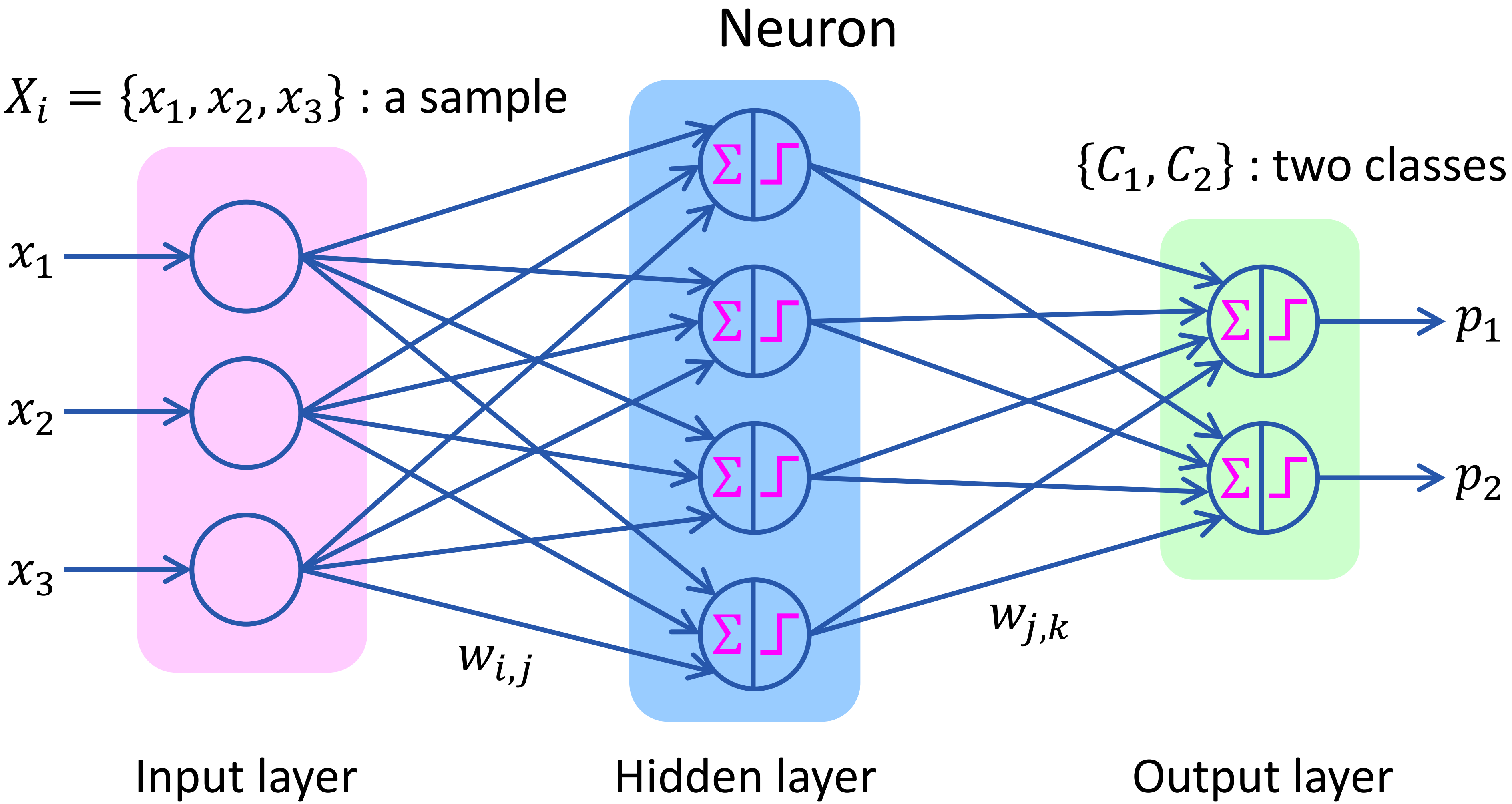
CSC 4740 / 6740 Data Mining

Spring 2024

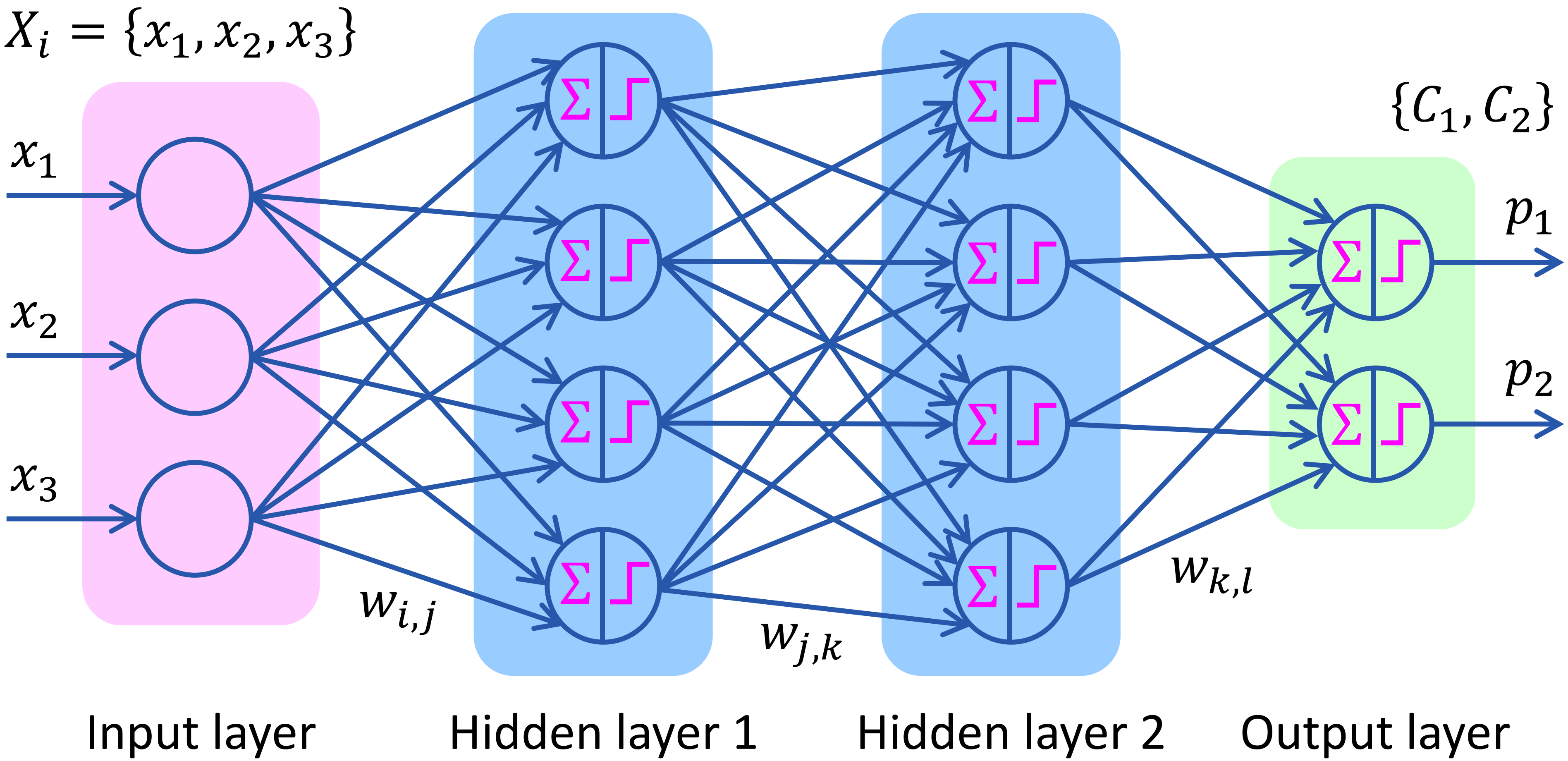
Chapter 9 Classification: Advanced Methods

GeorgiaStateUniversity

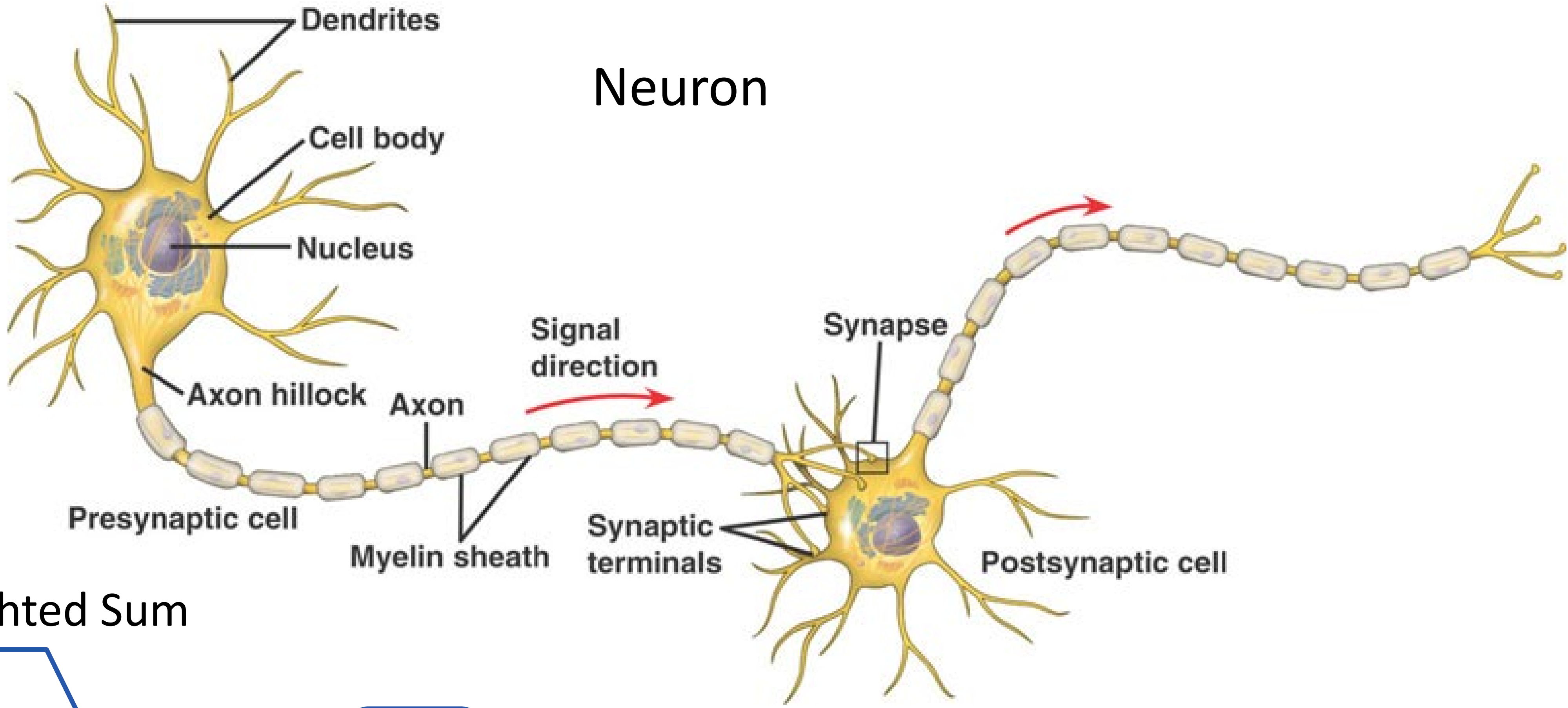
Neural Network

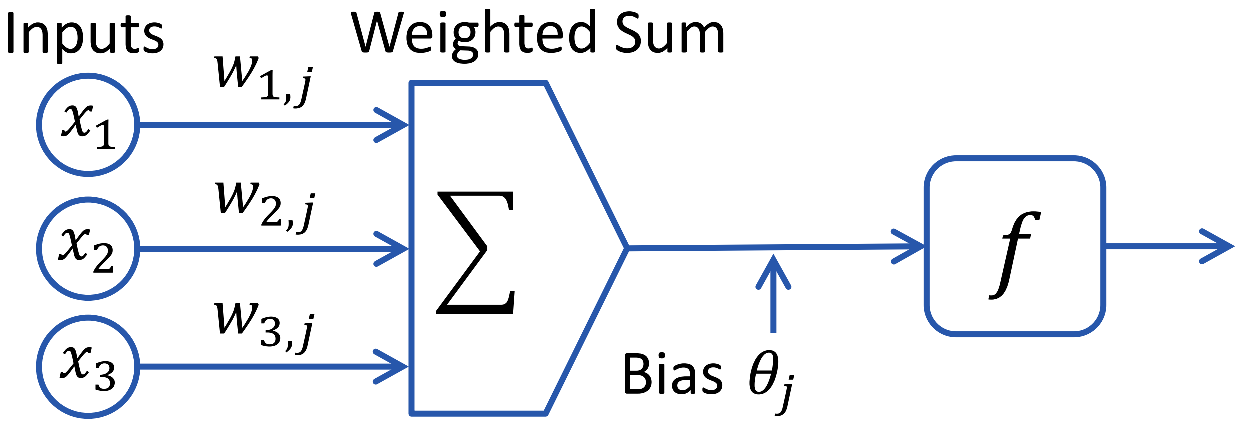


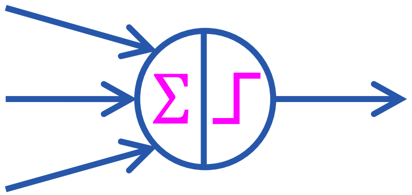
Neural Network



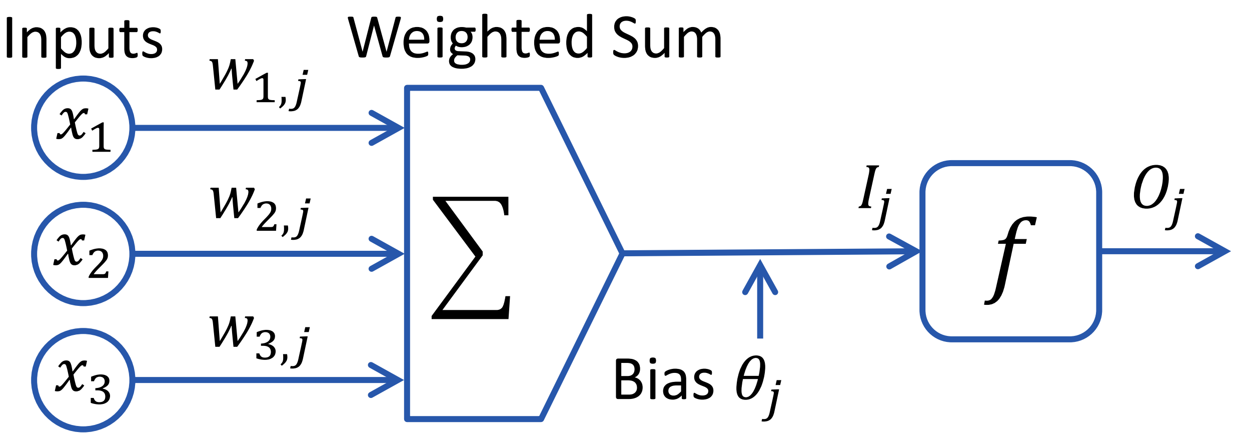
Neuron

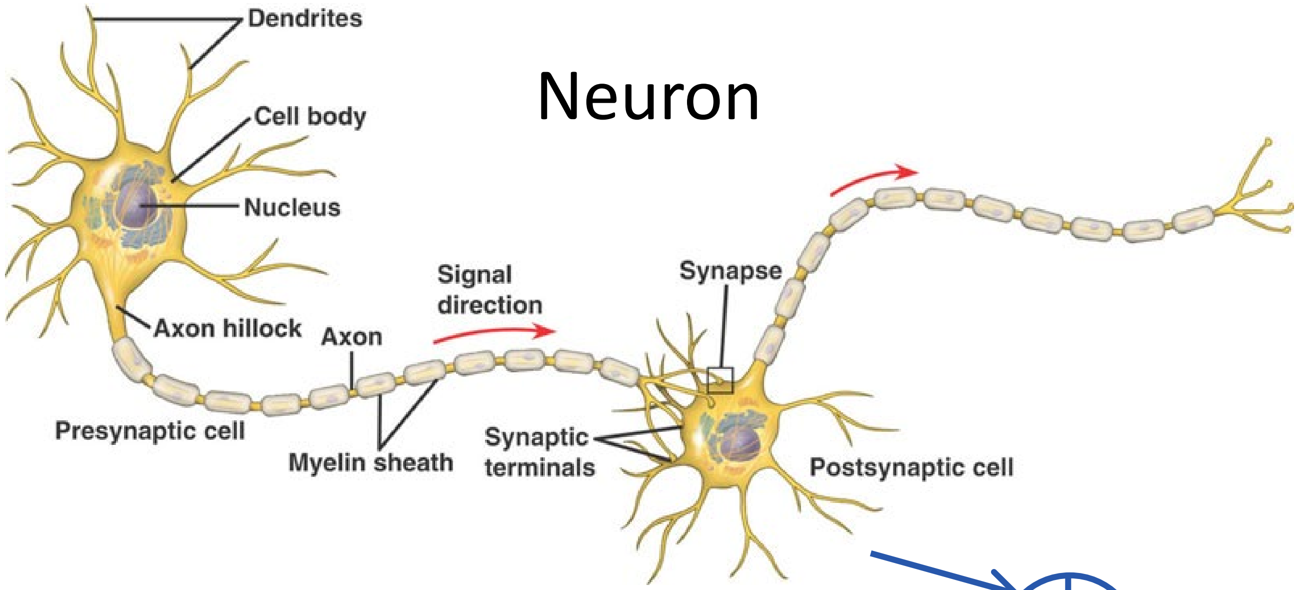


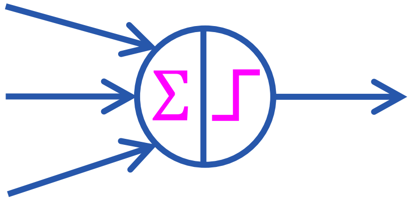




Perceptron



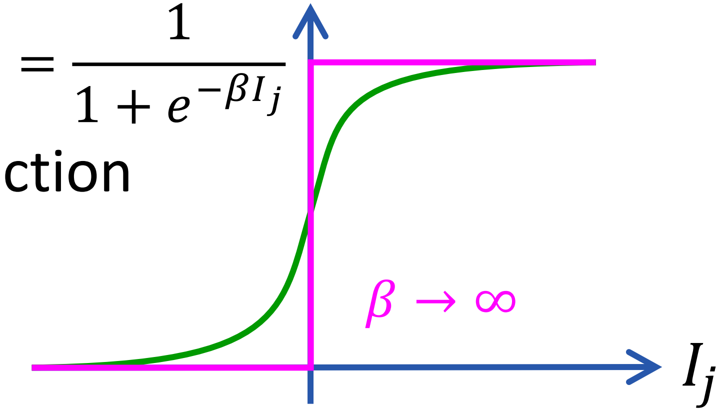




Logistic function

$$f(I_j) = \frac{1}{1 + e^{-\beta I_j}}$$

Sigmoid function



$$I_j = \sum_i w_{i,j} x_i + \theta_j$$

$$O_j = f(I_j) = \frac{1}{1 + e^{-\beta I_j}}$$

$$\beta \to \infty : \quad f(I_j) = \mathrm{sign}(I_j)$$

Neural Network

Topology:

# of units in the input layer

# of hidden layers

# of units in each hidden layer

# of units in the output layer

Parameters:

$w_{i,j}$ for each connection

β, θ_j for each hidden or output unit

Neural networks can closely approximate any function

Given enough hidden units and enough training samples

Neural Network as a Classifier

Weakness	Strength
Long learning time	High tolerance to noisy data
Some parameters are determined empirically, e.g., the network topology or “structure”	Well-suited for continuous-values inputs and outputs
Poor interpretability: Difficult to interpret the weights of the hidden units	Successful on an array of real-world data, e.g., hand-written letters
	Inherently parallel

Neural Network	SVM
Non-deterministic algorithm	Deterministic algorithm
Can easily be learned in incremental fashion	Hard to learn: learned in batch mode using quadratic programming techniques
To learn complex functions—use multilayer perceptron (nontrivial)	Using kernels can learn very complex functions

How to Train the Neural Network?

Backpropagation Algorithm: A neural network learning algorithm

- For each training data object, the weights $w_{i,j}$ are adjusted to minimize the mean squared error between prediction and ground truth

- Adjustments are made in the "**backwards**" direction: from the output layer , to the hidden layer

How to Train the Neural Network?

Backpropagation Algorithm: A neural network learning algorithm

Steps:

1. Initialize weights $w_{i,j}$ and biases θ_j to small random numbers
2. For each training data object
   1) Propagate the inputs forward
   2) Backpropagate the error by updating weights $w_{i,j}$ and biases θ_j
3. Terminating condition : when the error is very small, etc.

Backpropagation Algorithm

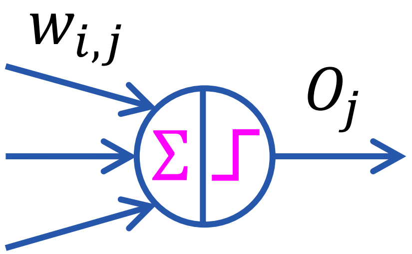
The error:

$$\mathrm{Err}_j = O_j(1 - O_j)(T_j - O_j)$$

where, O_j is the actual output

T_j is the known value

$O_j(1 - O_j)$ is the derivative of the logistic function



Unit j in the output layer

Update the weights:

$$\Delta w_{i,j} = l \cdot \mathrm{Err}_j \cdot O_i$$
$$w_{i,j} = w_{i,j} + \Delta w_{i,j}$$

Update the bias:

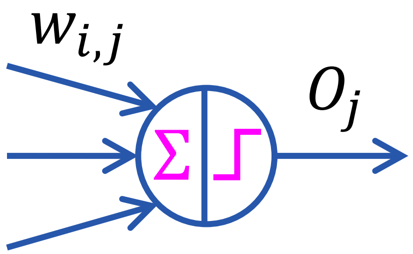
$$\Delta \theta_j = l \cdot \mathrm{Err}_j$$
$$\theta_j = \theta_j + \Delta \theta_j$$

$l \in (0,1)$: learning rate

Rule of thumb: $l = \dfrac{1}{t}$

t is # of iterations through the training set so far

Backpropagation Algorithm



Unit j in the hidden layer

The error:

$$\mathrm{Err}_j = O_j(1 - O_j) \sum_k w_{j,k} \cdot \mathrm{Err}_k$$

where, O_j is the actual output

$w_{j,k}$ is the weight of the connection from unit j to k in higher layer

Err_k is the error of unit k

Update the weights:

$$\Delta w_{i,j} = l \cdot \mathrm{Err}_j \cdot O_i$$
$$w_{i,j} = w_{i,j} + \Delta w_{i,j}$$

Update the bias:

$$\Delta \theta_j = l \cdot \mathrm{Err}_j$$
$$\theta_j = \theta_j + \Delta \theta_j$$

$l \in (0,1)$: learning rate

Rule of thumb: $l = \frac{1}{t}$

t is # of iterations through the training set so far

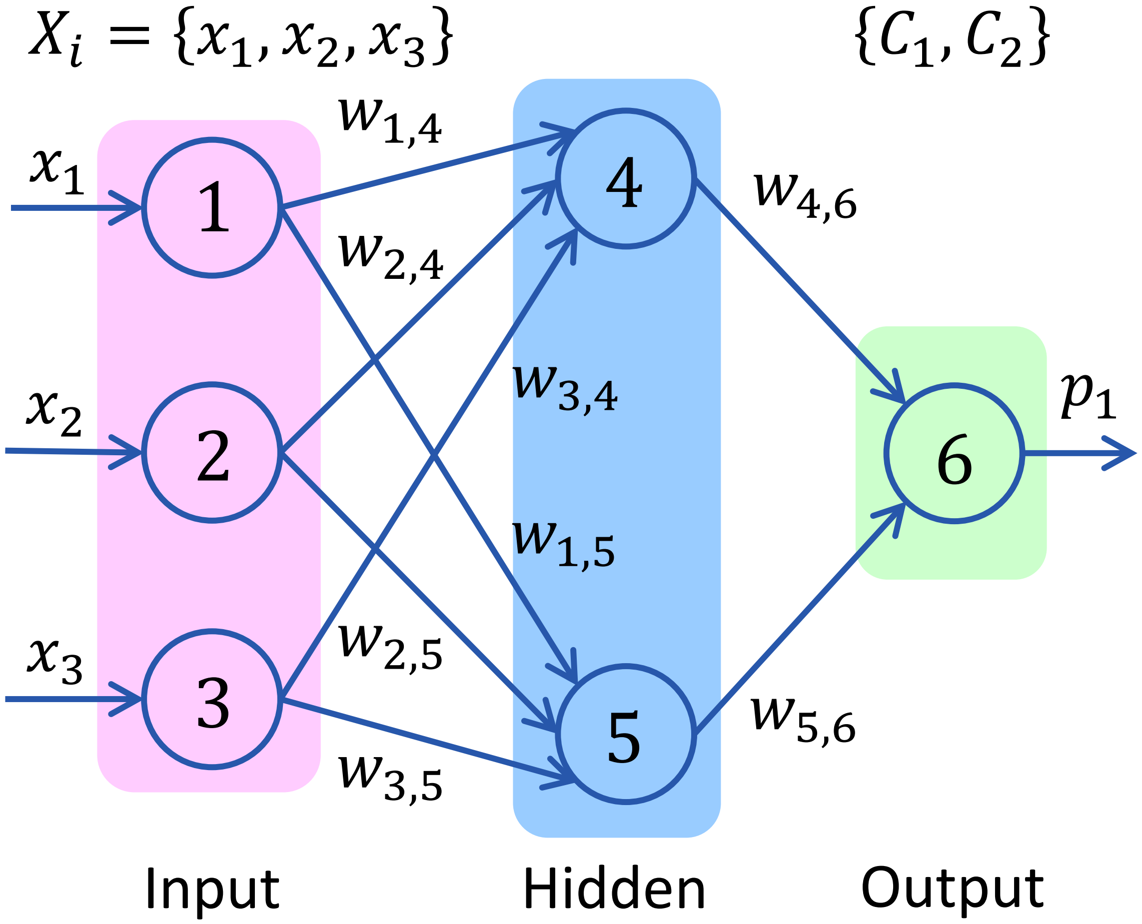
Training data object:

$X_i = \{1, 0, 1\}$

class label: 1

Initial values:

$w_{1,4}$	0.2
$w_{1,5}$	-0.3
$w_{2,4}$	0.4
$w_{2,5}$	0.1
$w_{3,4}$	-0.5
$w_{3,5}$	0.2
$w_{4,6}$	-0.3
$w_{5,6}$	-0.2
θ_4	-0.4
θ_5	0.2
θ_6	0.1



Multilayer feed-forward networks

Learning rate $l = 0.9$

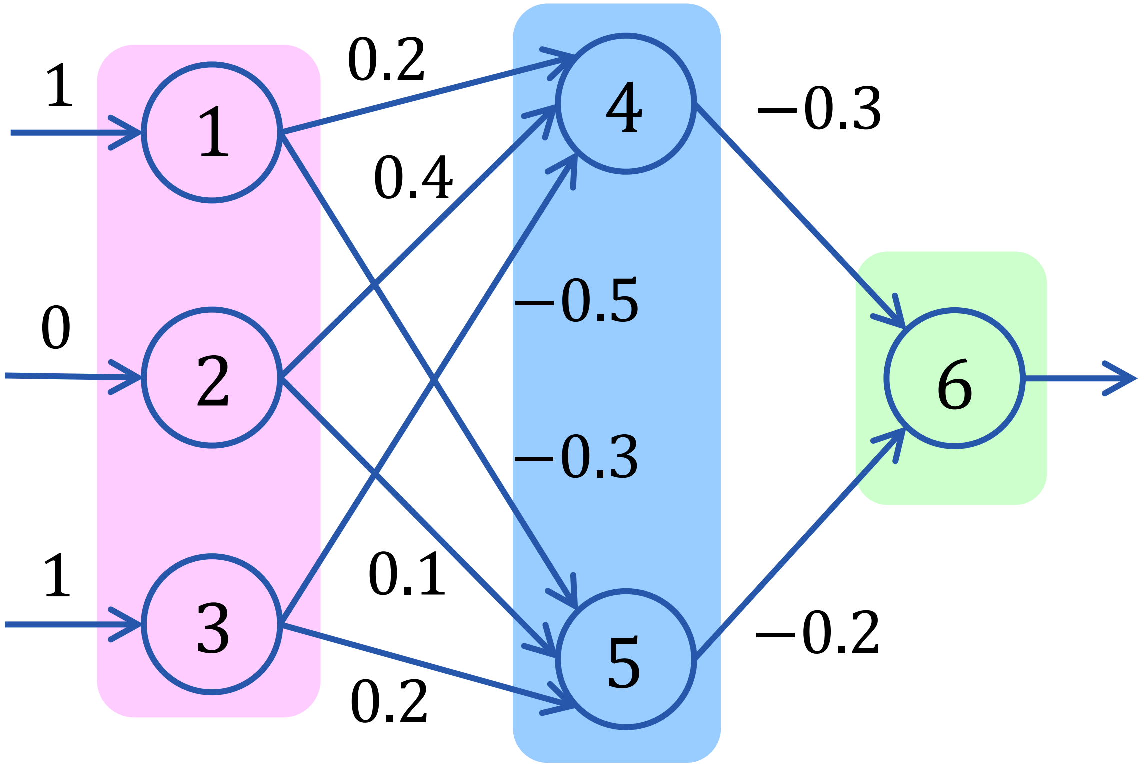
Training data object:

$X_i = \{1, 0, 1\}$

class label: 1

Initial values:

$w_{1,4}$	0.2
$w_{1,5}$	-0.3
$w_{2,4}$	0.4
$w_{2,5}$	0.1
$w_{3,4}$	-0.5
$w_{3,5}$	0.2
$w_{4,6}$	-0.3
$w_{5,6}$	-0.2
θ_4	-0.4
θ_5	0.2
θ_6	0.1



Unit j	**Net Input I_j**	**Output O_j**
4	$0.2 + 0 - 0.5 - 0.4 = -0.7$	$\frac{1}{1+e^{0.7}} = 0.332$
5	$-0.3 + 0 + 0.2 + 0.2 = 0.1$	$\frac{1}{1+e^{-0.1}} = 0.525$
6	$-0.3 \times 0.332 - 0.2 \times 0.525 + 0.1 = -0.105$	$\frac{1}{1+e^{0.105}} = 0.474$

Propagate the inputs forward $I_j = \sum_i w_{i,j} x_i + \theta_j$ $O_j = f(I_j) = \frac{1}{1+e^{-\beta I_j}}$

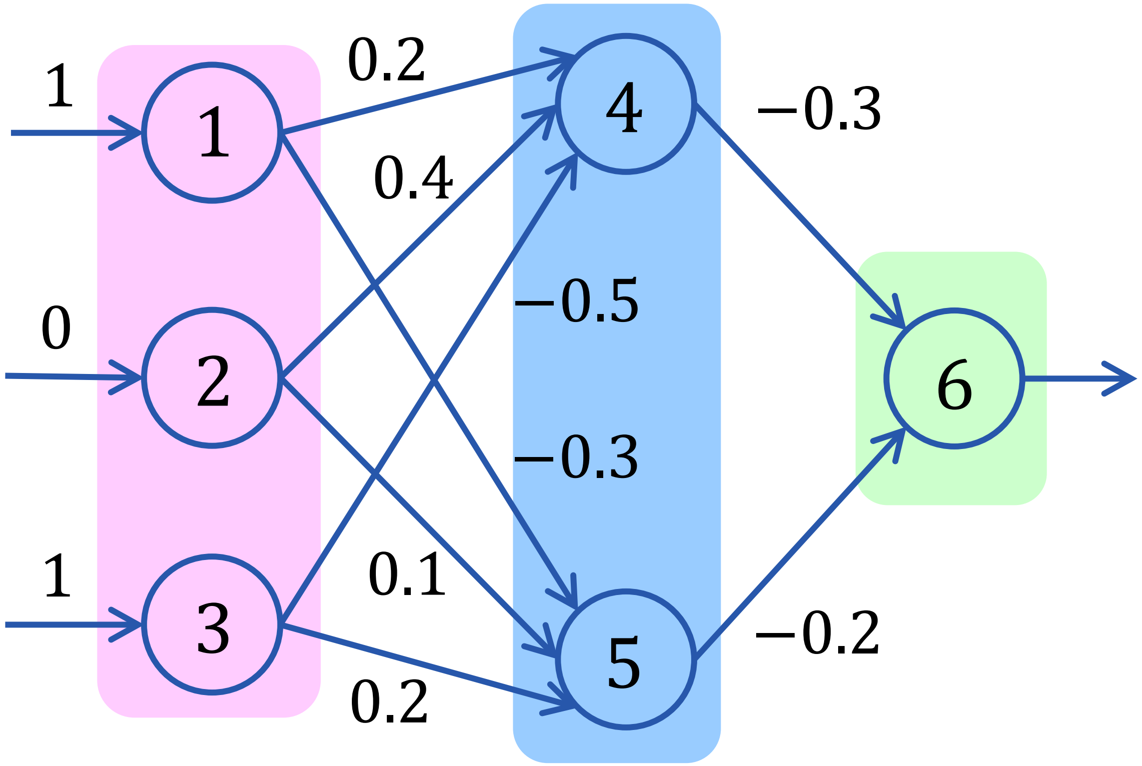
Training data object:

$X_i = \{1, 0, 1\}$

class label: 1

Initial values:

$w_{1,4}$	0.2
$w_{1,5}$	-0.3
$w_{2,4}$	0.4
$w_{2,5}$	0.1
$w_{3,4}$	-0.5
$w_{3,5}$	0.2
$w_{4,6}$	-0.3
$w_{5,6}$	-0.2
θ_4	-0.4
θ_5	0.2
θ_6	0.1



Unit j	Error Err_j
6	$0.474 \times (1 - 0.474) \times (1 - 0.474) = 0.1311$
5	$0.525 \times (1 - 0.525) \times 0.1311 \times (-0.2) = -0.0065$
4	$0.332 \times (1 - 0.332) \times 0.1311 \times (-0.3) = -0.0087$

Backpropagate the errors

Output layer: $\mathrm{Err}_j = O_j(1 - O_j)(T_j - O_j)$

Hidden layer: $\mathrm{Err}_j = O_j(1 - O_j)\sum_k w_{j,k} \cdot \mathrm{Err}_k$

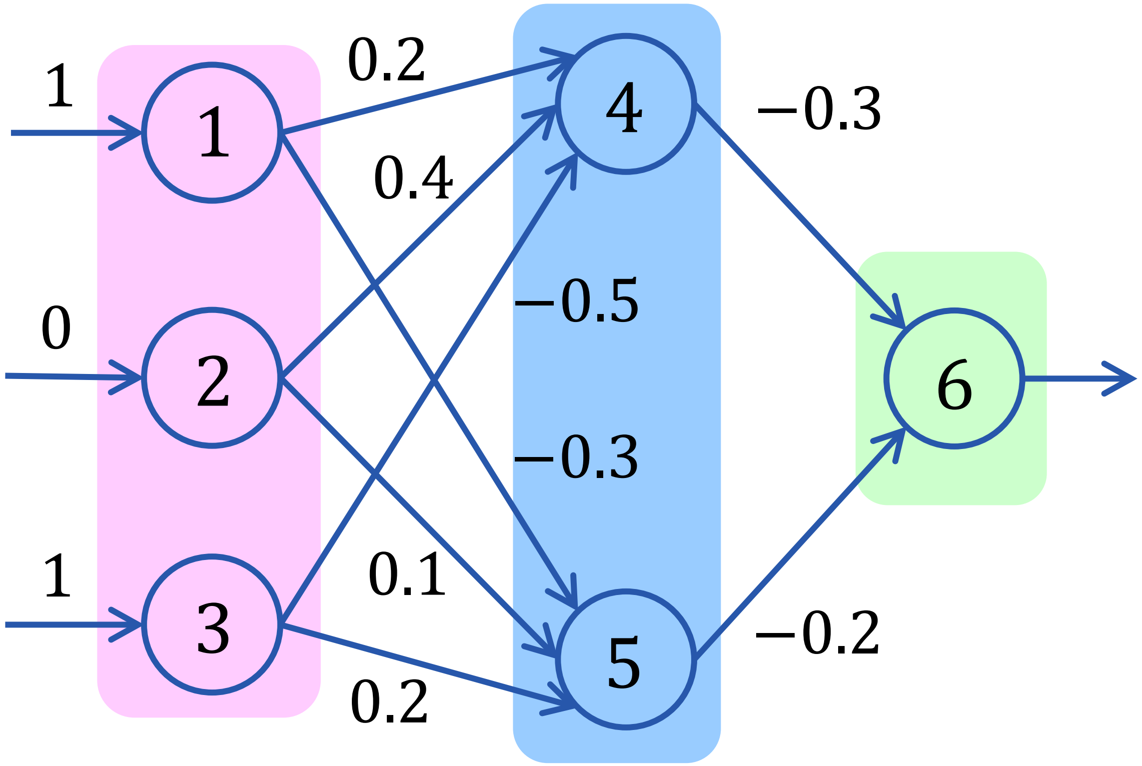
Training data object:

$X_i = \{1, 0, 1\}$

class label: 1

Initial values:

$w_{1,4}$	0.2
$w_{1,5}$	-0.3
$w_{2,4}$	0.4
$w_{2,5}$	0.1
$w_{3,4}$	-0.5
$w_{3,5}$	0.2
$w_{4,6}$	-0.3
$w_{5,6}$	-0.2
θ_4	-0.4
θ_5	0.2
θ_6	0.1



weights	**Error** Err_j
$w_{4,6}$	$-0.3 + 0.9 \times 0.1311 \times 0.332 = -0.261$
$w_{5,6}$	$-0.2 + 0.9 \times 0.1311 \times 0.525 = -0.138$

Backpropagate the errors

Learning rate $l = 0.9$

Update the weights: $\Delta w_{i,j} = l \cdot \mathrm{Err}_j \cdot O_i$

$w_{i,j} = w_{i,j} + \Delta w_{i,j}$

Ge

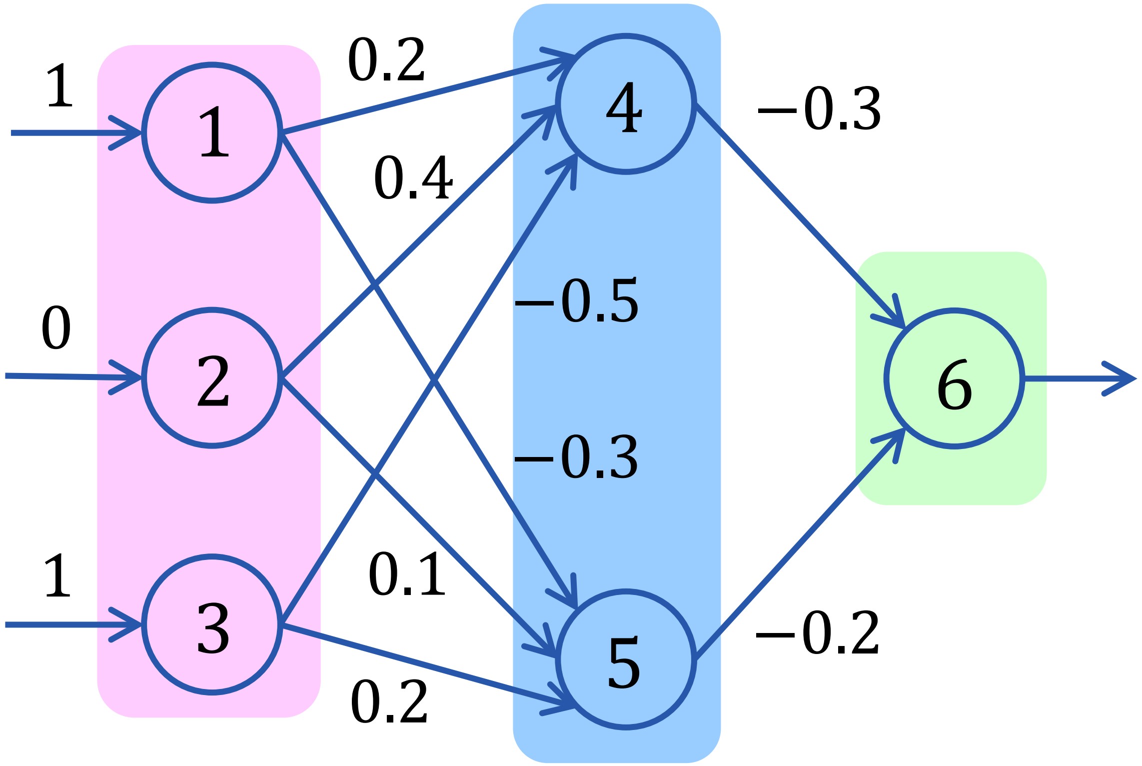
Training data object:

$X_i = \{1, 0, 1\}$

class label: 1

Initial values:

$w_{1,4}$	0.2
$w_{1,5}$	-0.3
$w_{2,4}$	0.4
$w_{2,5}$	0.1
$w_{3,4}$	-0.5
$w_{3,5}$	0.2
$w_{4,6}$	-0.3
$w_{5,6}$	-0.2
θ_4	-0.4
θ_5	0.2
θ_6	0.1



weights	Error Err_j
$w_{1,4}$	$0.2 + 0.9 \times (-0.0087) \times 1 = 0.192$
$w_{2,4}$	$0.4 + 0.9 \times (-0.0087) \times 0 = 0.4$
$w_{3,4}$	$-0.5 + 0.9 \times (-0.0087) \times 1 = -0.508$

Backpropagate the errors

Learning rate $l = 0.9$

Update the weights: $\Delta w_{i,j} = l \cdot \mathrm{Err}_j \cdot O_i$

$w_{i,j} = w_{i,j} + \Delta w_{i,j}$

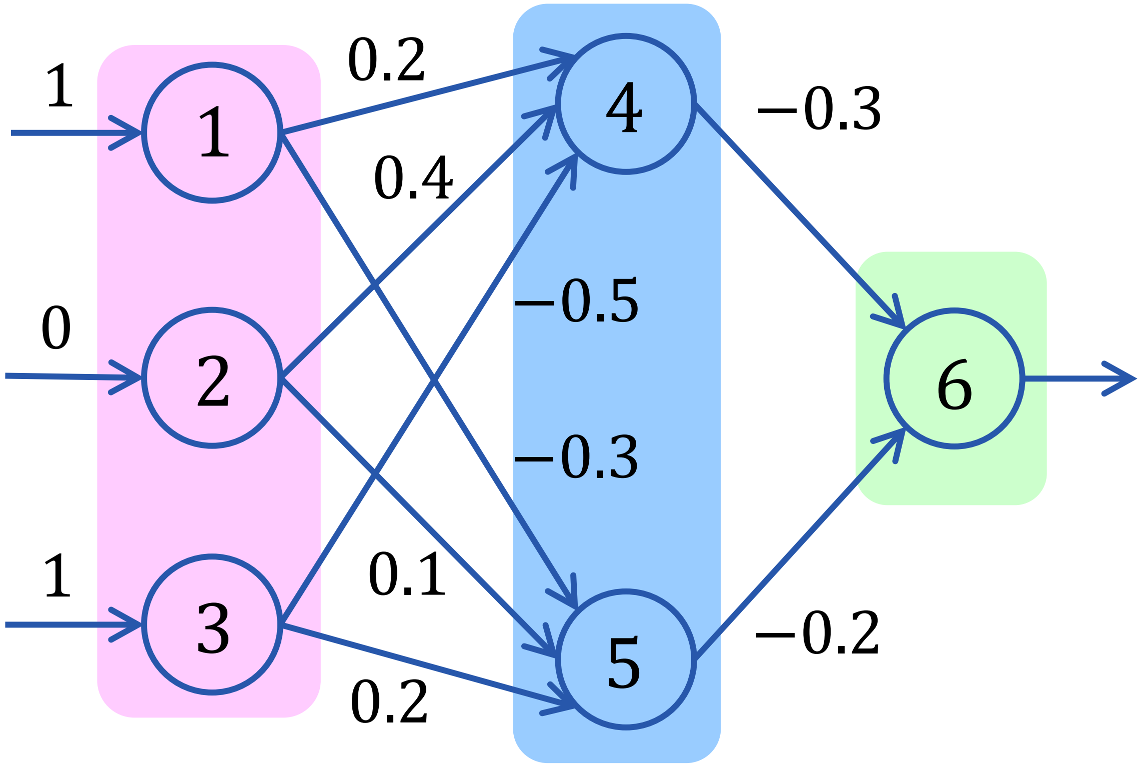
Training data object:

$X_i = \{1, 0, 1\}$

class label: 1

Initial values:

$w_{1,4}$	0.2
$w_{1,5}$	-0.3
$w_{2,4}$	0.4
$w_{2,5}$	0.1
$w_{3,4}$	-0.5
$w_{3,5}$	0.2
$w_{4,6}$	-0.3
$w_{5,6}$	-0.2
θ_4	-0.4
θ_5	0.2
θ_6	0.1



weights	Error Err_j
$w_{1,5}$	$-0.3 + 0.9 \times (-0.0065) \times 1 = -0.306$
$w_{2,5}$	$0.1 + 0.9 \times (-0.0065) \times 0 = 0.1$
$w_{3,5}$	$0.2 + 0.9 \times (-0.0065) \times 1 = 0.194$

Backpropagate the errors

Learning rate $l = 0.9$

Update the weights: $\Delta w_{i,j} = l \cdot \mathrm{Err}_j \cdot O_i$

$w_{i,j} = w_{i,j} + \Delta w_{i,j}$

Ge

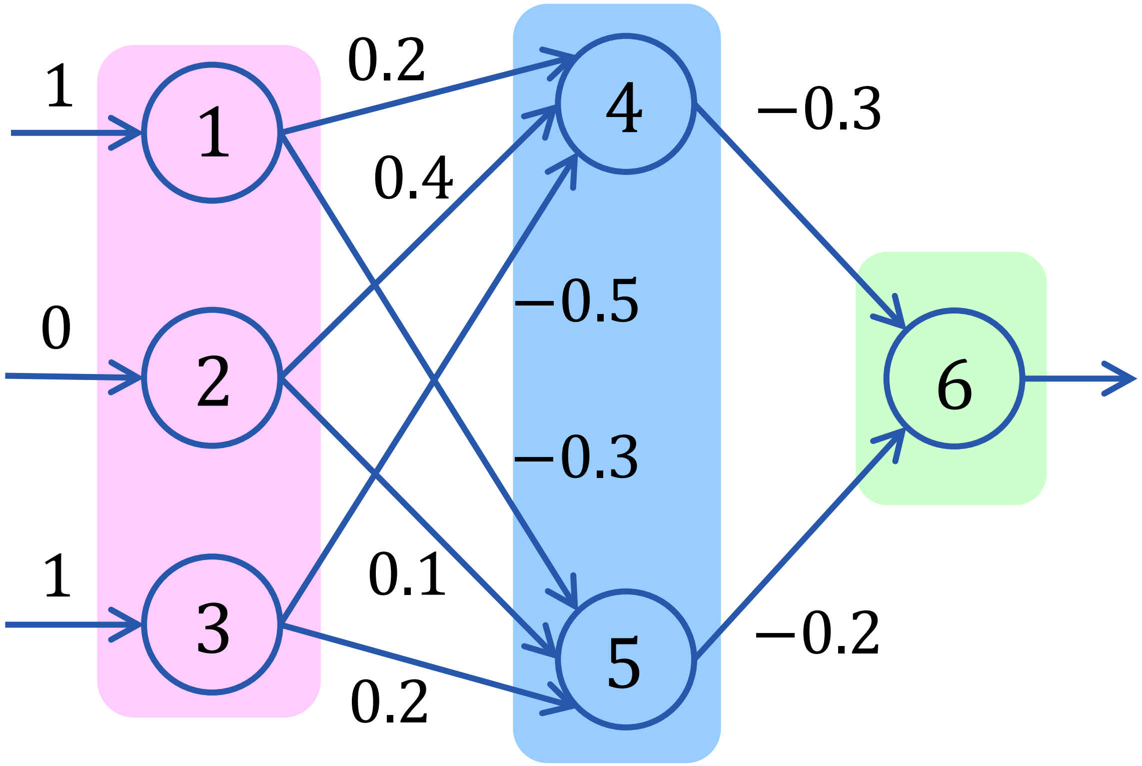
Training data object:

$X_i = \{1, 0, 1\}$

class label: 1

Initial values:

$w_{1,4}$	0.2
$w_{1,5}$	-0.3
$w_{2,4}$	0.4
$w_{2,5}$	0.1
$w_{3,4}$	-0.5
$w_{3,5}$	0.2
$w_{4,6}$	-0.3
$w_{5,6}$	-0.2
θ_4	-0.4
θ_5	0.2
θ_6	0.1



weights	Error Err_j
θ_6	$0.1 + 0.9 \times 0.1311 = 0.218$
θ_5	$0.2 + 0.9 \times (-0.0065) = 0.194$
θ_4	$-0.4 + 0.9 \times (-0.0087) = -0.408$

Backpropagate the errors

Learning rate $l = 0.9$

Update the biases: $\Delta\theta_j = l \cdot \mathrm{Err}_j$

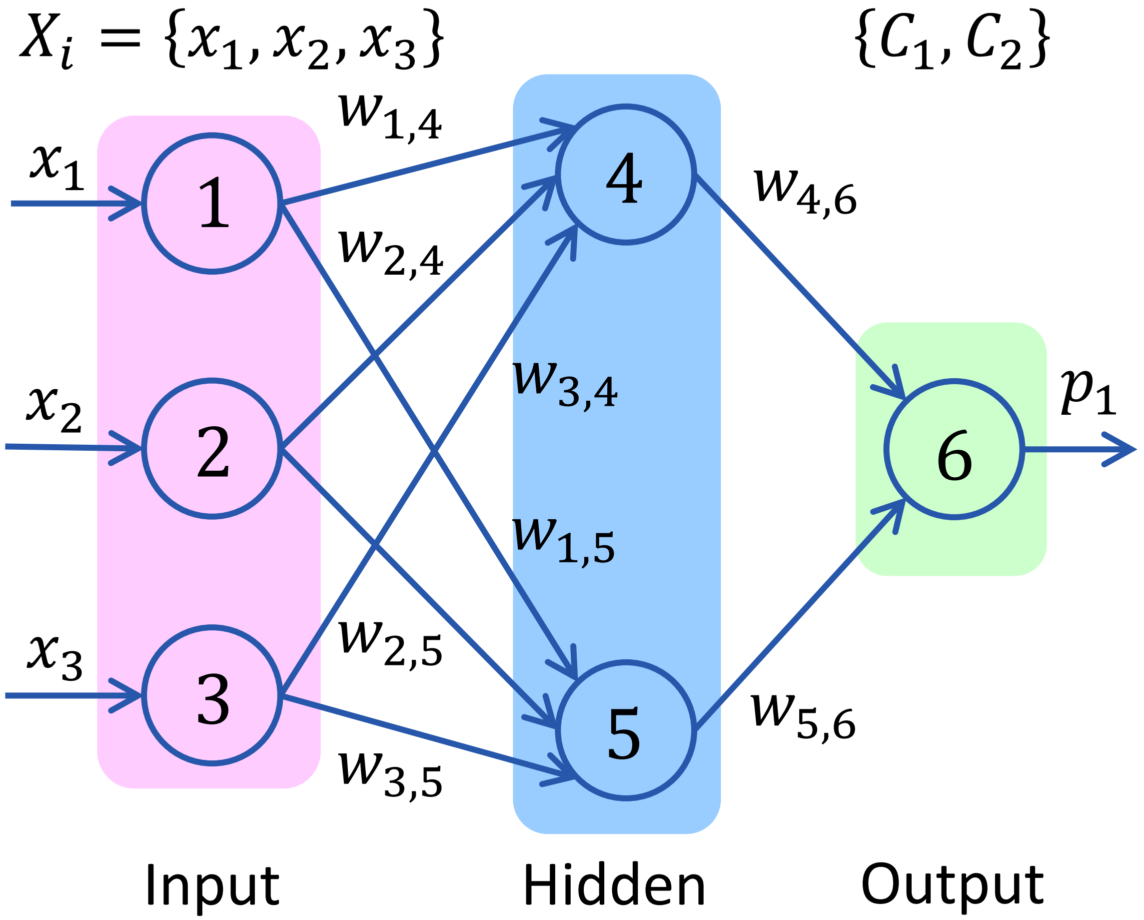
$\theta_j = \theta_j + \Delta\theta_j$

Training data object:

$X_i = \{1, 0, 1\}$ label: 1

Initial values:

weights	old	new
$w_{1,4}$	0.2	0.192
$w_{1,5}$	-0.3	-0.306
$w_{2,4}$	0.4	0.4
$w_{2,5}$	0.1	0.1
$w_{3,4}$	-0.5	-0.508
$w_{3,5}$	0.2	0.194
$w_{4,6}$	-0.3	-0.261
$w_{5,6}$	-0.2	-0.138
θ_4	-0.4	-0.408
θ_5	0.2	0.194
θ_6	0.1	0.218

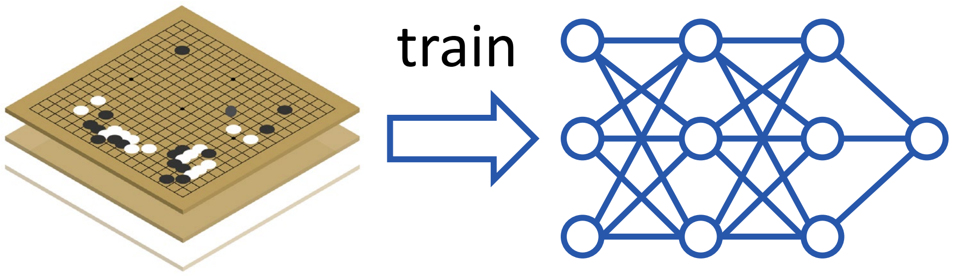


Multilayer feed-forward networks

Learning rate $l = 0.9$

Lee Sedol 9-dan vs AlphaGo

AlphaGo 4 – Lee Sedol 1



- Human expert positions
- Self-play positions

Mastering the game of Go with deep neural networks and tree search
David Silver, et al
Nature, 2016

Deep Learning Package Zoo

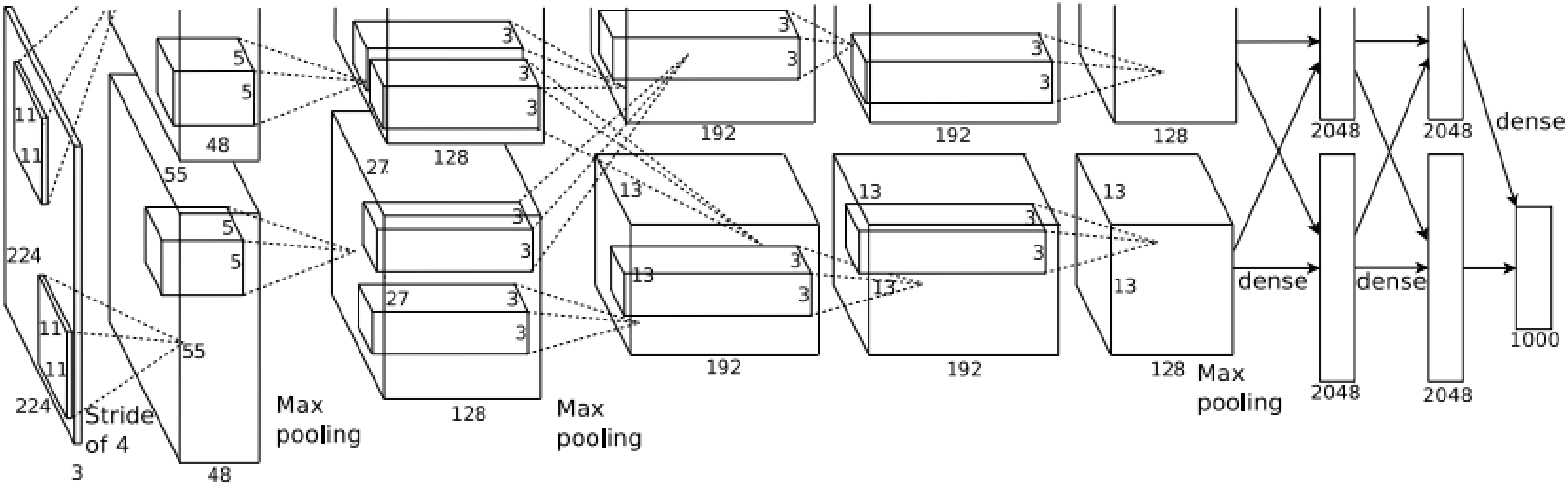
- Torch => PyTorch
- Caffe
- Theano (Keras, Lasagne)
- nVidia CuDNN
- Google TensorFlow
- Mxnet
- etc.

https://www.tensorflow.org/tutorials
https://cs224d.stanford.edu/lectures/CS224d-Lecture7.pdf
https://cbmm.mit.edu/sites/default/files/documents/Tensorflow%202_0%20slides.pdf
https://www.slideshare.net/databricks/introduction-to-tensorflow-20

Pre-Trained Models

- AlexNet
- VGG-16 (Visual Geometry Group - University of Oxford)
- BERT (Bidirectional Encoder Representations from Transformers)
- GPT (Generative Pre-trained Transformer) / GPT2 / GPT3

Architecture of AlexNet CNN



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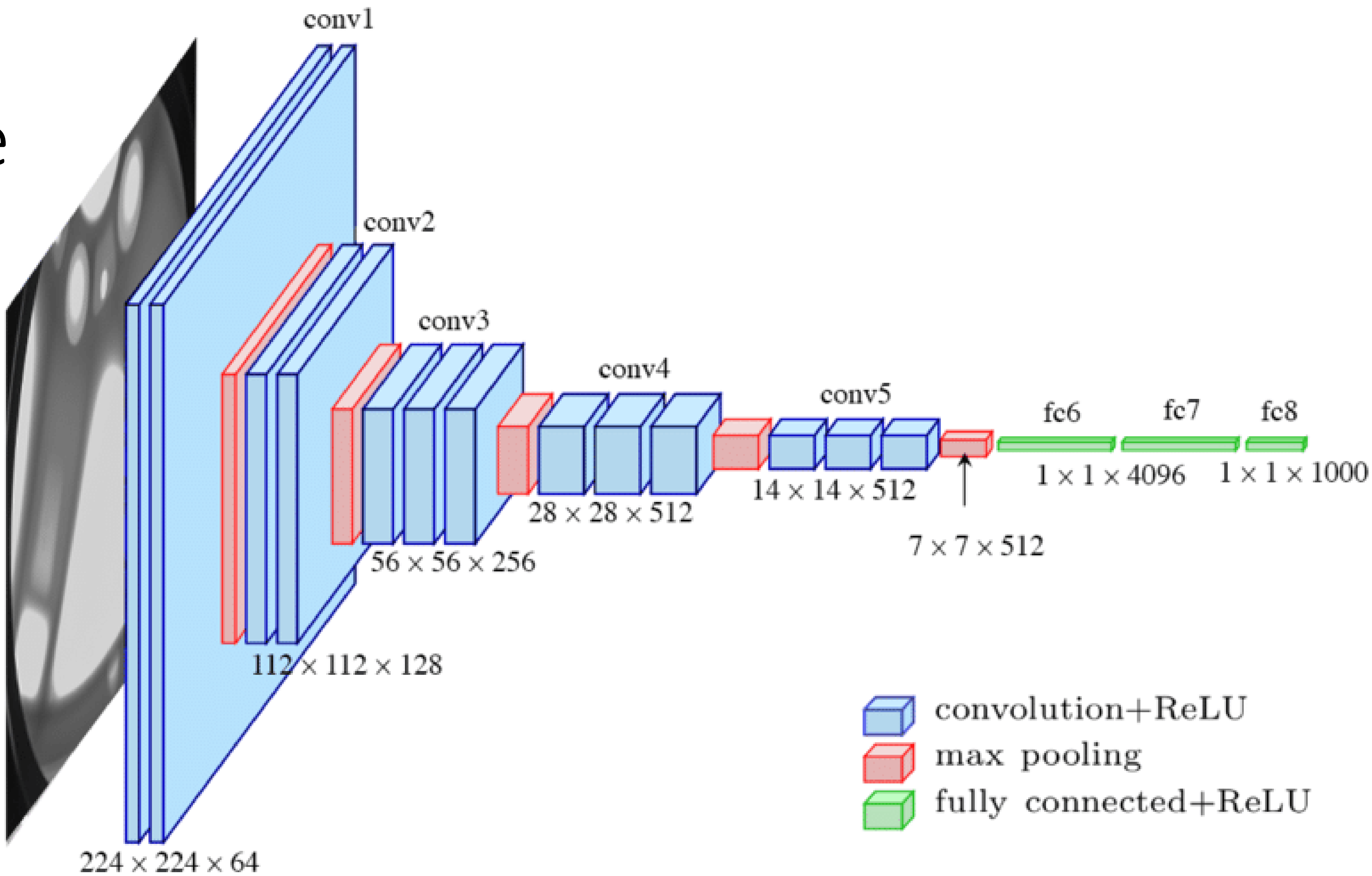
Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. "Imagenet classification with deep convolutional neural networks." Advances in neural information processing systems 25 (2012): 1097-1105.

VGG-16 Architecture



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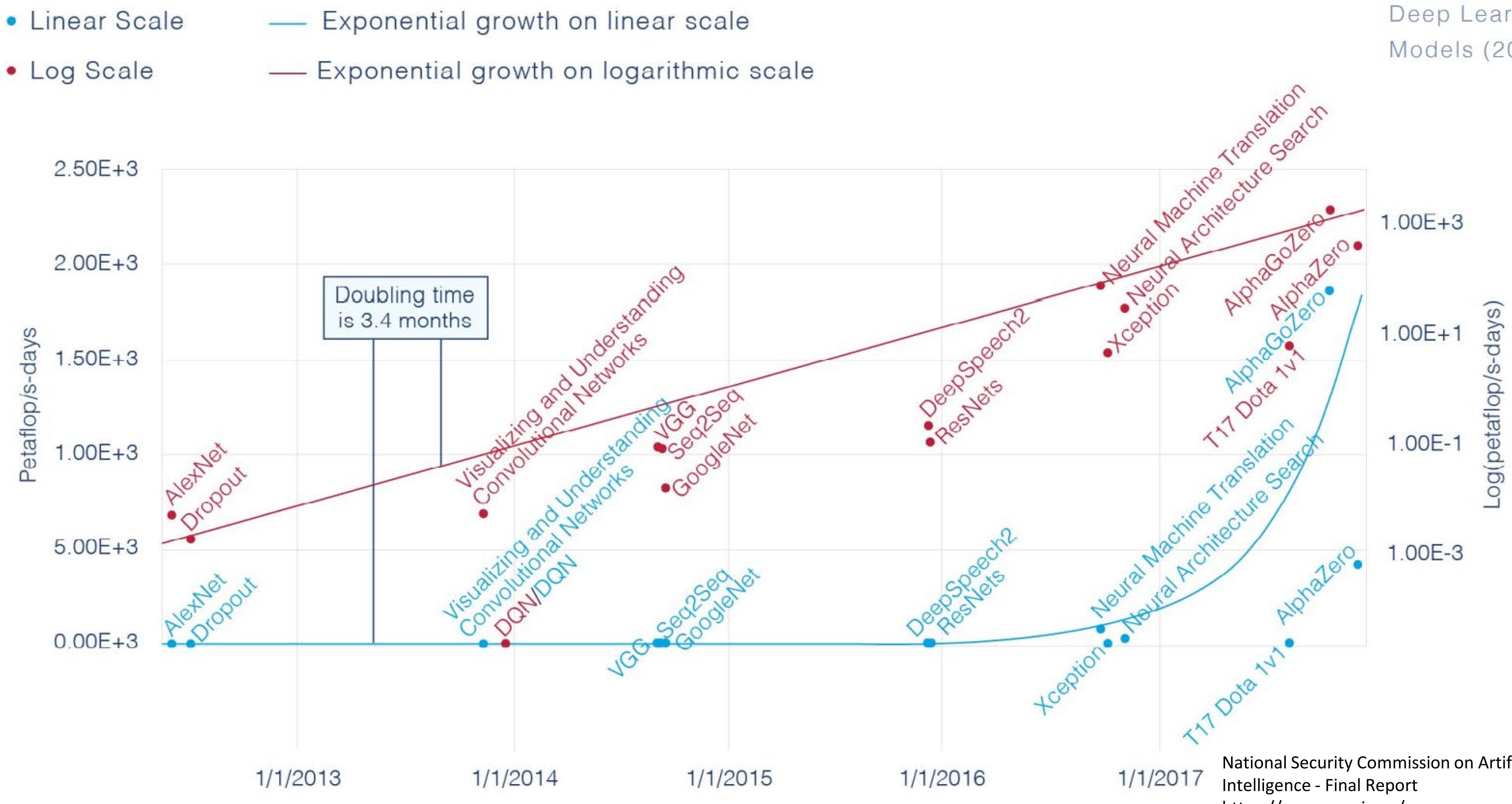
Ferguson, Max, Ronay Ak, Yung-Tsun Tina Lee, and Kincho H. Law. "Automatic localization of casting defects with convolutional neural networks." In 2017 IEEE international conference on big data (big data), pp. 1726-1735. IEEE, 2017.

Compute Required to Train Largest Deep Learning Models (2012-2017)

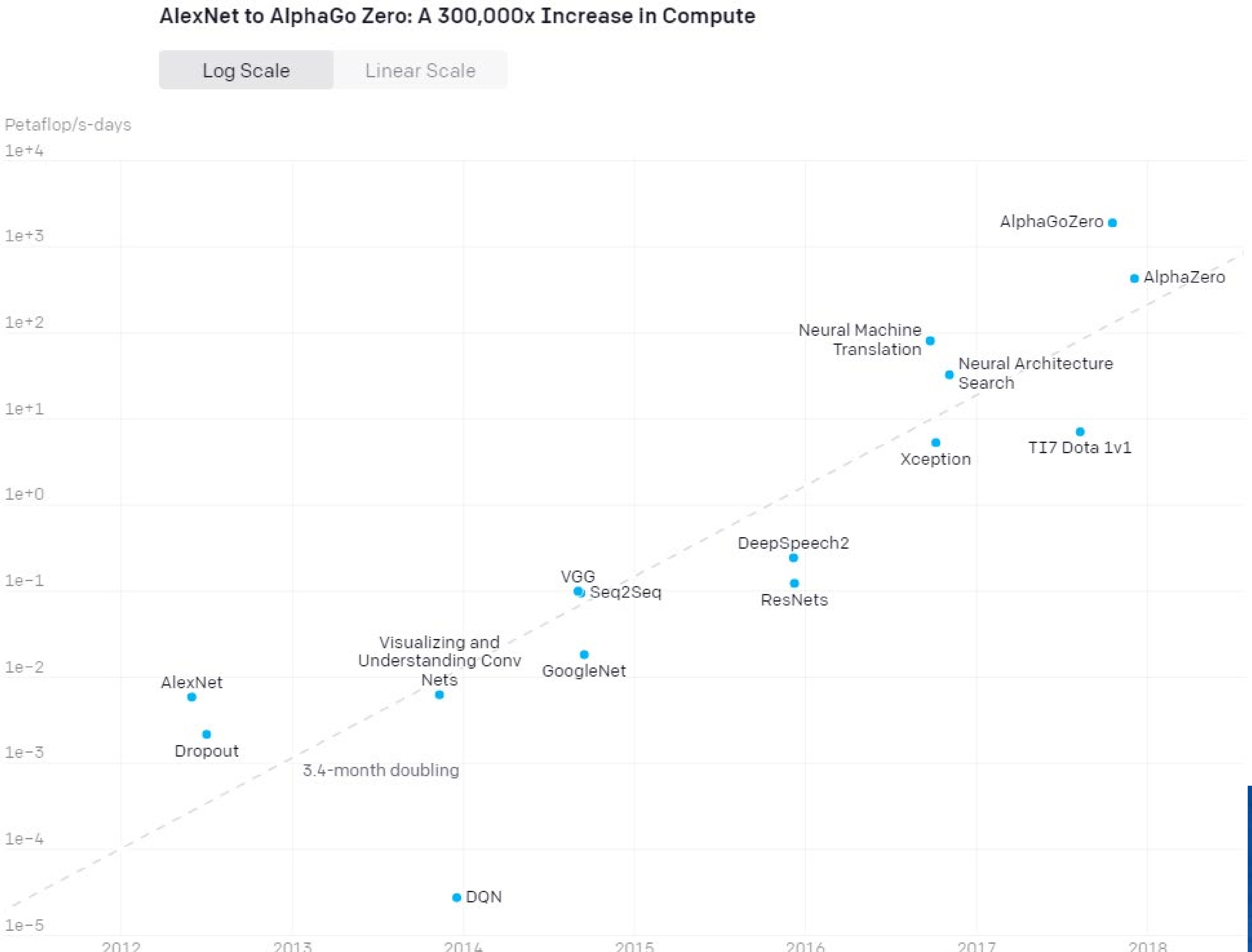
Compute Required to Train Largest Deep Learning Models (2012-2017)



Source: OpenAI, AI and Compute (May 16, 2018), https://openai.com/blog/ai-and-compute/

National Security Commission on Artificial Intelligence - Final Report
https://www.nscai.gov/wp-content/uploads/2021/03/Full-Report-Digital-1.pdf

AI & Compute



AI and Compute - OpenAI https://openai.com/blog/ai-and-compute/

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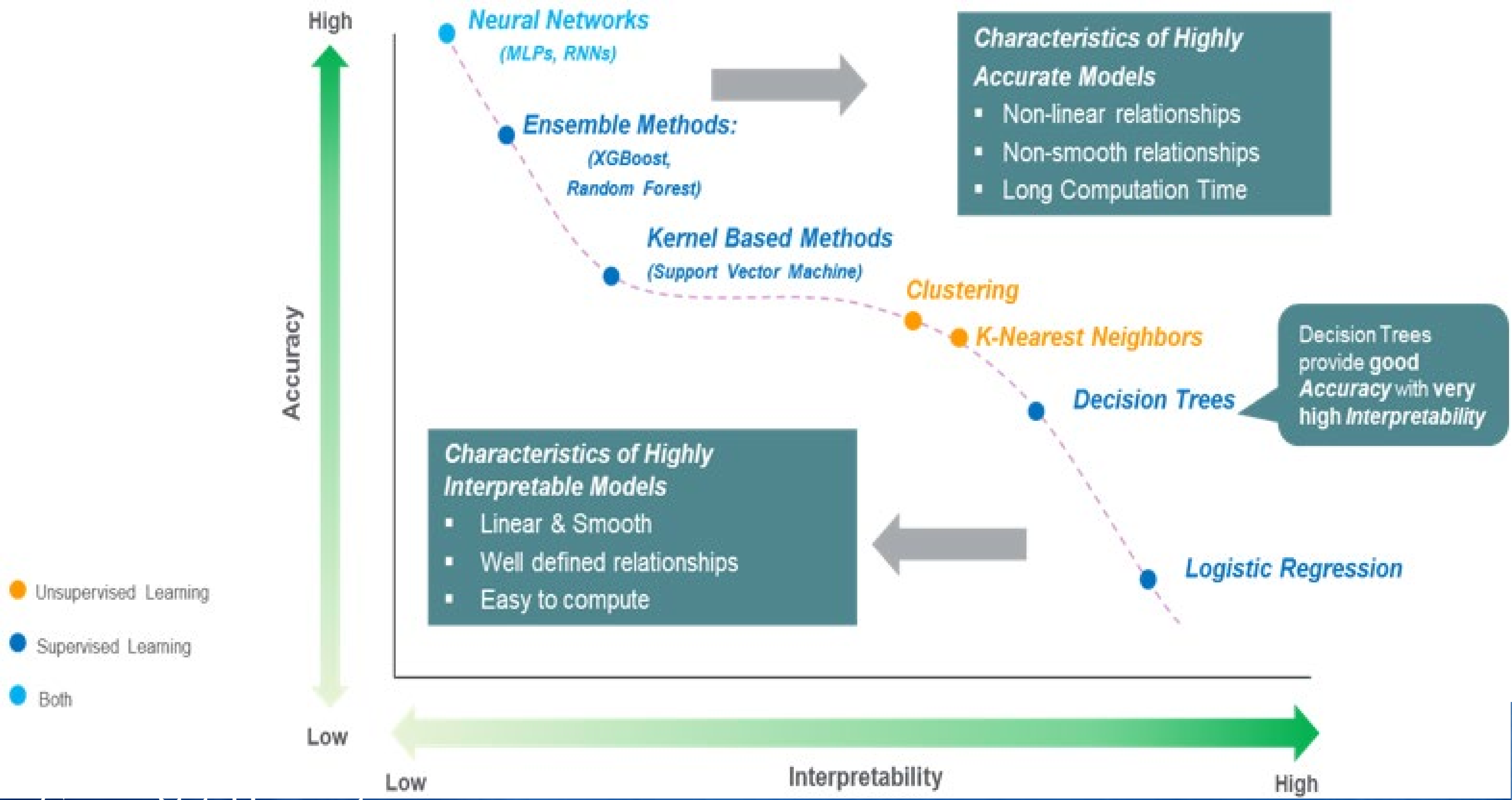

High
Accuracy
Low
Neural Networks
(MLPs, RNNs)
Ensemble Methods:
(XGBoost,
Random Forest)
Kernel Based Methods
(Support Vector Machine)
Clustering
K-Nearest Neighbors
Decision Trees
Logistic Regression
Characteristics of Highly Accurate Models
Non-linear relationships
Non-smooth relationships
Long Computation Time
Decision Trees provide good Accuracy with very high Interpretability
Characteristics of Highly Interpretable Models
Linear & Smooth
Well defined relationships
Easy to compute
Unsupervised Learning
Supervised Learning
Both
Low
Interpretability
High

k-Nearest Neighbor (k-NN) Classifier

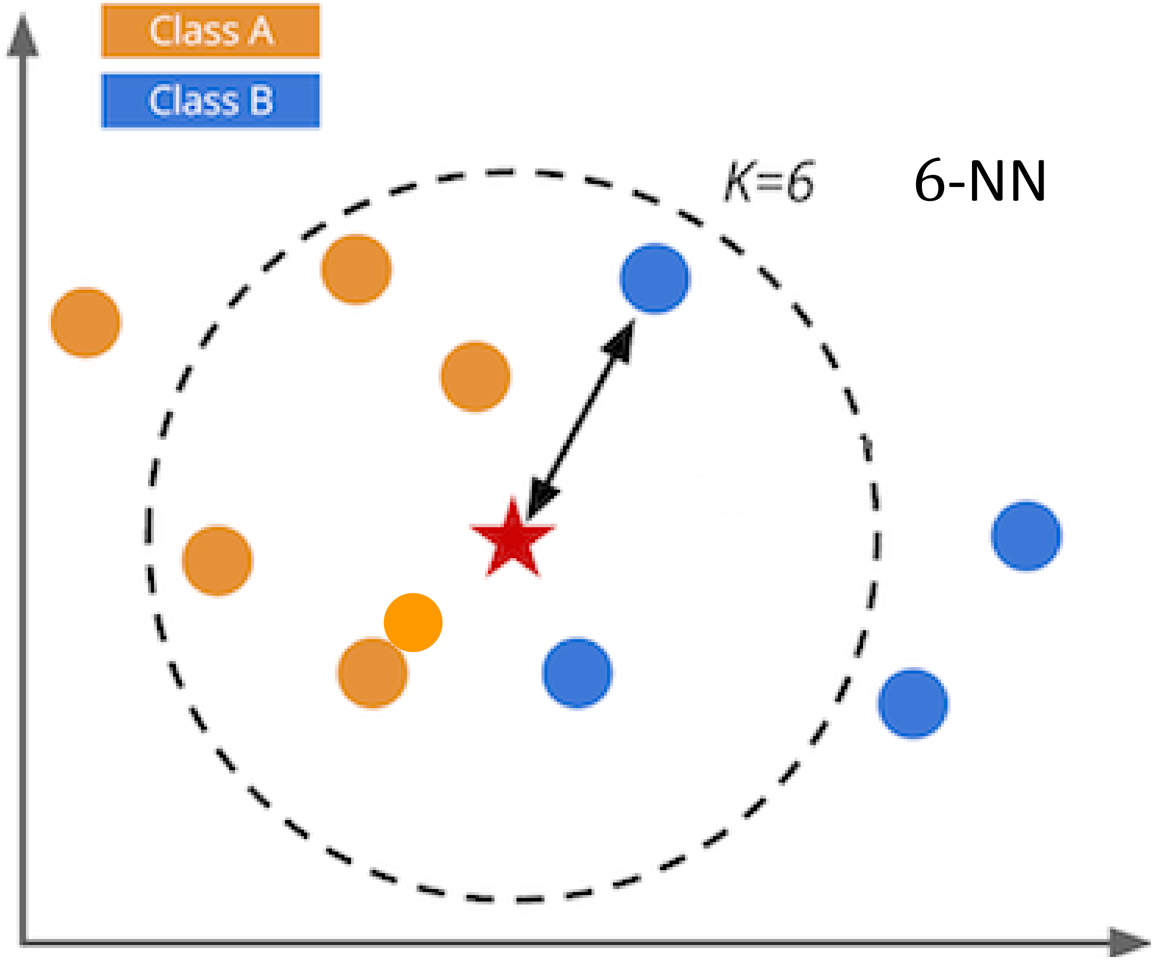
1. Compute the Distance/Similarity

$$d_{i,j} = \sqrt{\left(x_{i,1} - x_{j,1}\right)^2 + \left(x_{i,2} - x_{j,2}\right)^2}$$

2. Rank the remaining nodes

3. Select the Top-k nodes

4. Majority Vote

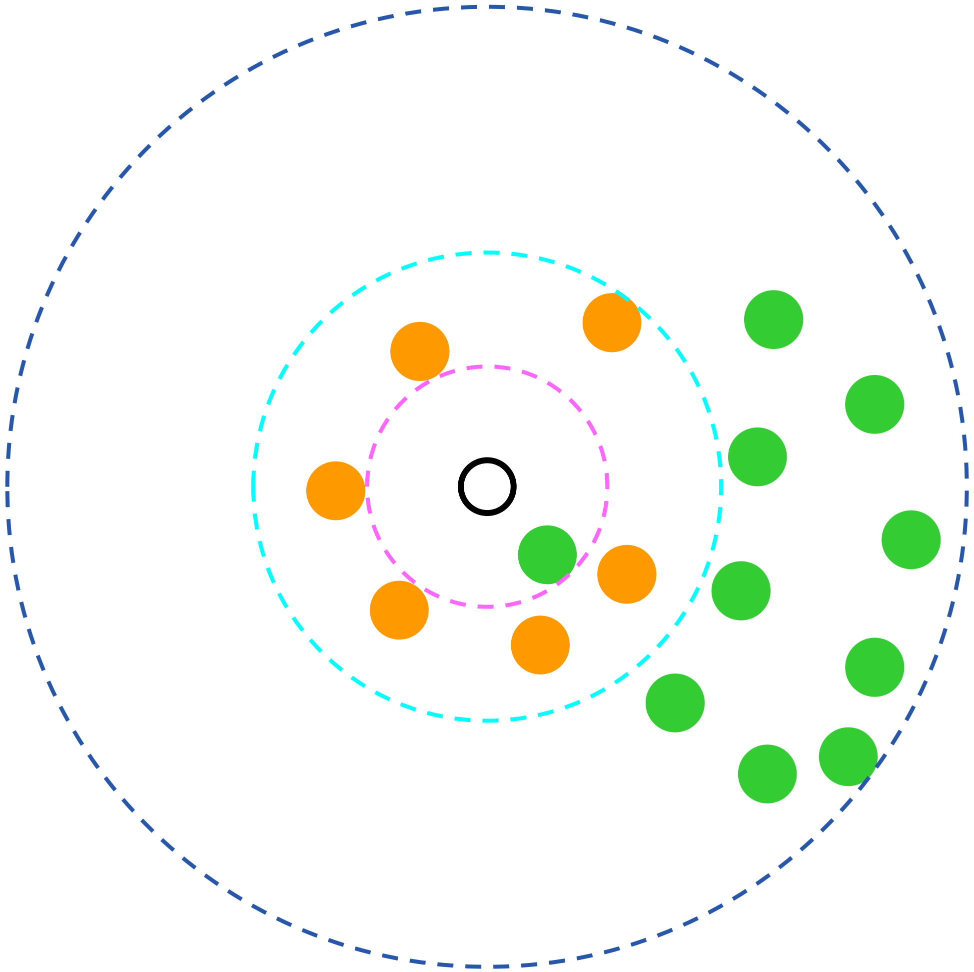


How to choose parameter k?

"too small" k: sensitive to outliers

"too large" k: many objects from other classes

medium k: highest accuracy



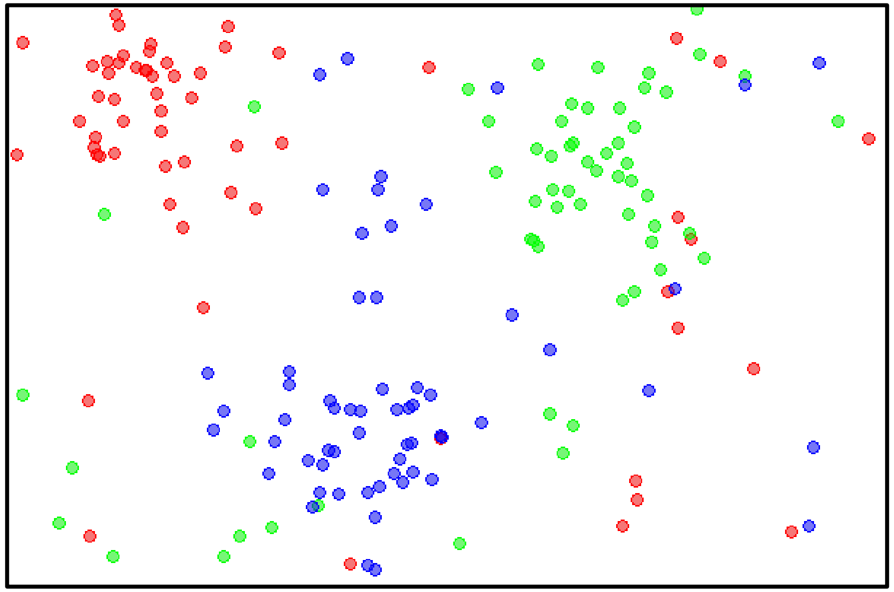
Decision set for $k = 1$

Decision set for $k = 7$

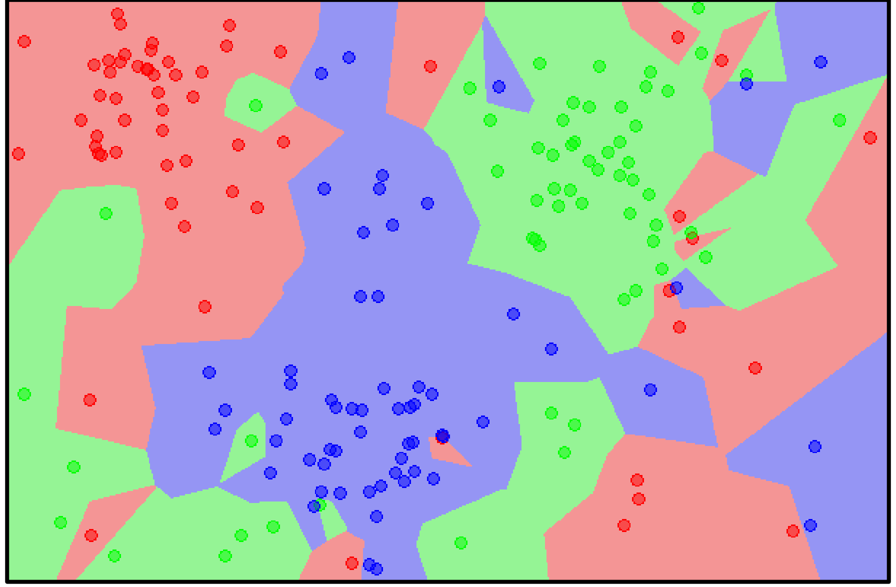
Decision set for $k = 16$

Difference Between 1-NN and 5-NN

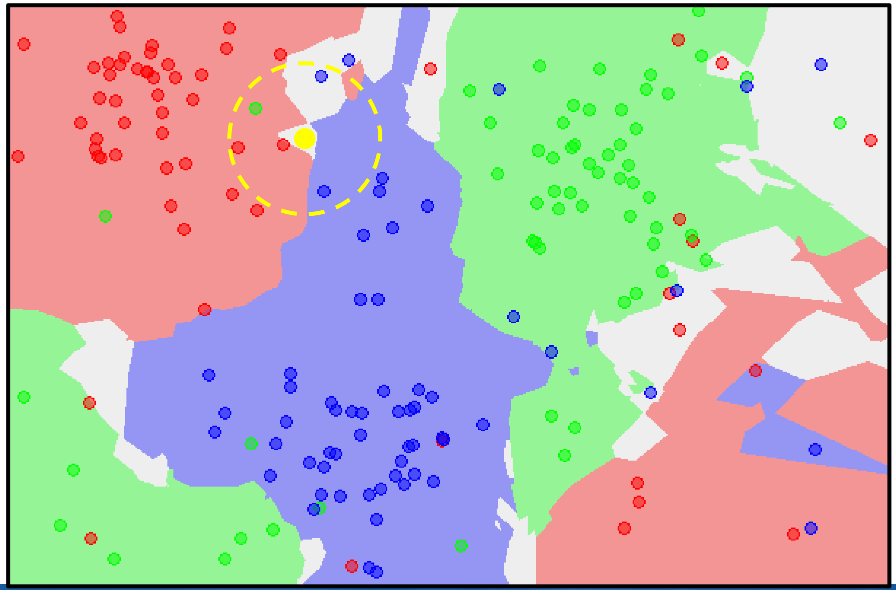
Original dataset



1-NN



5-NN



White Region: class votes are tied

{red, red, blue, blue, green}