Neural Networks: Introduction

Machine Learning

Based on slides and material from Geoffrey Hinton, Richard Socher, Dan Roth, Yoav Goldberg, Shai Shalev-Shwartz and Shai Ben-David, and others

Where are we?

Learning algorithms

- Decision Trees
- Perceptron
- AdaBoost
- Support Vector Machines
- Logistic Regression

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General learning principles

- Overfitting
- Mistake-bound learning
- PAC learning, sample complexity
- Hypothesis choice & VC dimensions
- Training and generalization errors
- Regularized Empirical Loss Minimization
- Bayesian Learning

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Produce *linear classifiers*

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Not really resolved

What if we want to train non-linear classifiers?

Where do the features come from?

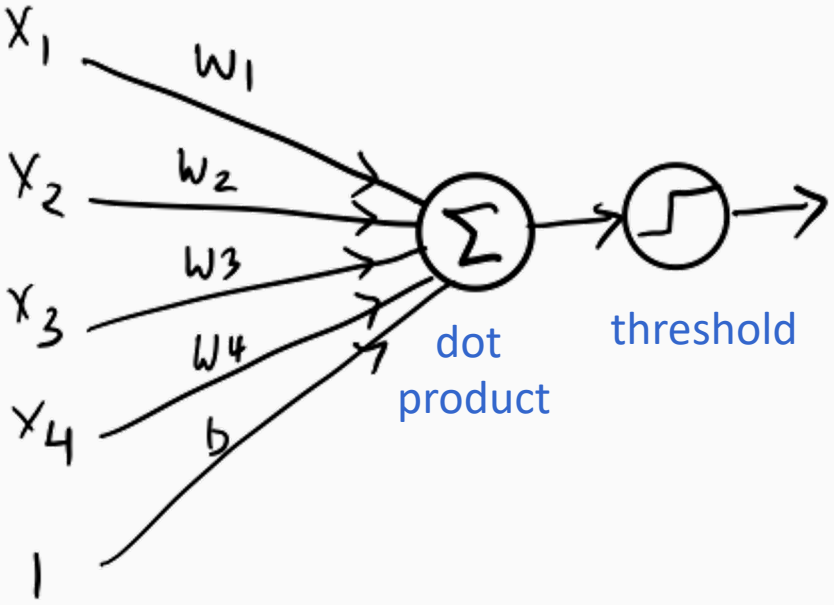
Neural Networks

- What is a neural network?
- Predicting with a neural network
- Training neural networks
- Practical concerns

This lecture

- What is a neural network?
  - The hypothesis class
  - Structure, expressiveness
- Predicting with a neural network
- Training neural networks
- Practical concerns

We have seen linear threshold units



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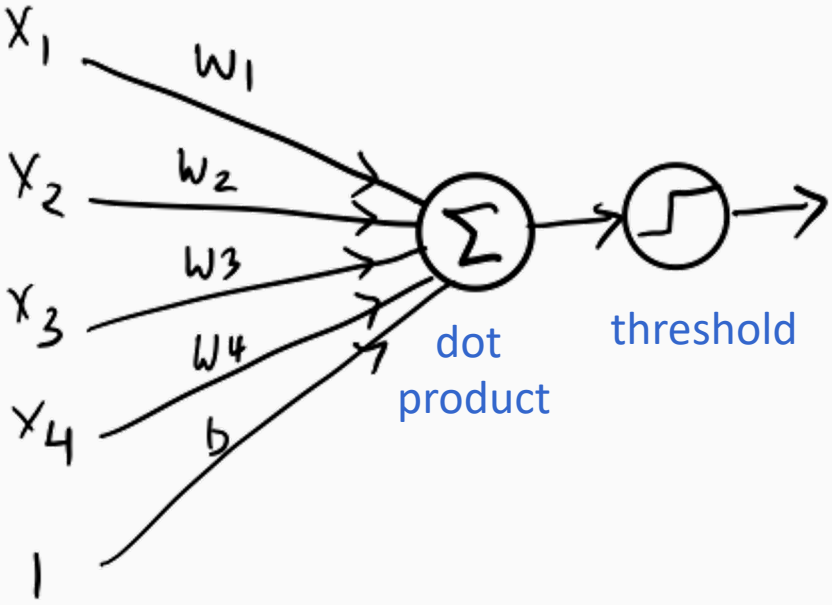

Prediction

$$\text{sgn}\,(\boldsymbol{w}^T\boldsymbol{x} + b) = \text{sgn}(\sum w_i x_i + b)$$

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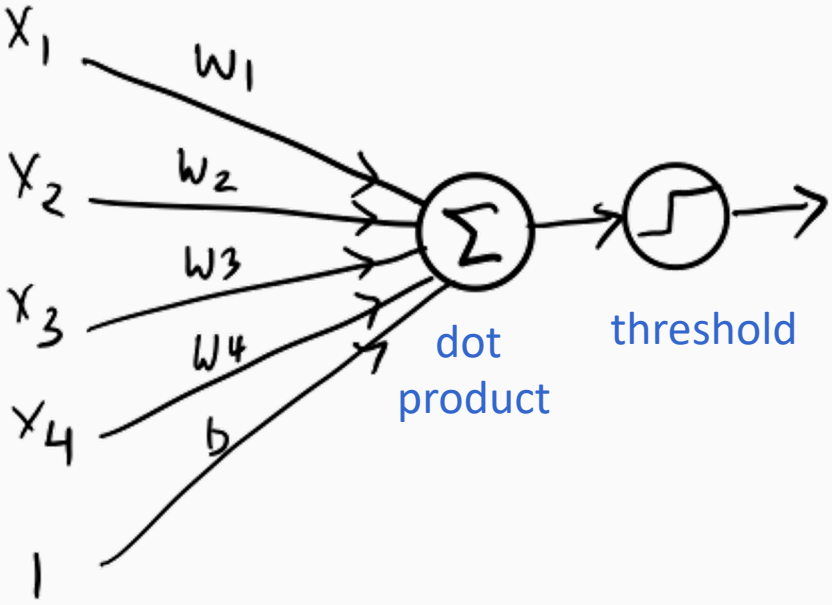

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various algorithms

perceptron, SVM, logistic regression,…

in general, minimize loss

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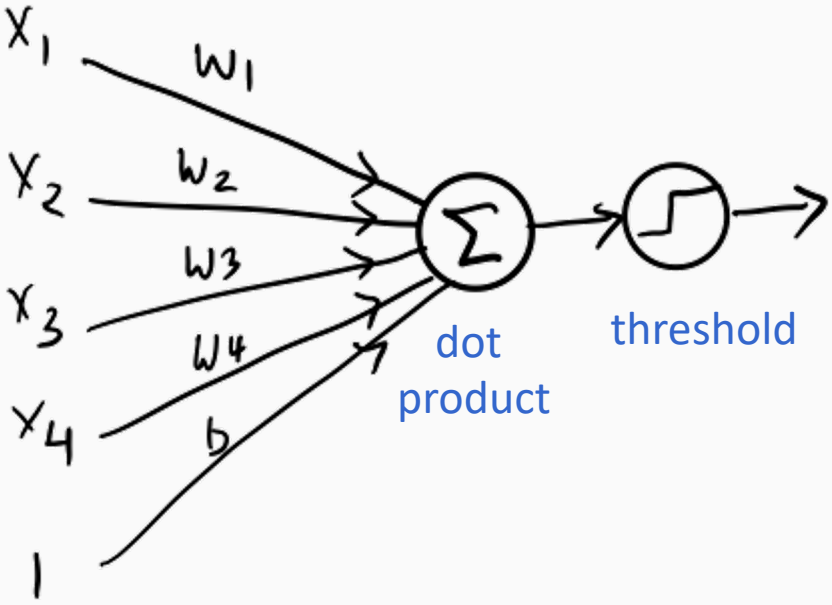

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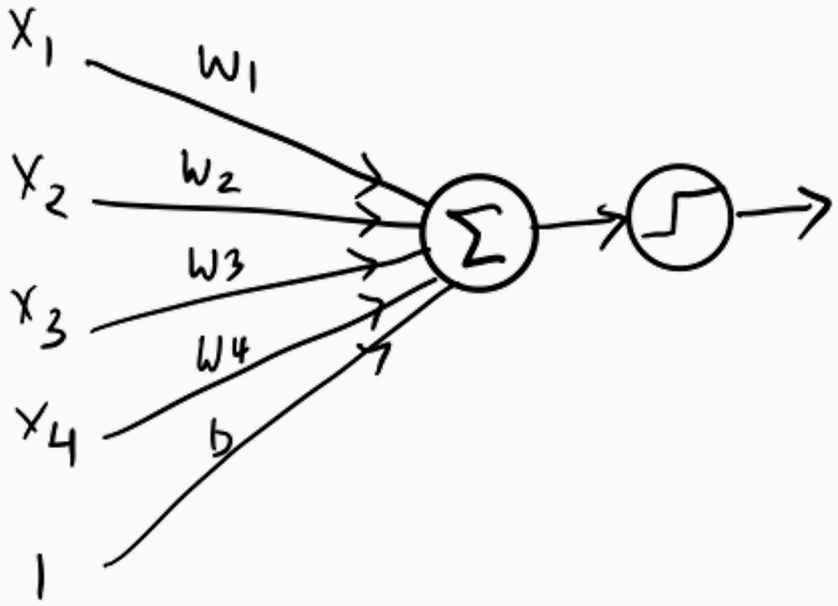
But where do these input features come from?

What if the features were outputs of another classifier?

Features from classifiers



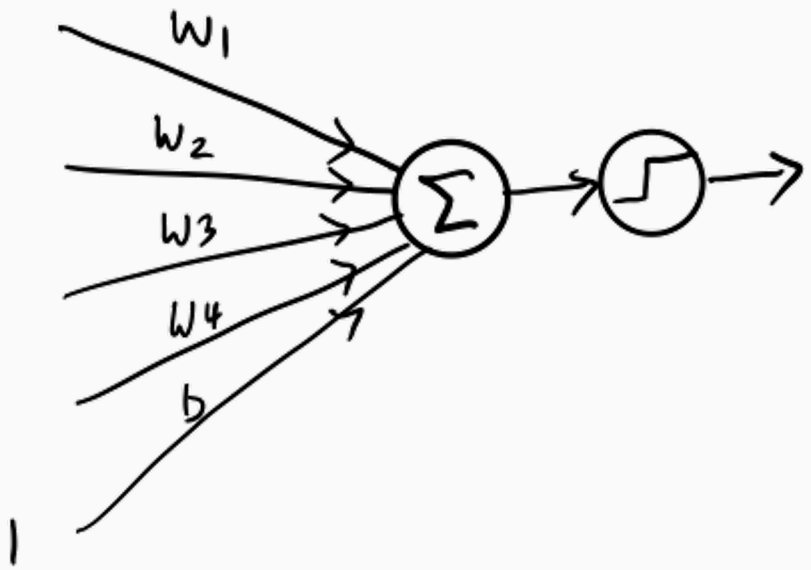
Features from classifiers

x_1

x_2

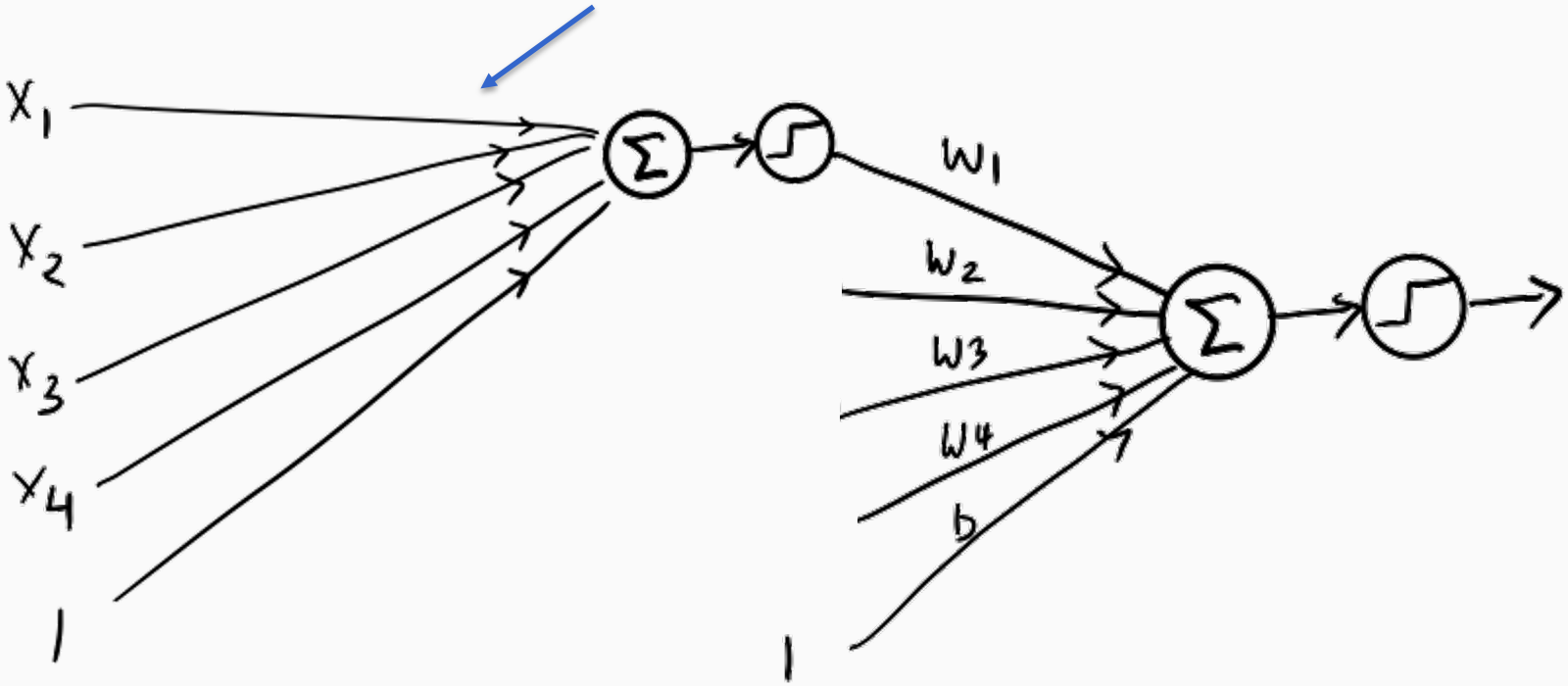
x_3

x_4



Features from classifiers

Each of these connections have their own weights as well



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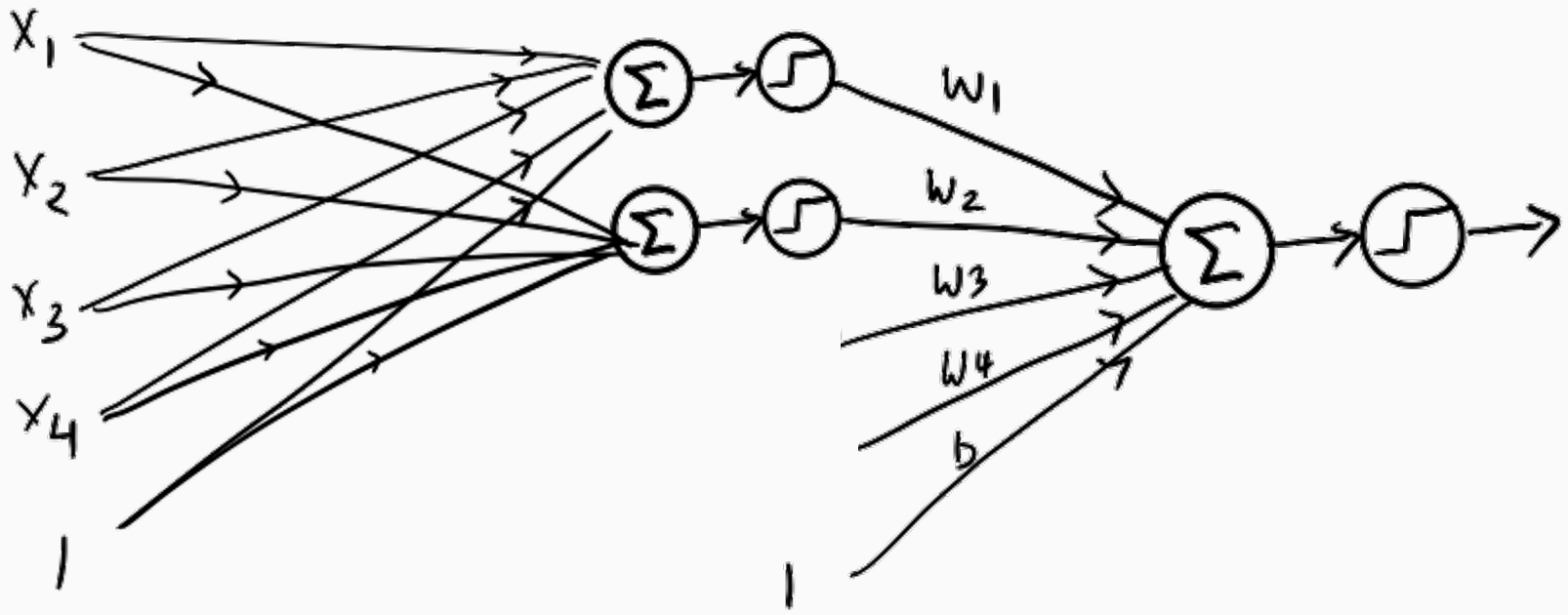
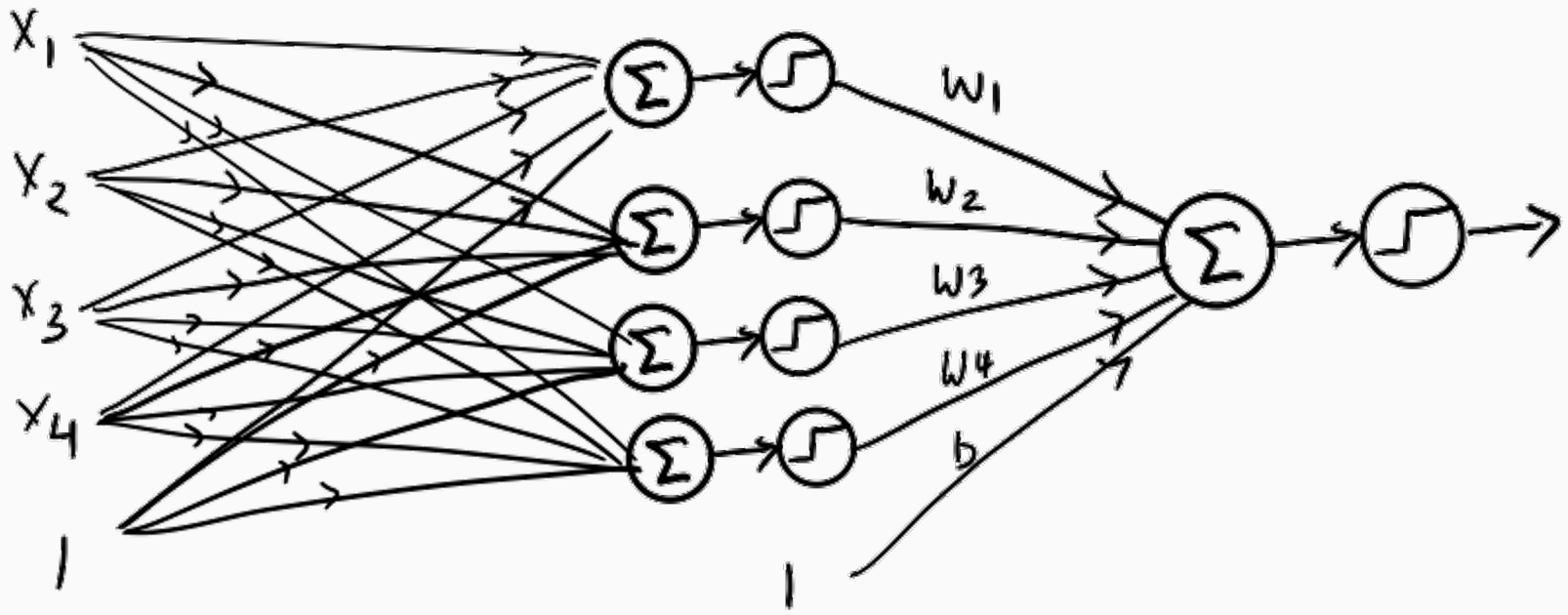


Features from classifiers

This is a **two layer** feed forward neural network



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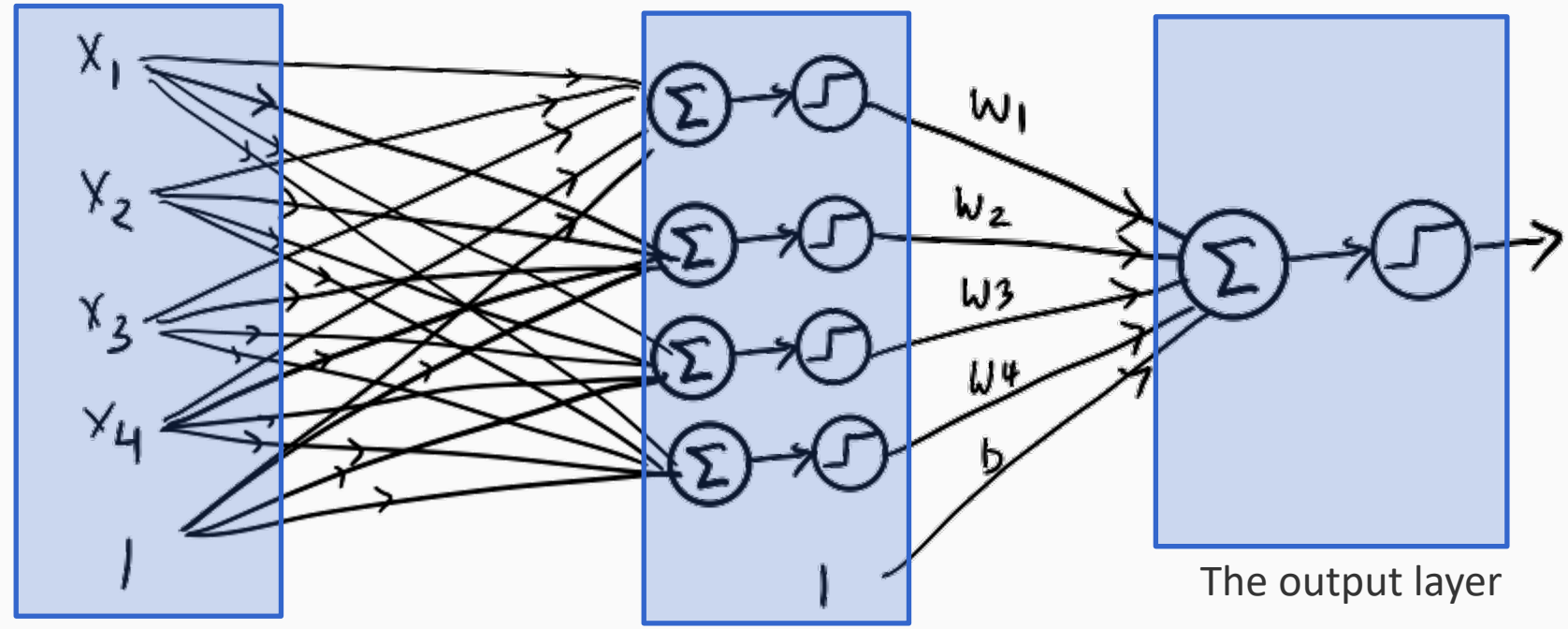

Think of the hidden layer as learning a good **representation** of the inputs

Features from classifiers

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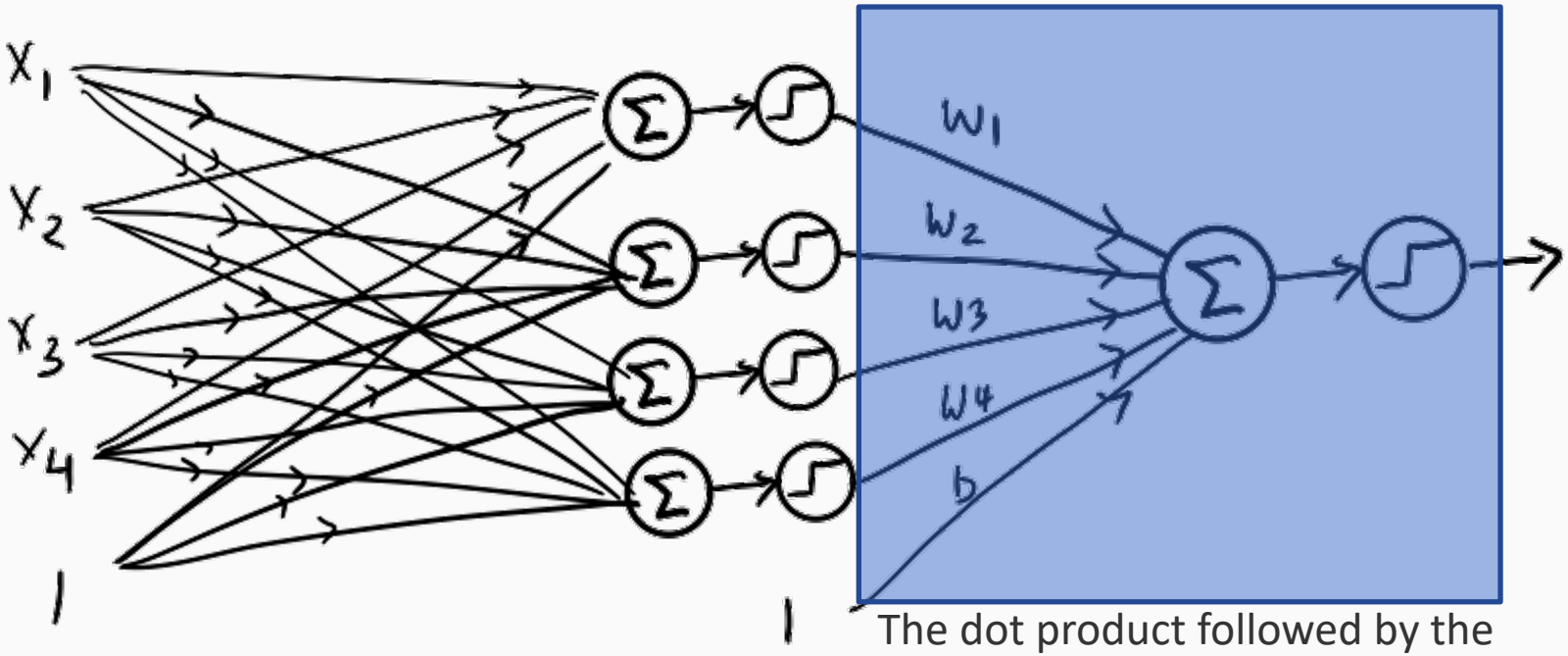

The dot product followed by the threshold constitutes a ***neuron***

Features from classifiers

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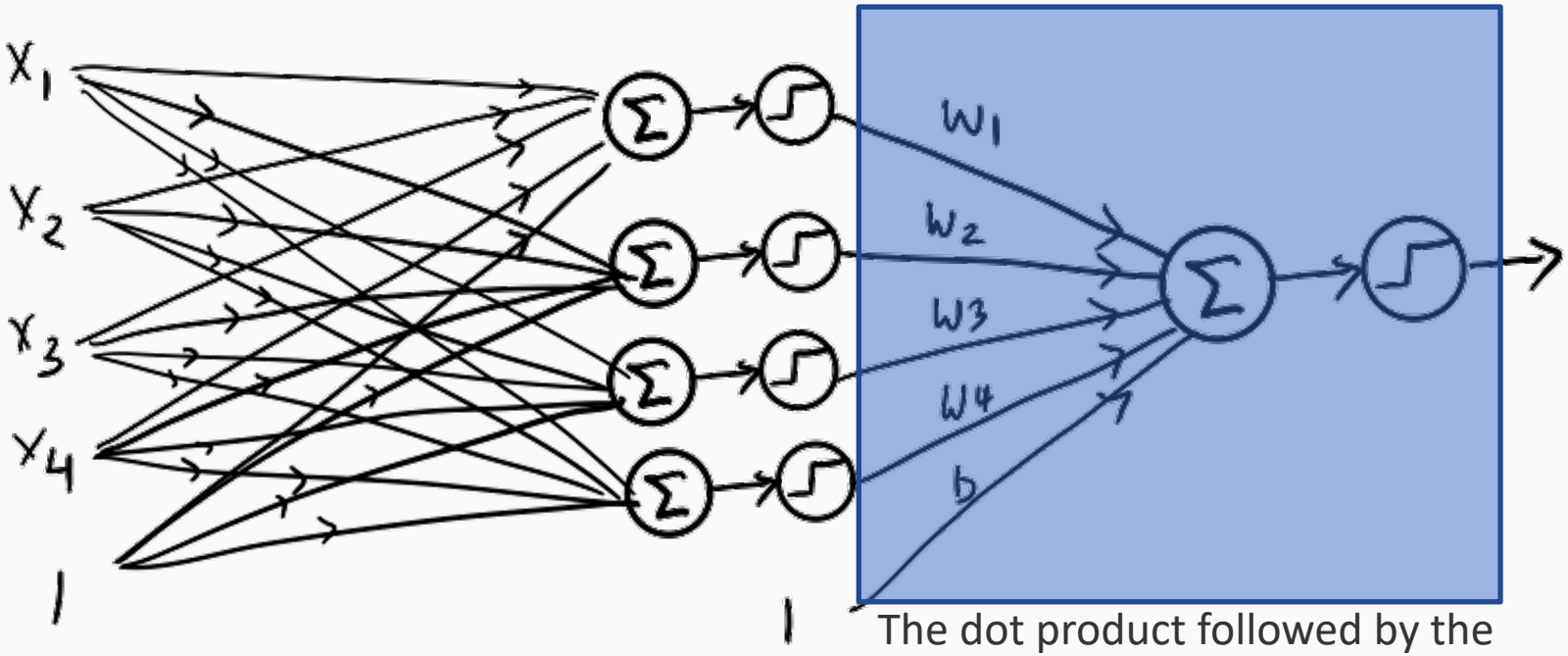

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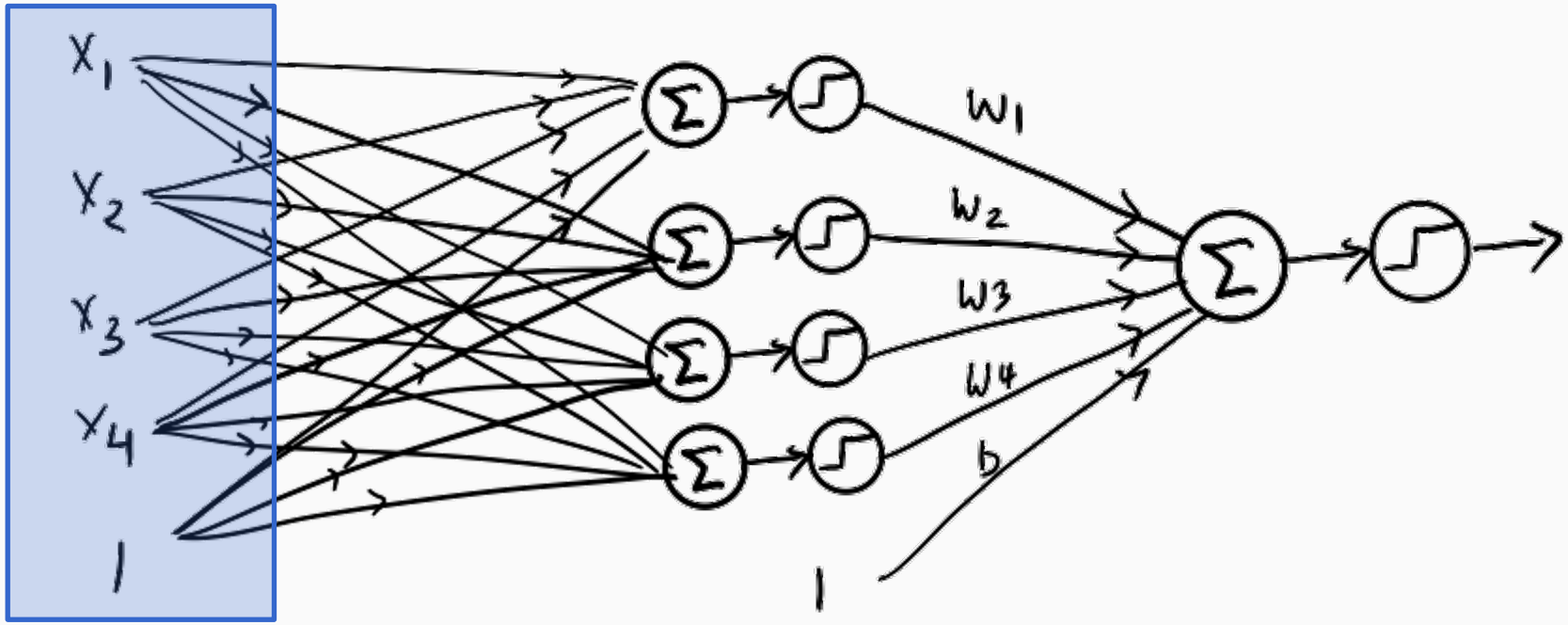
Five neurons in this picture (four in hidden layer and one output)

But where do the inputs come from?



The input layer

What if the inputs were the outputs of a classifier?

We can make a **three** layer network…. And so on.

Let us try to formalize this

Neural networks

A robust approach for approximating real-valued, discrete-valued or vector valued functions

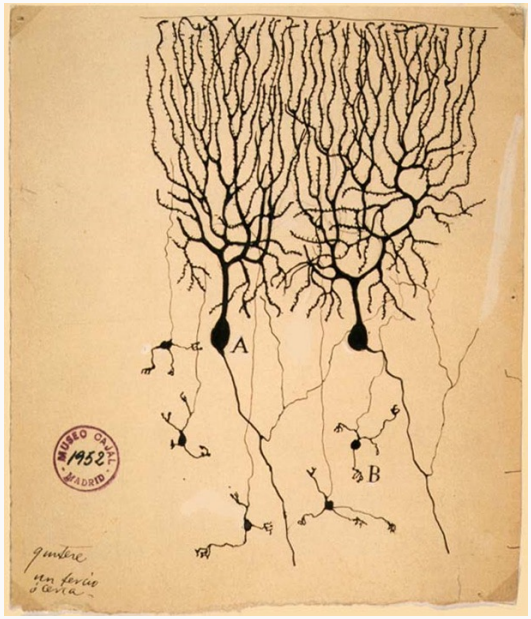
Among the most effective **general purpose** supervised learning methods currently known

- Especially for *complex and hard to interpret data* such as real-world sensory data

The Backpropagation algorithm to enable gradient-based learning of neural networks has been shown successful in many practical problems

- Across various application domains

Biological neurons

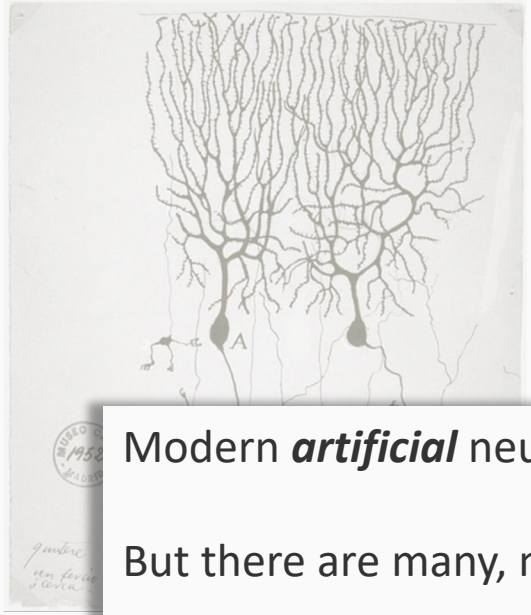


The first drawing of a brain cells by Santiago Ramón y Cajal in 1899

Neurons: core components of brain and the nervous system consisting of

1. Dendrites that collect information from other neurons
2. An axon that generates outgoing spikes

Biological neurons



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The
cells
Caja

Modern ***artificial*** neurons are **loosely** "inspired" by biological neurons

But there are many, many fundamental differences

Don't take the similarity seriously (as also claims in the news about the "emergence" of intelligent behavior)

Artificial neurons

*Functions that **very loosely** mimic a biological neuron*

A neuron accepts a collection of inputs (a vector **x**) and produces an output by:

1. Applying a dot product with weights **w** and adding a bias b
2. Applying a (possibly non-linear) transformation called an ***activation***

$$output = \text{activation}(\boldsymbol{w}^T \boldsymbol{x} + b)$$

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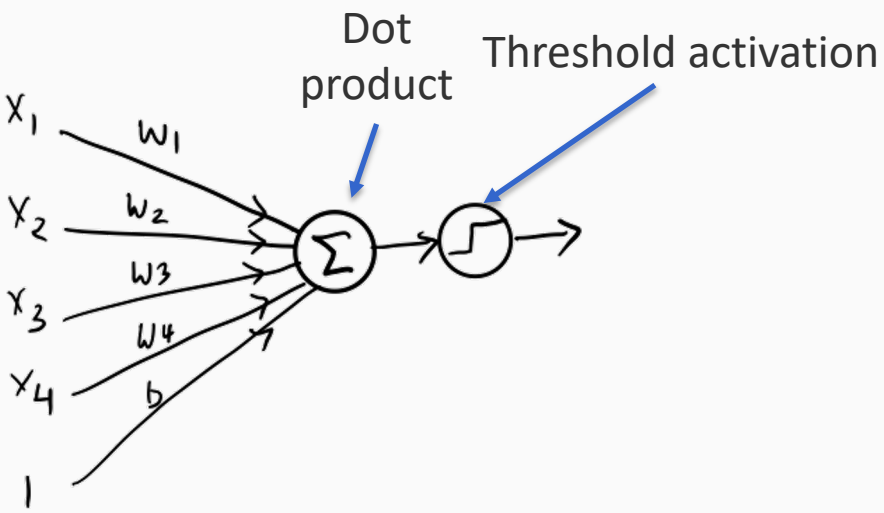

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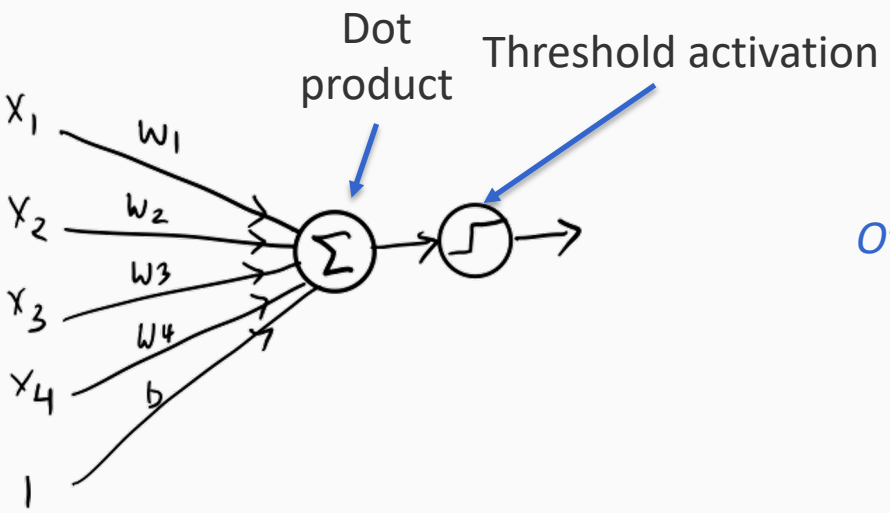

Other activations are possible

Activation functions

Also called transfer functions

$$output = \text{activation}(\boldsymbol{w}^T \boldsymbol{x} + b)$$

Name of the neuron	Activation function: $\text{activation}(z)$
Linear unit	z (i.e. no change to the input)
Threshold/sign unit	$\text{sgn}(z)$
Sigmoid unit	$\frac{1}{1 + \exp(-z)}$
Rectified linear unit (ReLU)	$\max(0, z)$
Tanh unit	$\tanh(z)$

Many more activation functions exist (sinusoid, sinc, gaussian, polynomial…)

A neural network

A function that converts inputs to outputs defined by a directed acyclic graph

- Nodes organized in layers, correspond to neurons
- Edges carry output of one neuron to another, associated with weights

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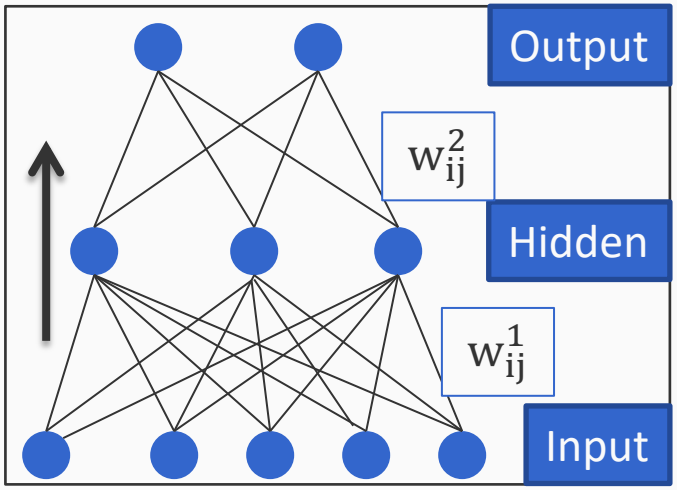

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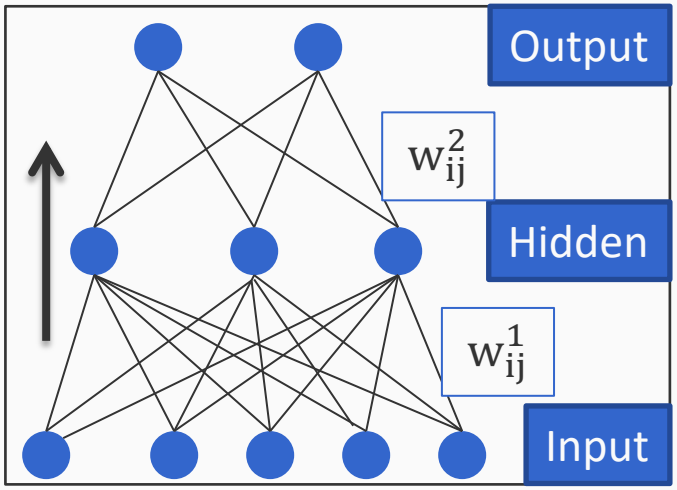

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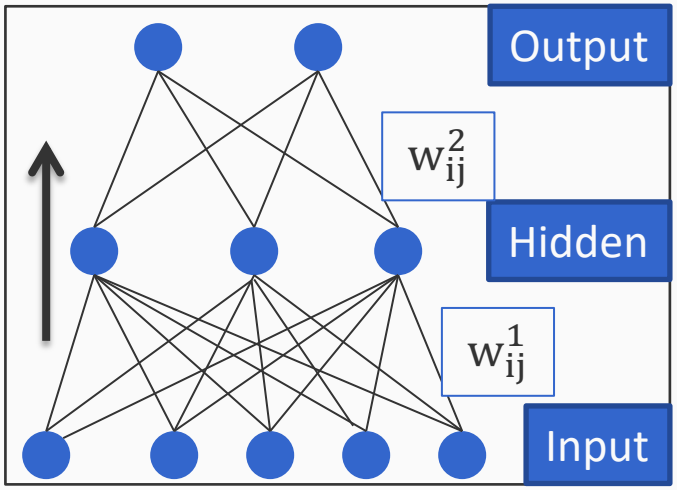

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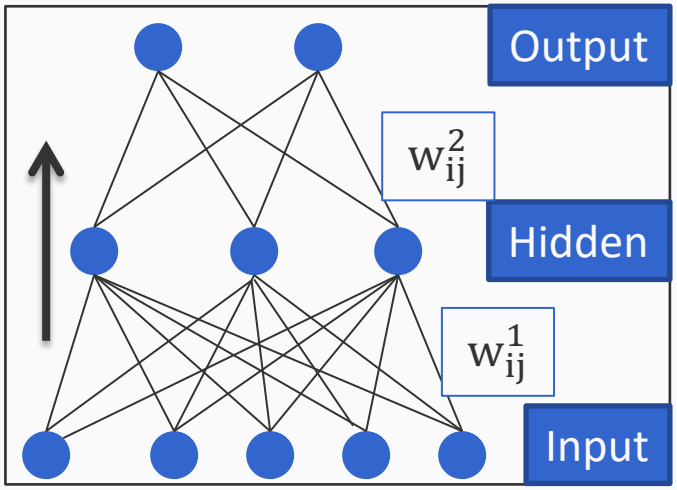

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  Learned from data

very

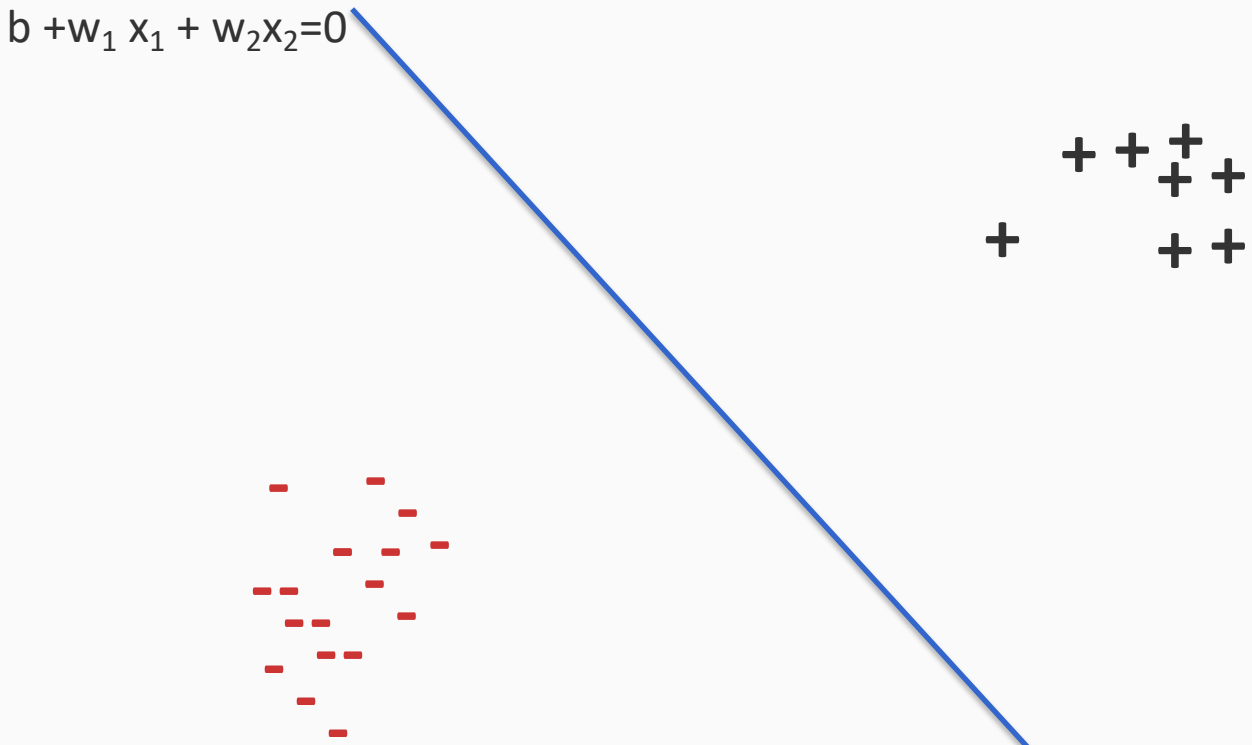
A brief history of neural networks

1943	McCullough and Pitts showed how linear threshold units can compute logical functions
1949	Hebb suggested a learning rule that has some physiological plausibility
1950	Rosenblatt, the Peceptron algorithm for a single threshold neuron
1969	Minsky and Papert studied the neuron from a geometrical perspective
1970s-90s	Convolutional neural networks (Fukushima, LeCun), the backpropagation algorithm (various), recurrent neural networks (various)
2000s-now	More compute, more data, more applications, deeper networks, better optimization, transformers, graph neural networks

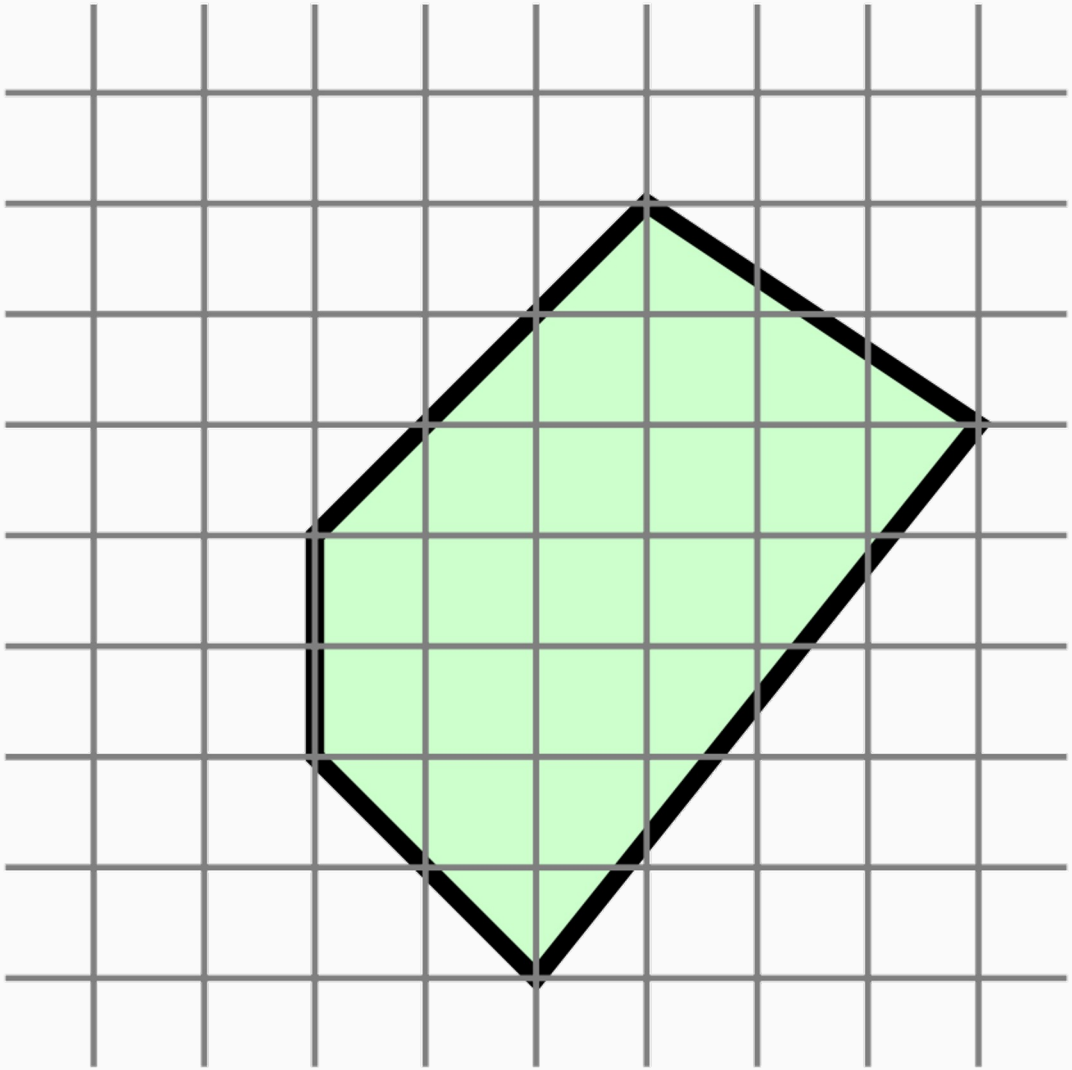
What functions do neural networks express?

A single neuron with threshold activation

Prediction = *sgn*$(b + w_1 x_1 + w_2 x_2)$



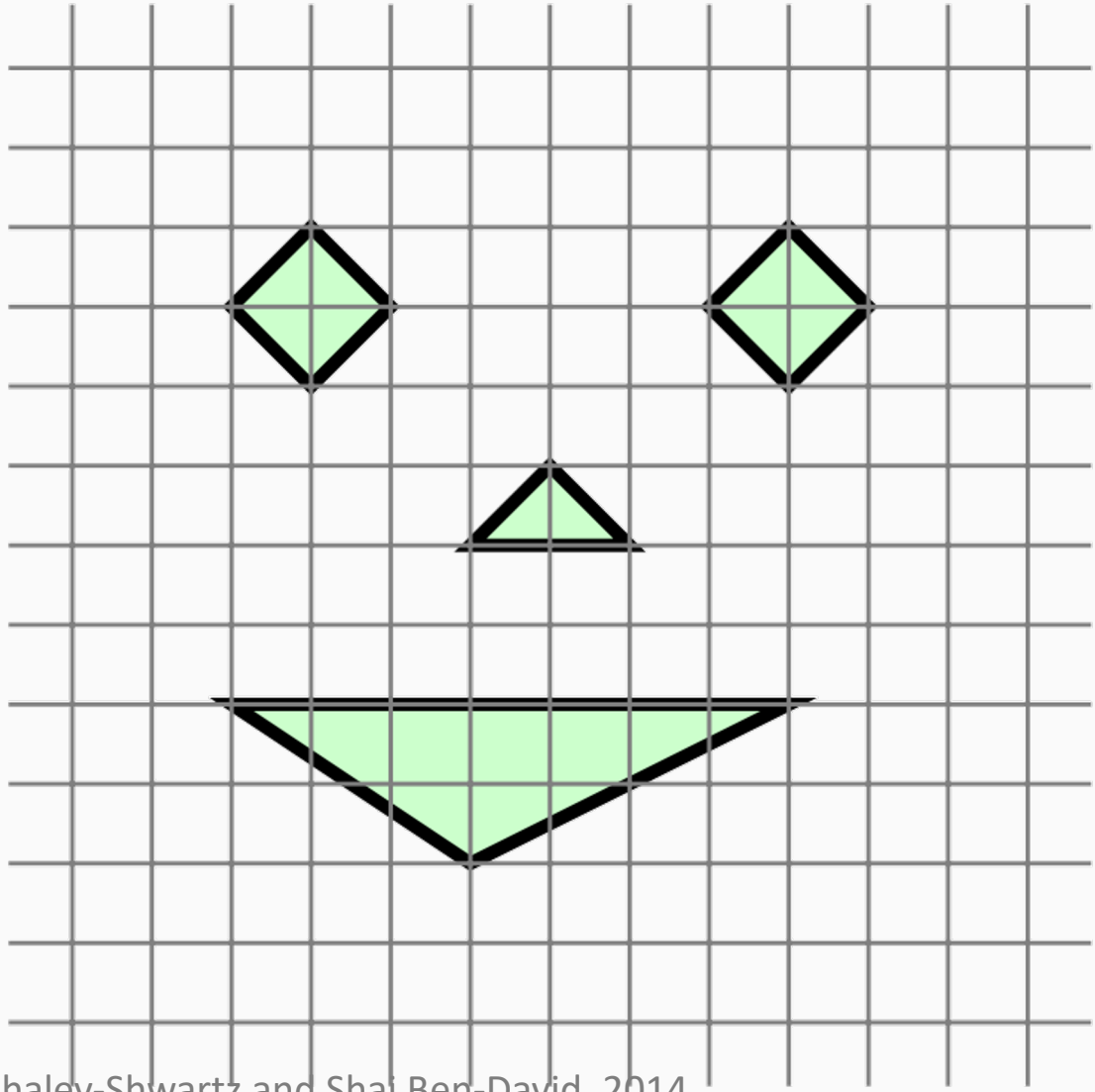
Two layers, with threshold activations



In general, convex polygons

Figure from Shai Shalev-Shwartz and Shai Ben-David, 2014

Three layers with threshold activations



In general, unions of convex polygons

Figure from Shai Shalev-Shwartz and Shai Ben-David, 2014

Neural networks are universal function approximators

- Any continuous function can be approximated to arbitrary accuracy using one hidden layer of sigmoid units [Cybenko 1989]
- Approximation error is insensitive to the choice of activation functions [DasGupta et al 1993]
- Two layer threshold networks can express *any* Boolean function
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- VC dimension of threshold network with edges E: $VC = O(|E| \log |E|)$
- VC dimension of sigmoid networks with nodes V and edges E:
  - Upper bound: $\mathrm{O}(|V|^2|E|^2)$
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Exercise: Show that if we have only linear units, then multiple layers does not change the expressiveness