Introduction

Outline

Basic Units

Nonlinearly Separable Problems

Backprop

Types of Units

Putting Things Together

CSCE 970 Lecture 2: Artificial Neural Networks and Deep Learning

Stephen Scott and Vinod Variyam

(Adapted from Ethem Alpaydin and Tom Mitchell)

sscott@cse.unl.edu

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Introduction

Deep learning is based in *artificial neural networks*

Consider humans:

- Total number of neurons $\approx 10^{10}$
- Neuron switching time $\approx 10^{-3}$ second (vs. 10^{-10})
- Connections per neuron $\approx 10^4$–10^5
- Scene recognition time ≈ 0.1 second
- 100 inference steps doesn't seem like enough

$\Rightarrow$ massive parallel computation

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Properties of artificial neural nets (ANNs):

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

Strong differences between ANNs for ML and ANNs for biological modeling

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- **The Beginning:** Linear units and the Perceptron algorithm (1940s)
  - Spoiler Alert: stagnated because of inability to handle data not *linearly separable*
  - Aware of usefulness of multi-layer networks, but could not train
- **The Comeback:** Training of multi-layer networks with Backpropagation (1980s)
  - Many applications, but in 1990s replaced by large-margin approaches such as support vector machines and boosting

Introduction
History of ANNs (cont'd)

- **The Resurgence:** Deep architectures (2000s)
  - Better hardware and software support allow for deep (> 5–8 layers) networks
  - Still use Backpropagation, but
    - Larger datasets, algorithmic improvements (new loss and activation functions), and deeper networks improve performance considerably
  - Very impressive applications, e.g., captioning images
- **The Problem:** Skynet (TBD)
  - Sorry.

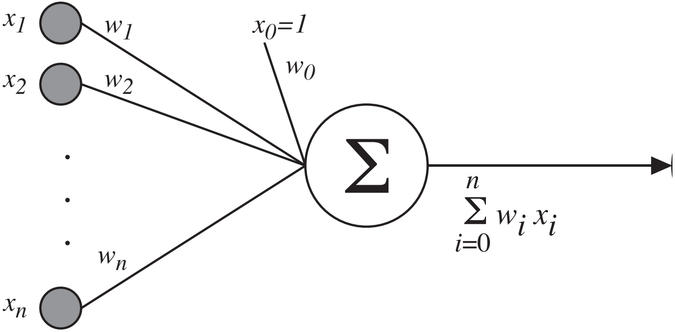
When to Consider ANNs

- 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
- Long training times acceptable

Outline

- Basic units
    - Linear unit
    - Linear threshold units
    - Perceptron training rule
- Nonlinearly separable problems and multilayer networks
- Backpropagation
- Putting everything together

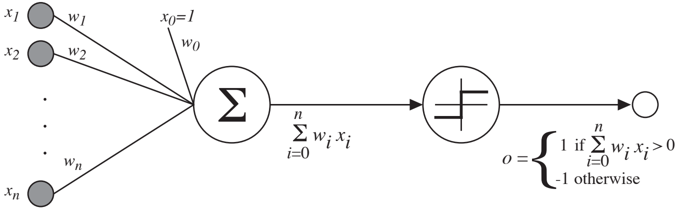
Linear Unit



$$\hat{y} = f(\mathbf{x}; \mathbf{w}, b) = \mathbf{x}^\top \mathbf{w} + b = w_1 x_1 + \cdots + w_n x_n + b$$

- If set $w_0 = b$, can simplify above
- Forms the basis for many other activation functions

Linear Threshold Unit



$$y = o(\mathbf{x}; \mathbf{w}, b) = \begin{cases} +1 & \text{if } f(\mathbf{x}; \mathbf{w}, b) > 0 \\ -1 & \text{otherwise} \end{cases}$$

(sometimes use 0 instead of -1)

Linear Threshold Unit
Decision Surface

(a) (b)

Represents some useful functions

- What parameters $(\mathbf{w}, b)$ represent $g(x_1, x_2; \mathbf{w}, b) = AND(x_1, x_2)$?

But some functions not representable

- I.e., those not **linearly separable**
- Therefore, we'll want **networks** of units

Perceptron Training Rule

$$w_j^{t+1} \leftarrow w_j^t + \Delta w_j^t \ , \text{ where } \Delta w_j^t = \eta \left(y^t - \hat{y}^t\right) x_j^t$$

and

- y^t is label of training instance t
- $\hat{y}^t$ is Perceptron output on training instance t
- η is small constant (e.g., 0.1) called **learning rate**

I.e., if $(y^t - \hat{y}^t) > 0$ then increase w_j^t w.r.t. x_j^t, else decrease

Can prove rule will converge if training data is linearly separable and η sufficiently small

Where Does the Training Rule Come From?

- Recall initial *linear unit*, where output

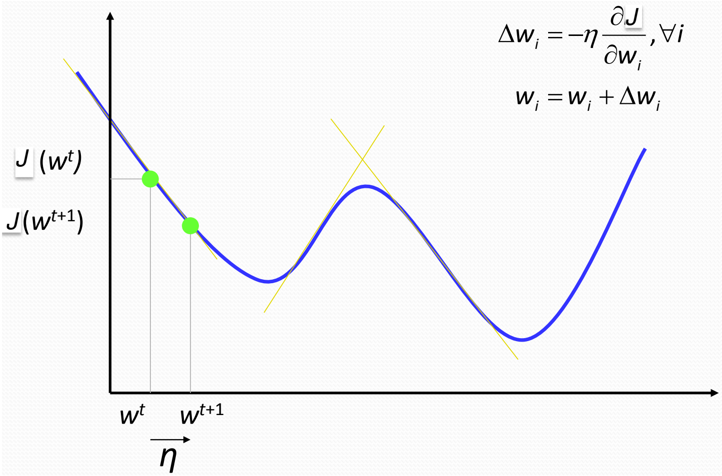
$$\hat{y}^t = f(\mathbf{x}; \mathbf{w}, b) = \mathbf{x}^\top \mathbf{w} + b$$

(i.e., no threshold)

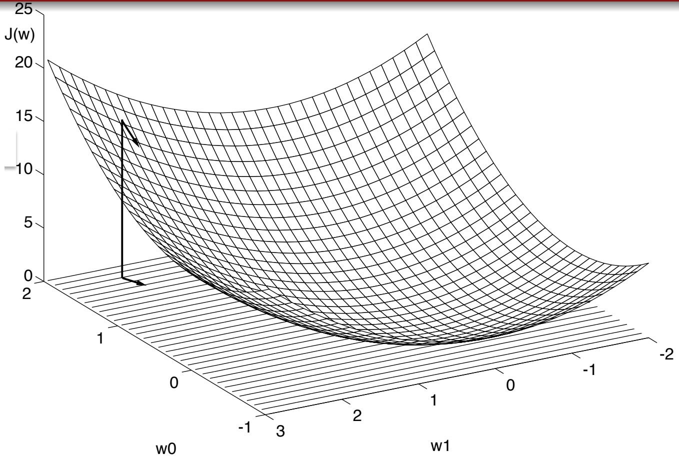
- For each training example, compromise between **correctiveness** and **conservativeness**
  - **Correctiveness:** Tendency to improve on $\mathbf{x}^t$ (reduce loss)
  - **Conservativeness:** Tendency to keep $\mathbf{w}^{t+1}$ close to $\mathbf{w}^t$ (minimize distance)
- Use **cost function** that measures both (let $w_0 = b$):

$$J(\mathbf{w}) = dist\left(\mathbf{w}^{t+1}, \mathbf{w}^t\right) + \eta\, loss\left(y^t, \overbrace{\mathbf{w}^{t+1} \cdot \mathbf{x}^t}^{\text{curr ex, new wts}}\right)$$

Gradient Descent



Gradient Descent (cont'd)



$$\frac{\partial J}{\partial \mathbf{w}} = \left[\frac{\partial J}{\partial w_0}, \frac{\partial J}{\partial w_1}, \cdots, \frac{\partial J}{\partial w_n}\right]$$

Gradient Descent (cont'd)

$$\begin{aligned} J(\mathbf{w}) &= \overbrace{\|\mathbf{w}^{t+1} - \mathbf{w}^t\|_2^2}^{conserv.} + \overbrace{\eta}^{coef.} \overbrace{(y^t - \mathbf{w}^{t+1} \cdot \mathbf{x}^t)^2}^{corrective} \\ &= \sum_{j=1}^{n} \left(w_j^{t+1} - w_j^t\right)^2 + \eta \left(y^t - \sum_{j=1}^{n} w_j^{t+1} x_j^t\right)^2 \end{aligned}$$

Take gradient w.r.t. $\mathbf{w}^{t+1}$ (i.e., $\partial J / \partial w_i^{t+1}$) and set to $\mathbf{0}$:

$$0 = 2\left(w_i^{t+1} - w_i^t\right) - 2\eta \left(y^t - \sum_{j=1}^{n} {\color{red} w_j^{t+1}} x_j^t\right) x_i^t$$

Gradient Descent (cont'd)

Approximate with

$$0 = 2\left(w_i^{t+1} - w_i^t\right) - 2\eta\left(y^t - \sum_{j=1}^{n} w_j^t x_j^t\right) x_i^t \ ,$$

which yields

$$w_i^{t+1} = w_i^t + \overbrace{\eta\left(y^t - \hat{y}^t\right) x_i^t}^{\Delta w_i^t}$$

Given other loss function and unit activation function, can derive weight update rule

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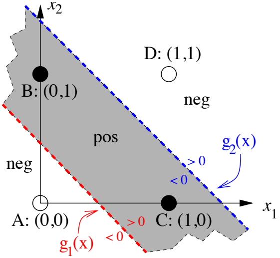
Using linear threshold units (book uses rectified linear units)



Represent with **intersection** of two linear separators

$$g_1(\mathbf{x}) = 1 \cdot x_1 + 1 \cdot x_2 - 1/2$$

$$g_2(\mathbf{x}) = 1 \cdot x_1 + 1 \cdot x_2 - 3/2$$

pos $= \{\mathbf{x} \in \mathbb{R}^2 : g_1(\mathbf{x}) > 0$ <u>AND</u> $g_2(\mathbf{x}) < 0\}$

neg $= \{\mathbf{x} \in \mathbb{R}^2 : g_1(\mathbf{x}), g_2(\mathbf{x}) < 0$ <u>OR</u> $g_1(\mathbf{x}), g_2(\mathbf{x}) > 0\}$

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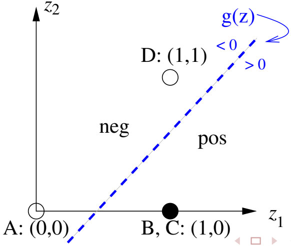
Let $z_i = \begin{cases} 0 & \text{if } g_i(\mathbf{x}) < 0 \\ 1 & \text{otherwise} \end{cases}$

Class	(x_1, x_2)	$g_1(\mathbf{x})$	z_1	$g_2(\mathbf{x})$	z_2
pos	B: $(0, 1)$	$1/2$	1	$-1/2$	0
pos	C: $(1, 0)$	$1/2$	1	$-1/2$	0
neg	A: $(0, 0)$	$-1/2$	0	$-3/2$	0
neg	D: $(1, 1)$	$3/2$	1	$1/2$	1

Now feed z_1, z_2 into $g(\mathbf{z}) = 1 \cdot z_1 - 2 \cdot z_2 - 1/2$



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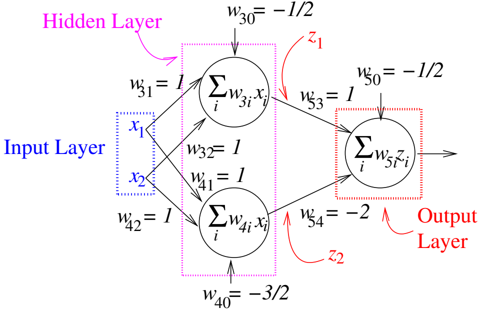
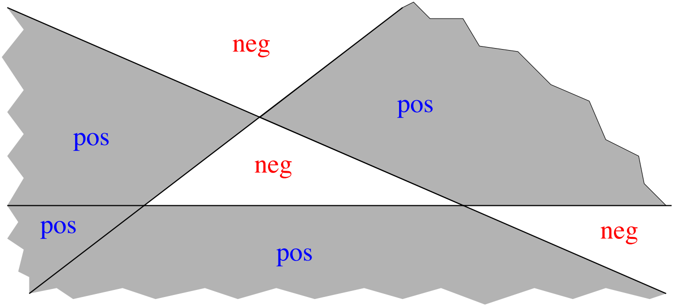
In other words, we **remapped** all vectors $\mathbf{x}$ to $\mathbf{z}$ such that the classes are linearly separable in the new vector space



This is a **two-layer perceptron** or **two-layer feedforward neural network**

Can use many **nonlinear** activation functions in hidden layer

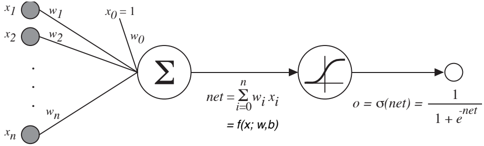
By adding up to 2 **hidden layers** of linear threshold units, can represent any **union** of **intersection of halfspaces**



First hidden layer defines halfspaces, second hidden layer takes intersection (AND), output layer takes union (OR)

The Sigmoid Unit

[Rarely used in deep ANNs, but continuous and differentiable]



$\sigma(net)$ is the **logistic function**

$$\sigma(net) = \frac{1}{1 + e^{-net}}$$

(a type of **sigmoid** function)

Squashes net into $[0, 1]$ range

Nice property:

$$\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$$

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Again, use squared loss for correctiveness:

$$E(\mathbf{w}^t) = \frac{1}{2}\left(y^t - \hat{y}^t\right)^2$$

(folding $1/2$ of correctiveness into loss func)

Thus $\dfrac{\partial E}{\partial w_j^t} = \dfrac{\partial}{\partial w_j^t}\dfrac{1}{2}\left(y^t - \hat{y}^t\right)^2$

$$= \frac{1}{2}\, 2\left(y^t - \hat{y}^t\right)\frac{\partial}{\partial w_j^t}\left(y^t - \hat{y}^t\right) = \left(y^t - \hat{y}^t\right)\left(-\frac{\partial \hat{y}^t}{\partial w_j^t}\right)$$

Sigmoid Unit
Gradient Descent (cont'd)

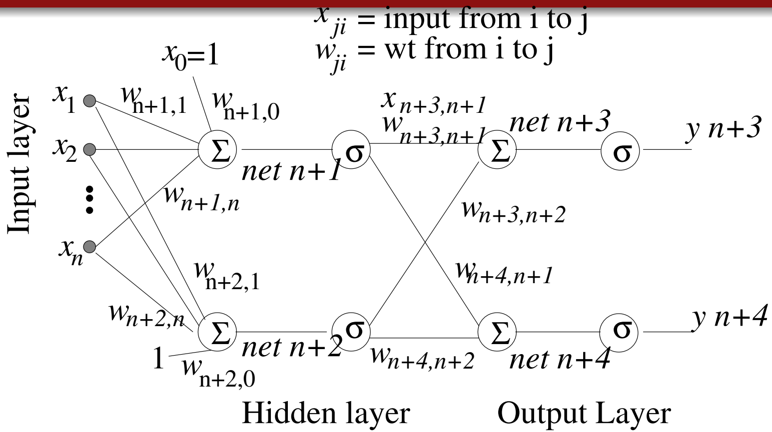
Since $\hat{y}^t$ is a function of $f(\mathbf{x}; \mathbf{w}, b) = net^t = \mathbf{w}^t \cdot \mathbf{x}^t$,

$$\begin{aligned}\frac{\partial E}{\partial w_j^t} &= -\left(y^t - \hat{y}^t\right) \frac{\partial \hat{y}^t}{\partial net^t} \frac{\partial net^t}{\partial w_j^t} \\ &= -\left(y^t - \hat{y}^t\right) \frac{\partial \sigma\left(net^t\right)}{\partial net^t} \frac{\partial net^t}{\partial w_j^t} \\ &= -\left(y^t - \hat{y}^t\right) \hat{y}^t \left(1 - \hat{y}^t\right) x_j^t\end{aligned}$$

Update rule:

$$\boxed{w_j^{t+1} = w_j^t + \eta\, \hat{y}^t \left(1 - \hat{y}^t\right) \left(y^t - \hat{y}^t\right) x_j^t}$$

Multilayer Networks



For now, using sigmoid units

$$E^t = E(\mathbf{w}^t) = \frac{1}{2} \sum_{k \in outputs} \left(y_k^t - \hat{y}_k^t\right)^2$$

Adjust weight w_{ji}^t according to E^t as before

For output units, this is easy since contribution of w_{ji}^t to E^t when j is an output unit is the same as for single neuron case[1], i.e.,

$$\frac{\partial E^t}{\partial w_{ji}^t} = -\left(y_j^t - \hat{y}_j^t\right) \hat{y}_j^t \left(1 - \hat{y}_j^t\right) x_{ji}^t = -\delta_j^t \, x_{ji}^t$$

where $\delta_j^t = -\frac{\partial E^t}{\partial net_j^t} =$ **error term** of unit j

[1] This is because all other outputs are constants w.r.t. w_{ji}^t

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- How can we compute the error term for hidden layers when there is no target output $\mathbf{r}^t$ for these layers?
- Instead **propagate back** error values from output layer toward input layers, scaling with the weights
- Scaling with the weights characterizes how much of the error term each hidden unit is "responsible for"

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The impact that w_{ji}^t has on E^t is only through net_j^t and units immediately "downstream" of j:

$$\frac{\partial E^t}{\partial w_{ji}^t} = \frac{\partial E^t}{\partial net_j^t} \frac{\partial net_j^t}{\partial w_{ji}^t} = x_{ji}^t \sum_{k \in down(j)} \frac{\partial E^t}{\partial net_k^t} \frac{\partial net_k^t}{\partial net_j^t}$$

$$= x_{ji}^t \sum_{k \in down(j)} -\delta_k^t \frac{\partial net_k^t}{\partial net_j^t} = x_{ji}^t \sum_{k \in down(j)} -\delta_k^t \frac{\partial net_k^t}{\partial \hat{y}_j} \frac{\partial \hat{y}_j}{\partial net_j^t}$$

$$= x_{ji}^t \sum_{k \in down(j)} -\delta_k^t \, w_{kj} \frac{\partial \hat{y}_j}{\partial net_j^t} = x_{ji}^t \sum_{k \in down(j)} -\delta_k^t \, w_{kj} \, \hat{y}_j \, (1 - \hat{y}_j)$$

Works for arbitrary number of hidden layers

Backpropagation Algorithm

Initialize all weights to small random numbers

Until termination condition satisfied do

- For each training example $(\mathbf{y}^t, \mathbf{x}^t)$ do
  1. Input $\mathbf{x}^t$ to the network and compute the outputs $\hat{\mathbf{y}}^t$
  2. For each output unit k

$$\delta_k^t \leftarrow \hat{y}_k^t \, (1 - \hat{y}_k^t) \, (y_k^t - \hat{y}_k^t)$$

  3. For each hidden unit h

$$\delta_h^t \leftarrow \hat{y}_h^t \, (1 - \hat{y}_h^t) \sum_{k \in down(h)} w_{k,h}^t \, \delta_k^t$$

  4. Update each network weight $w_{j,i}^t$

$$w_{j,i}^t \leftarrow w_{j,i}^t + \Delta w_{j,i}^t$$

where

$$\Delta w_{j,i}^t = \eta \, \delta_j^t \, x_{j,i}^t$$

Backpropagation Algorithm

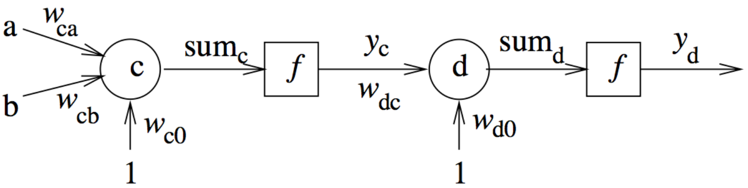
Example

target = r

$f(x) = 1 / (1 + \exp(-x))$

trial 1: a = 1, b = 0, r = 1

trial 2: a = 0, b = 1, r = 0



eta	0.3		
	trial 1	trial 2	
w_ca	0.1	0.1008513	0.1008513
w_cb	0.1	0.1	0.0987985
w_c0	0.1	0.1008513	0.0996498
a	1	0	
b	0	1	
const	1	1	
sum_c	0.2	0.2008513	
y_c	0.5498340	0.5500447	
w_dc	0.1	0.1189104	0.0964548
w_d0	0.1	0.1343929	0.0935679
sum_d	0.1549834	0.1997990	
y_d	0.5386685	0.5497842	

target	1	0
delta_d	0.1146431	-0.136083
delta_c	0.0028376	-0.004005

delta_d(t) = y_d(t) * (r(t) - y_d(t)) * (1 - y_d(t))

delta_c(t) = y_c(t) * (1 - y_c(t)) * delta_d(t) * w_dc(t

w_dc(t+1) = w_dc(t) + eta * y_c(t) * delta_d(t)

w_ca(t+1) = w_ca(t) + eta * a * delta_c(t)

Types of Output Units

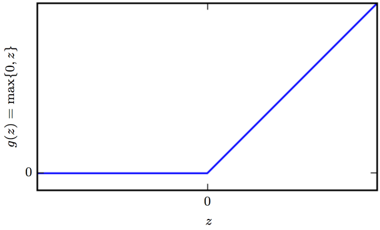
Given hidden layer outputs $\mathbf{h}$

- Linear unit (Sec 6.2.2.1): $\hat{y} = \mathbf{w}^\top \mathbf{h} + b$
  - Minimizing square loss with this output unit maximizes **log likelihood** when labels from normal distribution
    - I.e., find a set of parameters θ that is most likely to generate the labels of the training data
  - Works well with GD training
- Sigmoid (Sec 6.2.2.2): $\hat{y} = \sigma(\mathbf{w}^\top \mathbf{h} + b)$
  - Approximates non-differentiable threshold function
  - More common in older, shallower networks
  - Can be used to predict probabilities
- Softmax unit (Sec 6.2.2.3): Start with $\mathbf{z} = W^\top \mathbf{h} + \mathbf{b}$
  - Predict probability of label i to be $\text{softmax}(z)_i = \exp(z_i) / \left(\sum_j \exp(z_j) \right)$
  - Continuous, differentiable approximation to argmax

Types of Hidden Units

Rectified linear unit (ReLU) (Sec 6.3.1): $\max\{0, W^\top \mathbf{x} + \mathbf{b}\}$

- Good default choice
- Second derivative is 0 almost everywhere and derivatives large
- In general, GD works well when functions nearly linear



Logistic sigmoid (done already) and tanh (6.3.2)

- Nice approximation to threshold, but don't train well in deep networks
- Still potentially useful when piecewise functions inappropriate

Softmax (occasionally used as hidden)

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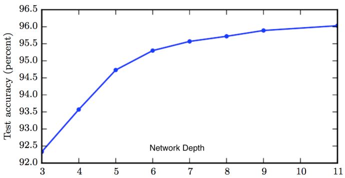
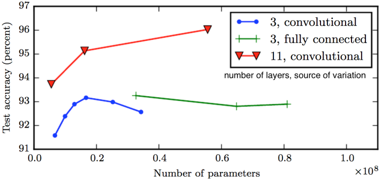
Hidden Layers

- How many layers to use?
  - Deep networks tend to build potentially useful representations of the data via composition of simple functions
  - Performance improvement not simply from more complex network (number of parameters)
  - Increasing number of layers still increases chances of overfitting, so need significant amount of training data with deep network; training time increases as well

Accuracy vs Depth



Accuracy vs Complexity



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- Any boolean function can be represented with two layers
- Any bounded, continuous function can be represented with arbitrarily small error with two layers
- Any function can be represented with arbitrarily small error with three layers

Only an **EXISTENCE PROOF**

- Could need exponentially many nodes in a layer
- May not be able to find the right weights