

255	128	128	240	1	128	24	255
255	**178**	245	240	1	128	24	255
245	128	245	240	1	128	128	128
24	24	24	255	255	0	0	0
0	0	0	0	0	0	0	0
245	245	128	128	128	128	245	245
245	245	245	240	240	240	255	240
255	240	128	240	240	128	240	255

Image Filtering via Convolution 4/5

New pixel value = (1*128+ 1*128+ 1*240+ 1*178+ 4*245+ 1*240+ 1*128+ 1*245+ 1*240)/12= 2507/12 =209

255	128 1	128 1	240 1	1	128	24	255
255	**178** 1	245 4	240 1	1	128	24	255
245	128 1	245 1	240 1	1	128	128	128
24	24	24	255	255	0	0	0
0	0	0	0	0	0	0	0
245	245	128	128	128	128	245	245
245	245	245	240	240	240	255	240
255	240	128	240	240	128	240	255

Image Filtering via Convolution 5/5

255	128	128	240	1	128	24	255
255	**178**	**209**	240	1	128	24	255
245	128	245	240	1	128	128	128
24	24	24	255	255	0	0	0
0	0	0	0	0	0	0	0
245	245	128	128	128	128	245	245
245	245	245	240	240	240	255	240
255	240	128	240	240	128	240	255

Image Filtering via Convolution: Kernels

- **By varying coefficients of the kernel, we can achieve different goals**
  - Smoothing, sharpening, detecting edges, etc.
- **Better yet: can we learn proper kernels? Part of CNN objective**
- **Examples of Kernels:**

1/12

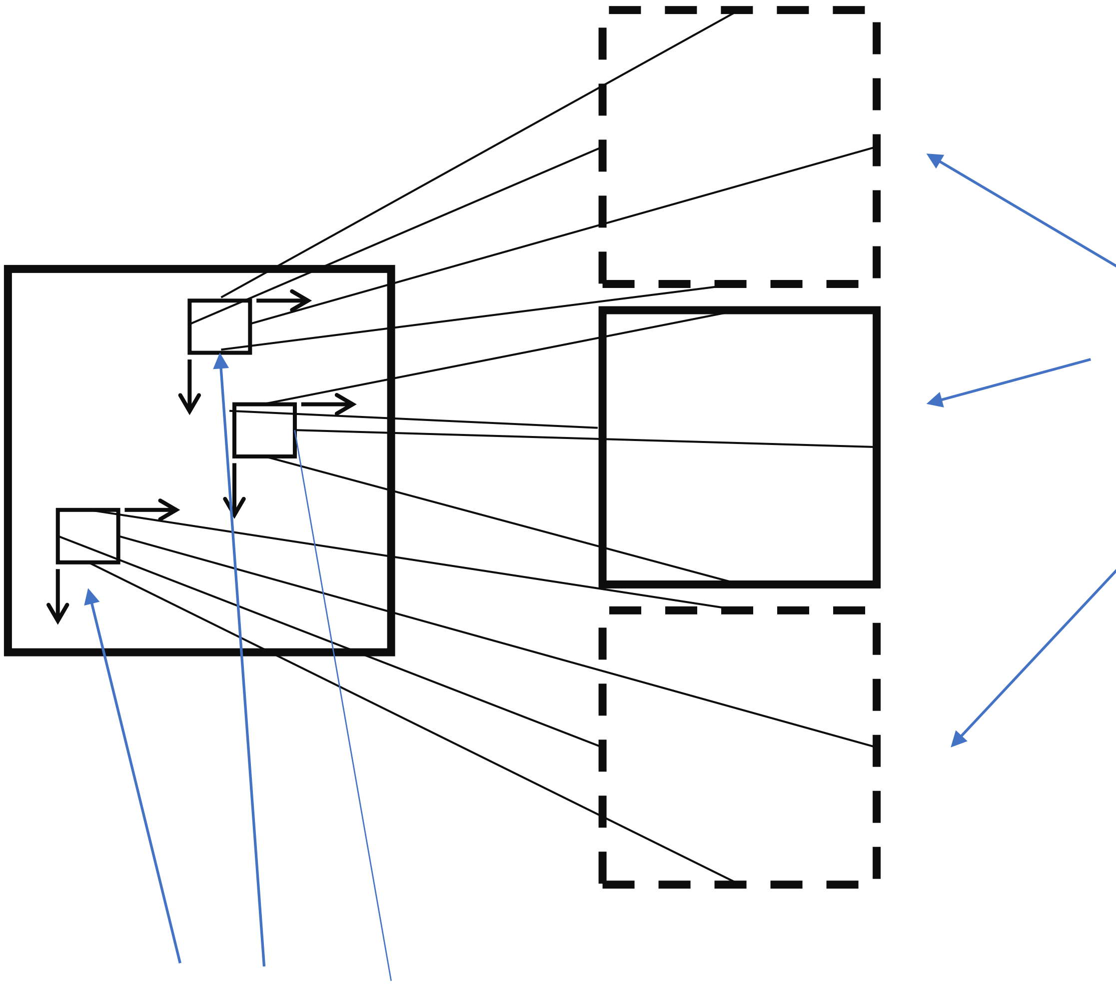
1	1	1
1	4	1
1	1	1

Smoothing/Noise-reduction

1	0	-1
1	0	-1
1	0	-1

(Vertical) Edge detection

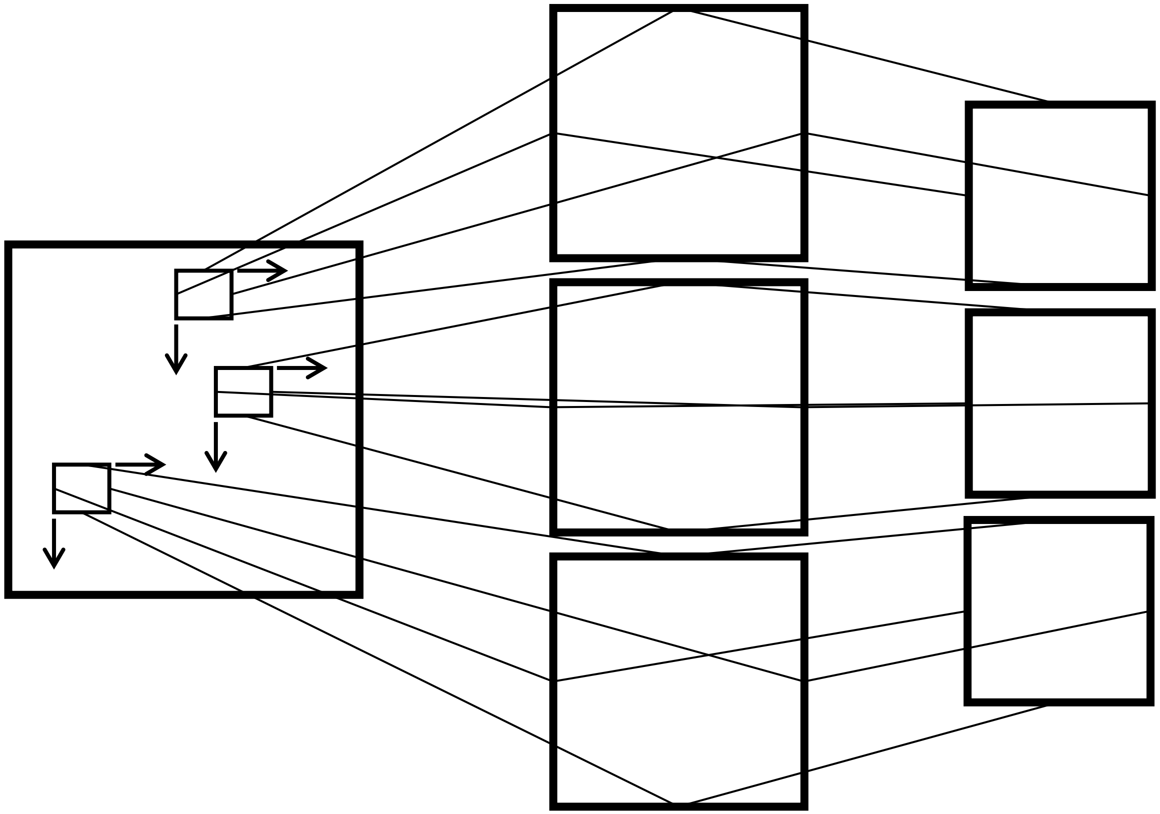
2D Convolutional Neuron



The number of kernels defines the number of *features maps* (*channels*).

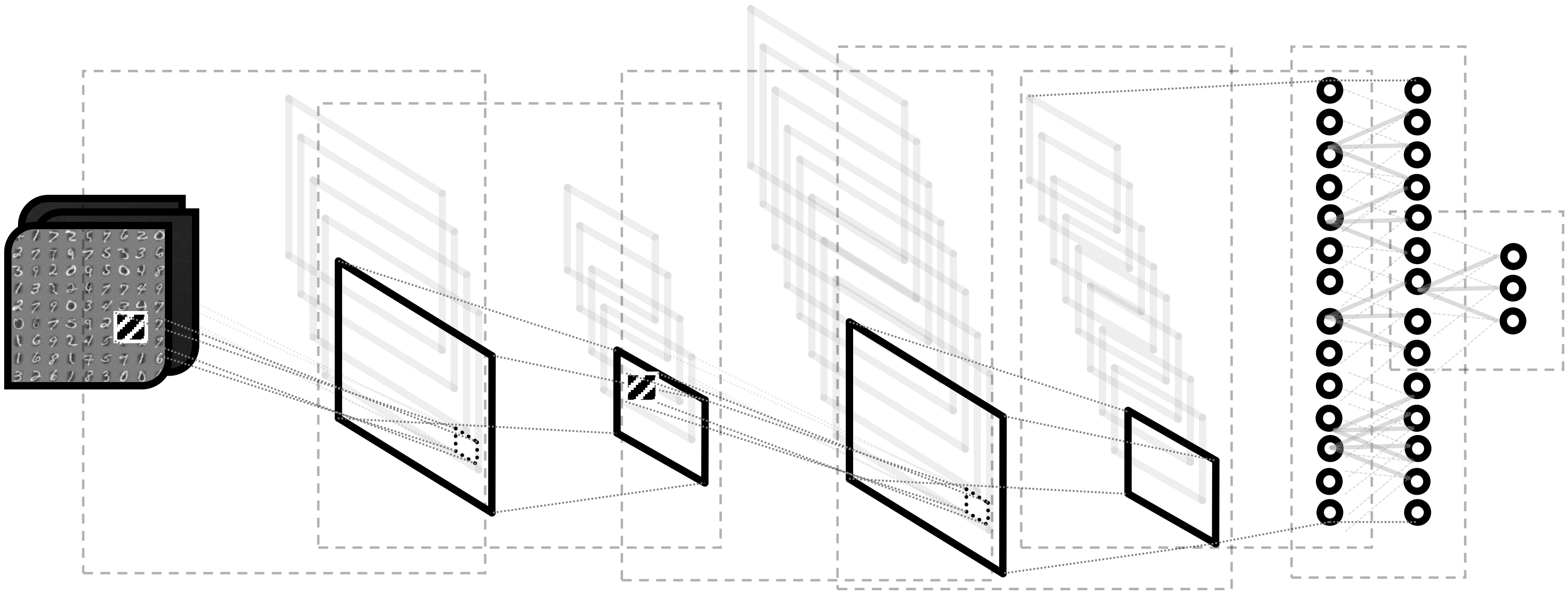
The sizes of the kernels define the *receptive fields*.

Convpool Layer



Convolution, pooling, and going through some activations

Illustrating A Simple CNN



Some convpool layers plus some fully-connected layers

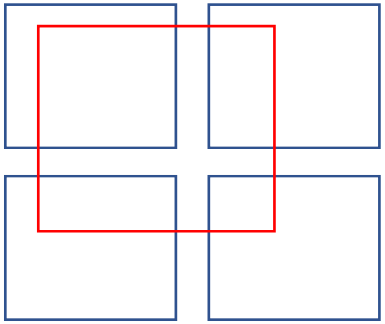
CNN Examples - Different Complexities

- LeNet
- AlexNet

LeNet

- Each pixel in layer 3 corresponds to 7/3 of a pixel in the input Second level
- Receptive field of layer 1 is 5X5

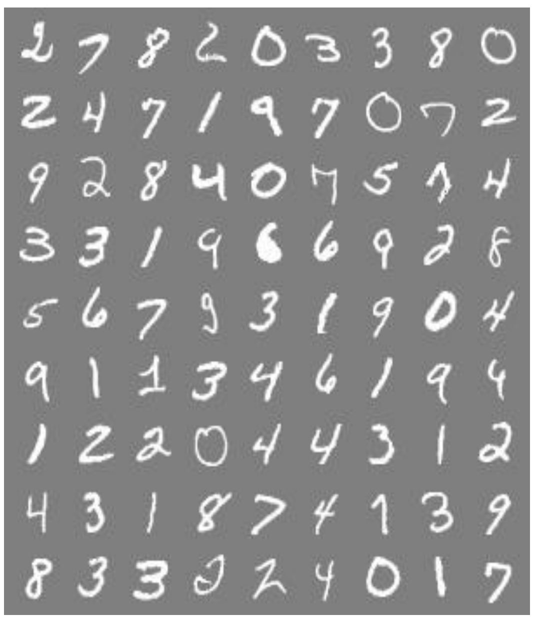
Layer Number	Input Shape	Receptive Field	Number of Feature Maps	Type of Neuron
1	28 X 28 X 1	5 X 5	20	Convolutional
2	24 X 24 X 20	2 X 2		Pooling
3	12 X 12 X 20	5 X 5	50	Convolutional
4	8 X 8 X 50	2 X 2		Pooling
5	800	1 X 1	500	Fully Connected
6	500		10	Softmax

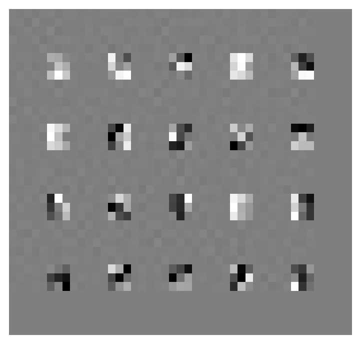


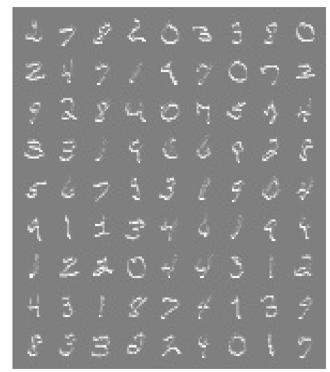
LeCun, Yann, et al. "Gradient-based learning applied to document recognition." *Proceedings of the IEEE* 86.11 (1998): 2278-2324.

Case Study: LeNet

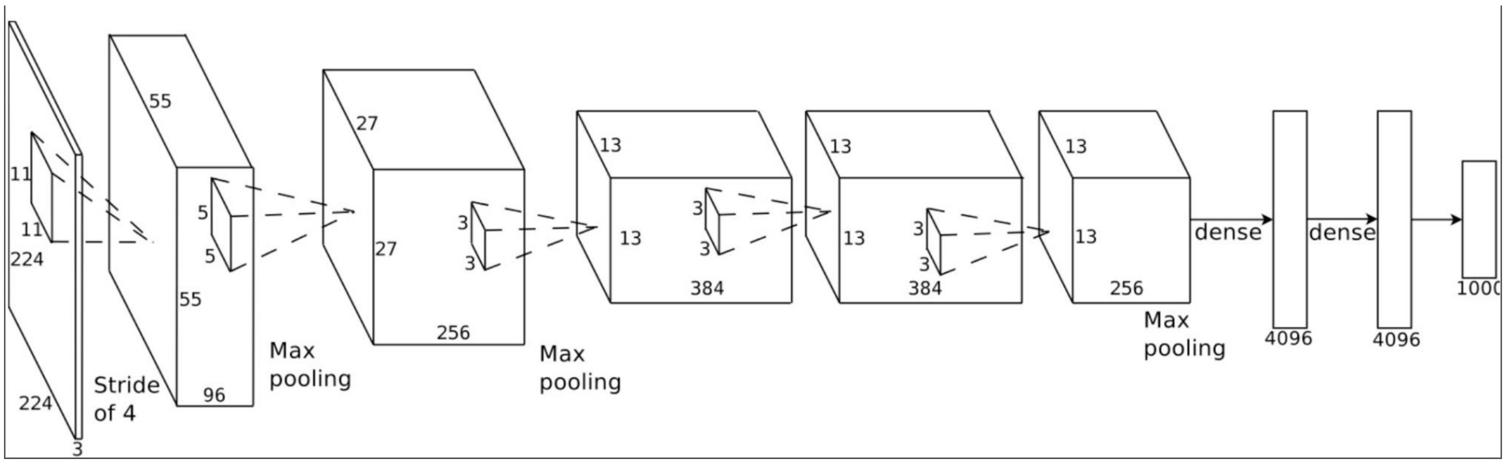
- This is after training the network for 75 epochs with a learning rate of 0.01
- Produces an accuracy of 99.38% on the MNIST dataset.

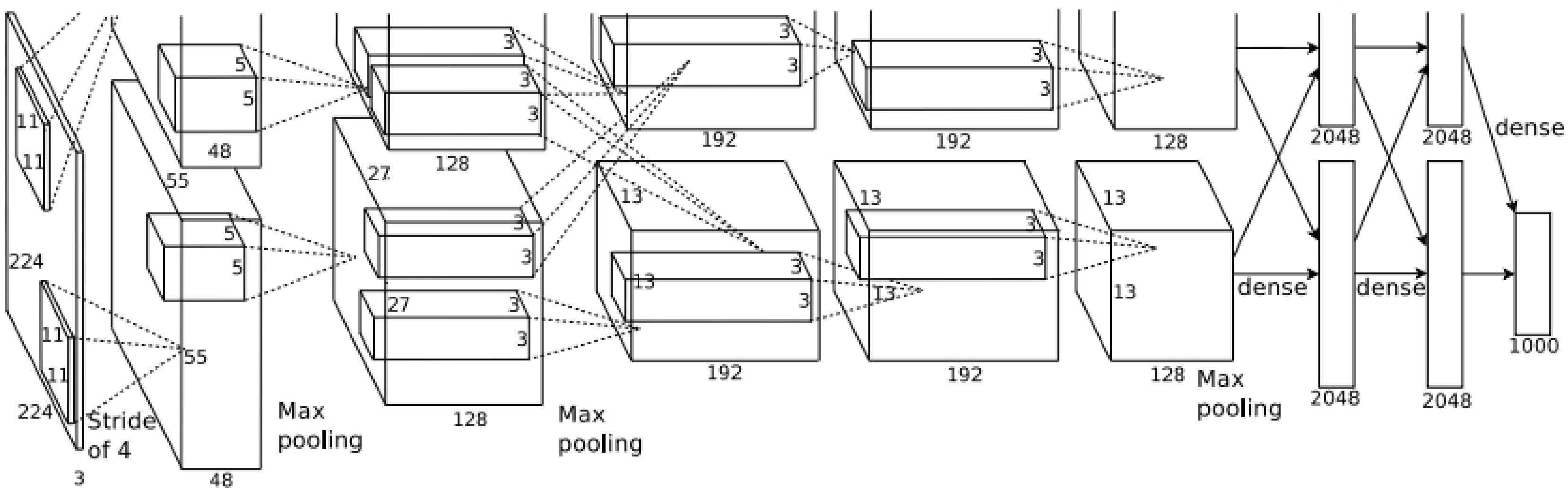






Case Study: AlexNet





Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. "Imagenet classification with deep convolutional neural networks." *Advances in neural information processing systems*. 2012.

Case Study: AlexNet 1/3

Layer Number	Input Shape	Receptive Field	Number of Kernels	Type of Neuron
1	224 X 224 X 3	11 X 11, stride 4	96	Convolutional
2		3 X 3, stride 2		Pooling
3	55 X 55 X 96	5 X 5	256	Convolutional
4		3 X 3, stride 2		Pooling
5	13 X 13 X 256	3 X 3, padded	384	Convolutional
6	13 X 13 X 384	3 X 3, padded	384	Convolutional
7	13 X 13 X 384	3 X 3	256	Convolutional
8	43264	1 X 1	4096	Fully Connected
9	4096	1 X 1	4096	Fully Connected
10	4096		1000	Softmax

Receptive field of the layer 7 is

~ 52 pixels !! which is almost as big as an object part (about one – fourth of the input image)

Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. "Imagenet classification with deep convolutional neural networks." *Advances in neural information processing systems*. 2012.

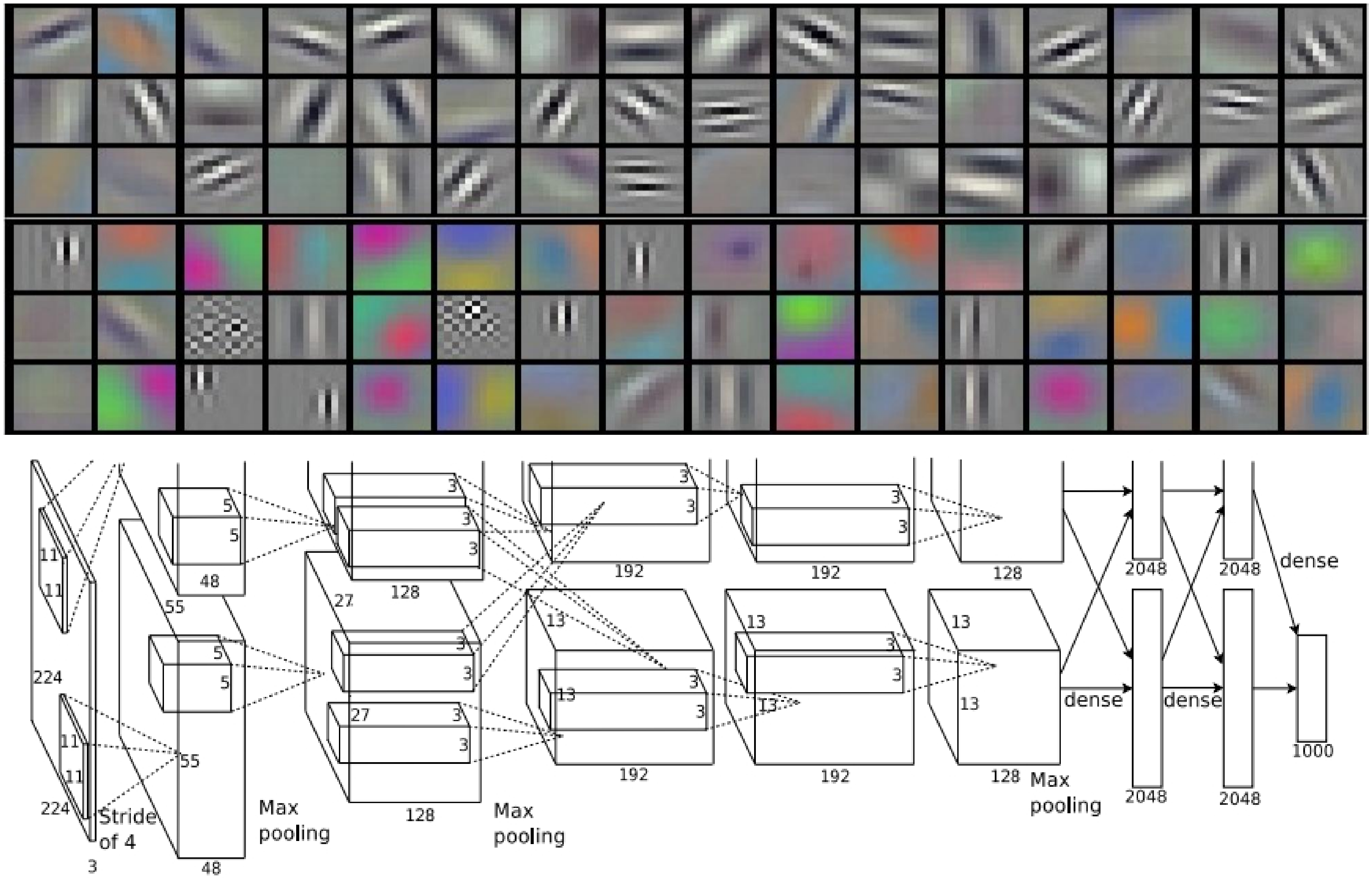
Case Study: AlexNet 2/3

- **Imagenet -15 million images in over 22,000 categories**
- **Imagenet categories are much more complicated than other datasets**
  - Often difficult even for humans to categorize perfectly
  - Average human-level performance is about 96% on this dataset
- **(ILSVRC), used about 1000 of these categories**
- **AlexNet was the earliest systems to break the 80% mark**
  - Non-neural conventional techniques were unable to achieve such performance

Case Study: AlexNet 3/3

- **AlexNet was huge at the time.**
  - The size could lead to instability during training or inability to learn, if without proper regularization
- **Some techniques were used to make it trainable**
  - AlexNet was the first prominent network to feature ReLU
  - Features multi-GPU training (originally trained the networks on two Nvidia GTX 580 GPUs with 3GB)

Case Study: AlexNet Filters



Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. "Imagenet classification with deep convolutional neural networks." *Advances in neural information processing systems*. 2012.

CNN Recap

- **The CNNs are similar to the basic MLP architecture illustrated earlier, but some key extensions include:**
  - The concept of weight-sharing through kernels
  - Weight-sharing enables learnable kernels, which in turn define feature maps
  - The idea of pooling

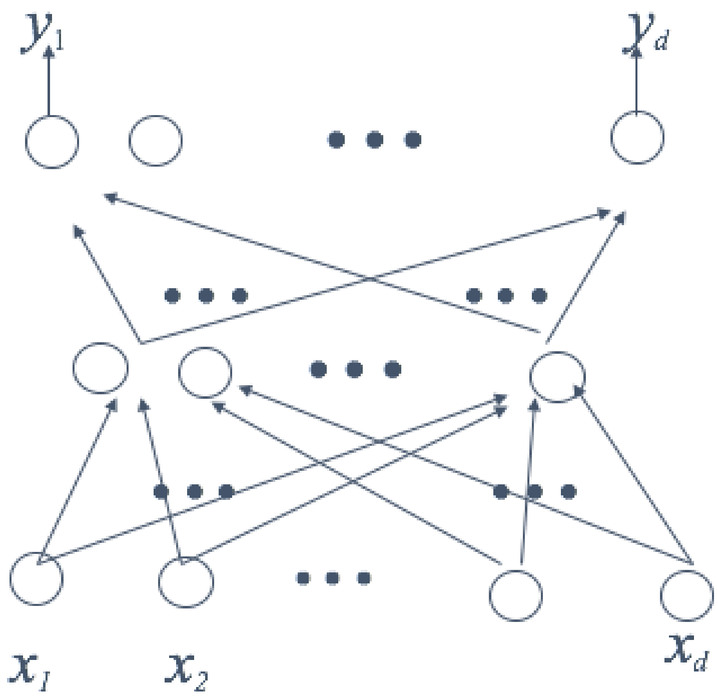
Auto-encoder 1/4

- **Networks seen thus far are all trained via supervised learning**

- **Sometimes we may need to train a network without supervision:**

  → Unsupervised learning

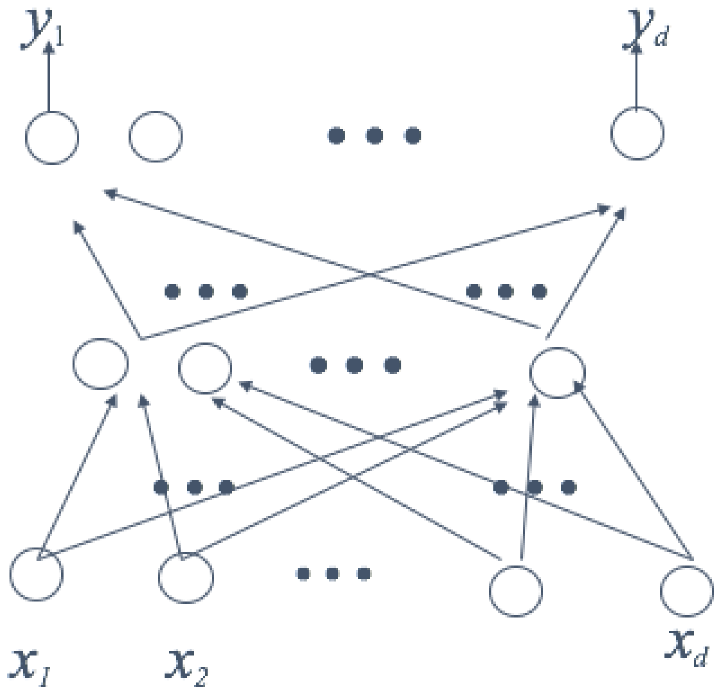
- **Auto-encoder is a such example**
  - Consider y_i being an approximation of x_i.



Auto-encoder 2/4

- Perfect auto-encoder would map x_i to x_i

- Learn good representations in the hidden layer



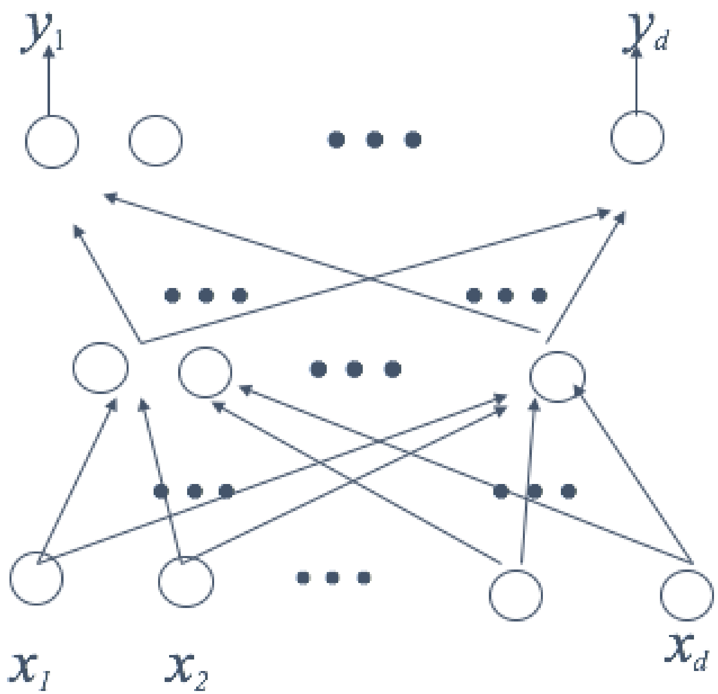
Auto-encoder 3/4

Consider two cases

- Much fewer hidden nodes than input nodes
- Many hidden nodes or more hidden nodes than input nodes

Case 1: Encoder for compressing input and compressed data should still be able to reconstruct the input

- Similar to, e.g., PCA



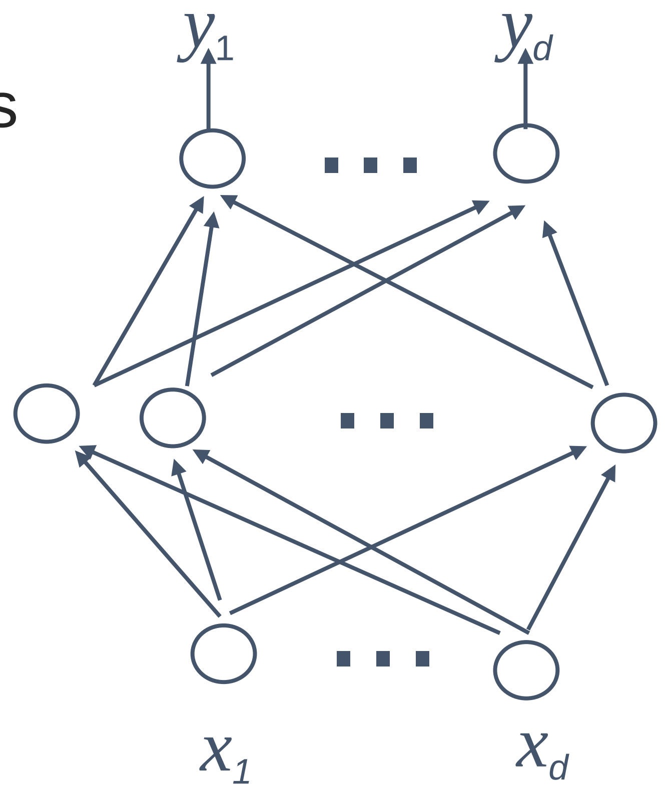
Auto-encoder 4/4

Consider two cases

- Fewer hidden nodes than input nodes
- More hidden nodes than input nodes

Case 2: Allow more hidden nodes than input

- Allow more freedom for the input-to-hidden layer mapping in exploring structure of the input
- Additional “regularization” will be needed in order to find meaningful results

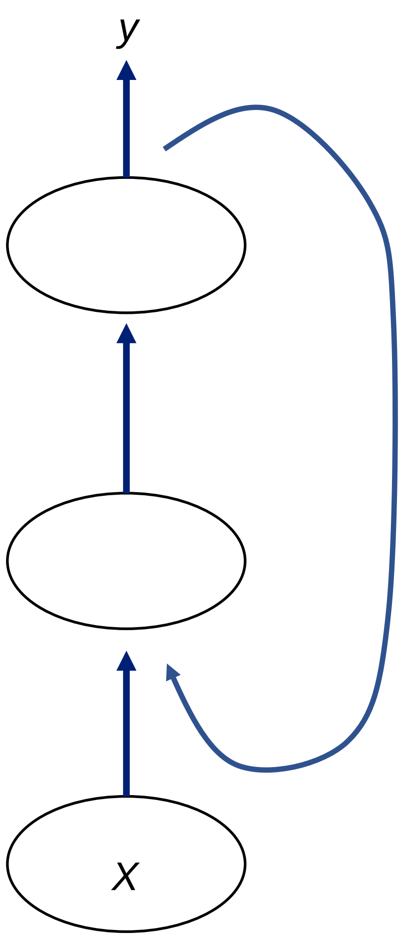


Recurrent Neural Networks (RNNs) 1/4

- ***Feedforward networks*: Neurons are interconnected without any cycle in the connection**
- ***Recurrent neural networks*: Allow directed cycles in connections between neurons**
  - Notion of “state” or temporal dynamics
  - Necessity of internal memory
- **One clear benefit: Such networks could naturally model variable-length sequential data**

Recurrent Neural Networks (RNNs) 2/4

- **A basic, illustrative architecture for RNN (showing only one node each layer)**
  - **QUESTION:** What is this network equivalent to, if we "unfold" the cycles for a given sequence of data?



Recurrent Neural Networks (RNNs) 3/4

- Training with BP algorithm may suffer from so-called *vanishing gradient problem*
- Some RNN variants have sophisticated "recurrence" structures, invented in part to address such difficulties faced by basic RNN models

Recurrent Neural Networks (RNNs) 4/4

- **Examples:**
- **The "Long short-term memory" (LSTM) model**
  - used to produce state-of-the-art results in speech and language applications
- **The Gated Recurrent Unit model, illustrated here:**