WELCOME TO TDT4171: Methods in AI

Before we start:

- Please turn off your microphone
- If you have a question or want to say something as we move along, first try getting my attention using the chat.
- If that doesn't work, then unmute and shout out

The lecture will be recorded, and made available on Blackboard

TDT4171 Artificial Intelligence Methods

Lecture 8 – Basic ANNs

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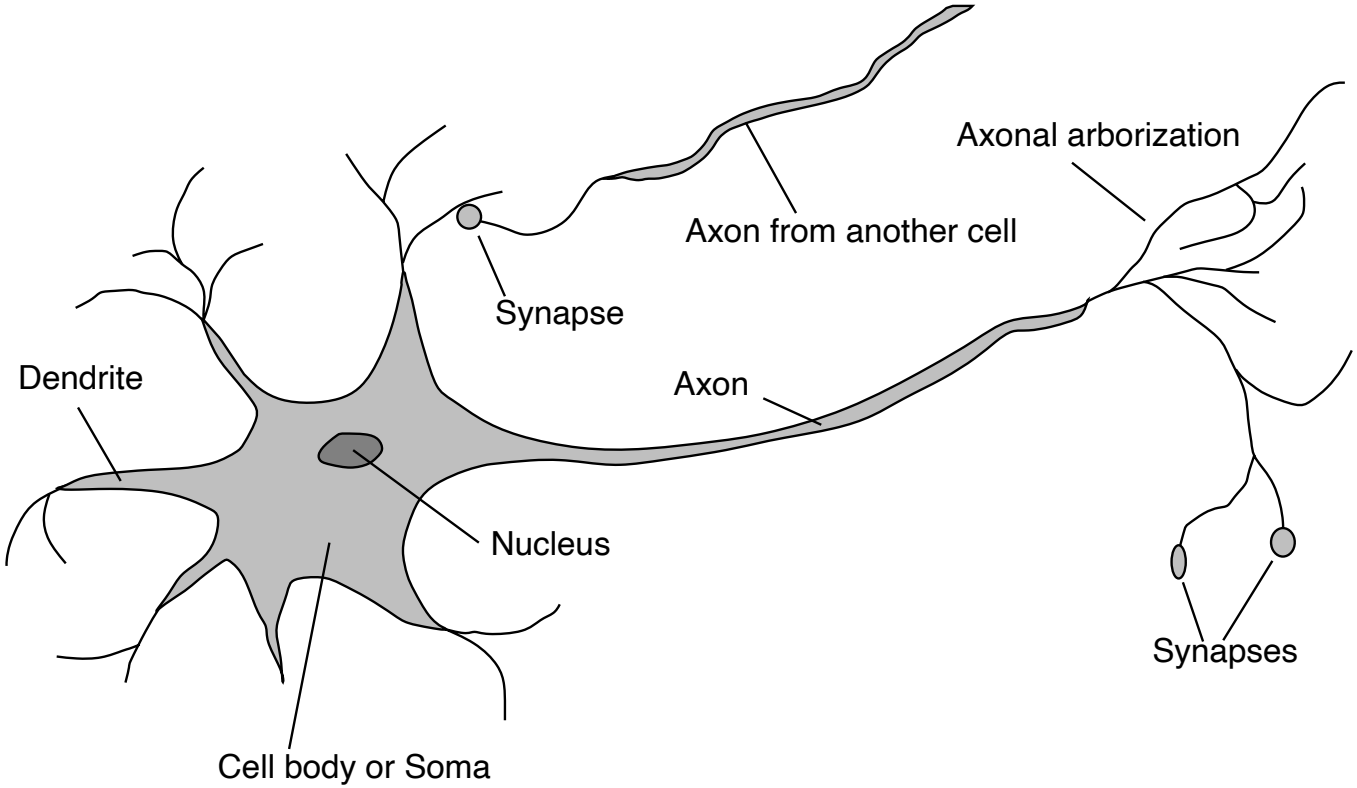
Outline

Summary from last time

- Learning needed for **unknown environments**, **lazy designers**
- **Learning agent = performance element + learning element**
- Learning method depends on **type of performance element**, available **feedback**, type of **component to be improved**, and its **representation**
- For **supervised learning**, the aim is to find a simple hypothesis that is approximately consistent with training examples
- Decision tree learning using **information gain**
- **Learning performance = prediction accuracy measured on test set**

Brains

10^{11} neurons of > 20 types, 10^{14} synapses
Signals are noisy "spike trains" of electrical potential



Connectionist Models

Some facts about the human brain:

- Number of neurons about 10^{11}
- Connections per neuron about 10^4 – 10^5
- Scene recognition time about $.1$ second
- Neuron switching time about $.001$ second
- 100 inference steps doesn't seem like enough for scene recognition $\rightarrow$ much parallel computation

Properties of artificial neural nets (ANN's):

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed process
- Emphasis on tuning weights automatically

When to Consider Neural Networks

- Input is high-dimensional discrete or real-valued (e.g. raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant

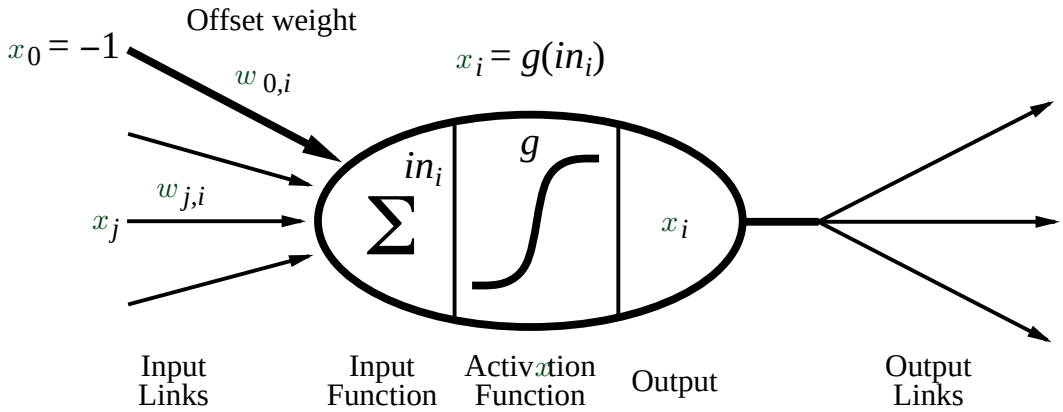
Examples:

- Speech recognition
- Image classification
- Text understanding
- Autonomous drivers
- Financial prediction

Perceptron

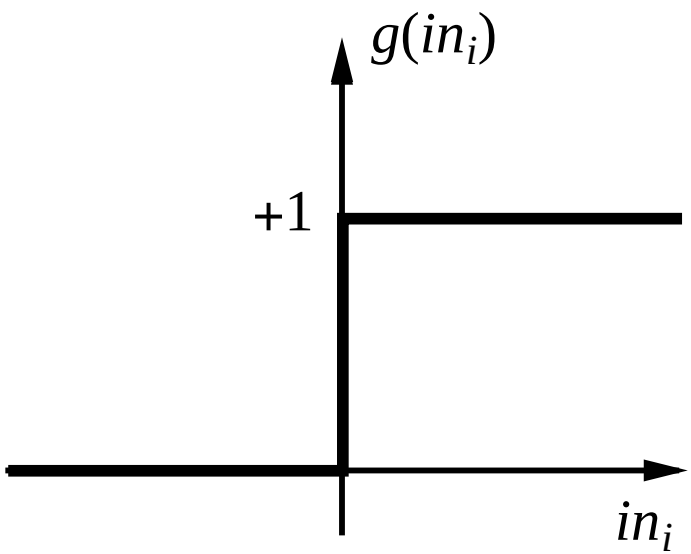
Output is typically a **non-linear function** of the inputs (e.g., a "squashed" one):

$$x_i \leftarrow g(in_i) = g\left(\sum_j w_{ji} x_j\right)$$

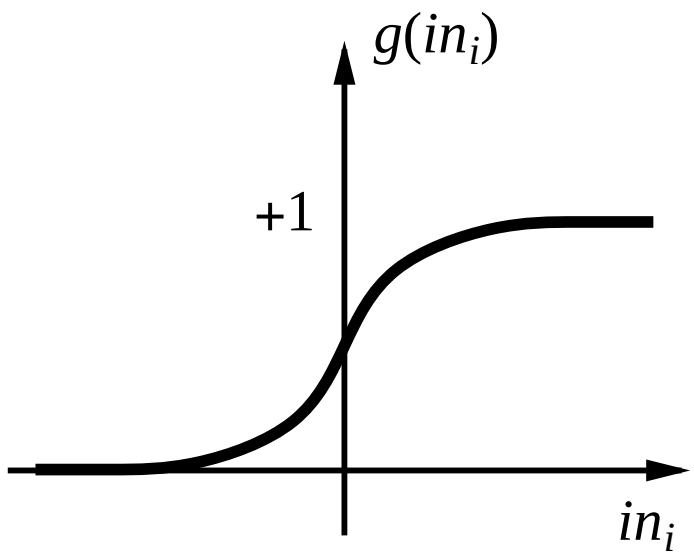


A gross **oversimplification** of real neurons, but its purpose is to develop understanding of what networks of simple units can do.

Activation functions



(a)



(b)

(a) is a **step function** or **threshold function**

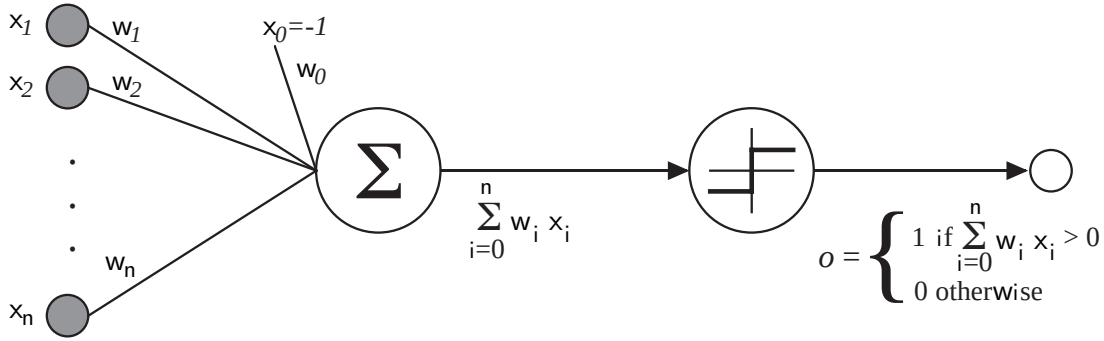
(b) is a **sigmoid** function $1/(1+e^{-x})$

(c) We will also consider **linear** functions today, and **rectified linear units** (ReLUs) when we get to deep learning.

Note! Changing the bias weight $w_{0,i}$ moves the threshold location

Perceptron activated by step-function

Start by looking at **single perceptron with step-function activation**:



$$\text{output}(x_1, \ldots, x_n) = \begin{cases} 1 & \text{if } w_0 x_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ 0 & \text{otherwise.} \end{cases}$$

Alternative vector notation:

$$\text{output}(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w}^{\mathsf{T}} \vec{x} > 0 \\ 0 & \text{otherwise.} \end{cases}$$

Decision Surface of a Perceptron

A perceptron activated by a **step-function** can represent some useful binary functions.

Discuss with your neighbour:

What weights (if any) represent $\text{output}(x_1, x_2) = \texttt{AND}(x_1, x_2)$?

$\text{output}(x_1, x_2) = \texttt{OR}(x_1, x_2)$?

$\text{output}(x_1, x_2) = \texttt{XOR}(x_1, x_2)$?

$\text{output}(x_1) = \texttt{NOT}(x_1)$?

XOR: Why only linearly separable decisions?

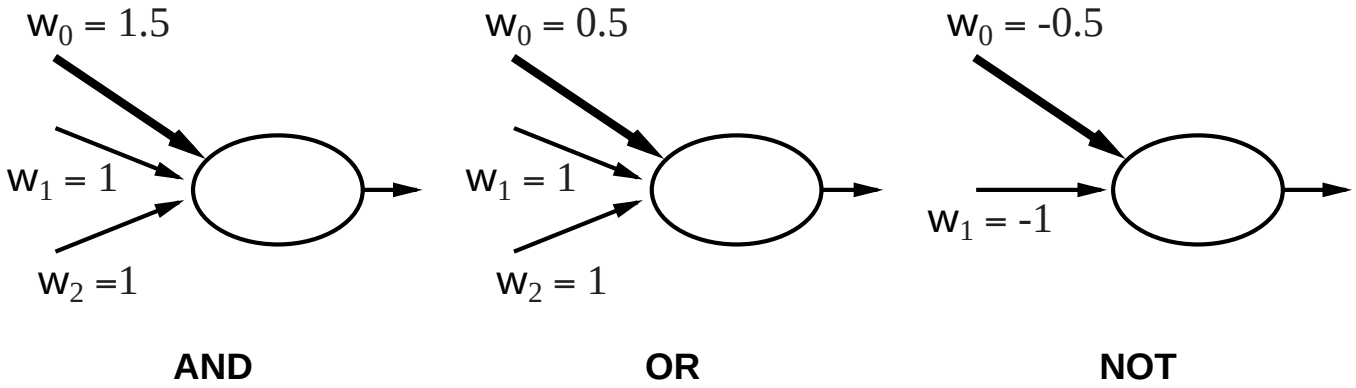
Let us consider the formulation for the "step" (i.e., the decision boundary) defined by $w_0 x_0 + w_1 x_1 + \cdots + w_n x_n = 0$.

- Pick out one of the data dimensions with non-zero weight, x_i (so $w_i \neq 0$; this is not a big deal because an x_i with corresponding $w_i = 0$ plays no role in the decision and can be thrown out).
- Wrt x_i, the decision boundary is given by

$$x_i = \sum_{j \neq i} \frac{-w_j}{w_i} x_j \underbrace{=}_{\gamma_j := -w_j/w_i} \sum_{j \neq i} \gamma_j \, x_j$$

  ... meaning that the decision boundary is a linear function in x_i, and this is true for any choice of i.

Implementing logical functions



- Some functions **not representable** by perceptrons, namely those that are **not linearly separable** (e.g., XOR).
- Can make it work by **"inventing" new inputs** to make it linearly separable (e.g., $x_3 \leftarrow |x_1 - x_2|$ for XOR).
- **Equivalentely**, if we have **networks** of perceptrons, **any Boolean function** can be implemented

Perceptron training rule (The "Delta-rule")

First we look at **learning weights of single perceptrons**:
From data $\langle \boldsymbol{x}, t \rangle$ (t is "target"), we want to tune $\vec{\boldsymbol{w}}$ automatically.

Let us consider simpler **linear unit**, where input is $\vec{\boldsymbol{x}}$ gives output $o = \vec{\boldsymbol{w}}^{\mathsf{T}} \vec{\boldsymbol{x}}$. The correct (observed) value is t.

Desiderata:

- Each weight w_i should be tuned separately.
- If $o = t$ there is no need to change any of the weights.
- If $o < t$ (too low):
  - If $x_i > 0$, we should **increase** w_i
  - If $x_i < 0$, we should **decrease** w_i
- If $o > t$ (too high):
  - If $x_i > 0$, we should **decrease** w_i
  - If $x_i < 0$, we should **increase** w_i
- The **more** we are off, the **larger** the change to the weights.

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Learning rule:

$$w_i \leftarrow w_i + \Delta w_i, \text{ where } \Delta w_i = \eta(t - o)x_i$$

Where:

- t is target value and o is perceptron output (as before)
- η is small constant called **the learning rate**.

Perceptron training rule (The "Delta-rule")

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- η is small constant called **the learning rate**.

Convergence:

- **Converges** if training data is linearly separable and η sufficiently small.
- **Result unclear when NOT linearly separable.**

Finding the optimal weights

We still consider **linear unit**, where input is $\vec{x}$ gives output

$$o = w_0 x_0 + w_1 x_1 + \cdots + w_n x_n = \vec{w}^{\mathsf{T}} \vec{x}$$

We learn w_i's that minimise the squared error

$$\mathbb{E}[\vec{w}] \equiv \frac{1}{2} \sum_{d \in \mathcal{D}} (t_d - o_d)^2,$$

where $\mathcal{D}$ is set of **training examples**, each of the form $d = \langle \boldsymbol{x}_d, t_d \rangle$.

Finding optimal weights – requirements

Description of our situation:

- We have a function $\mathbb{E}[\vec{w}]$ we want to minimise (wrt $\vec{w}$).
- **Why not just try a number of weight configurations $\vec{w}_i$, calculate $\mathbb{E}[\vec{w}_i]$ and see what happens?**

Finding optimal weights – requirements

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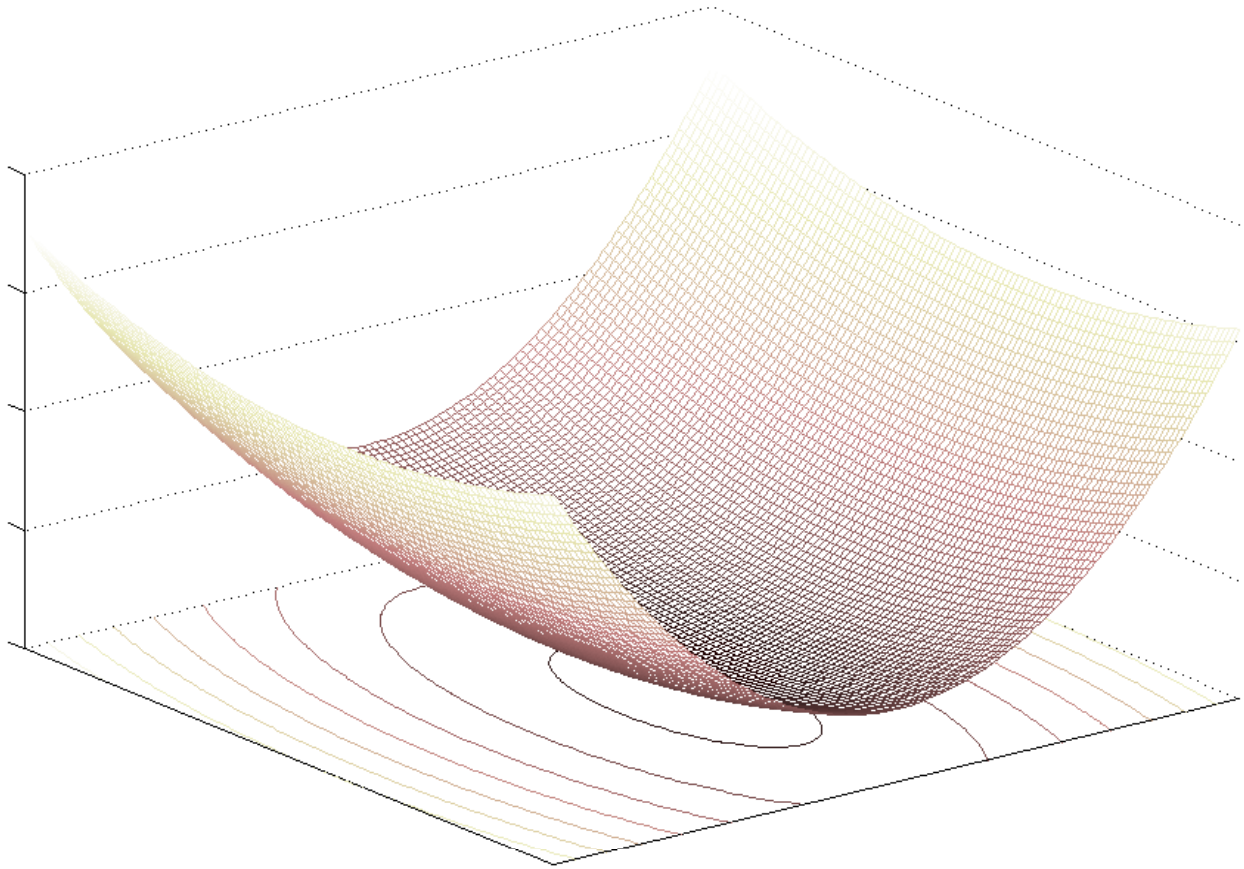
- We have a function $\mathbb{E}[\vec{w}]$ we want to minimise (wrt $\vec{w}$).
- **Why not just try a number of weight configurations $\vec{w}_i$, calculate $\mathbb{E}[\vec{w}_i]$ and see what happens?**
- There are infinitely many (even uncountably many) weight configurations.
- Minimization is typically in very high dimensional space.
- Evaluating $\mathbb{E}[\vec{w}]$ involves summing over all training examples – can be very expensive.

Thus, we cannot use a standard ("silly") Trial & Error approach here, but must devise a local search method.

Solution procedure



Discuss with your neighbour:

How can we minimise this function without knowing the whole shape?

We want a **general**, **quick**, and **robust** technique.

Gradient Descent – The setup

Let's begin by considering a function of a single variable:

- We want to find the value x which minimizes $f(x)$.
- To avoid evaluating the whole function we use an iterative approach:
  - Guess a value for x
  - Calculate the derivative at x.
  - Make a new guess for x based on the calculated information: If $f'(x) > 0$ our guess is too high; if $f'(x) < 0$ we are too low, and if $f'(x) \equiv 0$ we are just perfect.
  - . . . and keep going.

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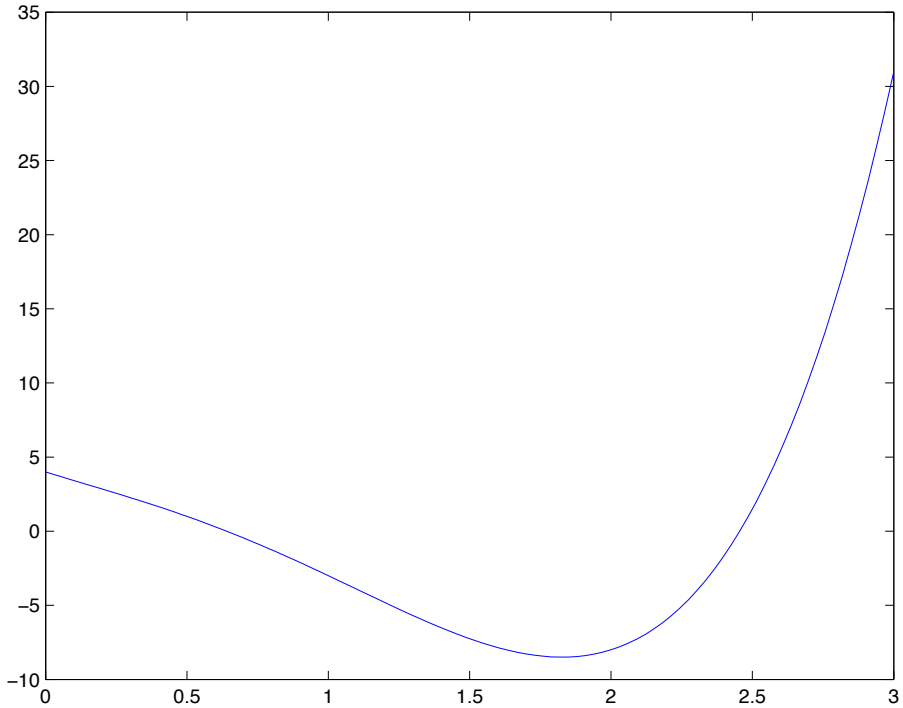
  - ...and keep going.
- **Intuition:**
  - If the derivative is small (in absolute value) we are close to the minimizing point
  - ...and if it is zero we are done
  - If it is large we are far away

Solution:
Use update rule $x_{i+1} \leftarrow x_i - \eta \cdot f'(x_i)$. $\eta > 0$ is the **learning rate**.

Gradient Descent – Example

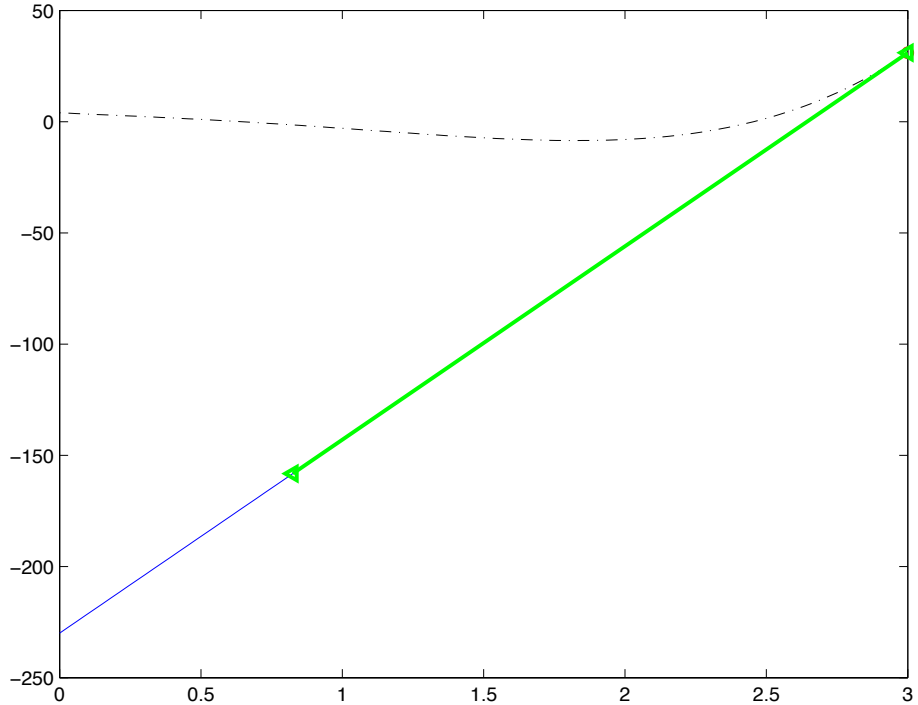
Minimize $f(x) = 2x^4 - 5x^3 + 2x^2 - 6x + 4$ with $\eta = 0.025$.



The $f(x)$ has a minimum at $x = 1.8261$. Let's try to find it...

Gradient Descent – Example

Minimize $f(x) = 2x^4 - 5x^3 + 2x^2 - 6x + 4$ with $\eta = 0.025$.

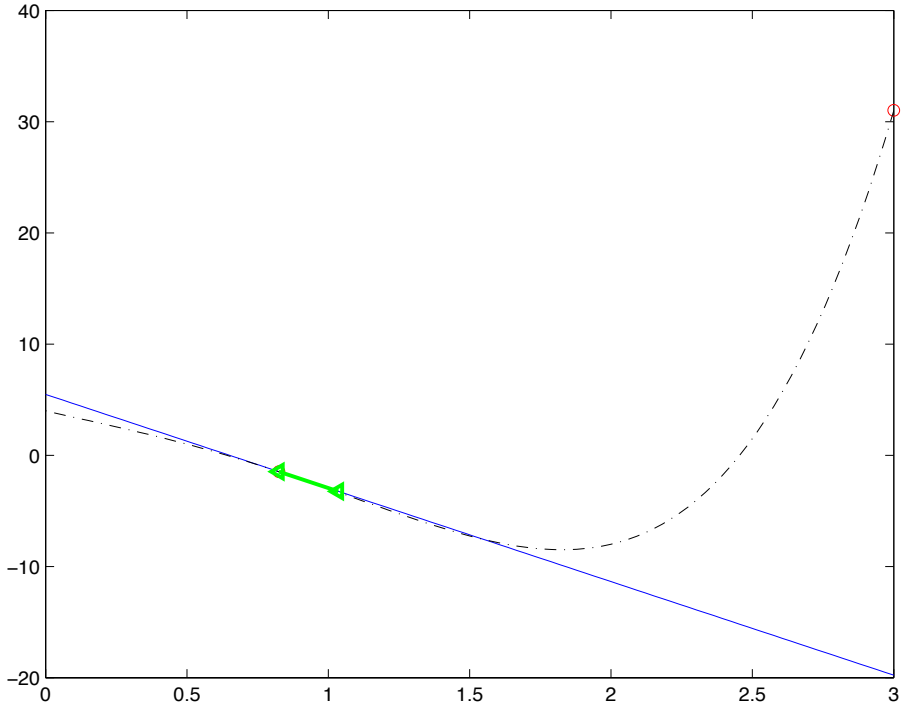


Starting from $x_0 = 3$ and finding $f'(3) = 87$:

$$\begin{aligned} x_1 &= x_0 - \eta f'(x_0) \\ &= 3 - 0.025 \cdot 87 = 0.8250 \end{aligned}$$

Gradient Descent – Example

Minimize $f(x) = 2x^4 - 5x^3 + 2x^2 - 6x + 4$ with $\eta = 0.025$.

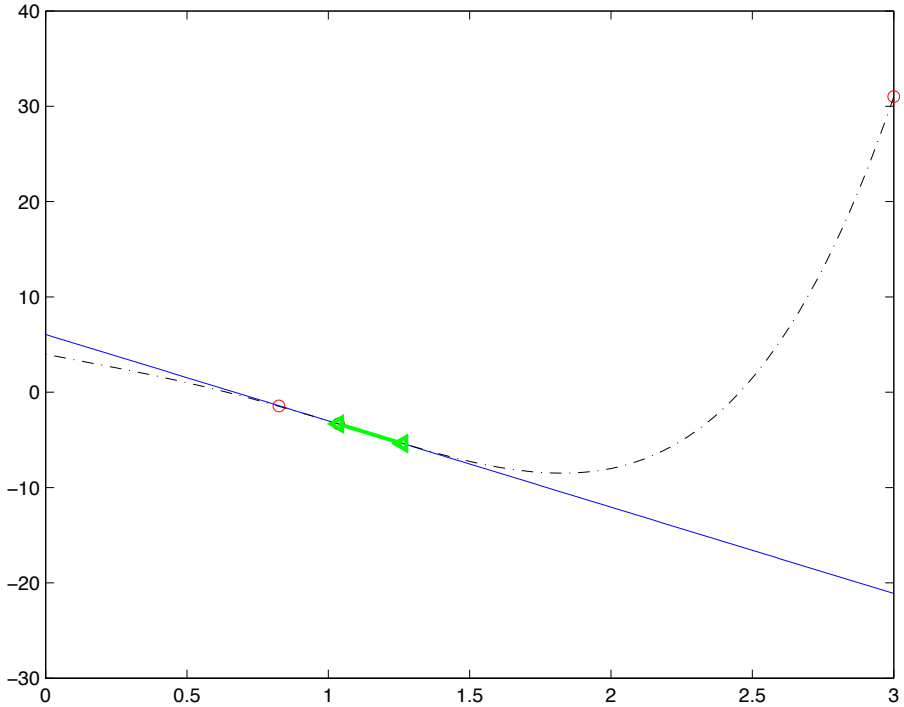


Going from $x_1 = 0.8250$ with $f'(0.8250) = -8.4172$:

$$\begin{aligned} x_2 &= x_1 - \eta f'(x_1) \\ &= 0.825 - 0.025 \cdot (-8.4172) = 1.0354 \end{aligned}$$

Gradient Descent – Example

Minimize $f(x) = 2x^4 - 5x^3 + 2x^2 - 6x + 4$ with $\eta = 0.025$.

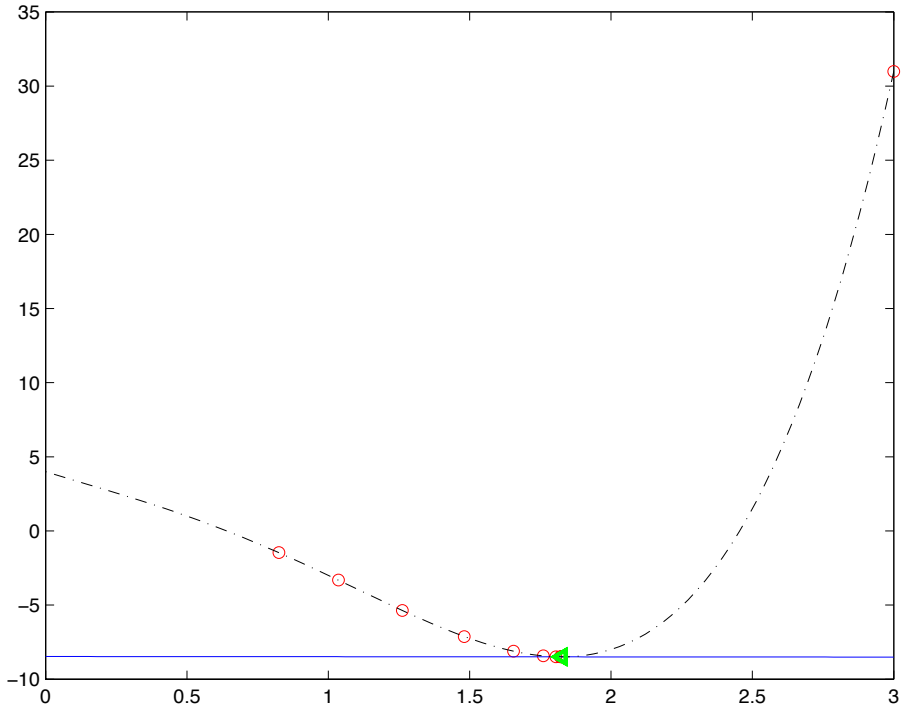


Going from $x_2 = 1.0354$ with $f'(1.0354) = -9.0592$:

$$x_3 = 1.0354 - 0.025 \cdot (-9.0592) = 1.2619$$

Gradient Descent – Example

Minimize $f(x) = 2x^4 - 5x^3 + 2x^2 - 6x + 4$ with $\eta = 0.025$.

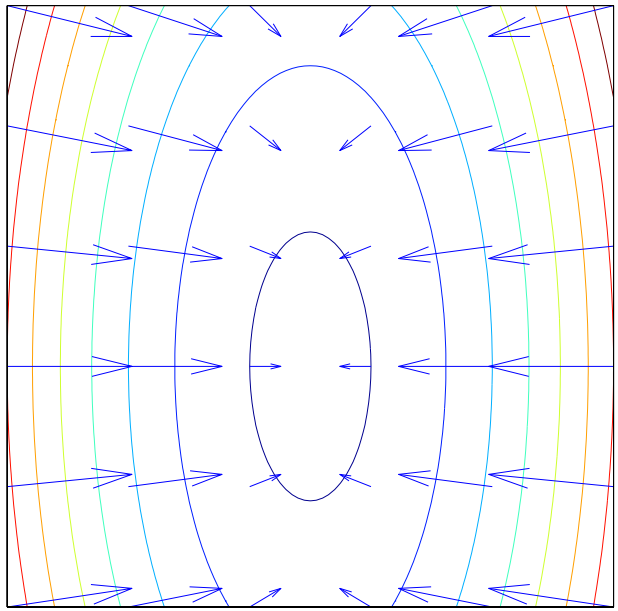


. . . and finally going from $x_{10} = 1.8260$ with $f'(1.8260) = -0.0034$:

$$x_{11} = 1.8260 - 0.025 \cdot (-0.0034) = 1.8261$$

. . . and we are done.

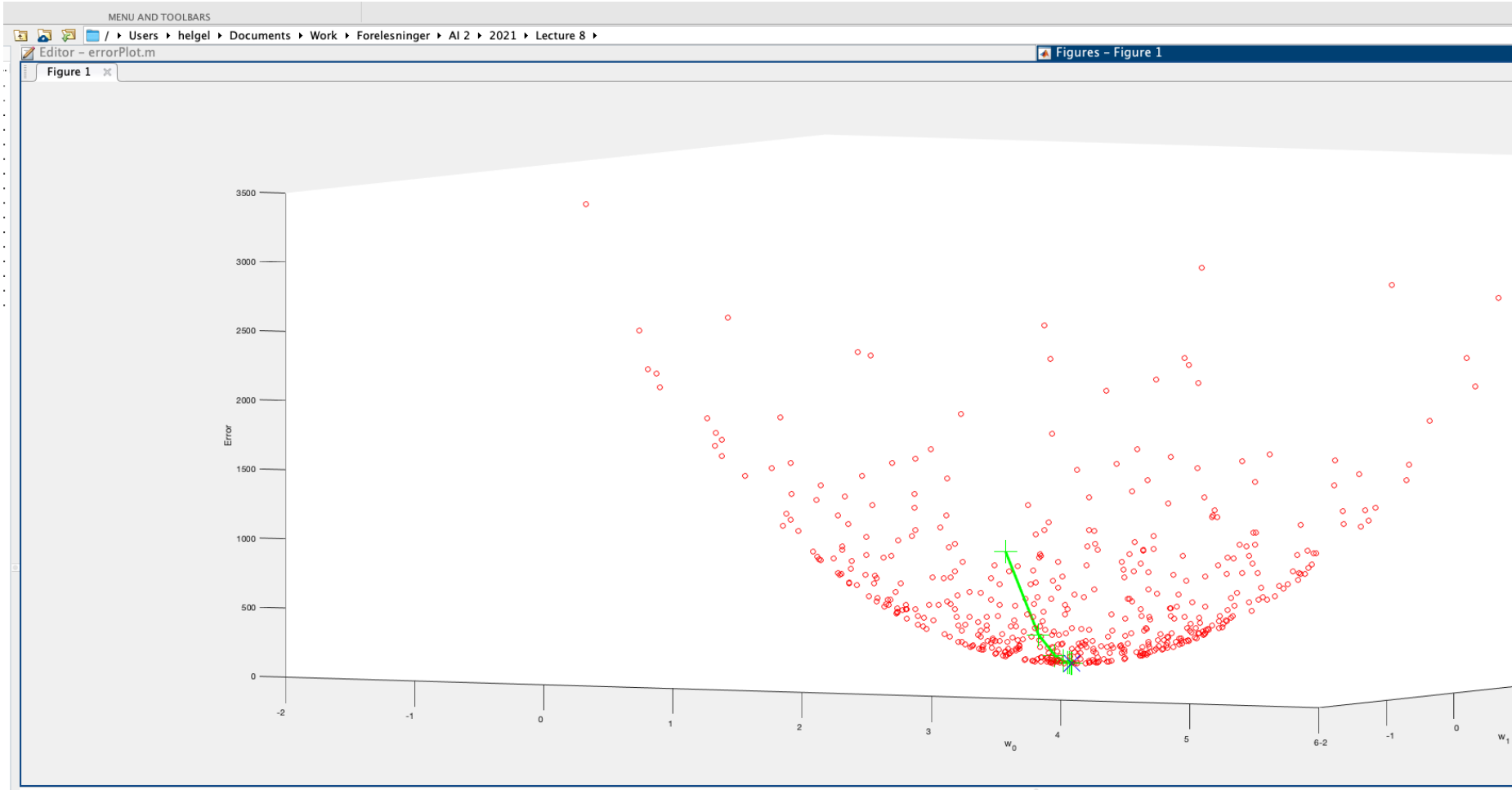
Gradient Descent – in higher dimensions



Recall that

- The **gradient** of a surface $\mathbb{E}[\vec{w}]$ is a vector in the direction the curve grows the most (calculated at $\vec{w}$).
- The gradient is calculated as $\nabla\mathbb{E}[\vec{w}] \equiv \left[\frac{\partial\mathbb{E}}{\partial w_0}, \frac{\partial\mathbb{E}}{\partial w_1}, \cdots \frac{\partial\mathbb{E}}{\partial w_n}\right]$.

Training rule: $\Delta\vec{w} = -\eta \cdot \nabla\mathbb{E}[\vec{w}]$, i.e., $\Delta w_i = -\eta \cdot \frac{\partial\mathbb{E}}{\partial w_i}$.



Command Window

```
First, do random evaluations
**************************************
After 500 evaluations: w_0 = 0.96 and w_1 = 2.92  with error 0.1725


Now, do gradient descent
**************************************
     Step  1: Error = 761.3351
     Step  2: Error = 184.7905
     Step  3: Error =  44.8960
     Step  4: Error =  10.9185
     Step  5: Error =   2.6579
     Step  6: Error =   0.6477
     Step  7: Error =   0.1580   --> Now we beat the result of random search
     Step  8: Error =   0.0386
     Step  9: Error =   0.0094
     Step 10: Error =   0.0023
```

Gradient Descent – Details for LINEAR activation function

$$
\begin{aligned}
\frac{\partial \mathbb{E}}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 \\
&= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\
&= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\
&= \sum_d (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{\boldsymbol{w}}^\mathsf{T} \vec{\boldsymbol{x}}_d) \\
\frac{\partial \mathbb{E}}{\partial w_i} &= -\sum_d x_{i,d} \cdot (t_d - o_d)
\end{aligned}
$$

Gradient Descent – The algorithm

Gradient-Descent($\mathcal{D}$, η)

Each training example is a pair of the form $\langle \vec{x}, t \rangle$, where $\vec{x}$ is the vector of input values, and t is the target output value. η is the learning rate (e.g., $.05$).

1. Initialize each w_i to some small random value
2. Until the termination condition is met:
   1. Initialize: $\Delta w_i \leftarrow 0$.
   2. For each $\langle \vec{x}, t \rangle$ in $\mathcal{D}$:
      - Input the instance $\vec{x}$ to the unit and compute the output o
      - For each linear unit weight w_i: $\Delta w_i \leftarrow \Delta w_i - \eta \cdot (-x_i \, (t - o))$
   3. For each linear unit weight w_i: $w_i \leftarrow w_i + \Delta w_i$

Same algorithm skeleton works for other activation functions, as long as we can calculate $\frac{\partial \mathbb{E}}{\partial w_i}$.

Gradient Descent with LOGISTIC activation functions

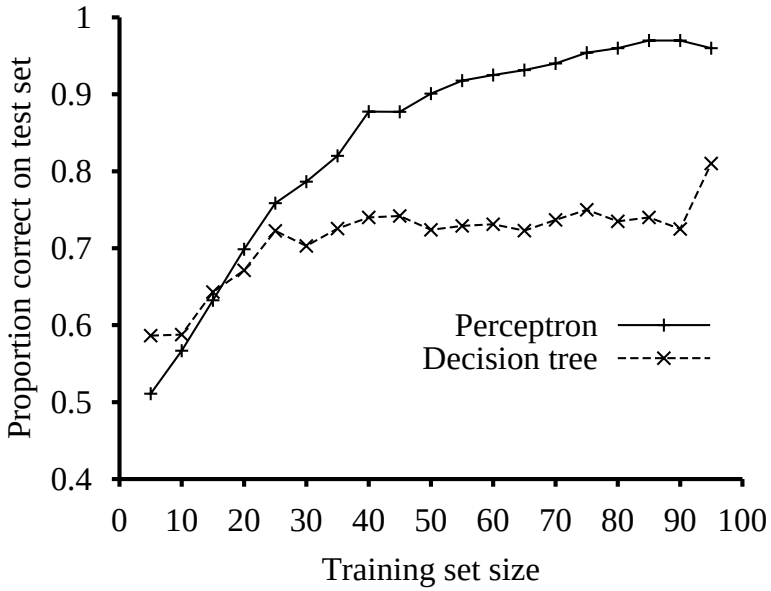
Assume the logistic activation function:

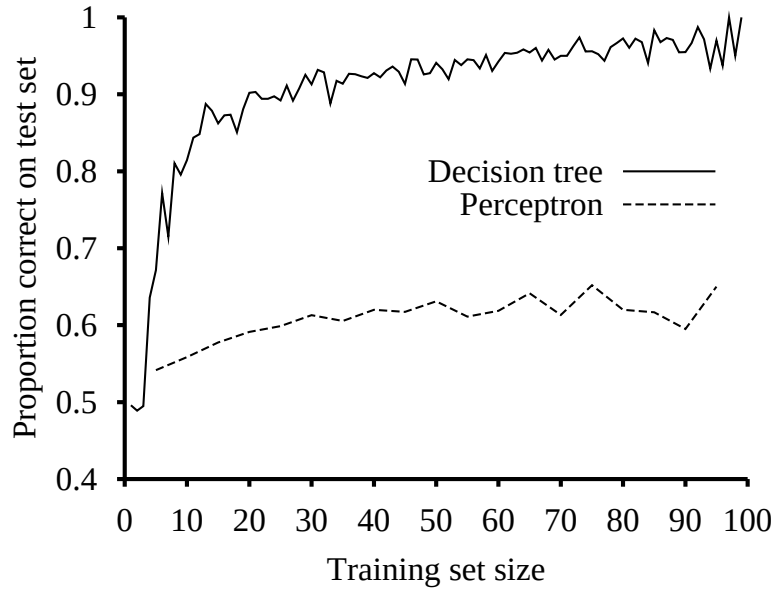
$$g(t) = \frac{1}{1+\exp(-t)}, \quad g'(t) = g(t) \cdot \left[1 - g(t)\right].$$

$$\begin{aligned}
\frac{\partial \mathbb{E}}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 \\
&= \sum_d (t_d - o_d) \frac{\partial}{\partial w_i} \left(t_d - g\left(\vec{\boldsymbol{w}}^\mathsf{T} \vec{\boldsymbol{x}}_d\right)\right) \\
&= \sum_d (t_d - o_d) \cdot (-1) \cdot x_{i,d} \cdot g'\left(\vec{\boldsymbol{w}}^\mathsf{T} \vec{\boldsymbol{x}}_d\right) \\
\frac{\partial \mathbb{E}}{\partial w_i} &= -\sum_d x_{i,d} \cdot (t_d - o_d) \cdot g\left(\vec{\boldsymbol{w}}^\mathsf{T} \vec{\boldsymbol{x}}_d\right) \left[1 - g\left(\vec{\boldsymbol{w}}^\mathsf{T} \vec{\boldsymbol{x}}_d\right)\right]
\end{aligned}$$

Perceptron learning – Does it work?

Perceptron learning rule converges to a consistent function **for any linearly separable data set**





`majority_11`: **Perceptron** OK, **DTL** hopeless

`restaurant`: **DTL** OK, **perceptron** cannot represent it

Summary - Perceptron

Perceptron delta-rule guaranteed to succeed if

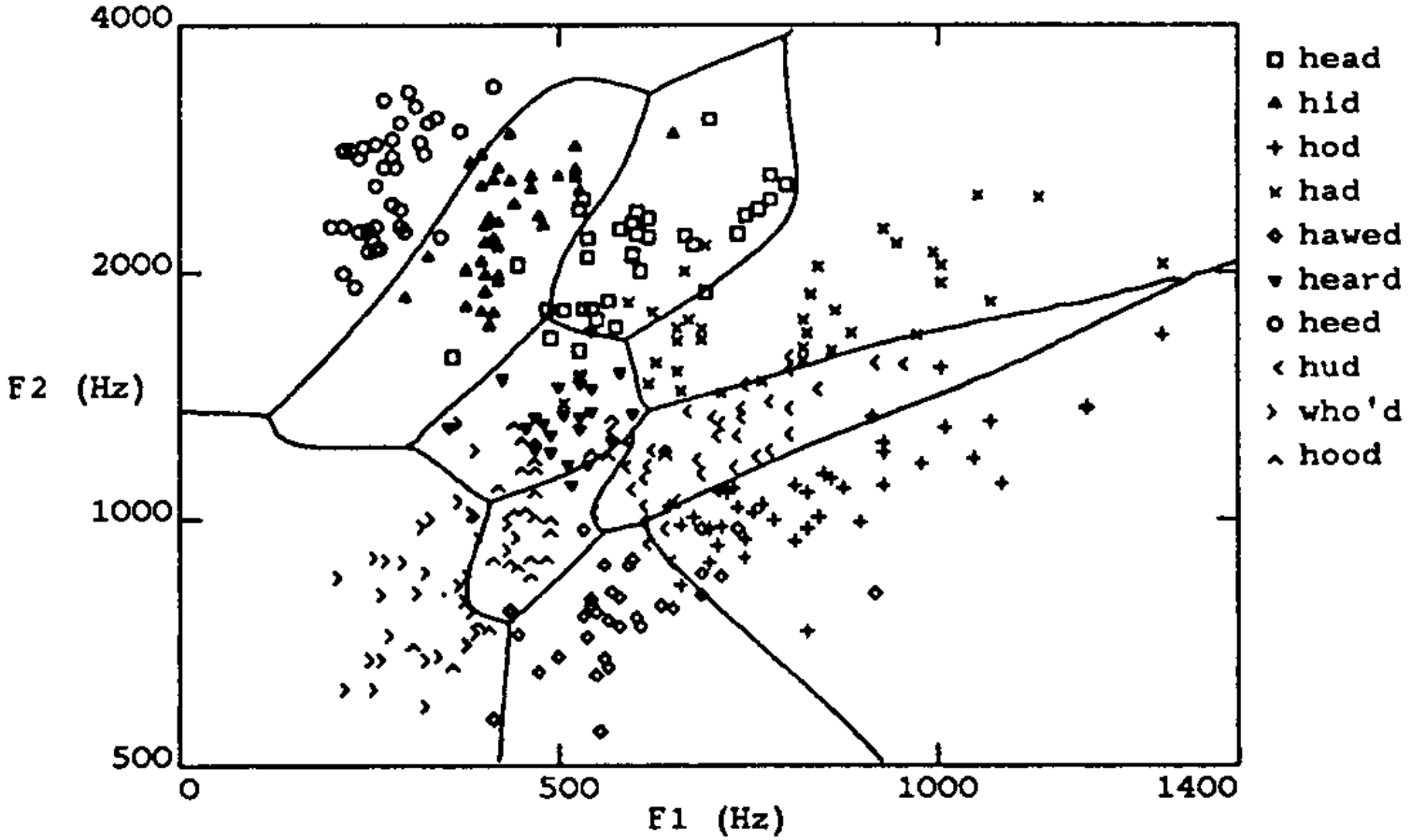
- Training examples are linearly separable
- Sufficiently small learning rate η

Linear unit training rule uses gradient descent

- Guaranteed to converge to $\boldsymbol{w}$ with minimum squared error
- Given sufficiently small learning rate η
- This is true even when training data contains **noise**, or the data is **not linearly separable**.
- **Gradient descent also works for other activation functions.**

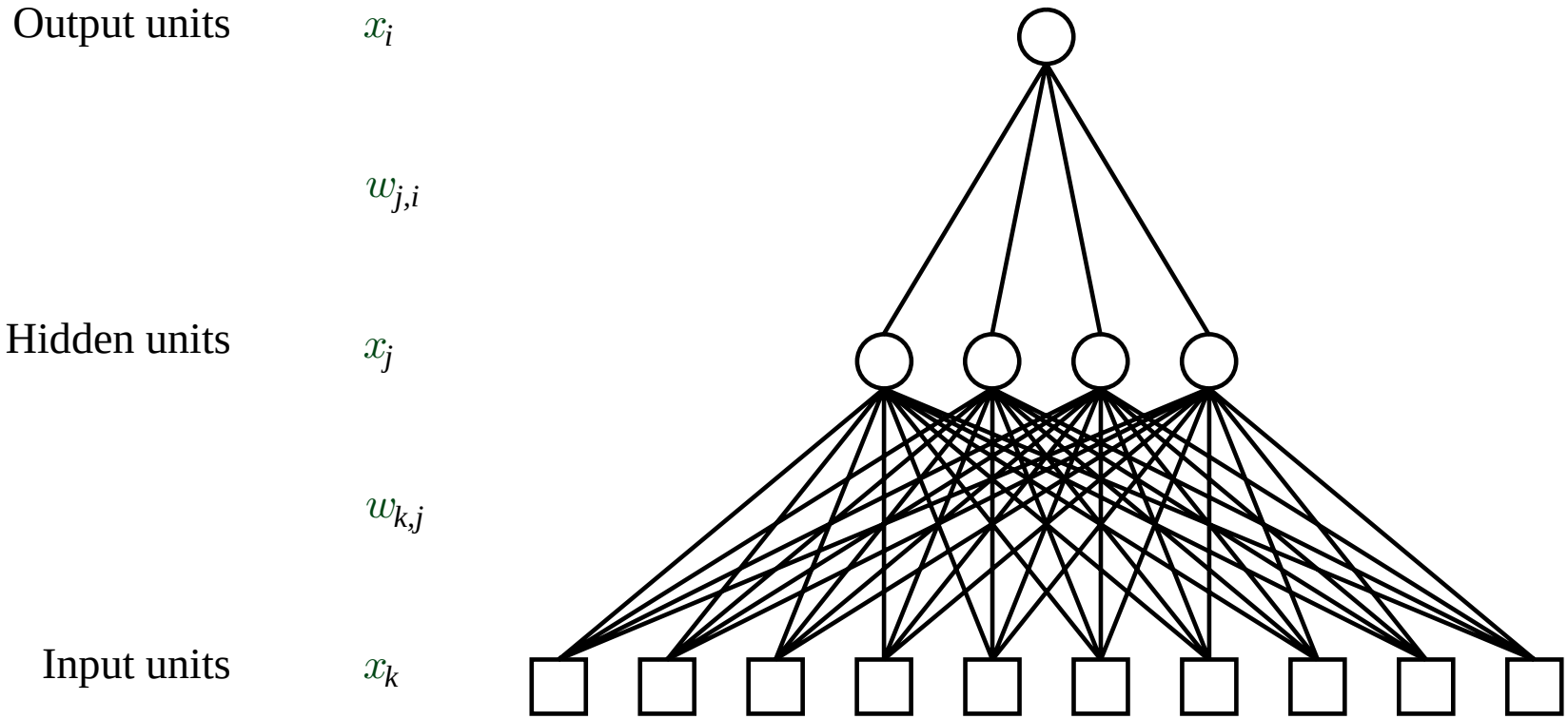
Perceptrons are unable to capture intricate patterns

Multilayer Networks of Sigmoid Units

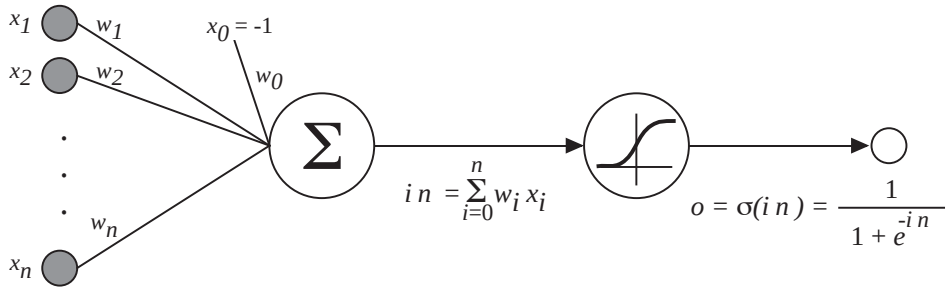


Multilayer perceptrons

Layers are usually fully connected; numbers of **hidden units** typically chosen "by hand" – doing a hyper-parameter search.



Sigmoid Unit Networks



Remember the sigmoid activation, often called $\sigma(\cdot)$, $\sigma(y) = \frac{1}{1+e^{-y}}$.

Remember also that it has the nice property that

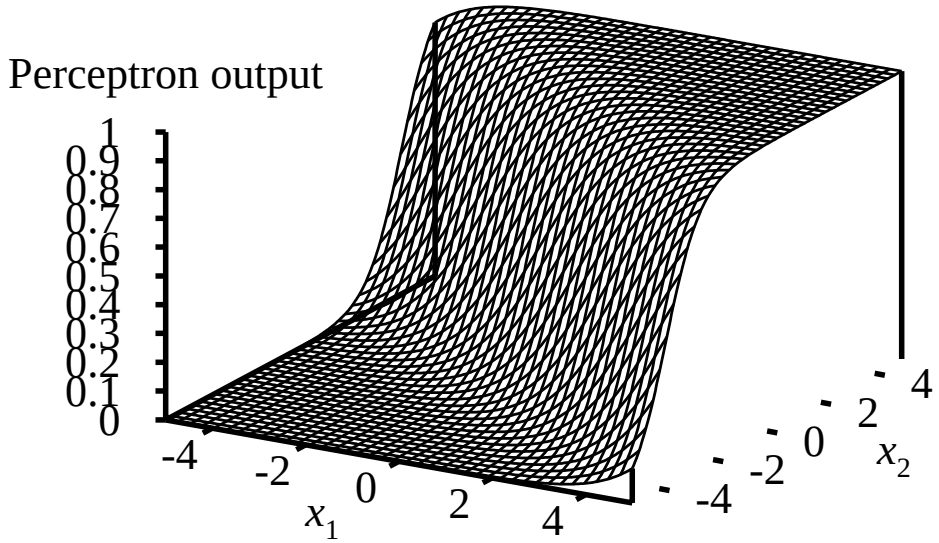
$$\frac{d\sigma(y)}{dy} = \sigma(y)(1 - \sigma(y)).$$

We can derive gradient decent rules to train

- **One** sigmoid unit → We (should) know how to do that.
- **Multilayer networks** of sigmoid units → Backpropagation

Sigmoids - expressibility

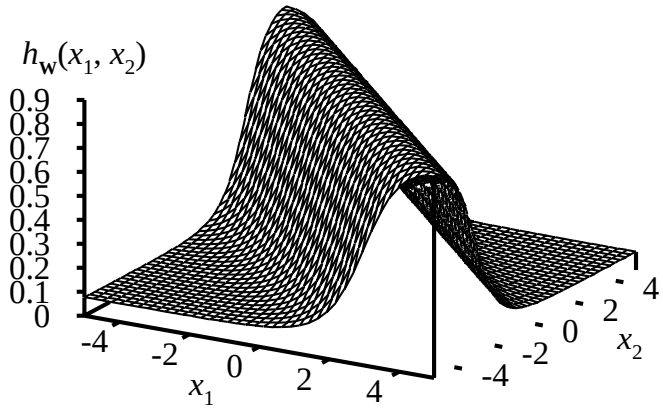
No hidden layer, input (x_1, x_2):

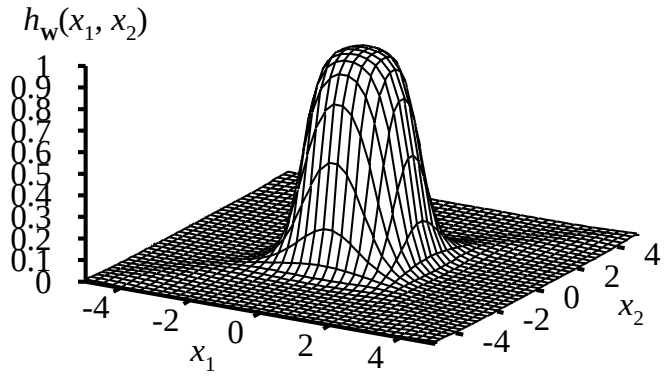


- Adjusting weights moves the location, orientation, and steepness of cliff
- Cannot tackle "correlation effects" of non-separable targets

Sigmoids - expressibility

Hidden layers:





- Combine two opposite-facing threshold functions to make a ridge
- Combine two perpendicular ridges to make a bump
- Add bumps of various sizes and locations to fit any surface

All continuous functions w/ 1 hidden layer, all functions w/ 2

Expressive Capabilities of ANNs

Boolean functions:

- Every boolean function can be represented by network with single hidden layer
- but might require exponential (in number of inputs) hidden units

Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers

Recall: Error Gradient for a Sigmoid Unit

Remember the perceptron learning, where we did the partial derivative of error wrt. weights:

$$\frac{\partial \mathbb{E}}{\partial w_i} = -\sum_d (t_d - o_d) \frac{\partial o_d}{\partial \text{in}_d} \frac{\partial \text{in}_d}{\partial w_i}$$

Now, activation is sigmoid, so $\frac{\partial o_d}{\partial \text{in}_d} = o_d(1 - o_d)$ and $\frac{\partial \text{in}_d}{\partial w_i} = x_{i,d}$. Therefore, $\frac{\partial \mathbb{E}}{\partial w_i}$ can easily be calculated in closed form.

Idea of Backprop

Do Gradient Descent for the full model:

$$w_i \leftarrow w_i - \eta \cdot \frac{\partial \mathbb{E}}{\partial w_i}$$

Weight updates are (typically – depending on $g(\cdot)$) easily available due to the restrictive structure of the feed forward model.

Backpropagation Algorithm – Sigmoid units

1. Initialize all weights to small random numbers.
2. Until satisfied:
   - For each training example
     1. Input the training example to the network and compute the network outputs and node activations along the way
     2. For each output unit k: $\delta_k \leftarrow \underbrace{o_k(1-o_k)}_{g'(o_k)} \times \underbrace{(t_k - o_k)}_{\text{Output error}}$
     3. For each hidden unit h:

$$\delta_h \leftarrow \underbrace{o_h(1-o_h)}_{g'(o_h)} \times \underbrace{\sum_{k \in \text{outputs}} w_{h,k} \cdot \delta_k}_{\text{Unit } h\text{'s contribution to next layer's error}}$$

     4. Update each network weight $w_{i,j}$: $w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}$, where $\Delta w_{i,j} = \eta \cdot \delta_j \cdot a_i$ and a_i is the activation of the node pushing information into $w_{i,j}$.

More on Backpropagation

- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight *momentum* $\alpha > 0$

$$\Delta w_{i,j}(n) = \eta \cdot \delta_j \cdot x_{i,j} + \alpha \cdot \Delta w_{i,j}(n-1)$$

- Minimizes error over *training* examples
  - Will it generalize well to subsequent examples? **Overfitting...**
- Training can take thousands of iterations $\rightarrow$ **slow!**
- Using network after training is very fast

Convergence of Backpropagation

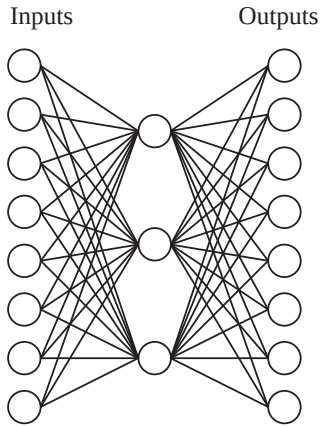
Gradient descent to some local minimum:

- Perhaps not global minimum ...
- Add momentum
- Train multiple nets with different initial weights

Nature of convergence – depending on g (here: logistic):

- Initialize weights near zero
  $\rightarrow$ Therefore, initial networks *near-linear*.
- Increasingly non-linear functions possible as training progresses.

Understanding Hidden Layer Representations – "XAI Light"



A target function:

Input		Output
10000000	→	10000000
01000000	→	01000000
00100000	→	00100000
00010000	→	00010000
00001000	→	00001000
00000100	→	00000100
00000010	→	00000010
00000001	→	00000001

Can this "auto-encoder" be learned with sigmoid activations??

Learning Hidden Layer Representations

Learned hidden layer representation:

Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.15	.99	.99	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.01	.11	.88	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

Do you recognize the encoding?

Learning Hidden Layer Representations

Learned hidden layer representation:

Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.15	.99	.99	→	01000000
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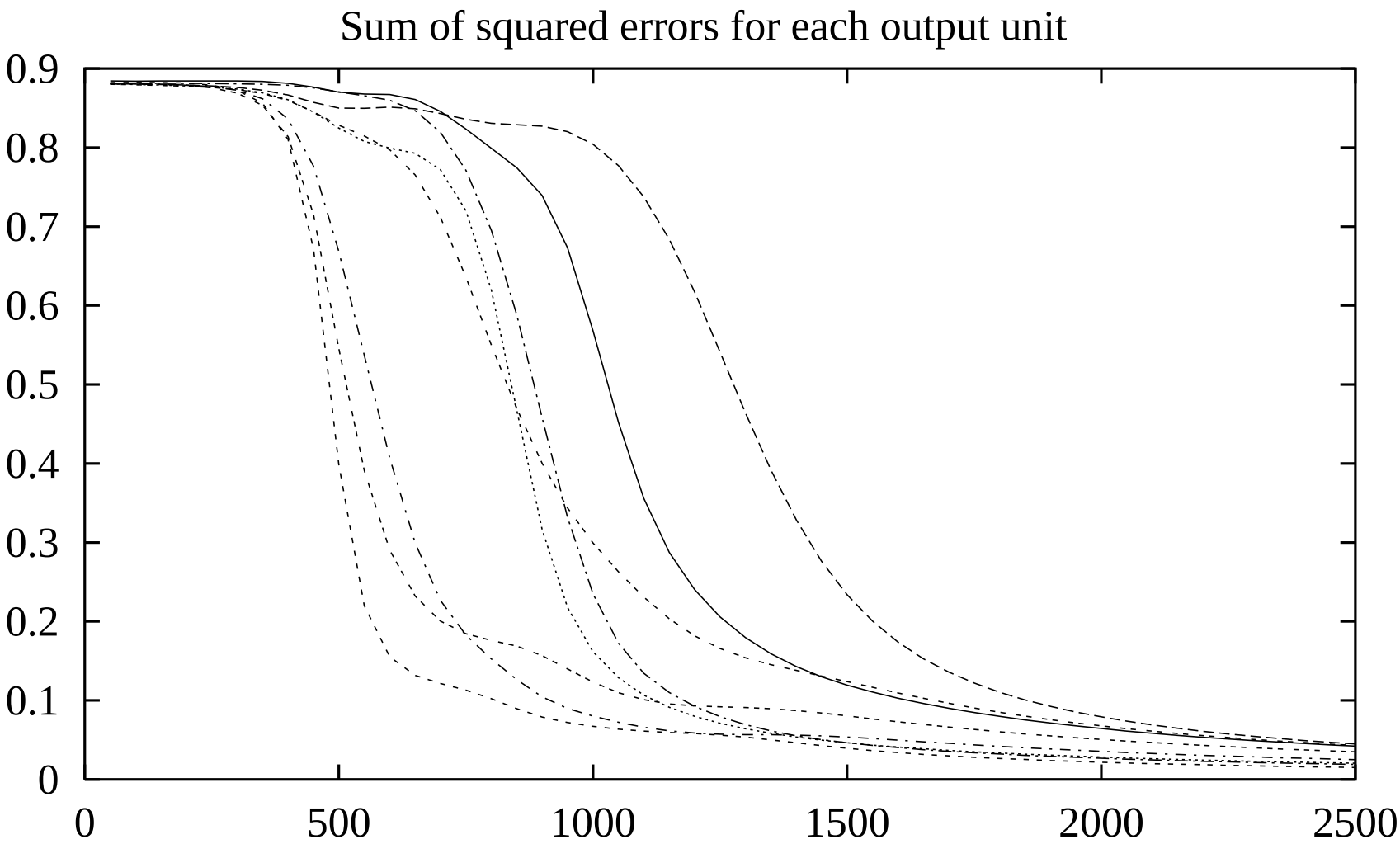
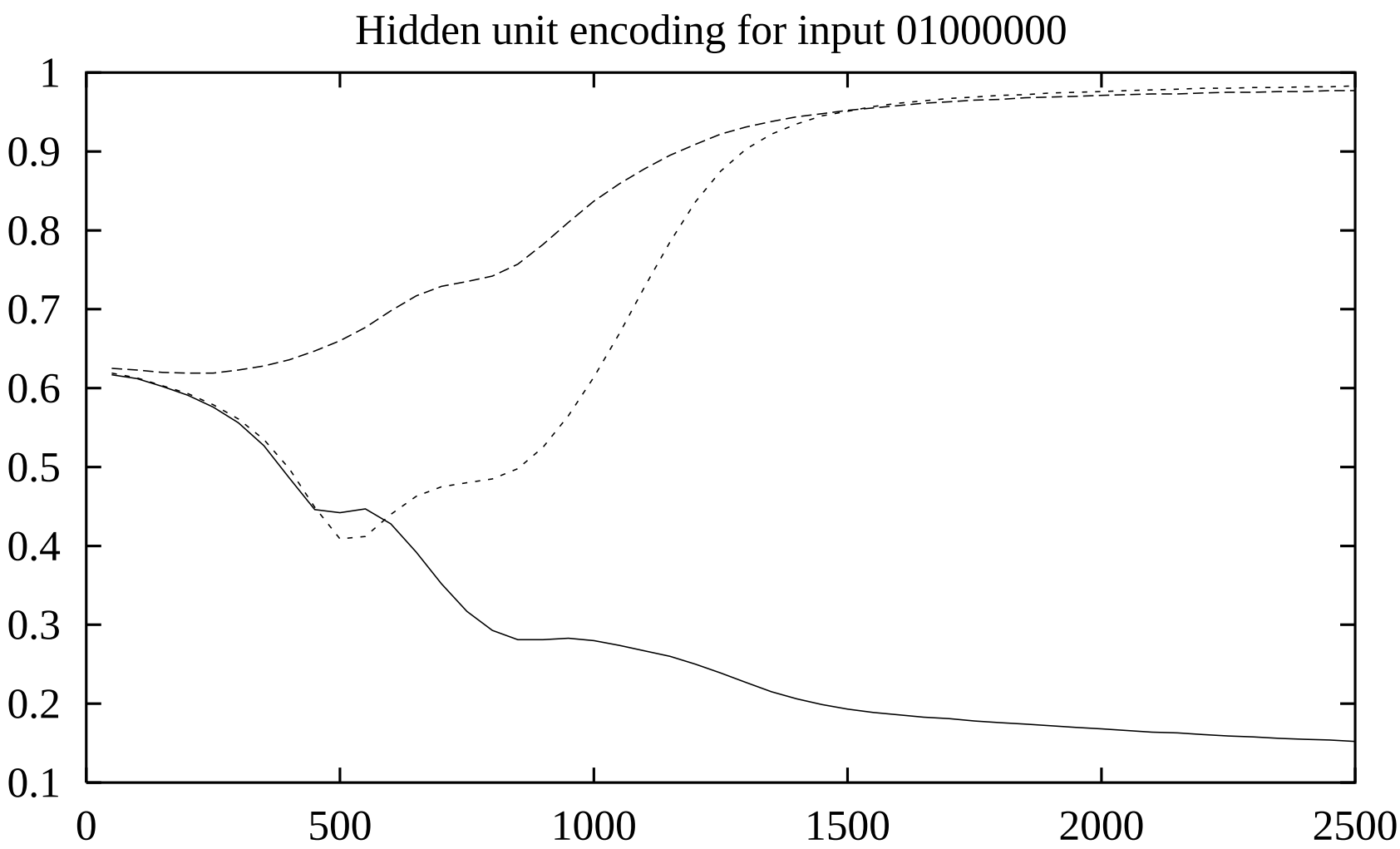
Do you recognize the encoding?

Training


Sum of squared errors for each output unit
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
500
1000
1500
2000
2500

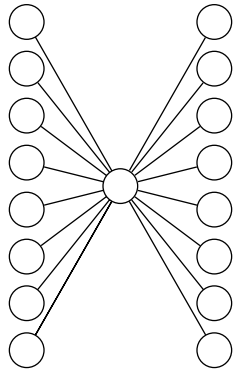
Training


Hidden unit encoding for input 01000000
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
500
1000
1500
2000
2500

Representative power of 8 - 1 - 8 sigmoid network

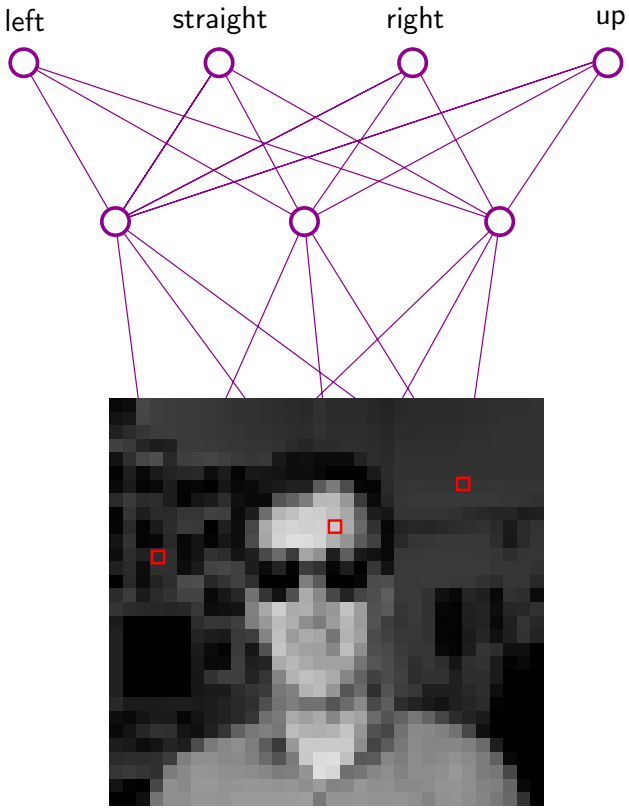
What is the capacity limit?

Representative power of 8 - 1 - 8 sigmoid network:



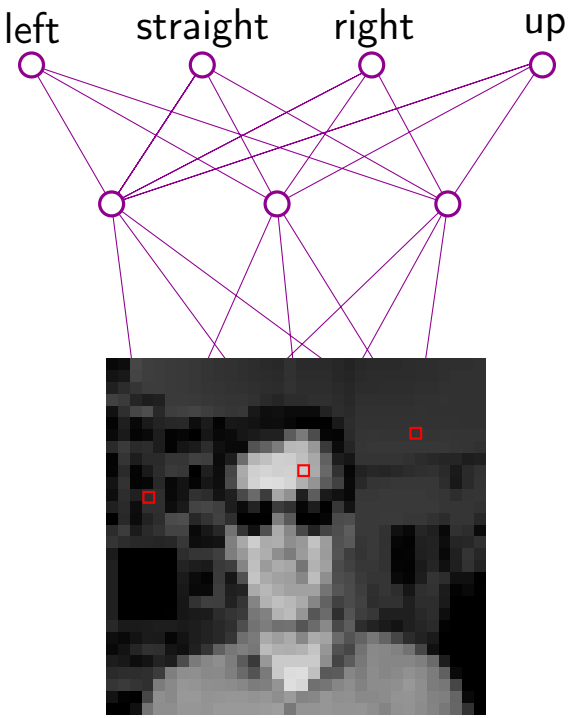
- Consider the same input $\rightarrow$ output mapping as last example (100000000 $\rightarrow$ 100000000, etc.)
- Can this be represented using the 8 - 1 - 8 structure?
  - Hidden node h can, e.g., take value $\alpha \cdot \sum_{i=1}^{8} 2^{i-1} \cdot x_i$
  - Can $h = f_1(\boldsymbol{x})$ be approximated using sigmoid functions?
  - Can $\boldsymbol{t} = f_2(h)$, be approximated using sigmoid functions?
  - If so: $\boldsymbol{t} = f_2(f_1(\boldsymbol{x}))$, and the answer is **YES!**
  - Unfortunately, f_2 is not monotone in h, therefore cannot be approximated without additional layers, and the answer is **NO!**

Neural Nets for Recognition of Viewing Direction

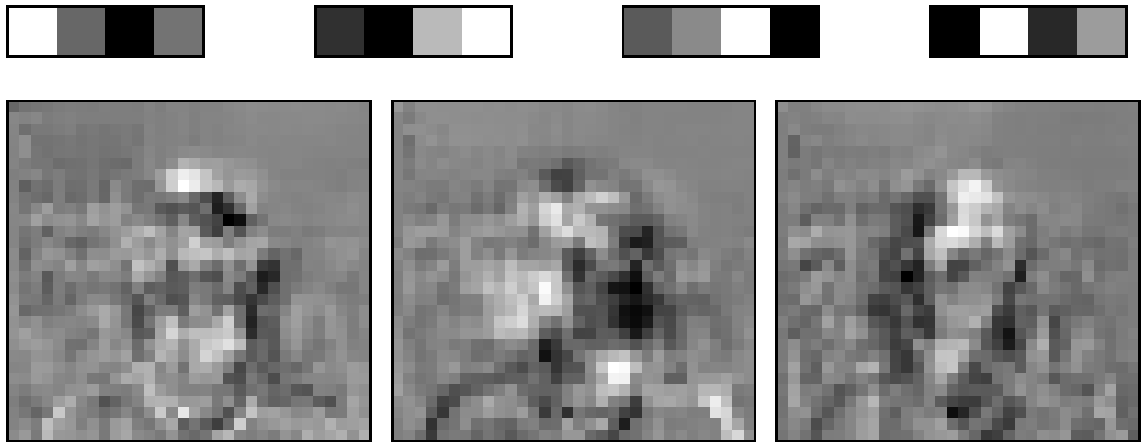


Typical input images (30×32 pixels)

Learned hidden unit weights



Learned Weights



Mostly "Up" | "Right"; **not** "Left" | Mostly "Straight"

Typical input images

Overfitting in ANNs – Why, and what to do...

The problem:

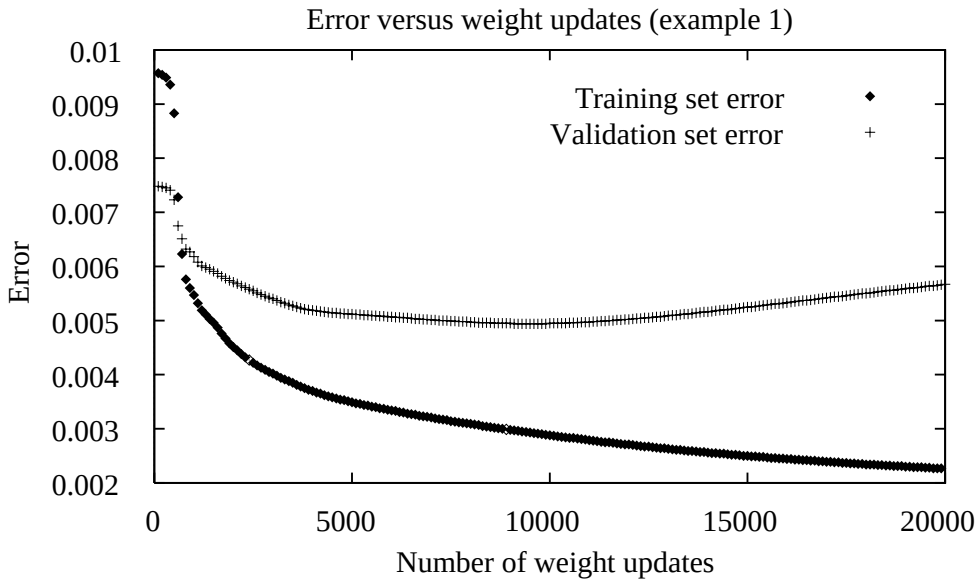
- Due to ANNs **universal approximation theorem**, overfitting is prominent in ANNs.
- Even a "relatively small" network has, if weights grow large in absolute value, the ability to construct **consistent hypothesis by memorizing** the training data.

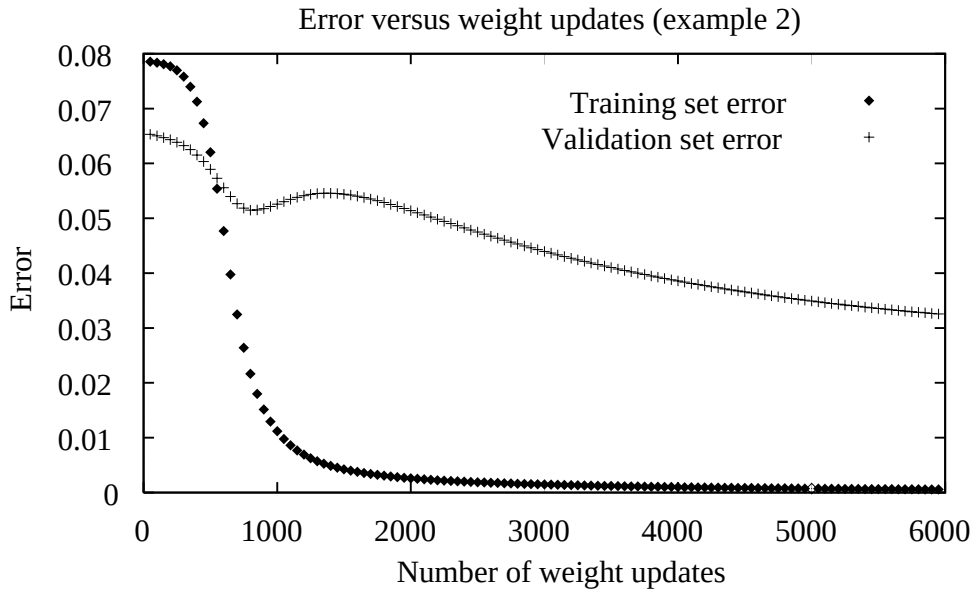
Some popular solutions:

Regularization: Define alternative error/loss functions, where we punish model complexity and/or extreme weights.

Validation: Monitor convergence/overfitting on a separate validation-set.

Overfitting in ANNs – validation loss





Summary

- Most brains have lots of neurons; each neuron $\approx$ linear–threshold unit (?)
- Perceptrons (one-layer networks) insufficiently expressive
- Multi-layer networks are sufficiently expressive; can be trained by gradient descent, i.e., error back-propagation
- Many applications: speech, driving, handwriting, fraud detection, etc.
- Engineering, cognitive modelling, and neural system modelling subfields have largely diverged