Artificial Neural Networks and Support Vector Machines

CS 486/686: Introduction to Artificial Intelligence

Outline

- What is a Neural Network?
  - Perceptron learners
  - Multi-layer networks
- What is a Support Vector Machine?
  - Maximum Margin Classification
  - The kernel trick
  - Regularization

Introduction

- Machine learning algorithms can be viewed as approximations of functions that describe the data
- In practice, the relationships between input and output can be **extremely** complex.

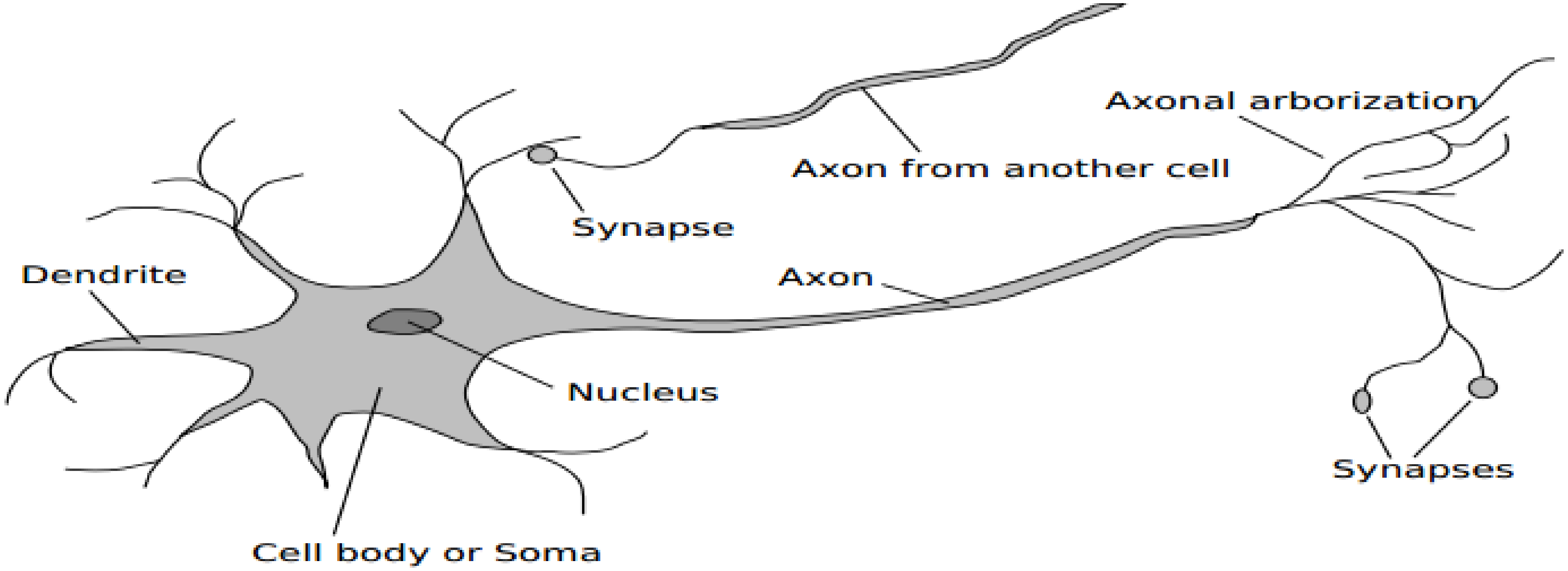
- We want to:
  - Design methods for learning arbitrary relationships
  - Ensure that our methods are efficient and do not overfit the data
- Today we'll discuss two modern techniques for learning arbitrary complex functions

Artificial Neural Nets

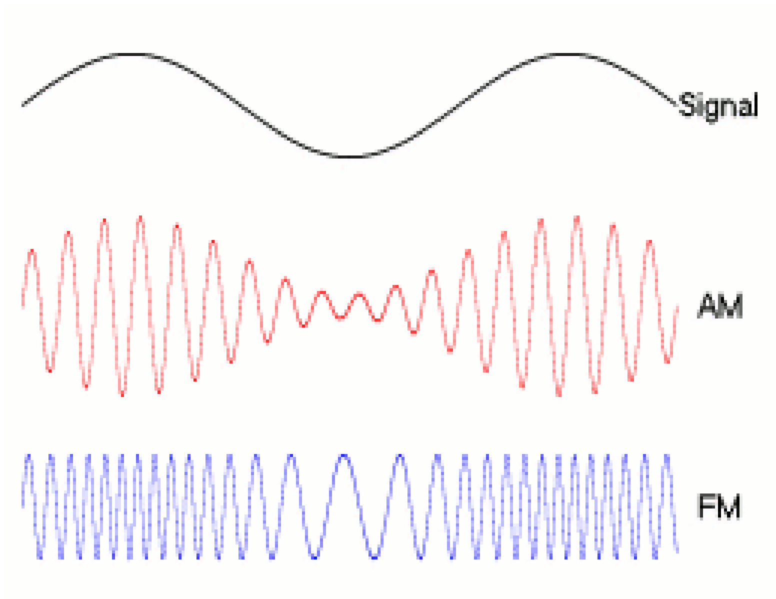
- Idea: The humans can often learn complex relationships very well.
- Maybe we can simulate human learning?

Human Brains

- A brain is a set of densely connected neurons.
- A neuron has several parts:
  - Dendrites: Receive inputs from other cells
  - Soma: Controls activity of the neuron
  - Axon: Sends output to other cells
  - Synapse: Links between neurons



Human Brains



- Neurons have two states
  - Firing, not firing
- All firings are the same
- Rate of firing communicates information (FM)
- Activation passed via chemical signals at the synapse between firing neuron's axon and receiving neuron's dendrite
- Learning causes changes in how efficiently signals transfer across specific synaptic junctions.

Artificial Brains?

- Artificial Neural Networks are based on very early models of the neuron.
- Better models exist today, but are usually used theoretical neuroscience, not machine learning

Artificial Brains?

- An artificial Neuron (McCulloch and Pitts 1943)

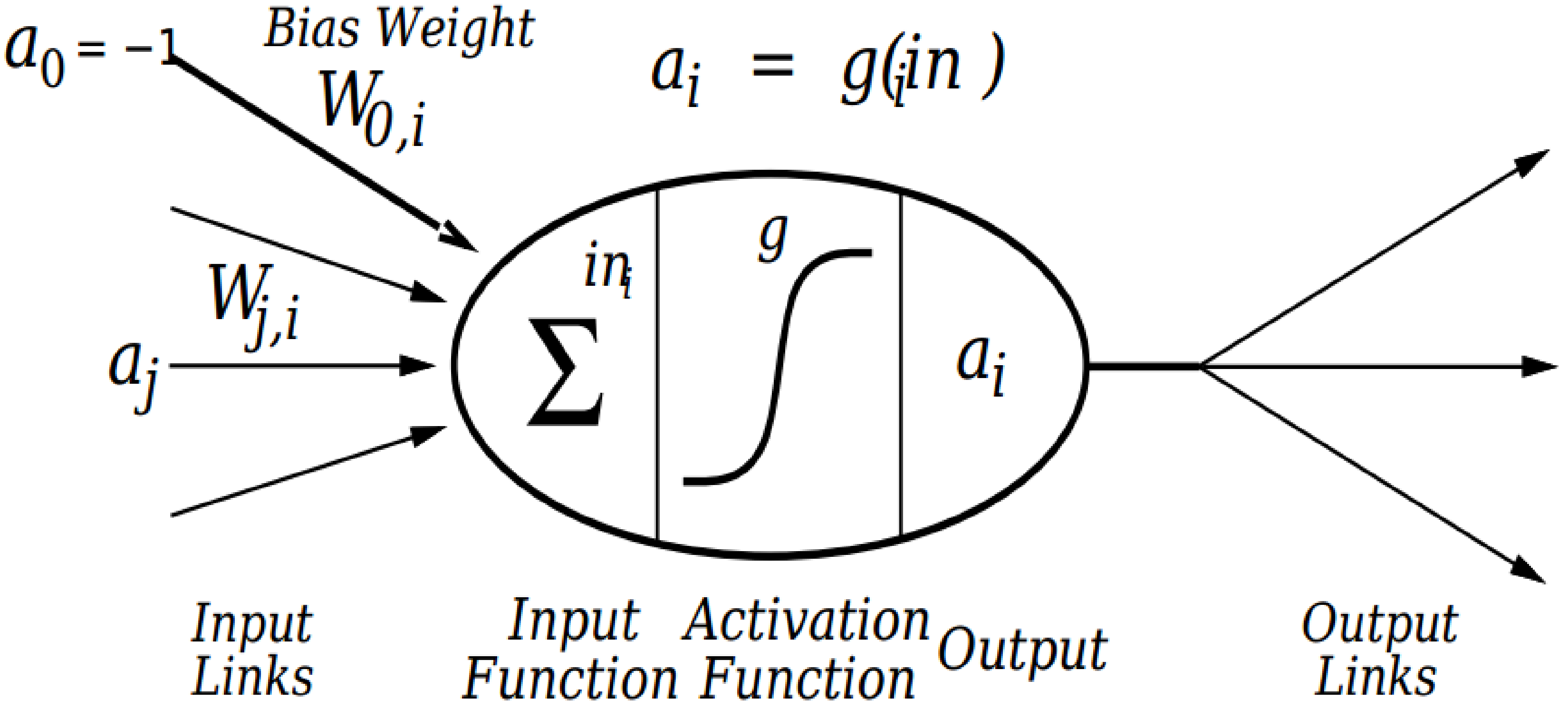
Link~ Synapse

Weight ~ Efficiency

Input Fun.~ Dendrite

Activation Fun.~ Soma

Output = Fire or not



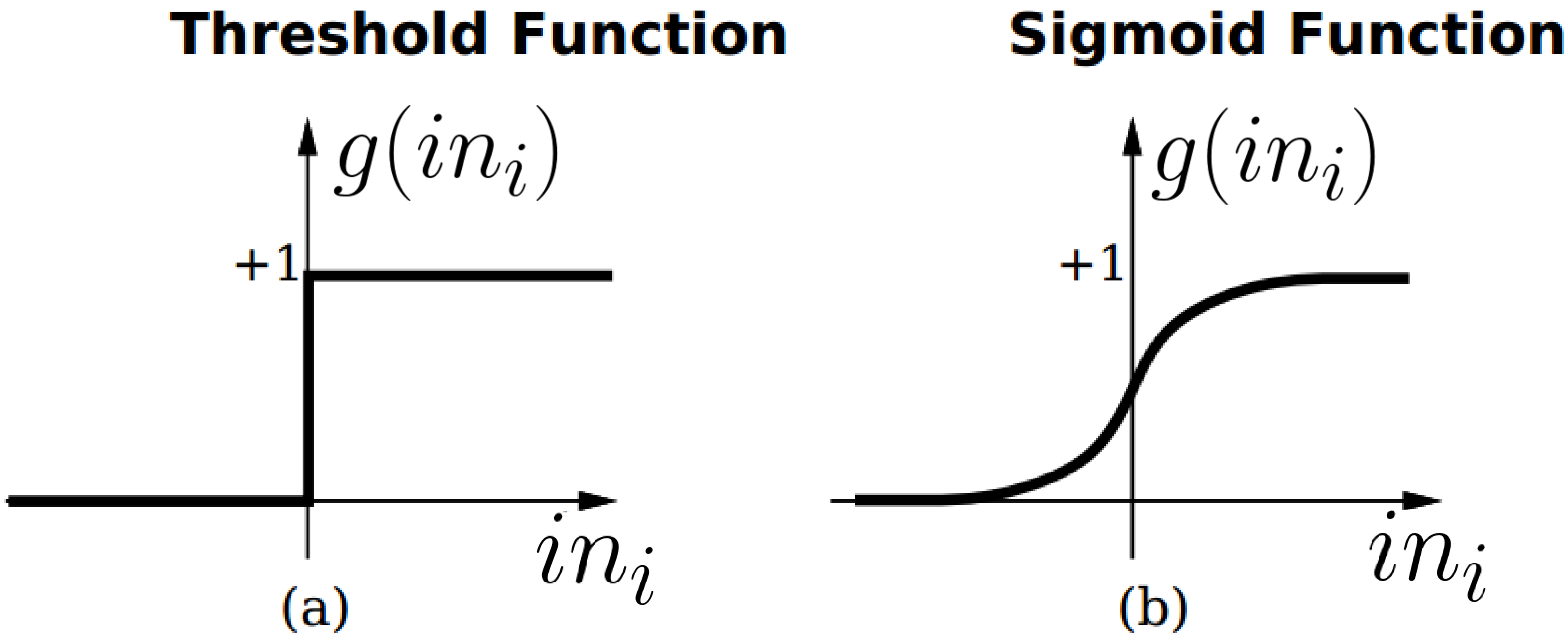
Artificial Neural Nets

- Collection of simple artificial neurons.
- Weights $W_{i,j}$ denote strength of connection from i to j
- Input function: $in_i = \sum_j W_{i,j} \times a_j$
- Activation Function: $a_i = g(in_i)$

Activation Function

- Activation Function: $a_i = g(in_i)$
- Should be non-linear (otherwise, we just have a linear equation)
- Should mimic firing in real neurons
  - Active (a_i ~ 1) when the "right" neighbors fire the right amounts
  - Inactive (a_i ~ 0) when fed "wrong" inputs

Common Activation Functions

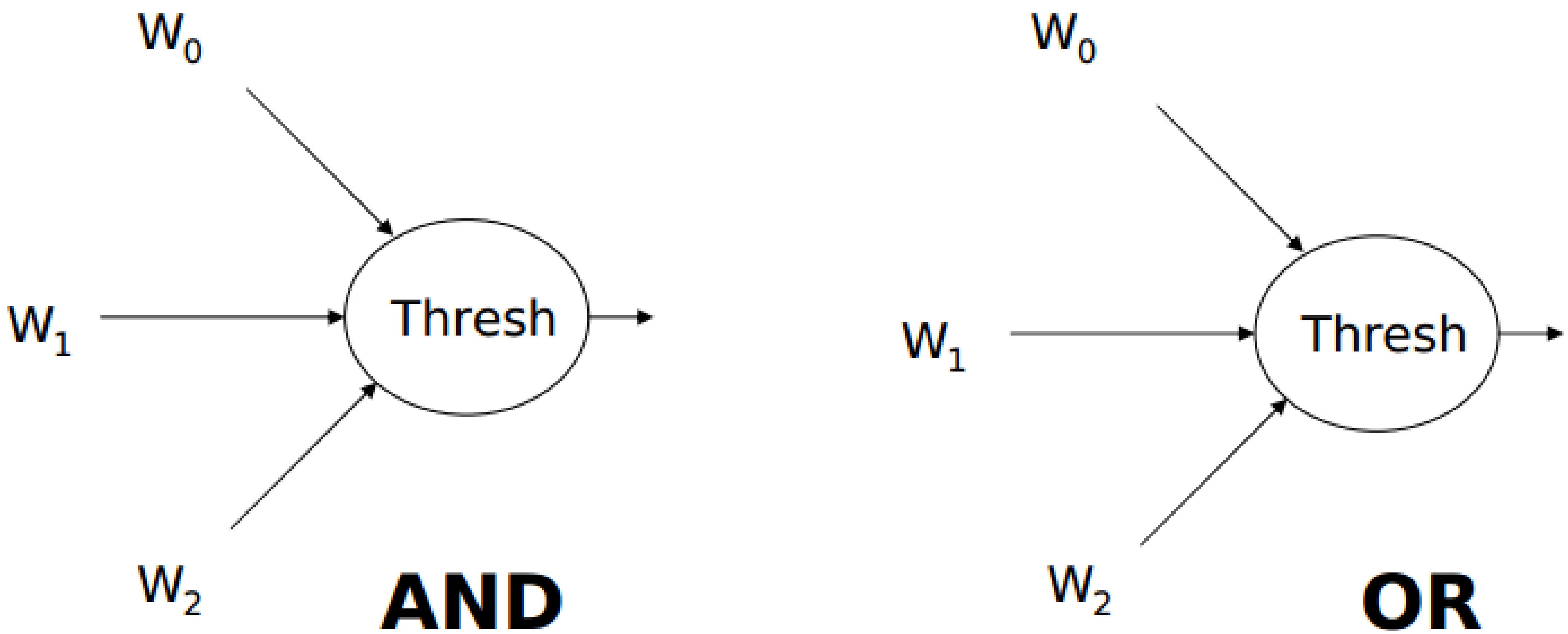


Weights determine threshold

$$g(in_i) = \frac{1}{1 + e^{-in_i}}$$

Logic Gates

- It is possible to construct a universal set of logic gates using the neurons described (McCulloch and Pitts 1943)



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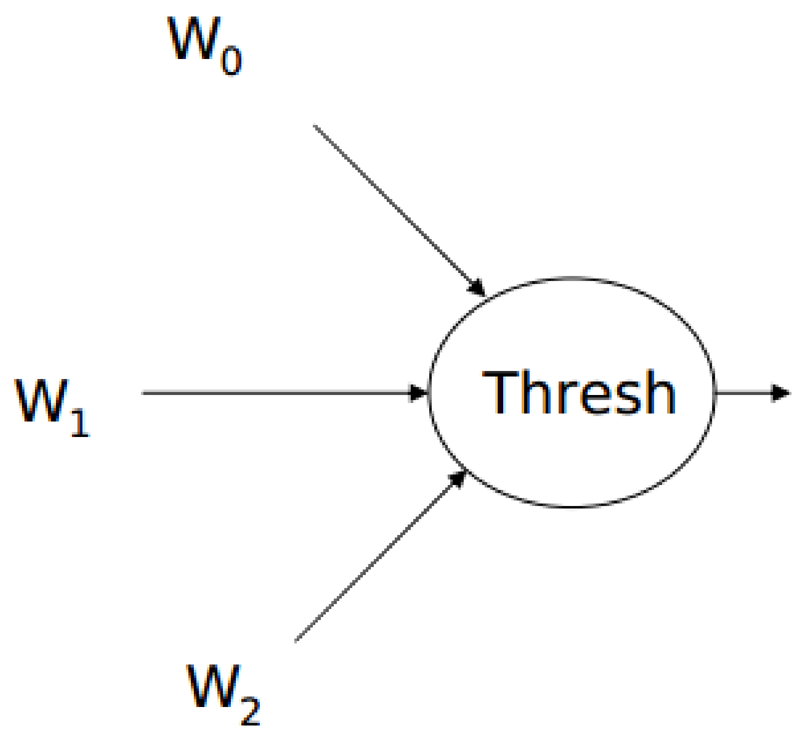
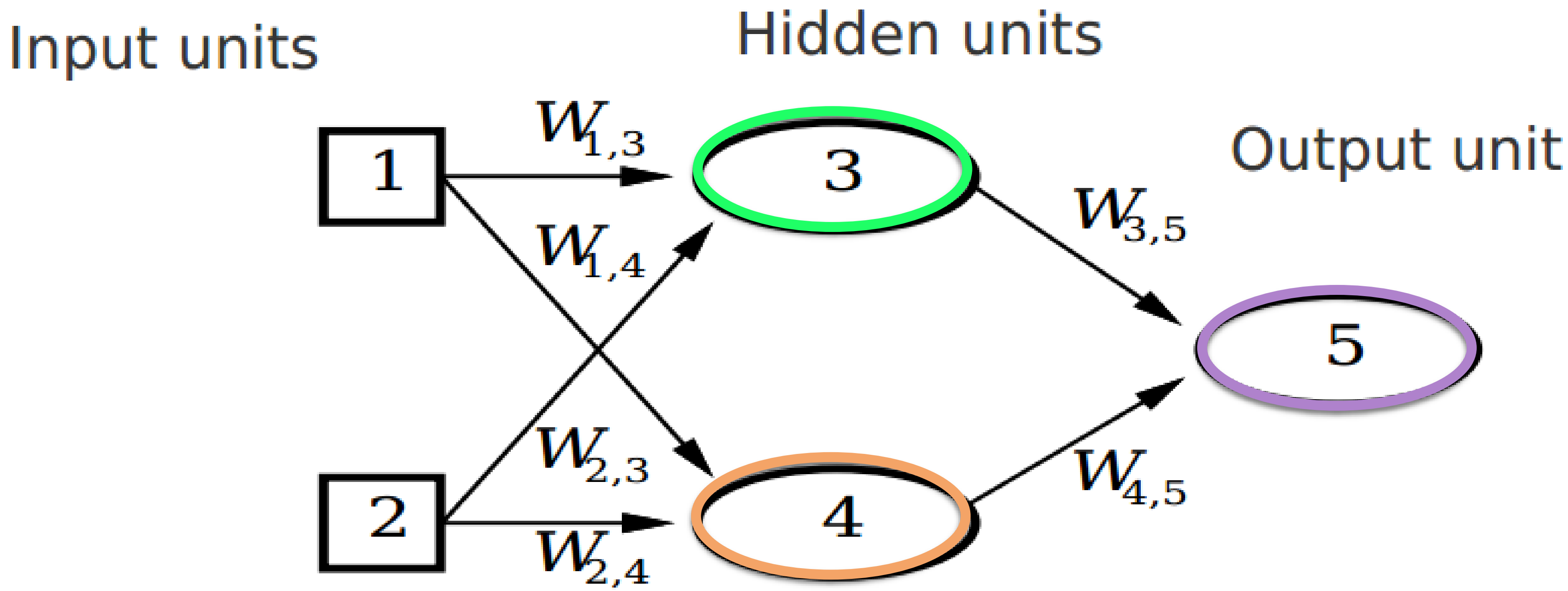


NOT

Network Structure

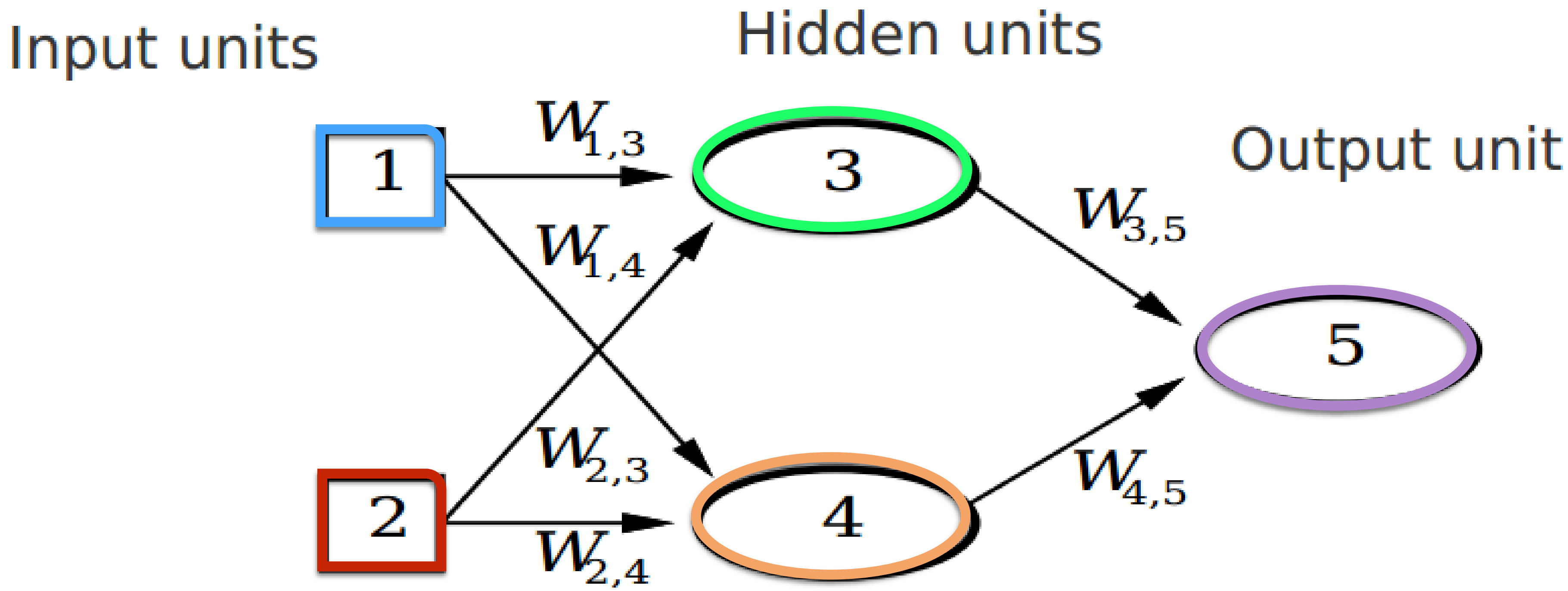
- Feed-forward ANN
  - Direct acyclic graph
  - No internal state: maps inputs to outputs.
- Recurrant ANN
  - Directed cyclic graph
  - Dynamical system with an internal state
  - Can remember information for future use

Example



$$a_5 = g(W_{3,5} \cdot a_5 + W_{4,5} \cdot a_4)$$

Example



$$a_5 = g(W_{3,5} \cdot a_5 + W_{4,5} \cdot a_4)$$

$$a_5 = g(W_{3,5} \cdot g(W_{1,3} \cdot a_1 + W_{2,3} \cdot a_2) + W_{4,5} \cdot g(W_{1,4} \cdot a_1 + W_{2,4} \cdot a_2))$$

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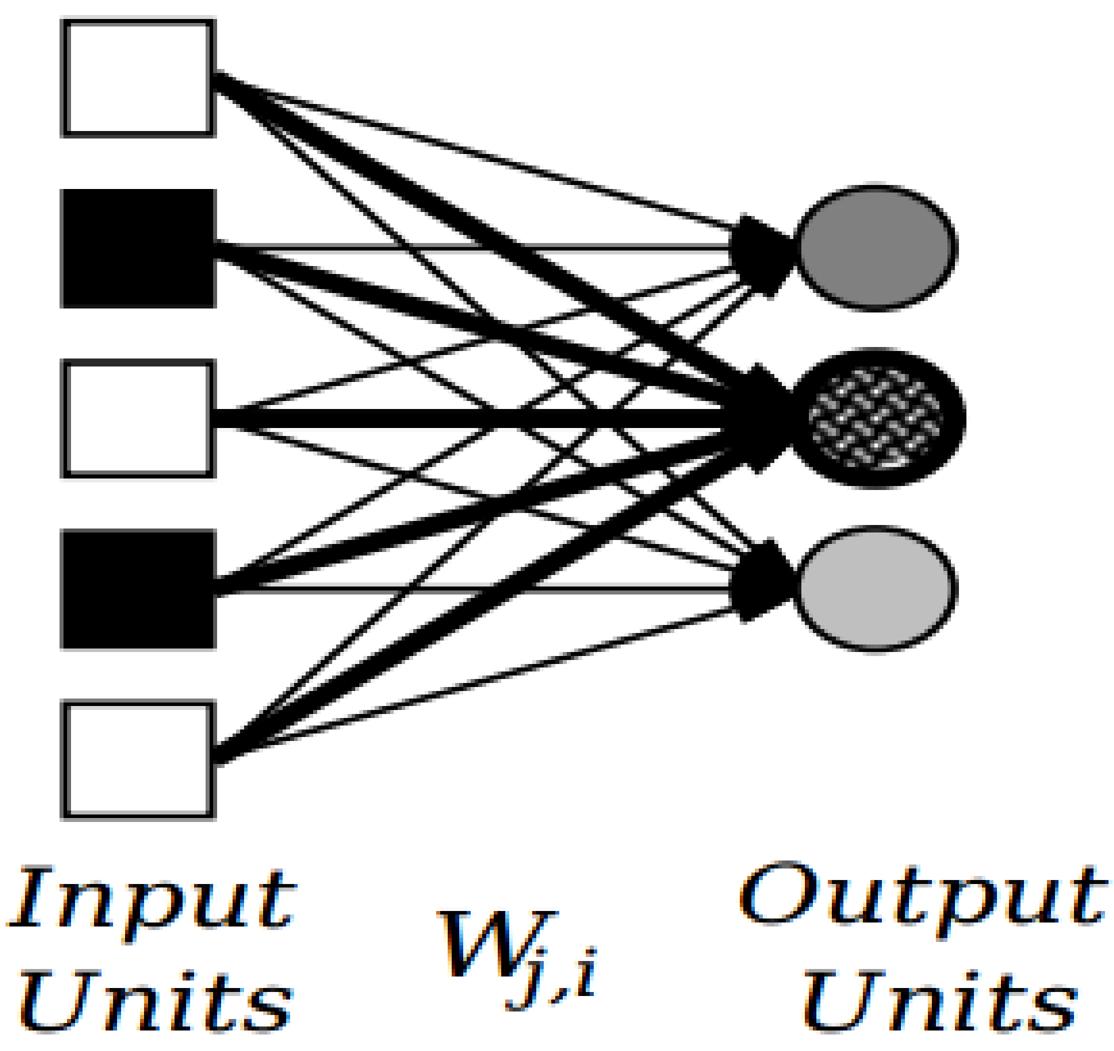
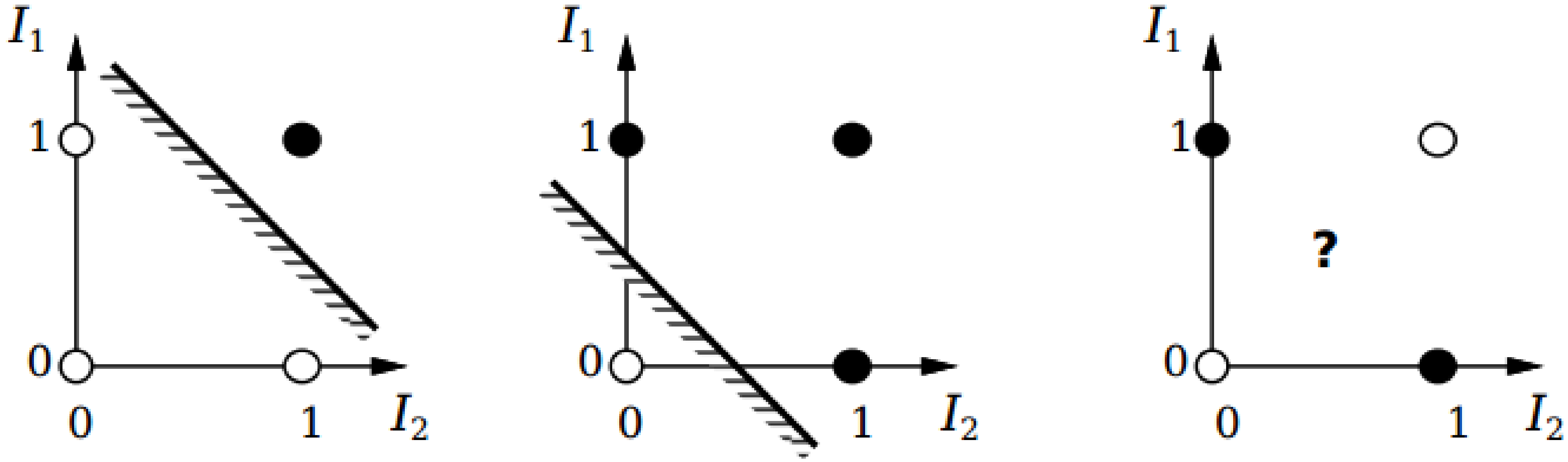
Perceptrons

Single layer feed-forward network



Perceptrons

Can learn only linear separators



(a) I_1 **and** I_2 (b) I_1 **or** I_2 (c) I_1 **xor** I_2

Training Perceptrons

- Learning means adjusting the weights
  - Goal: minimize loss of fidelity in our approximation of a function
- How do we measure loss of fidelity?
  - Often: Half the sum of squared errors of each data point

$$E = \sum_i 0.5(y_i - h_W(x_i))^2$$

Gradient Descent

$$\frac{\partial E}{\partial W_k} = \frac{\partial}{\partial W_k} \sum_i 0.5(y_i - h_W(\mathbf{x_i}))^2$$

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$$\frac{\partial E}{\partial W_k} = \sum_i 0.5 \cdot 2 \cdot (y_i - h_W(\mathbf{x_i})) \frac{\partial}{\partial W_k} (y\_g(\sum_j W_j x_{i,j}))$$

Gradient Descent

$$\frac{\partial E}{\partial W_k} = \frac{\partial}{\partial W_k}\sum_i 0.5(y_i - h_W(\mathbf{x_i}))^2$$

$$\frac{\partial E}{\partial W_k} = \sum_i \frac{\partial}{\partial W_k} 0.5(y_i - h_W(\mathbf{x_i}))^2$$

$$\frac{\partial E}{\partial W_k} = \sum_i 0.5 \cdot 2 \cdot (y_i - h_W(\mathbf{x_i}))\frac{\partial}{\partial W_k}(y_- g(\sum_j W_j x_{i,j}))$$

$$\frac{\partial E}{\partial W_k} = \sum_i (y_i - h_W(\mathbf{x_i}))(-g'(\mathbf{w}\cdot\mathbf{x_i})\frac{\partial}{\partial W_k}\mathbf{w}\cdot\mathbf{x_i})$$

Gradient Descent

$$\frac{\partial E}{\partial W_k} = \frac{\partial}{\partial W_k} \sum_i 0.5(y_i - h_W(\mathbf{x_i}))^2$$

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$$\frac{\partial E}{\partial W_k} = \sum_i (y_i - h_W(\mathbf{x_i}))(-g'(\mathbf{w} \cdot \mathbf{x_i}) \frac{\partial}{\partial W_k} \mathbf{w} \cdot \mathbf{x_i})$$

$$\frac{\partial E}{\partial W_k} = \sum_i (y_i - h_W(\mathbf{x_i}))(-g'(\mathbf{w} \cdot \mathbf{x_i}) \cdot x_{i,k})$$

Learning Algorithm

- Repeat for "some time"

- For each example i:

$$
\begin{aligned}
I &\leftarrow \mathbf{w} \cdot \mathbf{x_i} \\
E &\leftarrow y_i - g(I) \\
W_j &\leftarrow W_j + \alpha(E \cdot g'(I) \cdot x_{i,j}) \forall j
\end{aligned}
$$

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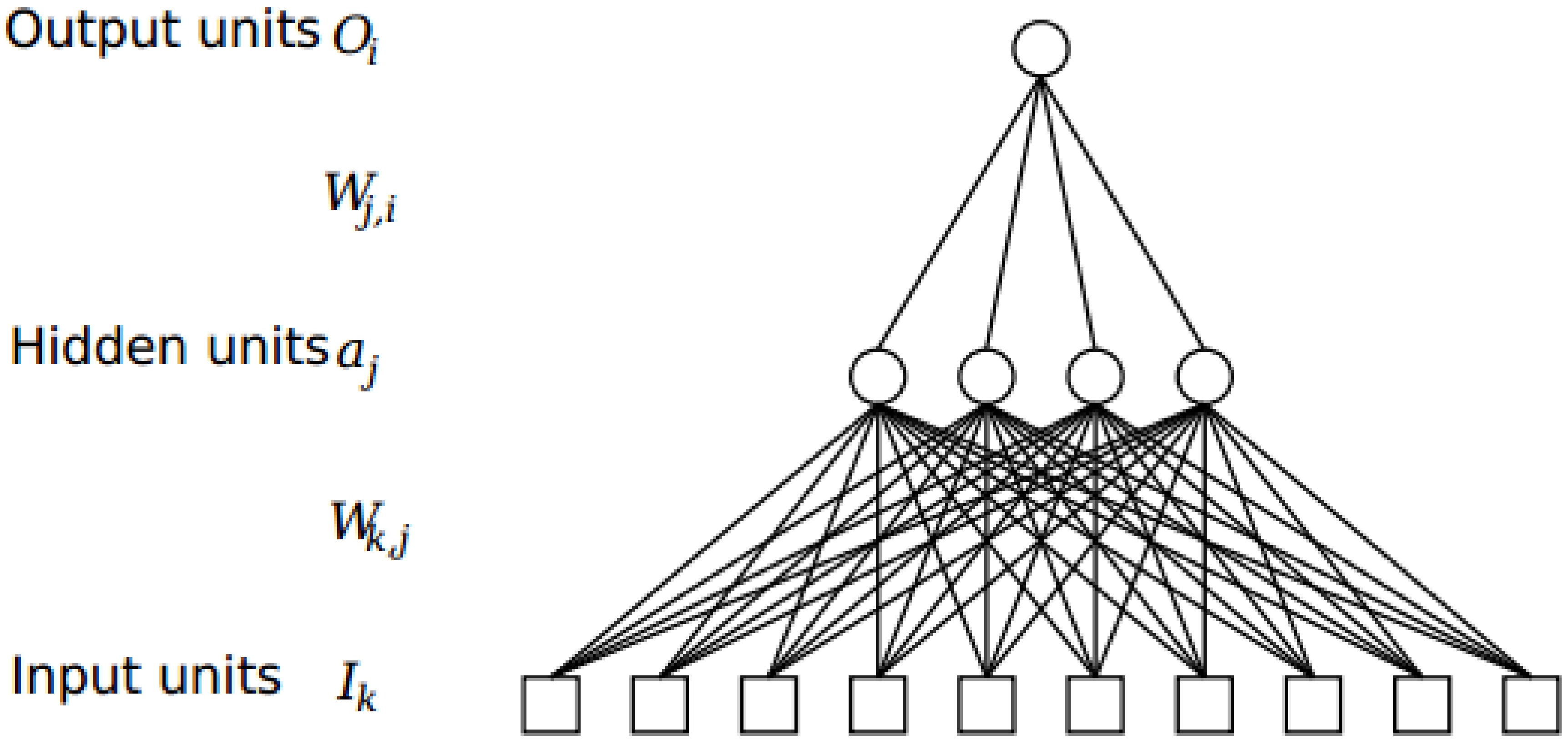
Multilayer Networks

- Minsky's 1969 book *Perceptrons* showed perceptrons could not learn XOR.
- At the time, no one knew how to train deeper networks.
- Most ANN research abandoned.

Multilayer Networks

- *Any* continuous function can be learned by an ANN with just one hidden layer (if the layer is large enough).



Training Multilayer Nets

- For weights from hidden to output layer, just use Gradient Descent, as before.

$$\Delta_i = E \cdot g'(I)$$
$$W_{j,i} = W_{j,i} + \alpha \Delta_i a_j$$

- For weights from input to hidden layer, we have a problem: What is y?

$$E = \sum_i 0.5(y_i - h_W(x_i))^2$$

Back Propigation

- Idea: Each hidden layer caused *some* of the error in the output layer.
- Amount of error caused should be proportionate to the connection strength.

$$\Delta_i = E \cdot g'(I)$$
$$W_{j,i} = W_{j,i} + \alpha \Delta_i a_j$$

$$\Delta_j = g'(I) \cdot \sum_i W_{j,i} \Delta_i$$

$$W_{k,j} = W_{k,j} + \alpha \Delta_j x_k$$

Back Propigation

- Repeat for "some time":
- Repeat for each example:
  - Compute Deltas and weight change for output layer, and update the weights .
  - Repeat until all hidden layers updated:
    - Compute Deltas and weight change for the deepest hidden layer not yet updated, and update it.

When to use ANNs

- When we have high dimensional or real-valued inputs, and/or noisy (e.g. sensor data)
- Vector outputs needed
- Form of target function is unknown (no model)
- Not import for humans to be able to *understand* the mapping

Drawbacks of ANNs

- Unclear how to interpret weights, especially in many-layered networks.
- How deep should the network be? How many neurons are needed?
- Tendency to overfit in practice (very poor predictions outside of the range of values it was trained on)

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SVMs

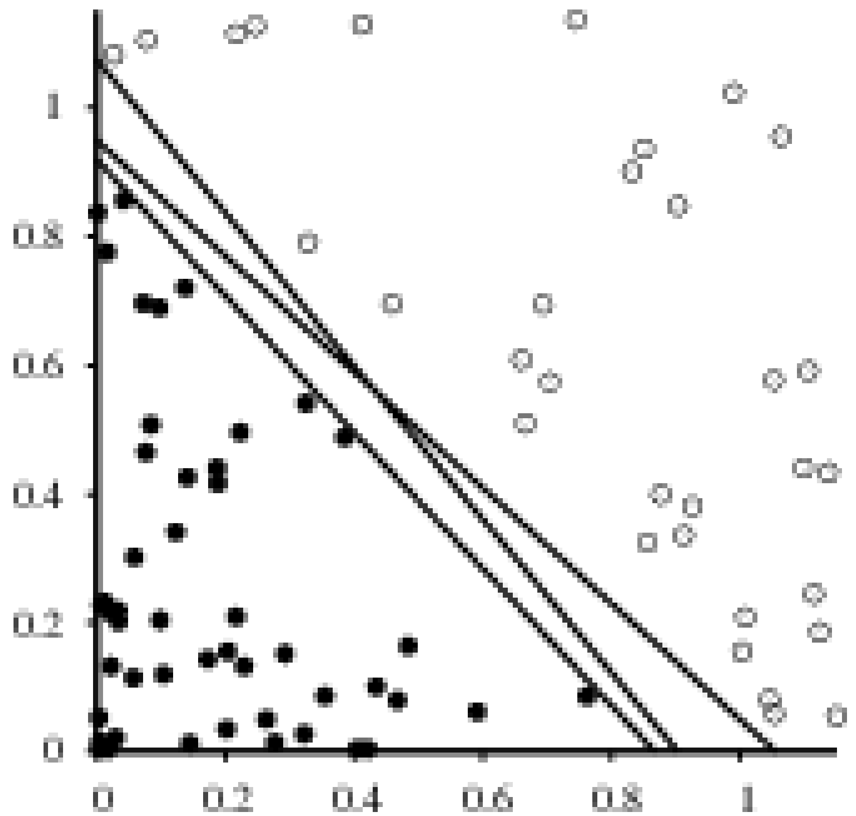
- We want an algorithm that can learn arbitrary functions (like multilayered ANNs)
- But, it shouldn't require picking a lot of parameters, and should extrapolate in a reasonable, predictable way.

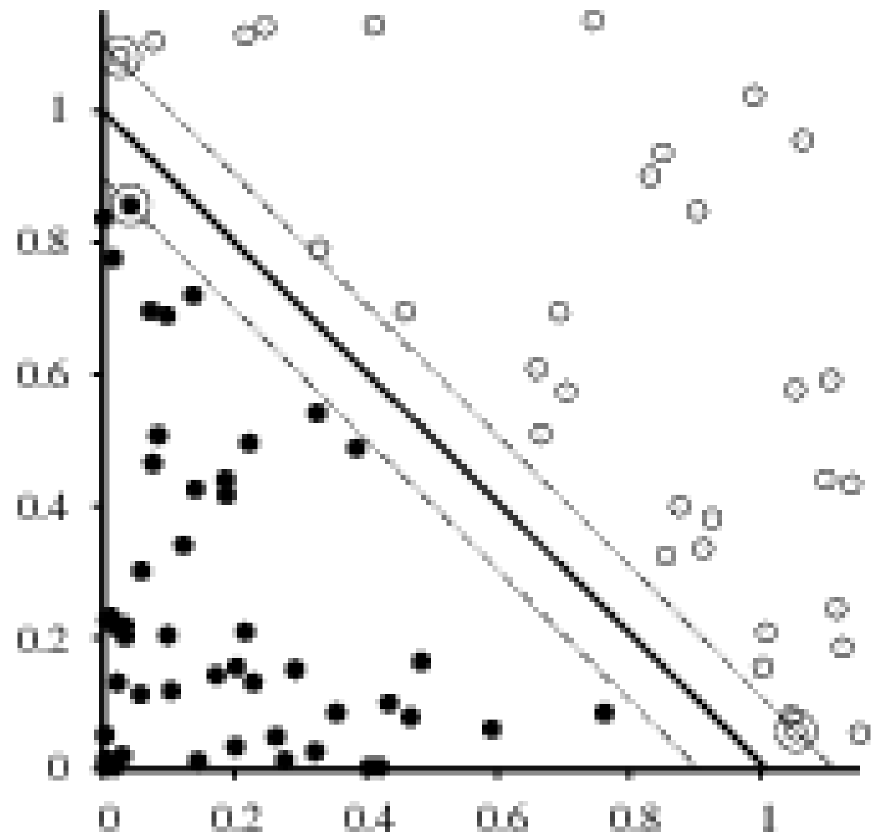
SVMs

- Support Vector Machines (SVMs) can learn arbitrary functions.
- SVMs also extrapolate in a predictable, controllable way, and have just two parameters to set.
- Often the first choice of modern practitioners.

Maximum Margin

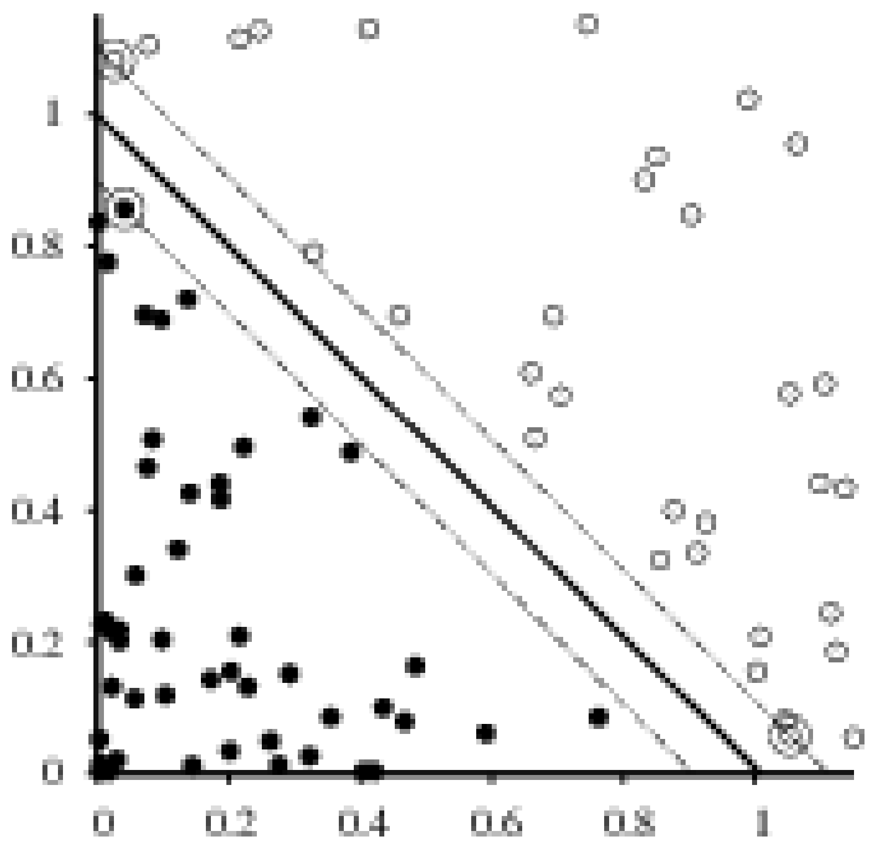
- Idea: We do not know where the exact decision boundary is, so pick "safest" one.
- Best separating hyperplane is furthest from any point, but still partitions cleanly





Support Vectors

- A maximum margin hyperplane is defined by its "Support Vectors"
- These are the points that "support" the plane on either side
- Find the optimal SVs using Quadratic Programming



Finding the SVs

- Find a weight α_j for each point.

$$\arg\max_{\alpha} \sum_j \alpha_j - \frac{1}{2} \sum_{j,k} \alpha_j \alpha_k y_j y_j (\mathbf{x_j} \cdot \mathbf{x_k})$$

$$s.t.$$

$$\alpha_j \geq 0 \forall j$$

$$\sum_j \alpha_j y_j = 0$$

- y_i = label of example i (-1 for negative, + 1 for positive)
- x_i = input vector for example i

Using the SVs

- To classify a new point, figure out whether it's above or below the plane

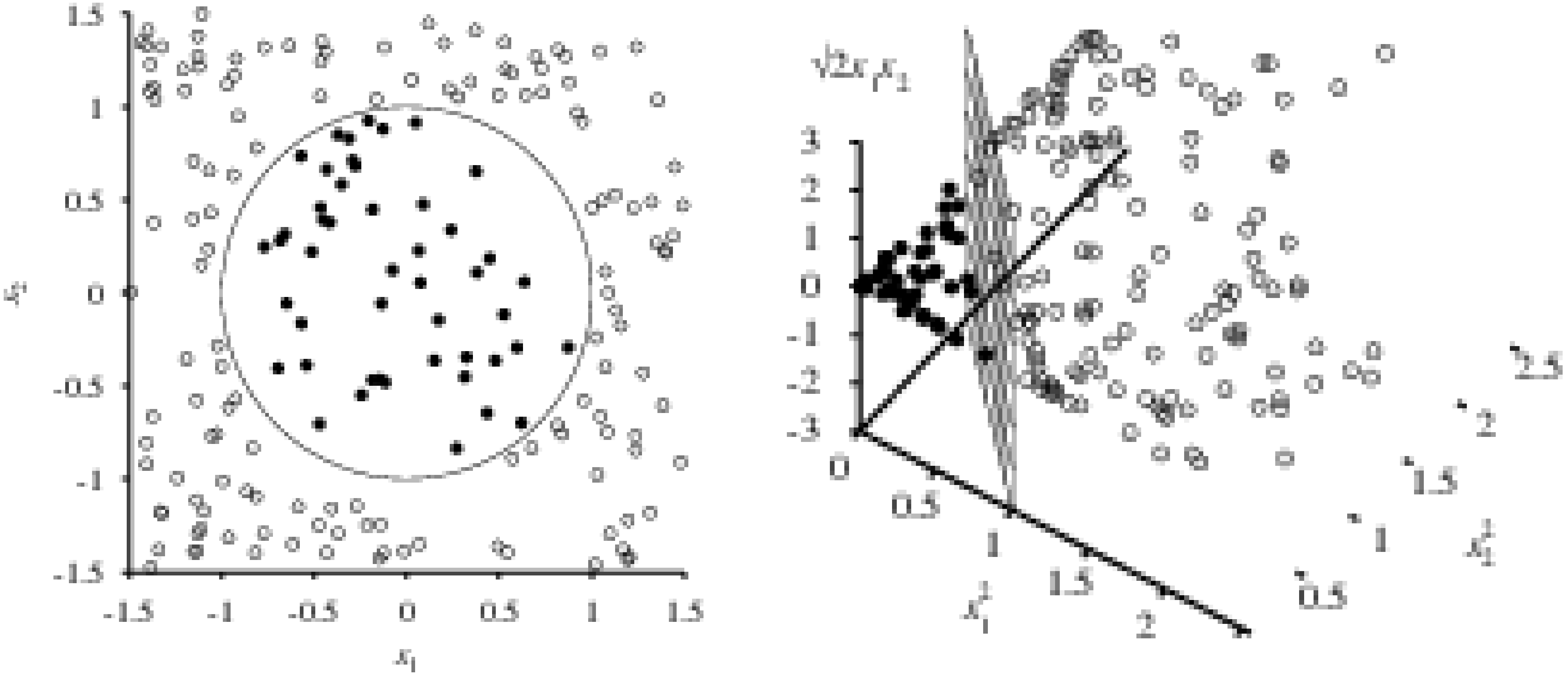
$$H(\mathbf{x}) = sign(\sum_j \alpha_j y_j (\mathbf{x} \cdot \mathbf{x_j}) - b)$$

- Only need to store x_j vectors for points with non-zero weight, so model can be compact.

Non-Linear Learning

- If we're just finding the best line, how can we learn arbitrary functions?
- Insight: A high-dimensional line can be projected into any shape in lower dimensions.

Non-Linear Learning



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The Kernel Trick

- Solution: Define a function F(x) that maps x to a new feature space. Learn an SVM using F(x) instead of x.
- Problems:
  - What should F(x) be?
  - If F(x) has many more dimensions than x, then the dot product will become expensive to compute.

The Kernel Trick

- We call any function of the inner product of two points a "kernel".

- Examples:
  - "Linear kernel": K(x_i,x_j)= $(\mathbf{x_i} \cdot \mathbf{x_j})$
  - Polynomial Kernel: $K(\mathbf{x_k}, \mathbf{x_j}) = (1 + \mathbf{x_j} \cdot \mathbf{x_k})^d$

The Kernel Trick

- Mercer's Theorem: Define a matrix K over every x_i, x_j in your data, such that

$$K_{i,j} = K(x_i, x_j)$$

- If K is positive definite, then there exists some feature space F(x) such that:

$$K(\mathbf{x_k}, \mathbf{x_j}) = F(\mathbf{x_j}) \cdot F(\mathbf{x_k})$$

Example

$$K(\mathbf{x_i}, \mathbf{x_j}) = (\mathbf{x_i} \cdot \mathbf{x_j})^2$$

Example

$$K(\mathbf{x_i}, \mathbf{x_j}) = (\mathbf{x_i} \cdot \mathbf{x_j})^2$$

$$K(\mathbf{x_i}, \mathbf{x_j}) = ((x_{i,1}x_{j,1}) + (x_{i,2}x_{j,2}))^2$$

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Example

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$$F([x_1, x_2]) = [x_1^2, x_2^2, \sqrt{2}x_1x_2)]$$

Example

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$$F([x_1, x_2]) = [x_1^2, x_2^2, \sqrt{2}x_1x_2)]$$

$$K(\mathbf{x_i}, \mathbf{x_j}) = F(\mathbf{x_i}) \cdot F(\mathbf{x_j})$$

The Kernel Trick

- Insight: data points themselves are never used in optimization, only $(\mathbf{x_i} \cdot \mathbf{x_j})$

- Mercer's Theorem means that, if we replace every $(\mathbf{x_i} \cdot \mathbf{x_j})$ by $K_{i,j} = K(x_i, x_j)$ then we are finding the optimal support vectors in some other feature space F(x)!

The Kernel Trick

- Since we never need to compute F(x) explicitly, the algorithm runs equally fast whether we use a kernel or not
- Not true of other methods. If a decision tree wants to work in a larger space, it needs to split on more attributes
- This is one of the main advantages of SVMs

Some Useful Kernels

- Polynomial kernel, F() exponentially larger as d increases:

$$K(\mathbf{x_k}, \mathbf{x_j}) = (1 + \mathbf{x_j} \cdot \mathbf{x_k})^d$$

- RBF kernel, F() has *infinite* dimensionality:

$$K(\mathbf{x_k}, \mathbf{x_j}) = exp(\gamma \sum_l (x_{k,l} - x_{j,l})^2)$$

Picking Kernels

- More dimensions is not always better
- RBF often good for image processing and related dense domains with smooth, circular or elliptical decision boundaries
- Linear kernel (d = 1) often better for sparse domains like text
- Depends on your problem

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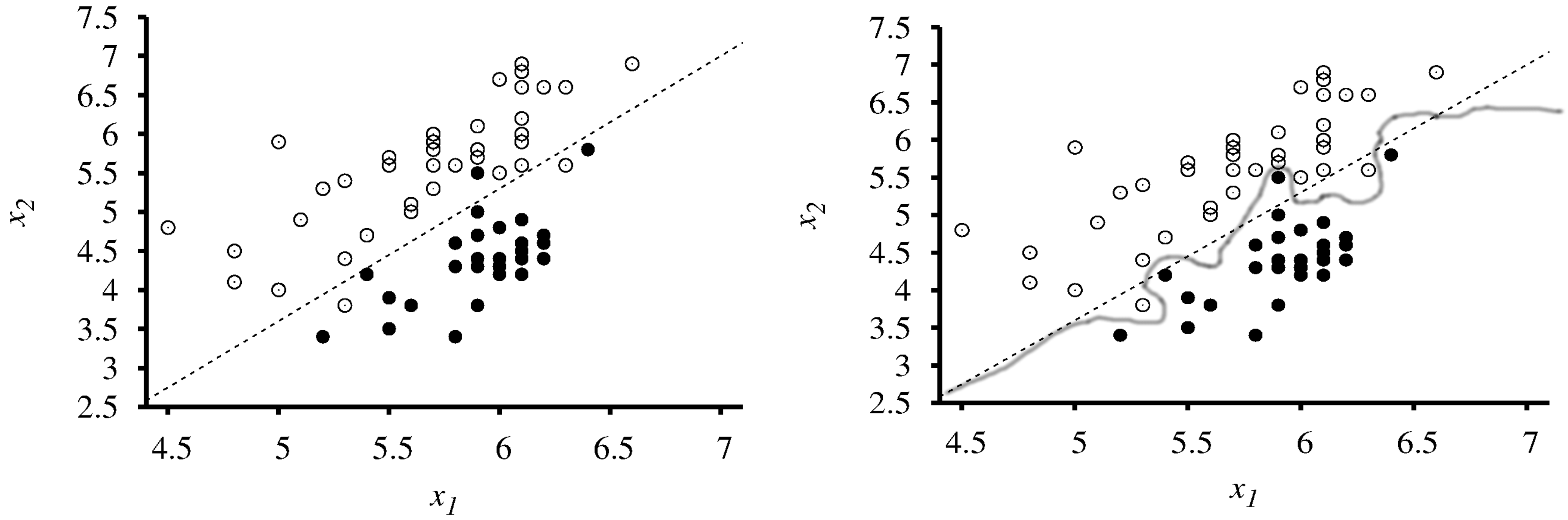
Regularization

- An SVM can usually find an exact decision boundary (if the feature space is big enough)
- But the exact boundary may over-fit the data

Example



7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
x_2
4.5
5
5.5
6
6.5
7
x_1
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
x_2
4.5
5
5.5
6
6.5
7
x_1

Regularization

- To avoid this, we add regularization parameter C
- Cost for misclassifying an example is C
- Cost for increasing total SV weight by 1 is 1/C.
- Right choice of C depends on your problem

Parameter Selection

- Pick a kernel
- Pick a *regularization cost C*, directly manipulates overfitting vs. underfitting

When to use an SVM

- Often a good first choice for classification
- Outcome is binary, and there are not too many features or data points
- Have some notion of the proper kernel

When to avoid an SVM

- "Big Data" problems (tons of data, speed is very important, QP too slow)
- Human interpretation is important
- Problem has many outputs

Summary

You should be able to:

- Describe what a Neural Network is, and how to train one from data using back-propagation.
- Describe what maximum margin hyperplanes are and support vectors are.
- Explain how an SVM can learn non-linear functions efficiently, using the kernel trick.

Announcements

- A5 Due Today
- A6 Out Today (Fun!)
- Thursday: Computational Learning Theory
  - R&N Ch 18.5
  - P & M Ch 7.7.2

Perceptrons

- Minsky's 1969 book *Perceptrons* showed perceptrons could not learn XOR.
- Led to collapse of neural approaches to AI, and the rise of symbolic approaches during the AI winter. Note that we already knew the neural model was Turing-complete though!
- Now thought to have been a *philosophically* motivated shift, rather than one required by the science.
- ***Olazaran, Mikel (August 1996). "A Sociological Study of the Official History of the Perceptrons Controversy". Social Studies of Science* 26**: 611–659.