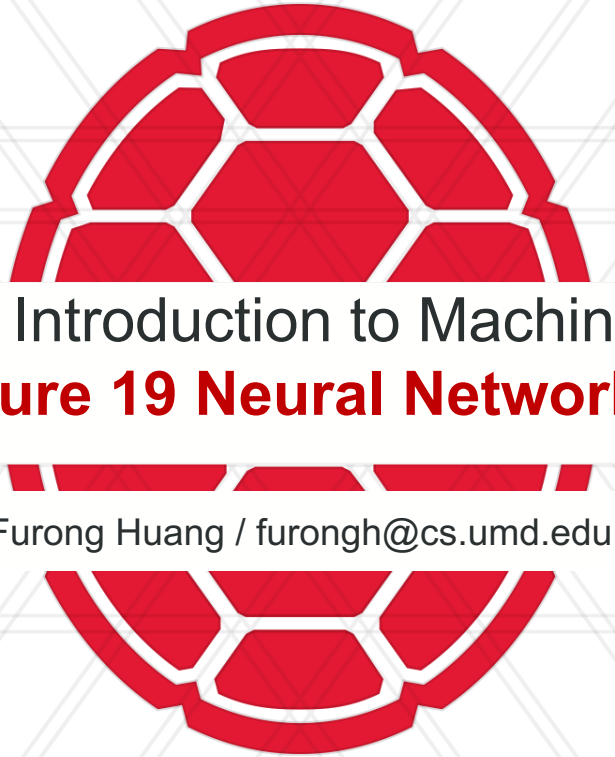
Slides adapted from Prof Carpuat and Duraiswami



CMSC 422 Introduction to Machine Learning

Lecture 19 Neural Networks II

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Neural Networks

Last time

What are Neural Networks? (key components)

How to make a prediction given an input?

Why are neural networks powerful?

Neural Networks

Last time

- What are Neural Networks?
  - Multilayer perceptron
- How to make a prediction given an input?
  - Simple matrix operations + nonlinearities
- Why are neural networks powerful?
  - Universal function approximators!

Today

- how to train neural networks?

Example: a neural network to solve the XOR problem

$\varphi_0(x_1) = \{-1, 1\}$ $\varphi_0(x_2) = \{1, 1\}$

$\varphi_1(x_3) = \{-1, 1\}$

$\varphi_0(x_3) = \{-1, -1\}$ $\varphi_0(x_4) = \{1, -1\}$

$\varphi_1(x_1) = \{-1, -1\}$ $\varphi_1(x_2) = \{1, -1\}$

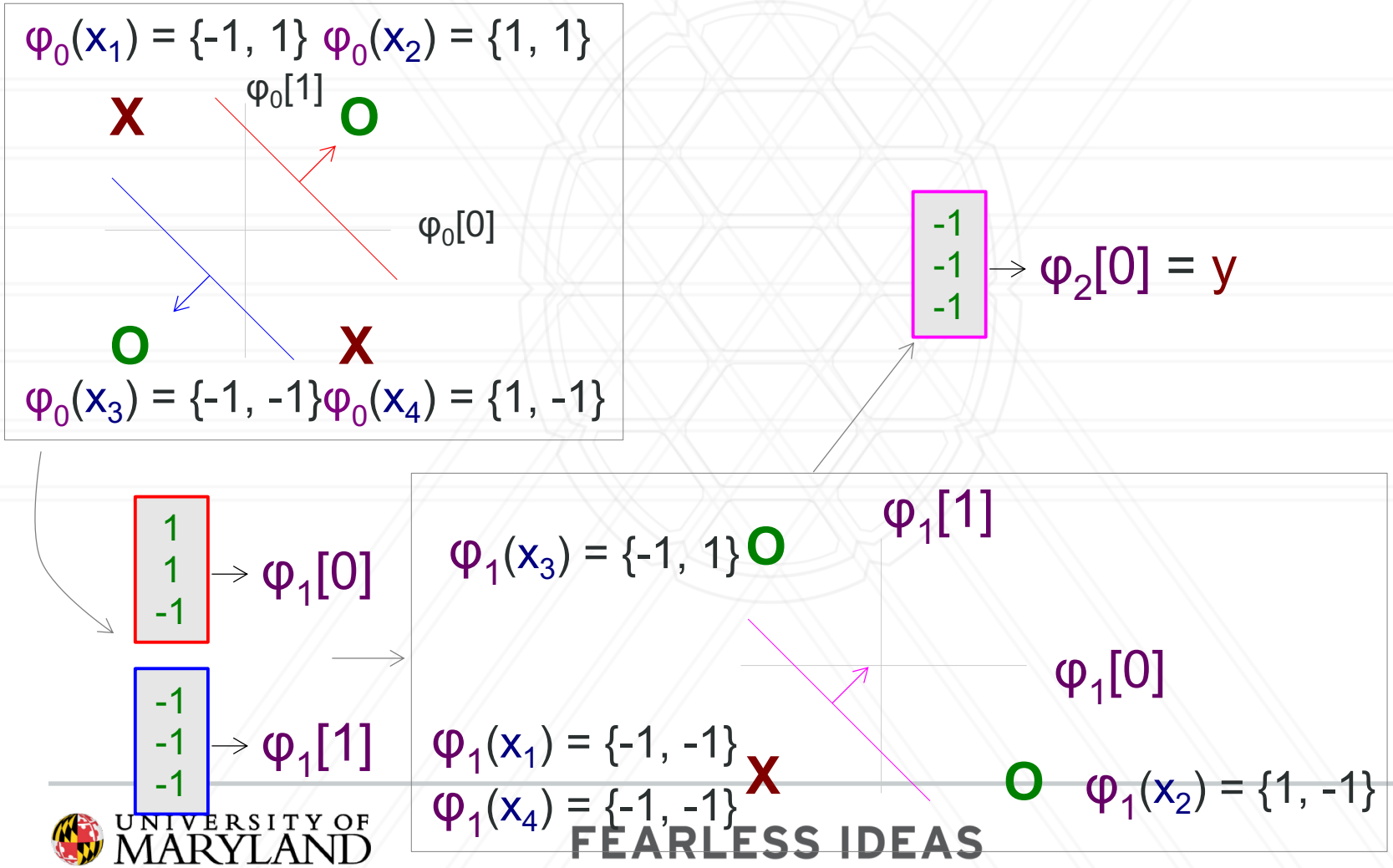
$\varphi_1(x_4) = \{-1, -1\}$

1
1
-1
→ $\varphi_1[0]$

-1
-1
-1
→ $\varphi_1[1]$

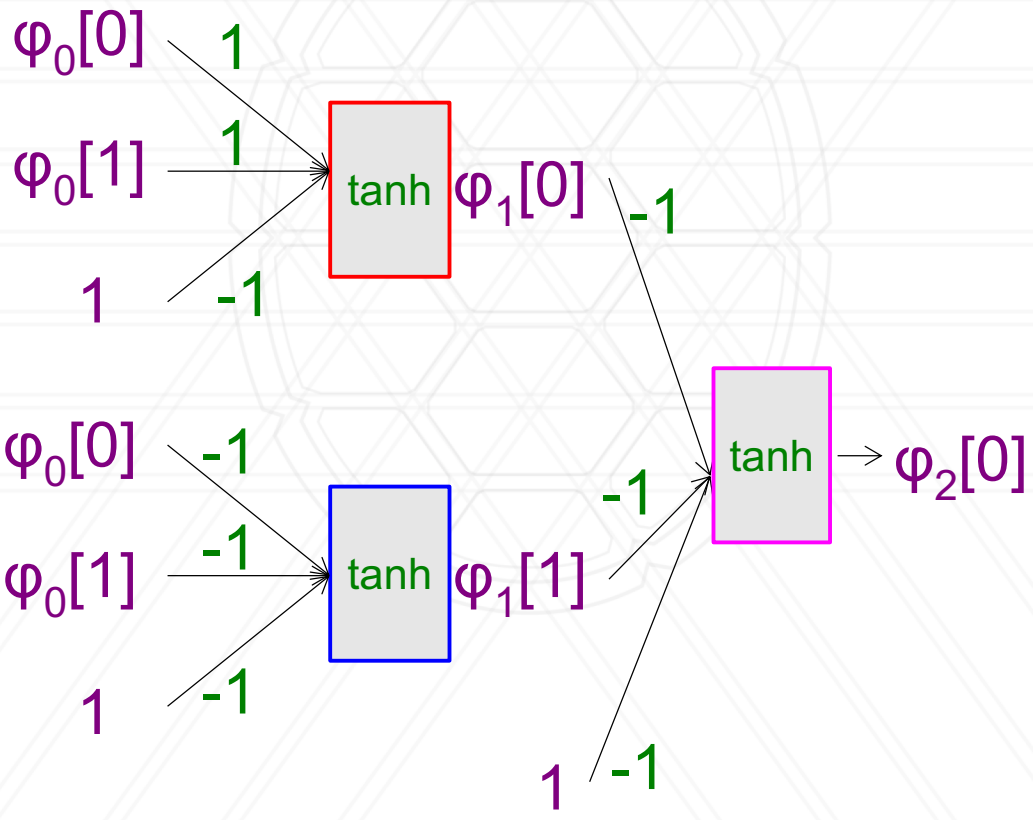
Example

- In new space, the examples are linearly separable!



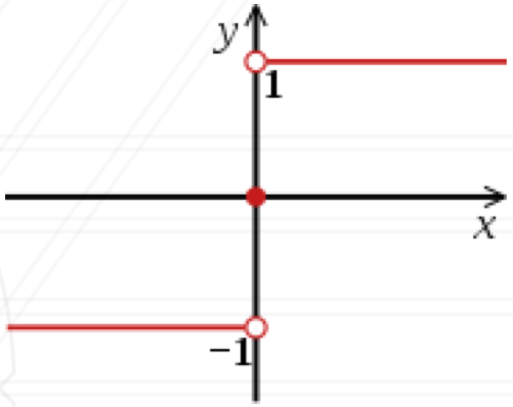
Example

- The final net

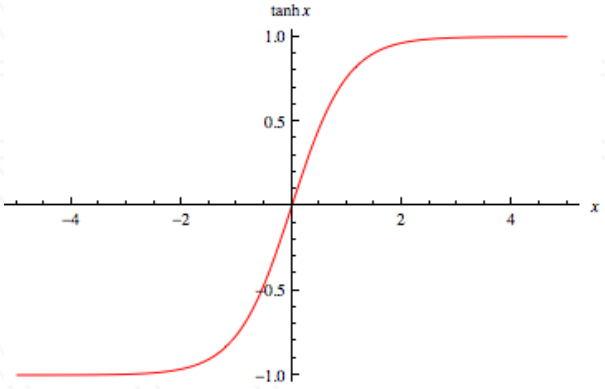


Activation Functions

- Examples:
  - Sign: $sign(x) = \begin{cases} -1, x < 0 \\ 0, x = 0 \\ 1, x > 0 \end{cases}$

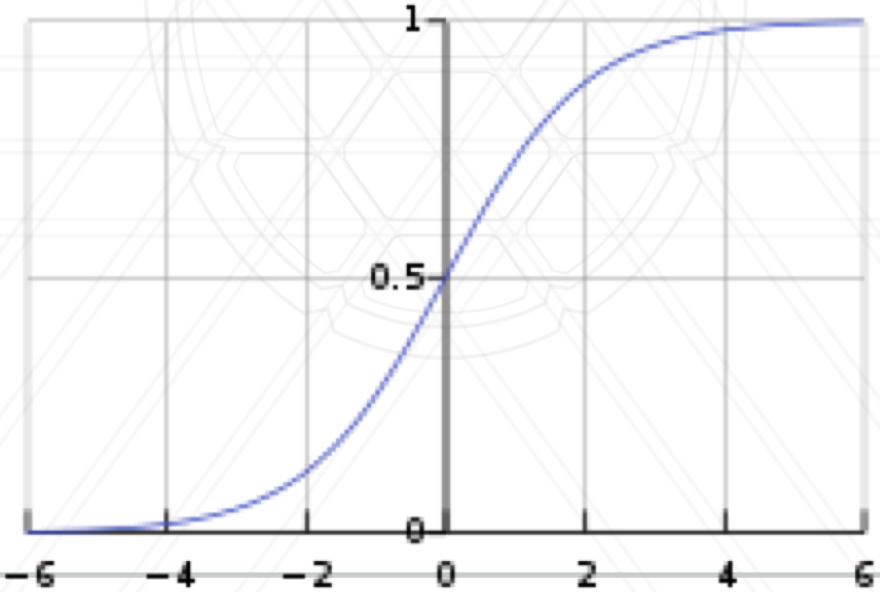


  - Tanh: $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{e^{2x} - 1}{e^{2x} + 1}$
    - Derivative: $\frac{\mathrm{d}}{dx}\tanh(x) = 1 - \tanh^2(x)$



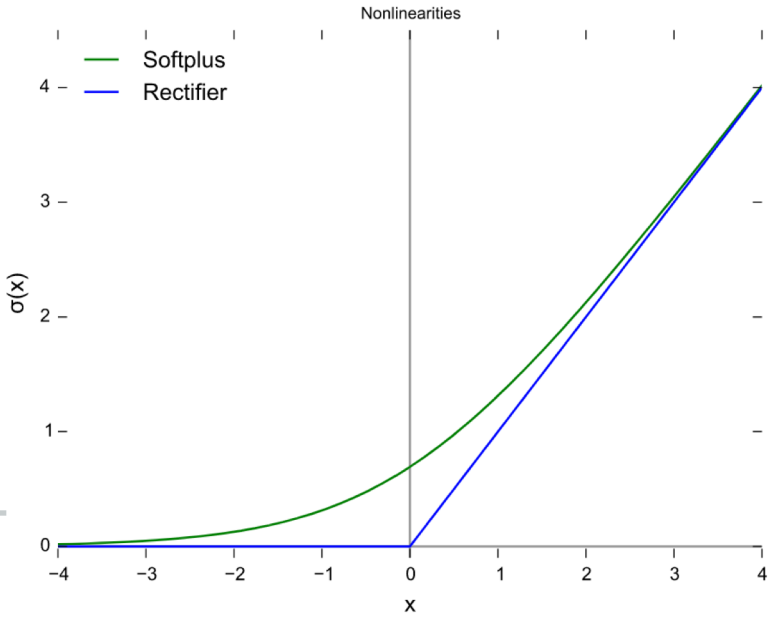
Activation Functions

- Sigmoid: $\sigma(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{1+e^x}$, logistic function
  - Derivative: $\frac{d}{dx}\sigma(x) = \frac{e^x}{1+e^x} = \sigma(x)\,(1-\sigma(x))$



Activation Functions

- Relu: $relu(x) = x^+ = \max(0, x)$ rectified linear unit
  - A smooth approximation: softplus
    $$f(x) = \log(1 + \exp x)$$
  - The derivative of softplus is logistic function $f'(x) = \frac{e^x}{1+e^x}$



Exercise

- Learn softmax function https://en.wikipedia.org/wiki/Softmax_function

Forward Propagation: given input x, compute network output

Algorithm 24 TwoLayerNetworkPredict($\mathbf{W}$, v, $\hat{x}$)

1: **for** $i = 1$ **to** *number of hidden units* **do**
2: $\quad h_i \leftarrow \tanh(w_i \cdot \hat{x})$ // compute activation of hidden unit i
3: **end for**
4: **return** $v \cdot h$ // compute output unit

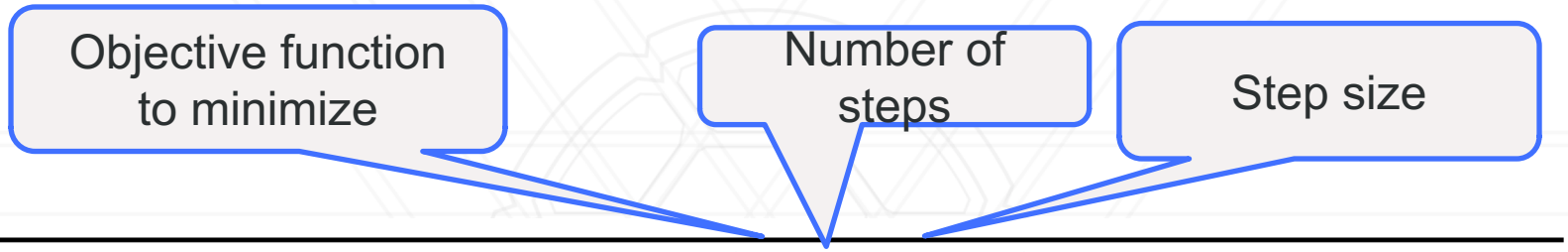
Neural Network Training

Backpropagation algorithm

=

Gradient descent + Chain rule

Recall: gradient descent for linear classifiers



Algorithm 22 GRADIENTDESCENT($\mathcal{F}$, K, η_1, ...)

1: $z^{(0)} \leftarrow \langle 0, 0, \ldots, 0 \rangle$ // initialize variable we are optimizing
2: **for** $k = 1 \ldots K$ **do**
3: $g^{(k)} \leftarrow \nabla_z \mathcal{F}|_{z^{(k-1)}}$ // compute gradient at current location
4: $z^{(k)} \leftarrow z^{(k-1)} - \eta^{(k)} g^{(k)}$ // take a step down the gradient
5: **end for**
6: **return** $z^{(K)}$

What's our Training Objective?

We'll consider the following objective

$$\min_{\mathbf{W},v} \sum_n \frac{1}{2}\left(y_n - \sum_i v_i f(\boldsymbol{w}_i \cdot \boldsymbol{x}_n)\right)^2$$

i.e. our goal is to find parameters **W**, v that minimize squared error

Other objectives are possible (e.g., other loss functions, add regularizer)

Backprop in a 2-layer network

Algorithm 25 TwoLayerNetworkTrain($\mathbf{D}$, η, K, *MaxIter*)

```
1:  W ← D×K matrix of small random values          // initialize input layer weights
2:  v ← K-vector of small random values            // initialize output layer weights
3:  for iter = 1 ... MaxIter do
4:      G ← D×K matrix of zeros                    // initialize input layer gradient
5:      g ← K-vector of zeros                      // initialize output layer gradient
6:      for all (x,y) ∈ D do
7:          for i = 1 to K do
8:              a_i ← w_i · x̂
9:              h_i ← tanh(a_i)                    // compute activation of hidden unit i
10:         end for
11:         ŷ ← v · h                              // compute output unit
12:         e ← y − ŷ                              // compute error
13:         g ← g − eh                             // update gradient for output layer
14:         for i = 1 to K do
15:             G_i ← G_i − e v_i (1 − tanh²(a_i)) x   // update gradient for input layer
16:         end for
17:     end for
18:     W ← W − ηG                                 // update input layer weights
19:     v ← v − ηg                                 // update output layer weights
20: end for
21: return W, v
```

Backprop in a 2-layer network

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4:      G ← D×K matrix of zeros                  // initialize input layer gradient
5:      g ← K-vector of zeros                    // initialize output layer gradient
6:
7:
8:
9:
10:
11:                  Compute Gradient G and g
12:
13:
14:
15:
16:
17:
18:     W ← W − ηG                               // update input layer weights
19:     v ← v − ηg                               // update output layer weights
20: end for
21: return W, v
```

What's our Training Objective?

We'll consider the following objective

$$\min_{\mathbf{W},v} \sum_n \frac{1}{2}\left(y_n - \sum_i v_i f(\boldsymbol{w}_i \cdot \boldsymbol{x}_n)\right)^2$$

i.e. our goal is to find parameters **W**, v that minimize squared error

Other objectives are possible (e.g., other loss functions, add regularizer)

Gradient of objective w.r.t. output layer weights v

$$\nabla_v = -\sum_n e_n \boldsymbol{h}_n$$

Error at example n: $y_n - \widehat{y_n}$

Vector of activations of hidden units for example n

Gradient of objective w.r.t. hidden unit weights w_i

$$\mathcal{L}(\mathbf{W}) = \frac{1}{2}\left(y - \sum_i v_i f(\boldsymbol{w}_i \cdot \boldsymbol{x})\right)^2$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}_i} = \frac{\partial \mathcal{L}}{\partial f_i}\frac{\partial f_i}{\partial \boldsymbol{w}_i}$$

Chain rule

$$\frac{\partial \mathcal{L}}{\partial f_i} = -\left(y - \sum_i v_i f(\boldsymbol{w}_i \cdot \boldsymbol{x})\right) v_i = -e v_i$$

$$\frac{\partial f_i}{\partial \boldsymbol{w}_i} = f'(\boldsymbol{w}_i \cdot \boldsymbol{x})\boldsymbol{x}$$

$$\nabla_{\boldsymbol{w}_i} = -e v_i f'(\boldsymbol{w}_i \cdot \boldsymbol{x})\boldsymbol{x}$$

 (This is on one example only)

Backprop in a 2-layer network

Algorithm 25 TwoLayerNetworkTrain($\mathbf{D}$, η, K, $MaxIter$)

1: $\mathbf{W} \leftarrow D \times K$ matrix of small random values // initialize input layer weights
2: $v \leftarrow K$-vector of small random values // initialize output layer weights
3: **for** $iter = 1 \ldots MaxIter$ **do**
4: $\mathbf{G} \leftarrow D \times K$ matrix of zeros // initialize input layer gradient
5: $g \leftarrow K$-vector of zeros // initialize output layer gradient
6: **for all** $(x, y) \in \mathbf{D}$ **do**
7: **for** $i = 1$ **to** K **do**
8: $a_i \leftarrow \boldsymbol{w}_i \cdot \hat{\boldsymbol{x}}$
9: $h_i \leftarrow \tanh(a_i)$ // compute activation of hidden unit i
10: **end for**
11: $\hat{y} \leftarrow \boldsymbol{v} \cdot \boldsymbol{h}$ // compute output unit
12: $e \leftarrow y - \hat{y}$ // compute error
13: $g \leftarrow g - e\boldsymbol{h}$ // update gradient for output layer
14: **for** $i = 1$ **to** K **do**
15: $\mathbf{G}_i \leftarrow \mathbf{G}_i - ev_i(1 - \tanh^2(a_i))\boldsymbol{x}$ // update gradient for input layer
16: **end for**
17: **end for**
18: $\mathbf{W} \leftarrow \mathbf{W} - \eta\mathbf{G}$ // update input layer weights
19: $v \leftarrow v - \eta g$ // update output layer weights
20: **end for**
21: **return** $\mathbf{W}$, v

Forward propagation

Update gradients

Update parameters

Tricky issues with neural network training

Sensitive to initialization

- Objective is non-convex, many local optima
- In practice: start with random values rather than zeros

Many other hyperparameters

- Number of hidden units (and potentially hidden layers)
- Gradient descent learning rate
- Stopping criterion

Neural networks vs. linear classifiers

Advantages of Neural Networks:

More expressive

Less feature engineering

Inconvenients of Neural Networks:

Harder to train

Harder to interpret

Neural Network Architectures

We focused on a **2-layer feedforward** network

Other architectures are possible

- More than 2 layers (aka deep learning)
- Recurrent network (i.e. network has cycles)
- Can still be trained with backpropagation
  - But more issues arise when networks get more complex (e.g., vanishing gradients)

Try different architectures and training parameters here:

http://playground.tensorflow.org

What you should know

- What are Neural Networks?
  - Multilayer perceptron
- How to make a prediction given an input?
  - Forward propagation: Simple matrix operations + nolinearities
- Why are neural networks powerful?
  - Universal function approximators!
- How to train neural networks?
  - The backpropagation algorithm

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