

ENGR-E 511; ENGR-E 399

# Machine Learning for Signal Processing

## Module 06: Neural Networks

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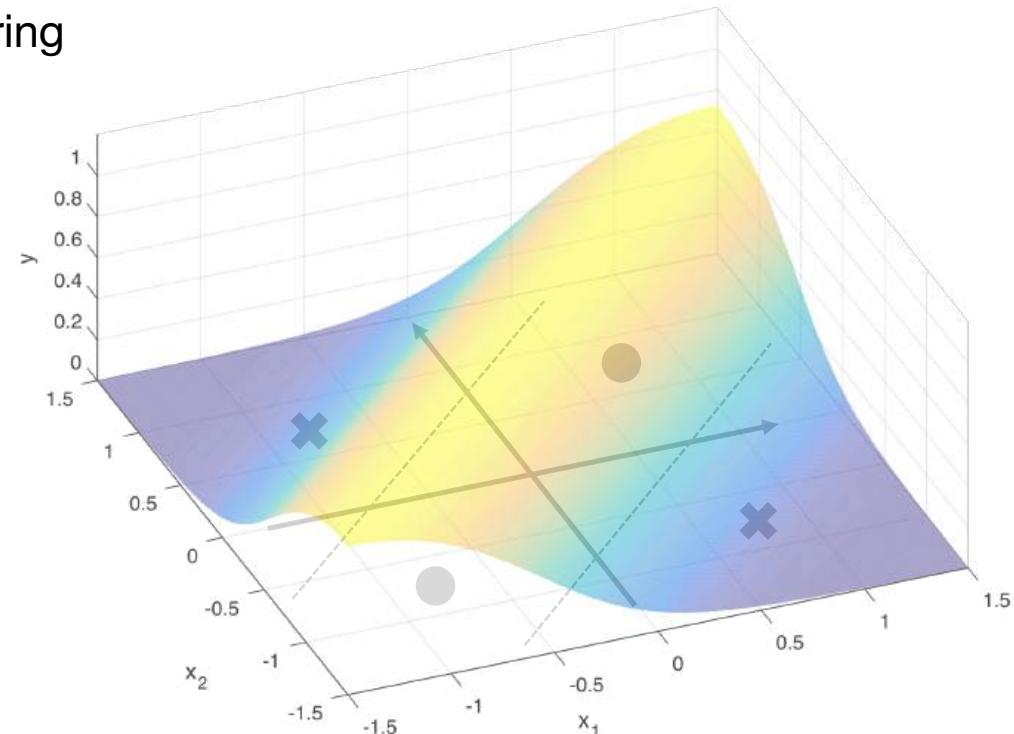
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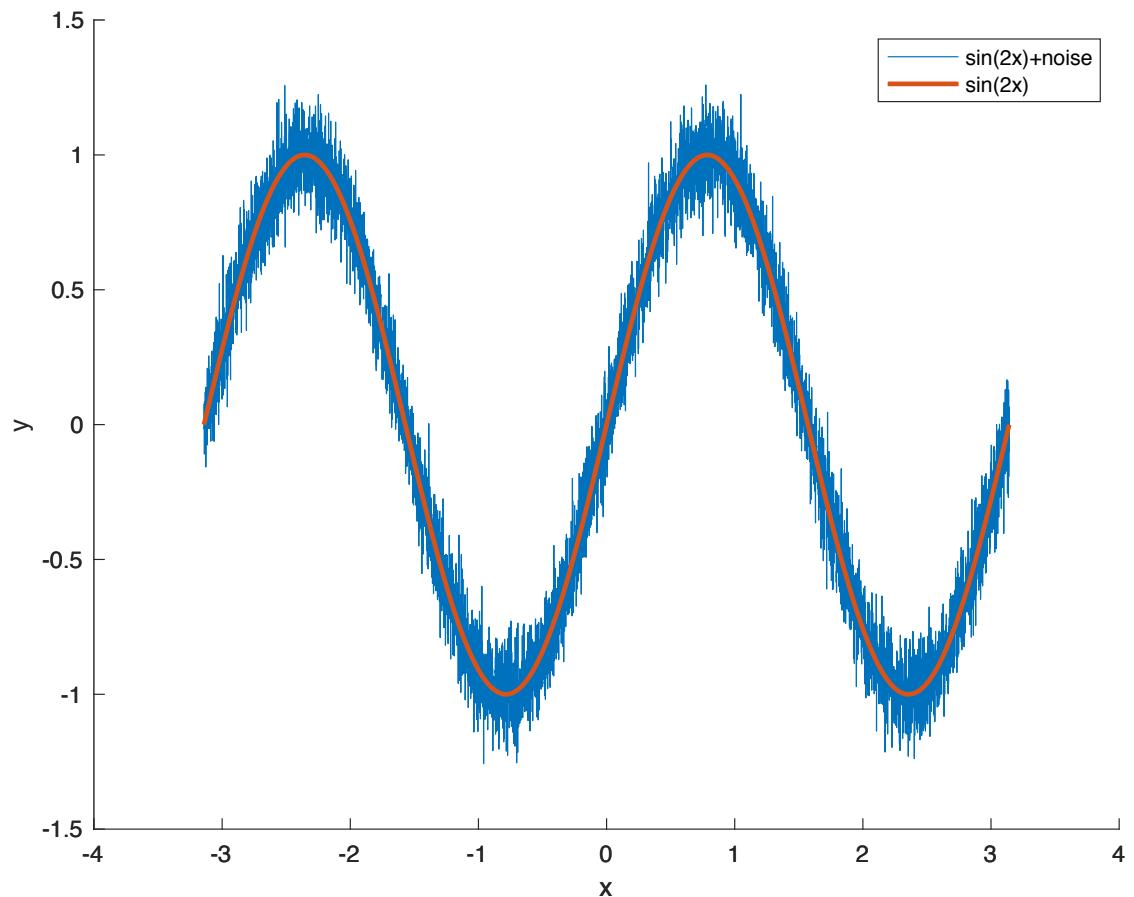
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# Denoising Revisited

## - A sine wave

- I observe a noisy signal (as always)
- I'm pretty sure that it is a sine wave
  - So I think my job is to find out its period



# Denoising Revisited

## - A sine wave

- We all are masters of optimization by now

- Let's formulate this as an optimization problem

- I start from a set of data points

$$[x_1, x_2, \dots, x_N]^\top \quad [y_1, y_2, \dots, y_N]^\top$$

- I don't know a lot about this data set, but I feel that there's a relationship

$$y_i \approx \sin(\omega x_i)$$

- The goal is to find  $\omega$  that minimizes the error

$$\mathcal{J} = \sum_i (y_i - \sin(\omega x_i))^2$$

- Is this a convex function?

$$\frac{\partial \mathcal{J}}{\partial \omega} = -2y_i x_i \cos(\omega x_i) + 2x_i \sin(\omega x_i) \cos(\omega x_i)$$

$$\frac{\partial \mathcal{J}^2}{\partial \omega^2} = 2y_i x_i^2 \sin(\omega x_i) + 2x_i^2 \cos(\omega x_i) \cos(\omega x_i) - 2x_i^2 \sin(\omega x_i) \sin(\omega x_i)$$

- Maybe not

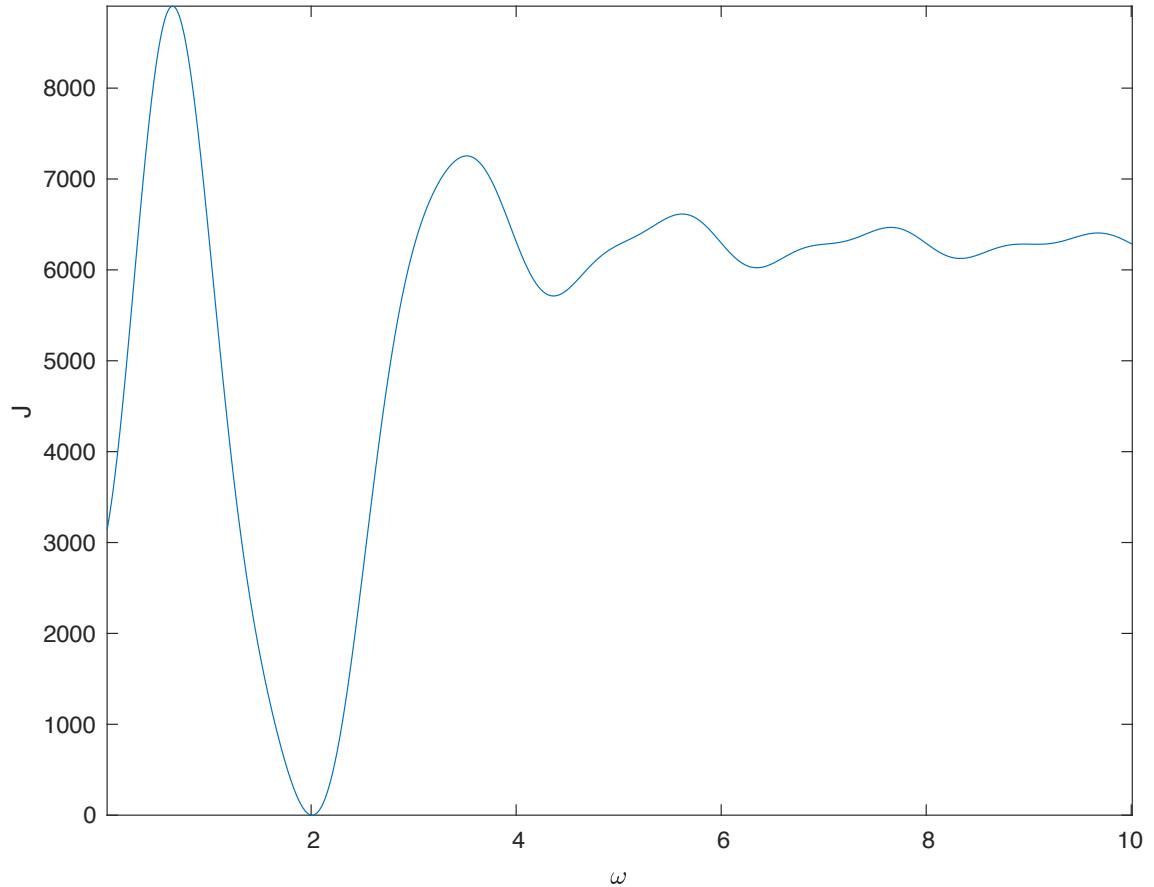


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# Denoising Revisited

- A sine wave
- $\mathcal{J}$  as a function of  $\omega$ 
  - Too complicated, and I don't know what to do



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# Denoising Revisited

## - A workaround: feature transform

- Even if we knew the ground truth (family of) function we are estimating, we give up
  - because a sine wave is too difficult for us to handle
- Instead, we're going to assume another trackable function

$$y_i \approx f(x_i; \Theta)$$

- Any candidate family of functions?
  - That might be able to replace a piece of sine wave?
- I'd use a 5<sup>th</sup> order polynomial function

$$y_i \approx f(x_i; \Theta) = a_5 x_i^5 + a_4 x_i^4 + a_3 x_i^3 + a_2 x_i^2 + a_1 x_i + a_0$$

- As there are 4 stationary points, it looks like a sine wave
- The new error function

$$\arg \min_{\Theta} \sum_i \mathcal{E}(y_i || f(x_i; \Theta)) = \arg \min_{a_5, a_4, a_3, a_2, a_1, a_0} \sum_i \left( y_i - (a_5 x_i^5 + a_4 x_i^4 + a_3 x_i^3 + a_2 x_i^2 + a_1 x_i + a_0) \right)^2$$

- Still look complicated?



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# Denoising Revisited

- A workaround: feature transform

- Let's form a new data matrix

$$\mathbf{X} = \begin{bmatrix} x_1^5 & x_2^5 & \cdots & x_N^5 \\ x_1^4 & x_2^4 & \cdots & x_N^4 \\ \vdots & & & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$

$x_i^j \leftarrow$  Sample index  
 $x_i^j \leftarrow$  Polynomial order

- Then, we can rewrite the function in a linear form

$$\mathbf{y}^\top \approx f(\mathbf{x}; \mathbf{a}) = \mathbf{a}^\top \mathbf{X} = [a_5 \ a_4 \ a_3 \ a_2 \ a_1 \ a_0]$$

$$\begin{bmatrix} x_1^5 & x_2^5 & \cdots & x_N^5 \\ x_1^4 & x_2^4 & \cdots & x_N^4 \\ \vdots & & & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$

- You can think of this procedure in two ways:

- Approximating a function with another tractable, yet non-linear function
- Converting the scalar input into a high-dim feature set and solve linearly



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# Denoising Revisited

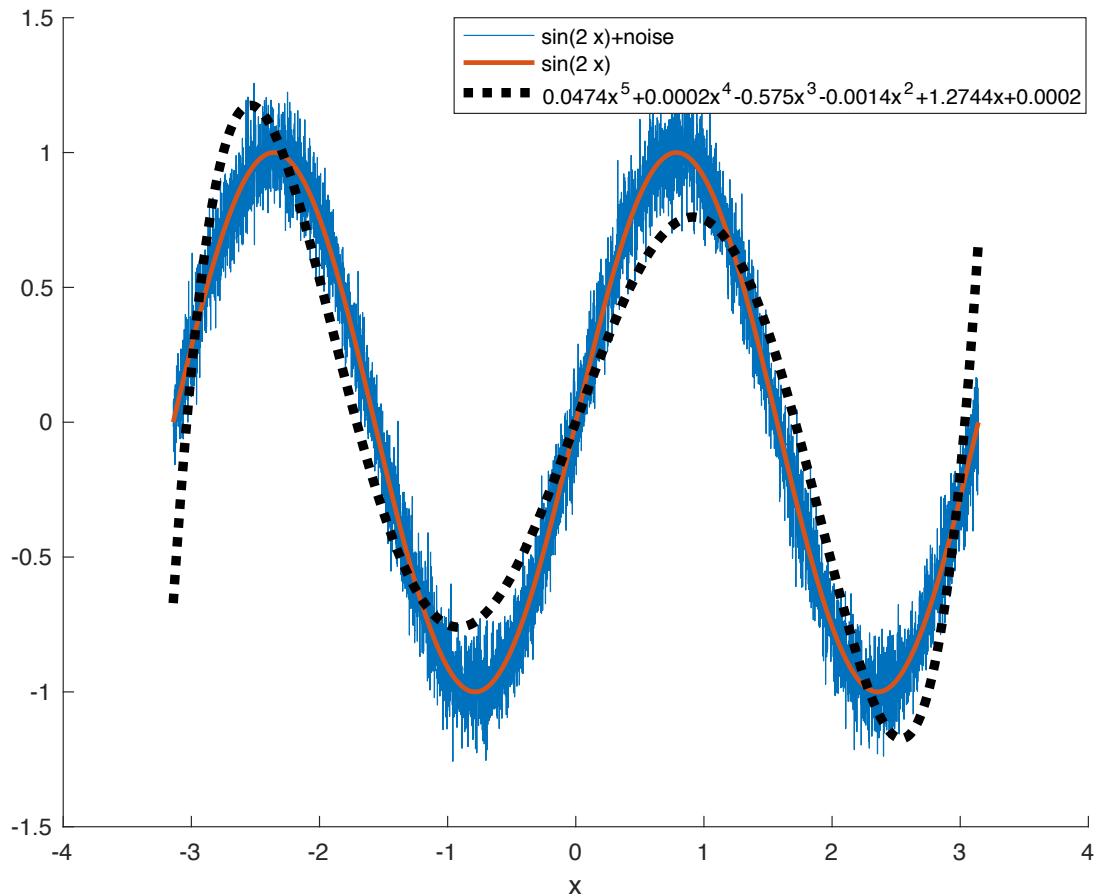
- A workaround: feature transform

- Now the error function is quadratic

$$\arg \min_{\mathbf{a}} (\mathbf{y}^\top - \mathbf{a}^\top \mathbf{X})(\mathbf{y}^\top - \mathbf{a}^\top \mathbf{X})^\top$$

- There's an analytic solution and we know how to solve it (see M01 L03)
- Long story short...

$$\begin{aligned}\mathbf{a}^* &= (\mathbf{X} \mathbf{X}^\top)^{-1} \mathbf{X} \mathbf{y} \\ &= [0.047, 0.0002, -0.575, -0.0014, 1.27, 0.0002]^\top\end{aligned}$$



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# Some Questions

- Are we good?
  - What if the signal is very long?
    - Many stationary points → polynomials with a high degree
  - What if the signal looks complicated?
    - Polynomials don't make sense anymore
  - Is there any parametric function that can potentially approximate any complicated target functions?
    - Universal approximation
    - This is our goal in learning neural networks
  - Hint: we converted the data and solved it linearly
    - We'll cover this part in the nonlinear modeling lecture
    - But, long story short, neural networks can do this job anyway
  - What's the difference between this denoising procedure and classification?
    - We'll cover it later in this lecture
    - But, long story short, they are not that different



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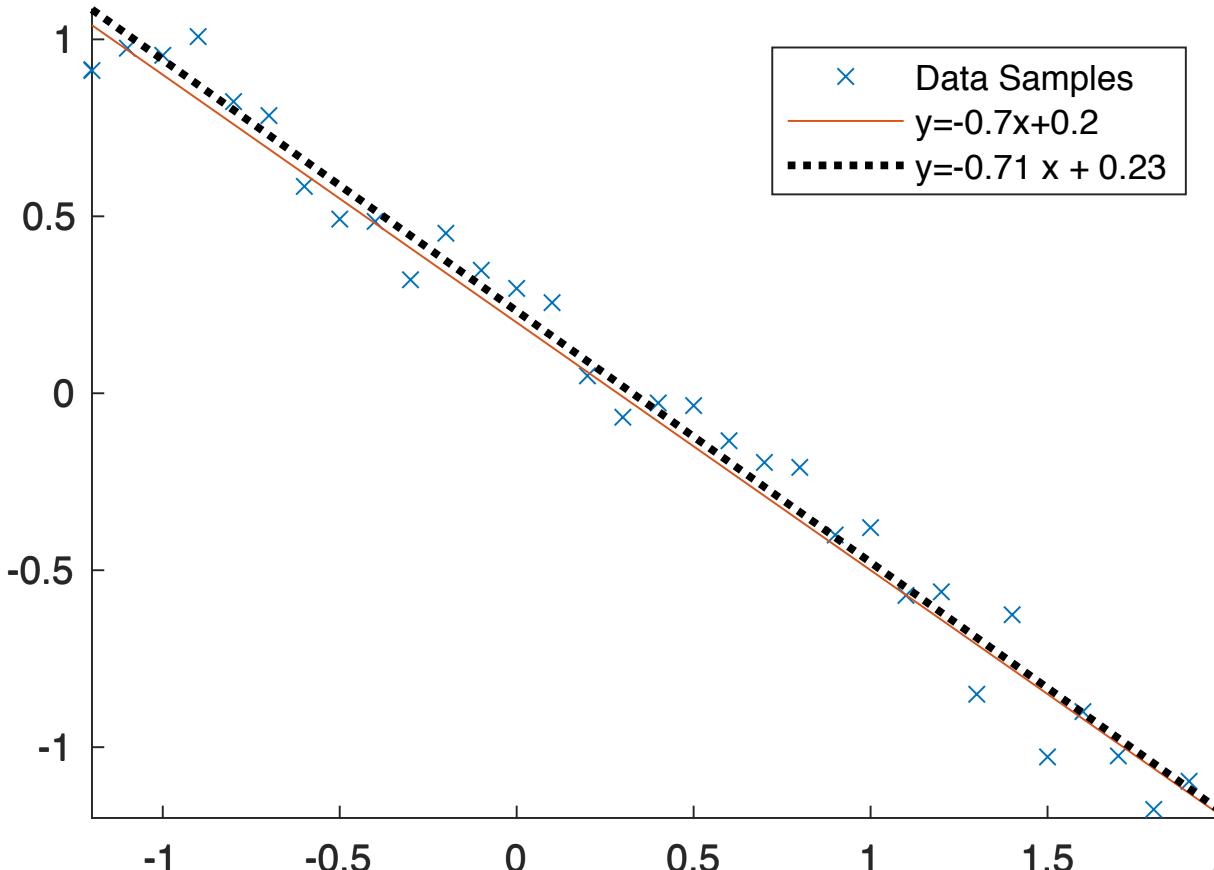
# Perceptron

- Linear line fitting
  - Let me solve a very simple regression problem

$$\mathbf{a} = [-0.7, 0.2]^\top$$

- The LMS solution:

$$\begin{aligned}\mathbf{a}^* &= (\mathbf{X}\mathbf{X}^\top)^{-1}\mathbf{X}\mathbf{y} \\ &= [-0.71, 0.23]^\top\end{aligned}$$

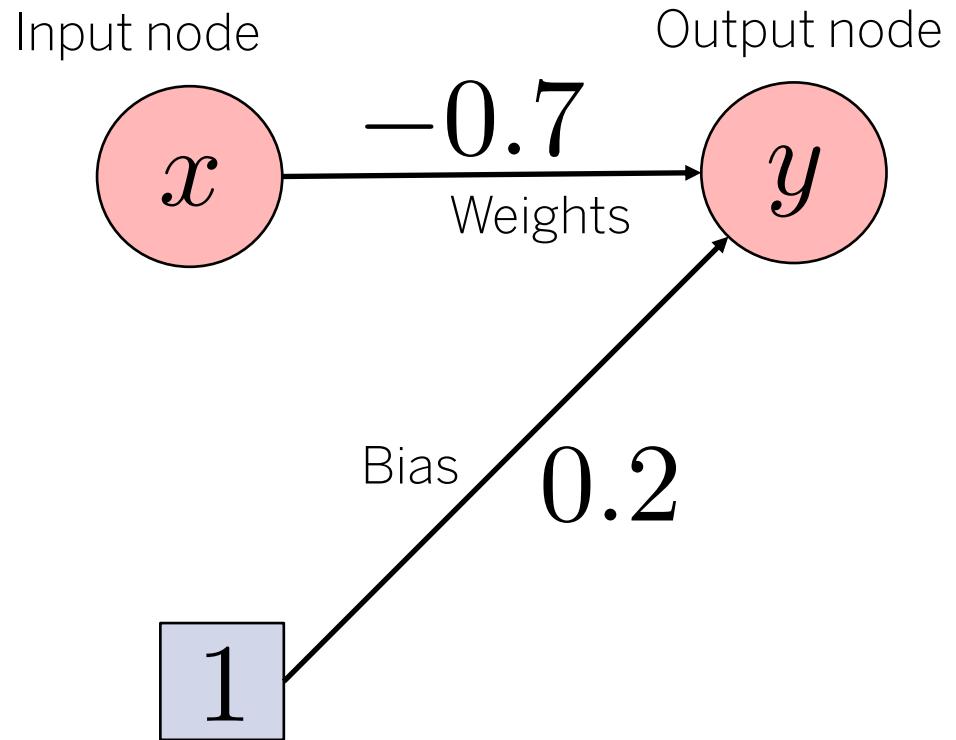


# Perceptron

- Linear line fitting

- You can represent this as a network

$$y_t = [a_1 \quad a_0] \cdot \begin{bmatrix} X_{(2,t)} \\ X_{(1,t)} \end{bmatrix}$$
$$y = \mathbf{a}^\top \mathbf{X}$$

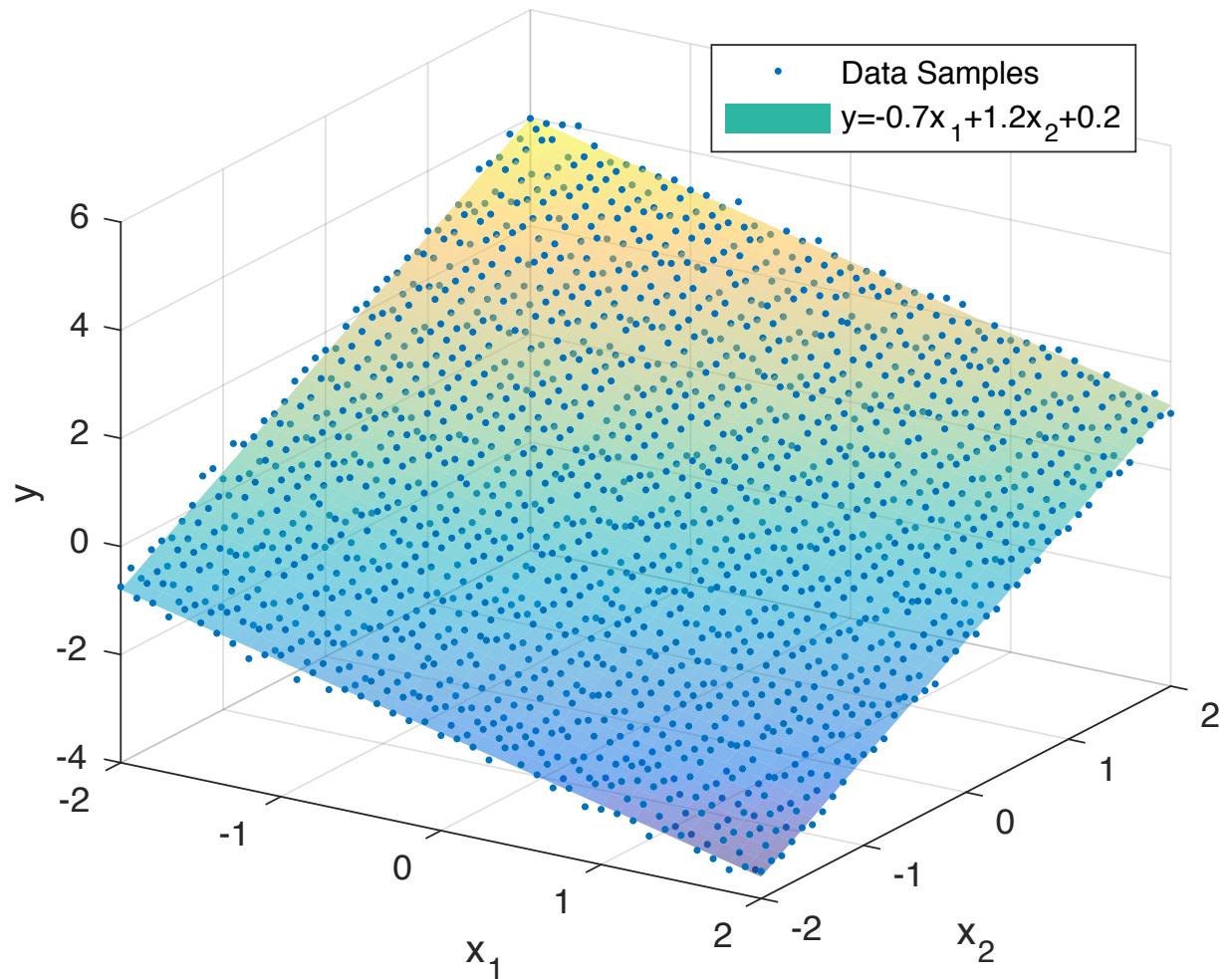


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# Perceptron

- Linear surface
- Two input dimensions? (fig)



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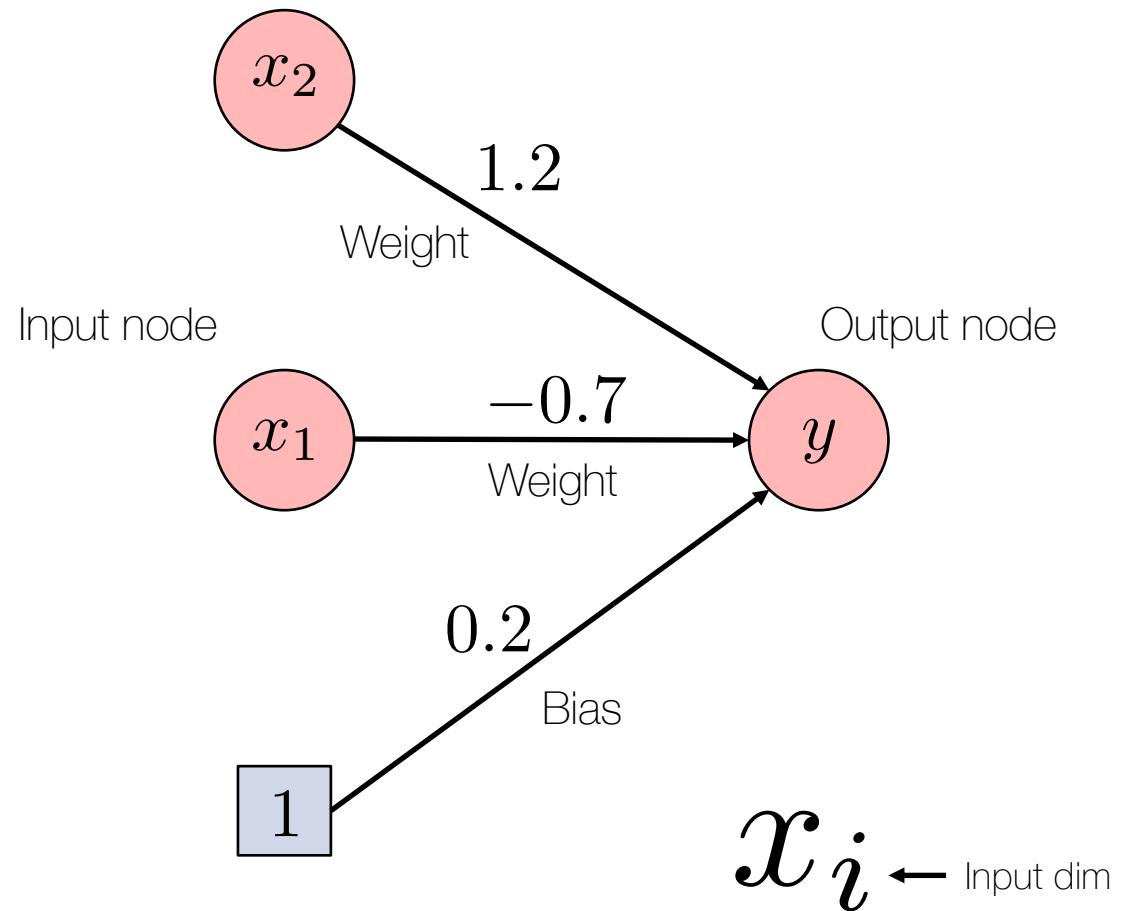
# Perceptron

- Linear surface

- You can represent this as a network as well

$$y_t = [a_2 \quad a_1 \quad a_0] \cdot \begin{bmatrix} X_{(2,t)} \\ X_{(1,t)} \\ 1 \end{bmatrix}$$

$$\mathbf{y} = \mathbf{a}^\top \mathbf{X}$$



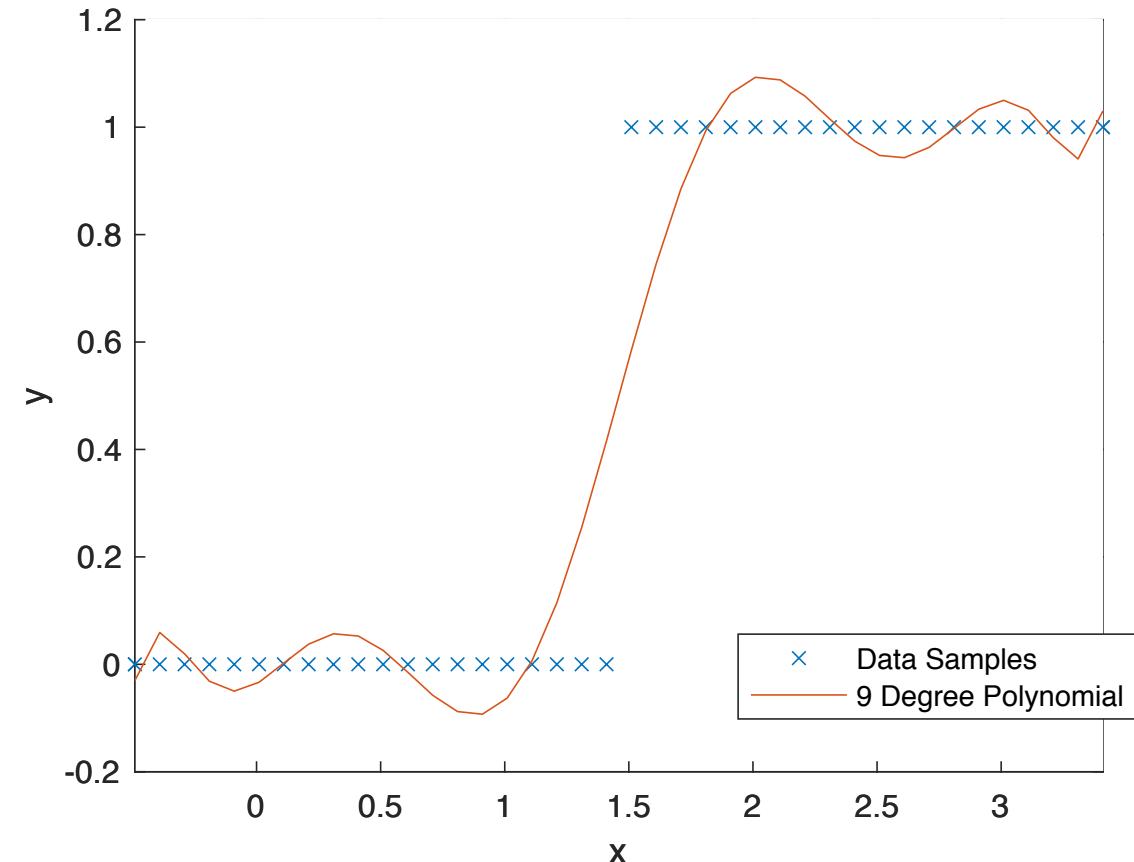
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# Decision Making with Perceptrons

## - Nonlinear?

- To remind you, we started from a set of observations (scalars for now)
- Each observation has a corresponding target variable
- We want to learn the mapping function
- Its not different from the linear line fitting cases
  - but the mapping function shouldn't be a dummy linear function anymore
  - How about another polynomial?



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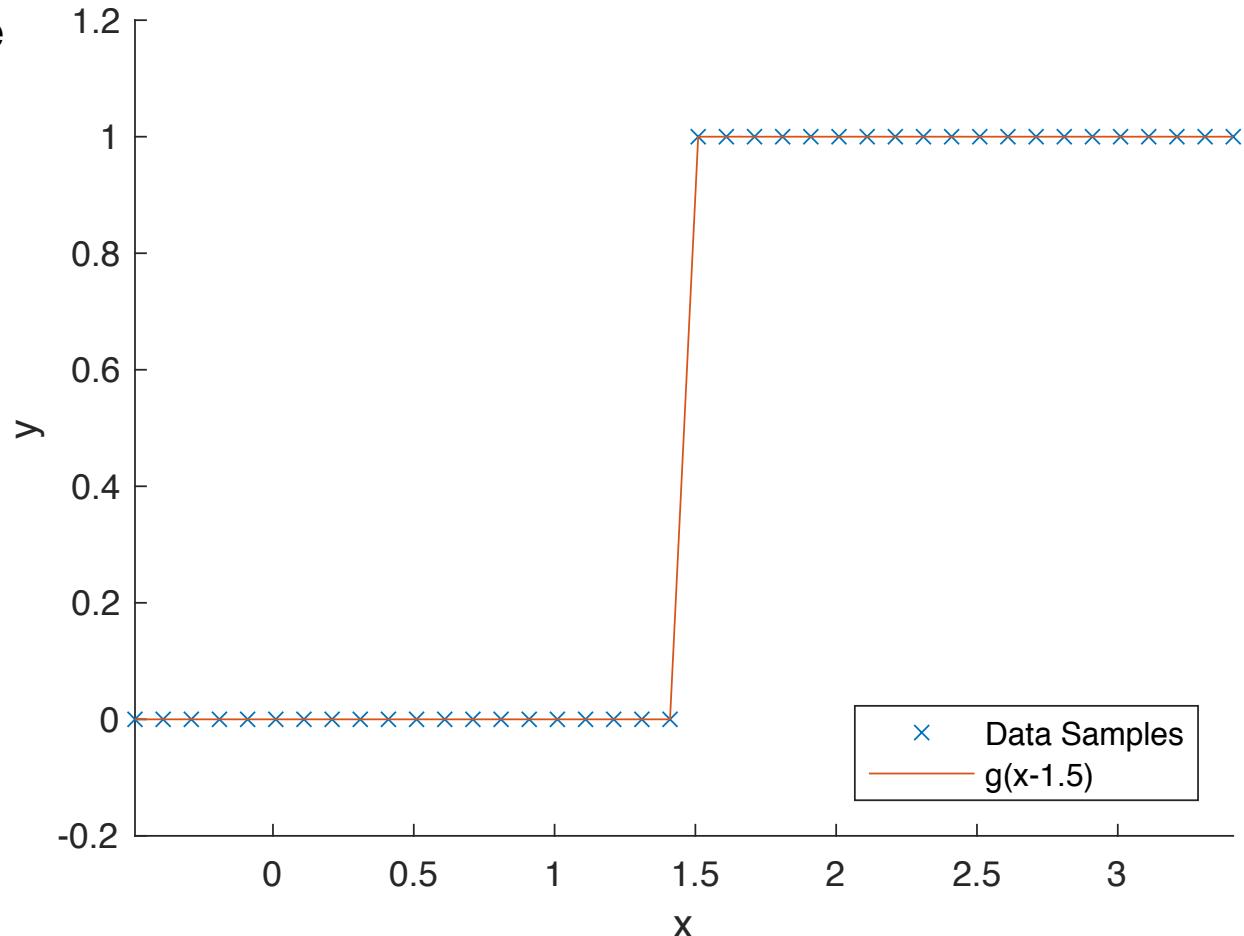
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# Decision Making with Perceptrons

- Nonlinear?

- A high degree polynomial works to some degree
- But what we see is a STEP!
  - Divided at around 1.5
- So, why don't we fit a step function?

$$g(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$



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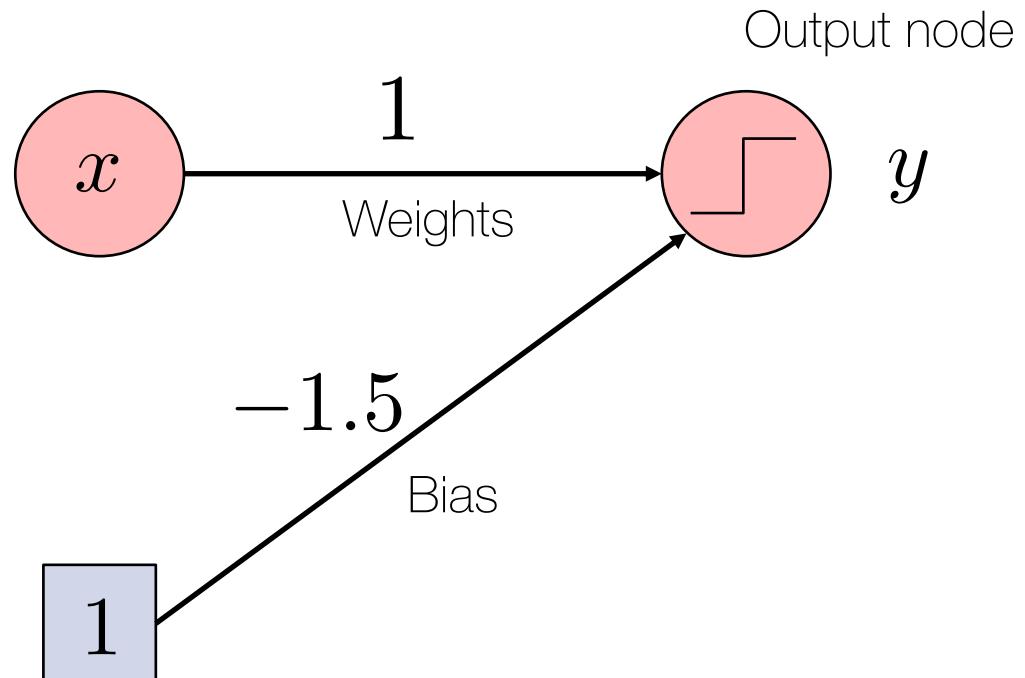
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# Decision Making with Perceptrons

- Nonlinear?
  - Once again, you can represent this as a network as well

$$\mathbf{y} = g(\mathbf{a}^\top \mathbf{X})$$

Input node

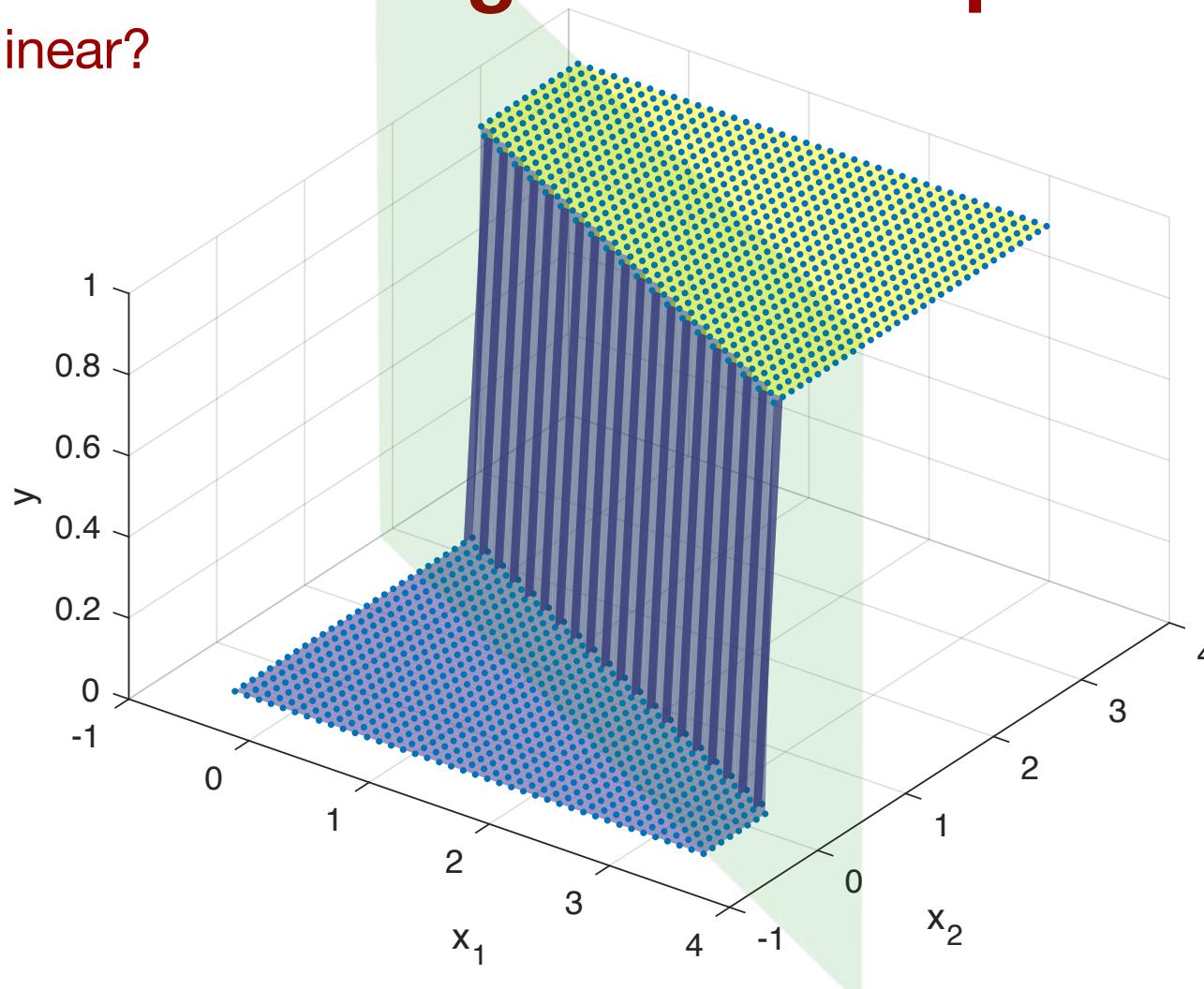


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# Decision Making with Perceptrons

- Nonlinear?



$$x_2 = -0.5x_1 + 2$$

$$0.5x_1 + x_2 - 2 = 0$$

$$g(x_2 + 0.5x_1 - 2)$$



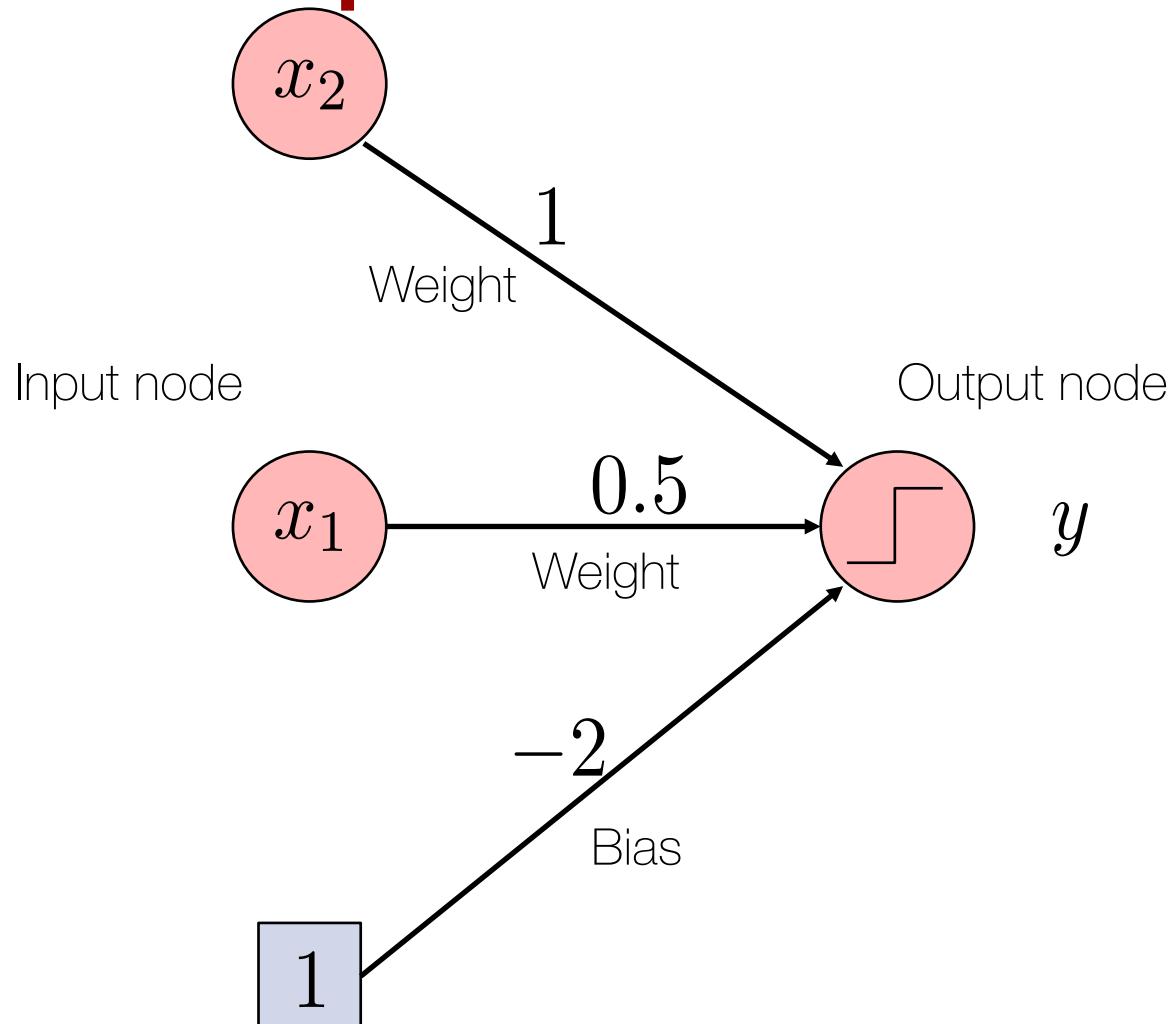
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# Decision Making with Perceptrons

- Nonlinear?
- Multi-dimensional step function

$$y = g(a^\top X)$$



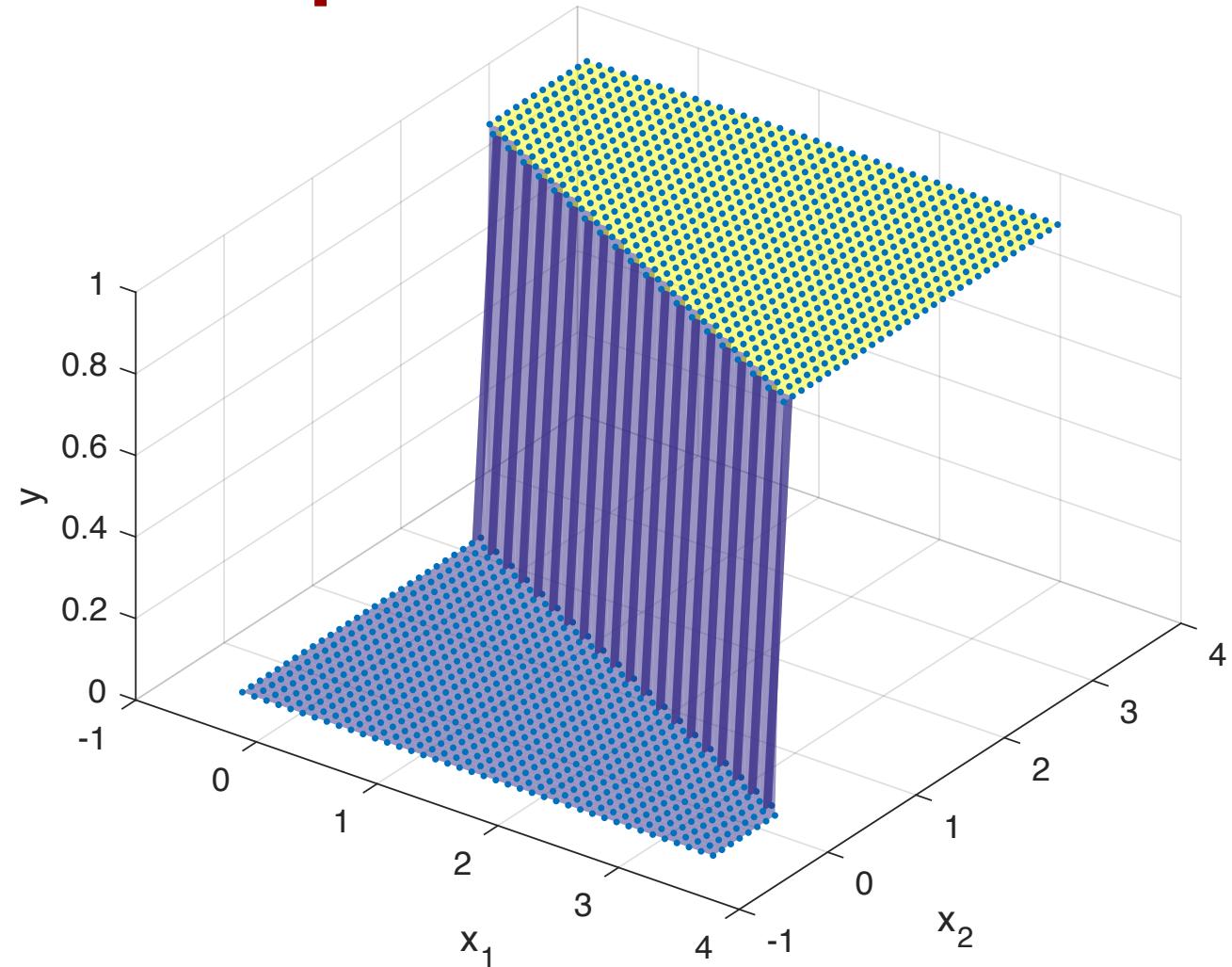
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# Decision Making with Perceptrons

## - Step functions

- I didn't tell you specifically, but
- The examples with step functions were for classification
  - e.g. This can be seen as a hyperplane
$$x_2 = -0.5x_1 + 2$$
  - Class 1 if  $x_2 \geq -0.5x_1 + 2$ 
$$\leftrightarrow g(x_2 + 0.5x_1 - 2) = 1$$
  - Class 2 if  $x_2 < -0.5x_1 + 2$ 
$$\leftrightarrow g(x_2 + 0.5x_1 - 2) = 0$$
- Classification is not different from another function approximation
  - Except for the fact that the model tries to approximate a step function



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# Logistic Regression

## - Step functions

- The data for training

- We start from a set of data samples, a matrix  $\mathbf{X} \in \mathbb{R}^{(D+1) \times N}$
  - We have another corresponding labeling information  $\mathbf{y} \in \mathbb{R}^{1 \times N}$

- The goal of the learning algorithm

- Estimate the parameters that minimize the error
    - Between the training label and the network output

$$\mathcal{E}(\mathbf{y} || g(\mathbf{a}^\top \mathbf{X})) = \frac{1}{2} \sum_{i=1}^N (y_i - g(\mathbf{a}^\top \mathbf{X}_{(:,i)}))^2 = \frac{1}{2} (\mathbf{y} - g(\mathbf{a}^\top \mathbf{X})) (\mathbf{y} - g(\mathbf{a}^\top \mathbf{X}))^\top$$

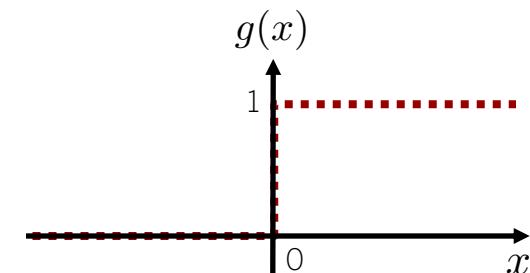
- Gradient descent?

- Partial differentiation w.r.t. the parameters

$$\frac{\partial \mathcal{E}}{\partial \mathbf{a}} = \mathbf{X} ((\mathbf{y} - g(\mathbf{a}^\top \mathbf{X})) \odot g'(\mathbf{a}^\top \mathbf{X}))^\top$$

- **The step function is not differentiable!**

$$g(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$



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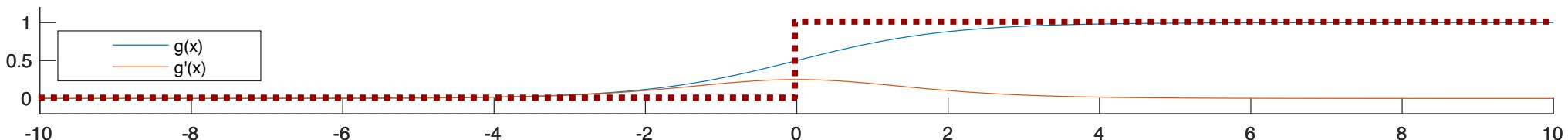
# Logistic Regression

## - Logistic function

- Step functions seem to be nice for classification, but it doesn't work
  - Because it's not differentiable
- What can we do?
  - Let's soften it up
  - Hint: you've already seen it!
- The logistic function

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

$$g'(x) = g(x)(1 - g(x))$$



- Gradient descent

$$\frac{\partial \mathcal{E}}{\partial \mathbf{a}} = \mathbf{X} \left( (\mathbf{y} - g(\mathbf{a}^\top \mathbf{X})) \odot g'(\mathbf{a}^\top \mathbf{X}) \right)^\top = \mathbf{X} \left( (\mathbf{y} - g(\mathbf{a}^\top \mathbf{X})) \odot [g(\mathbf{a}^\top \mathbf{X}) \odot ((1 - g(\mathbf{a}^\top \mathbf{X}))^\top] \right)$$

Derivative of logistic



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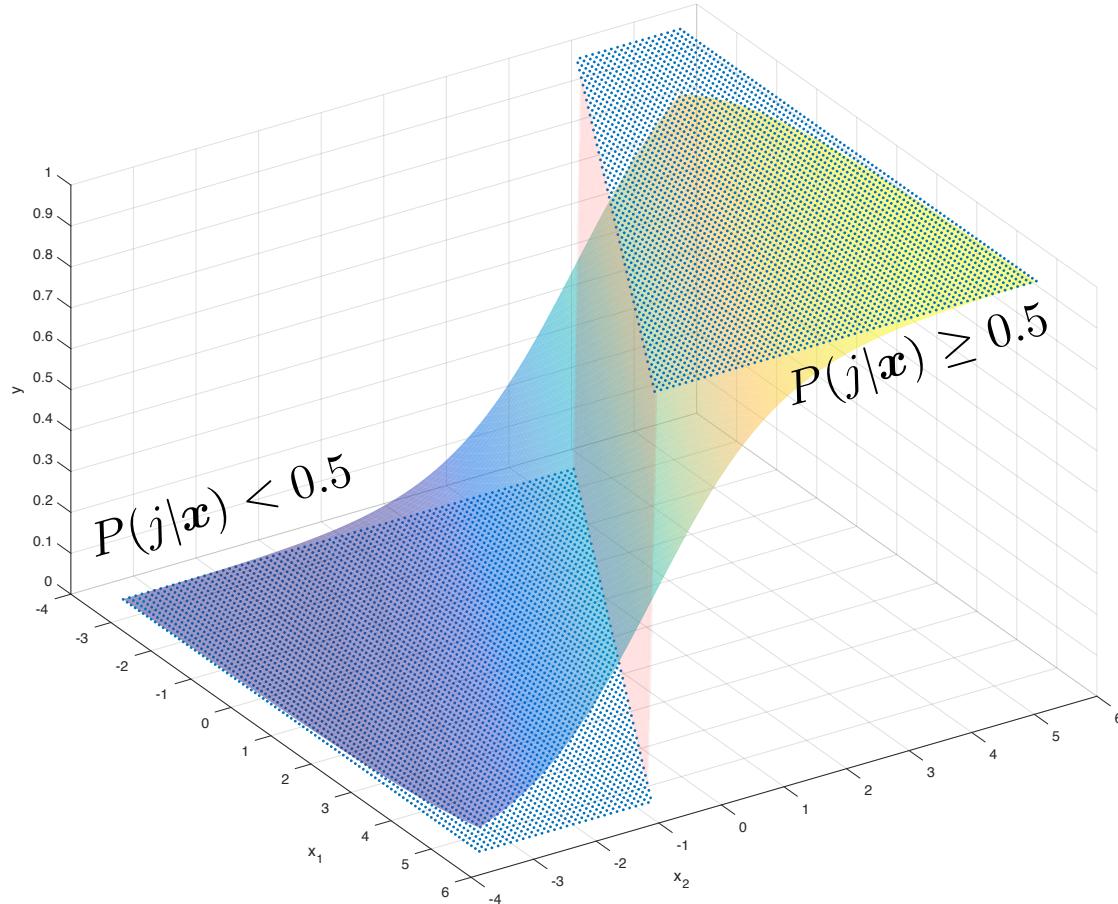
# Logistic Regression

## - Logistic function

- Now the decision is soft
  - and it works
- What the curved blanket says:
  - Corresponds to the posterior probability
- The decision boundary:

$$\log P(j|\mathbf{x}) = \log P(k|\mathbf{x})$$

$$g(x_2 + 0.5x_1 - 2) = 0.5$$



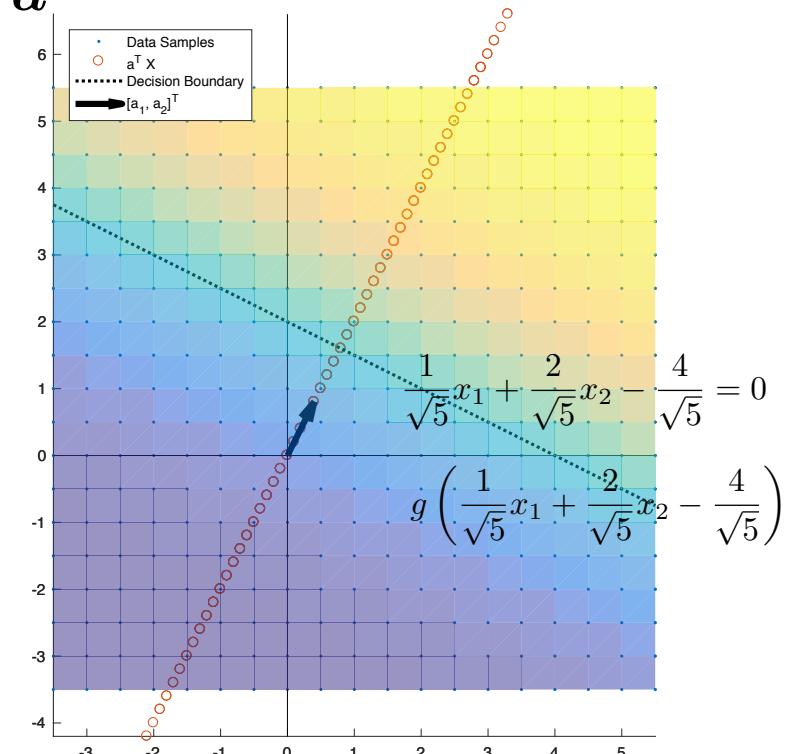
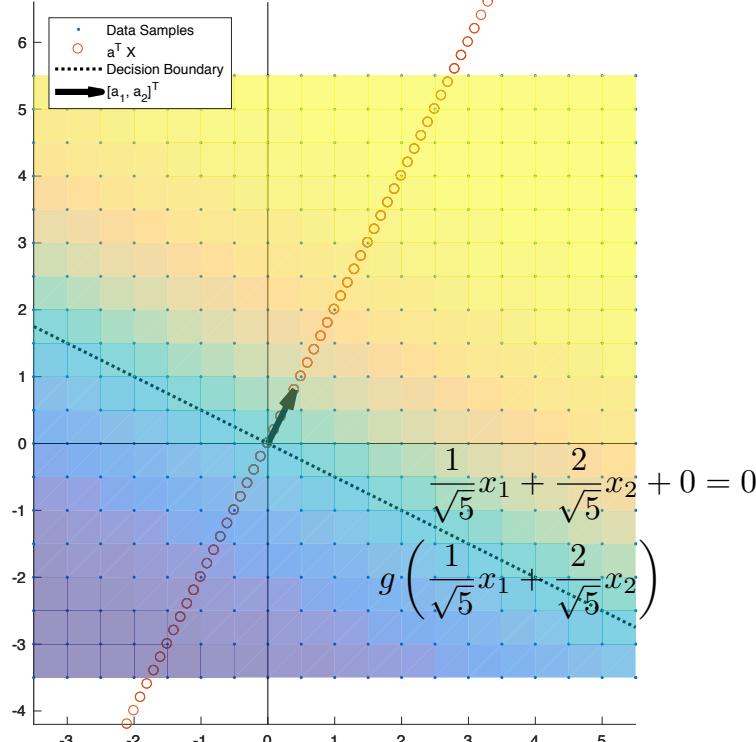
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# Logistic Regression

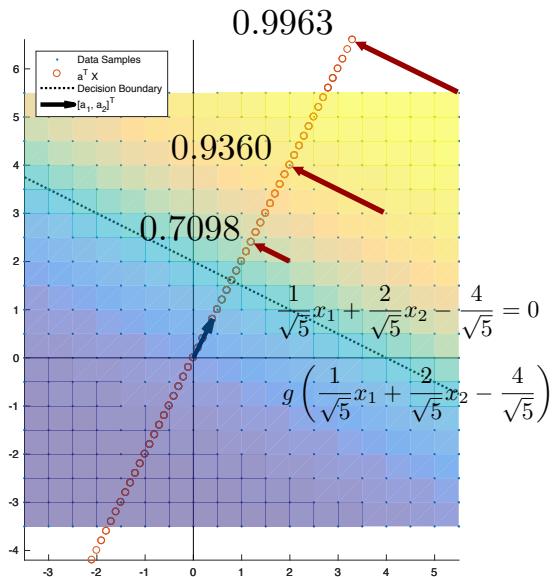
## - Analysis of decision boundaries

- Need a sharper decision?
  - It has something to do with your  $a$
- First example: decision boundaries with a normalized  $a$

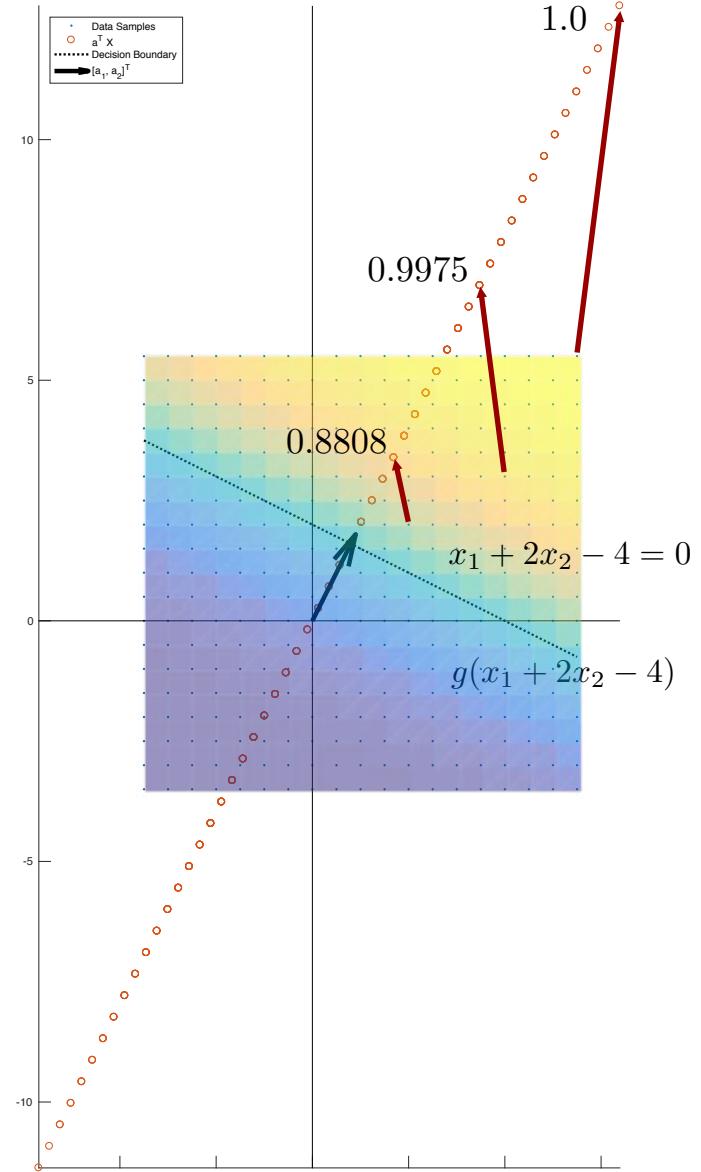


# Logistic Regression

## - Analysis of decision boundaries



- Scaling  $a$  doesn't change the decision boundary
$$1x_1 + 2x_2 - 4 = 1mx_1 + 2mx_2 - 4m = 0$$
- But it stretches or shrinks the data distribution after the projection
  - The same effect that makes the logistic function sharper or smoother



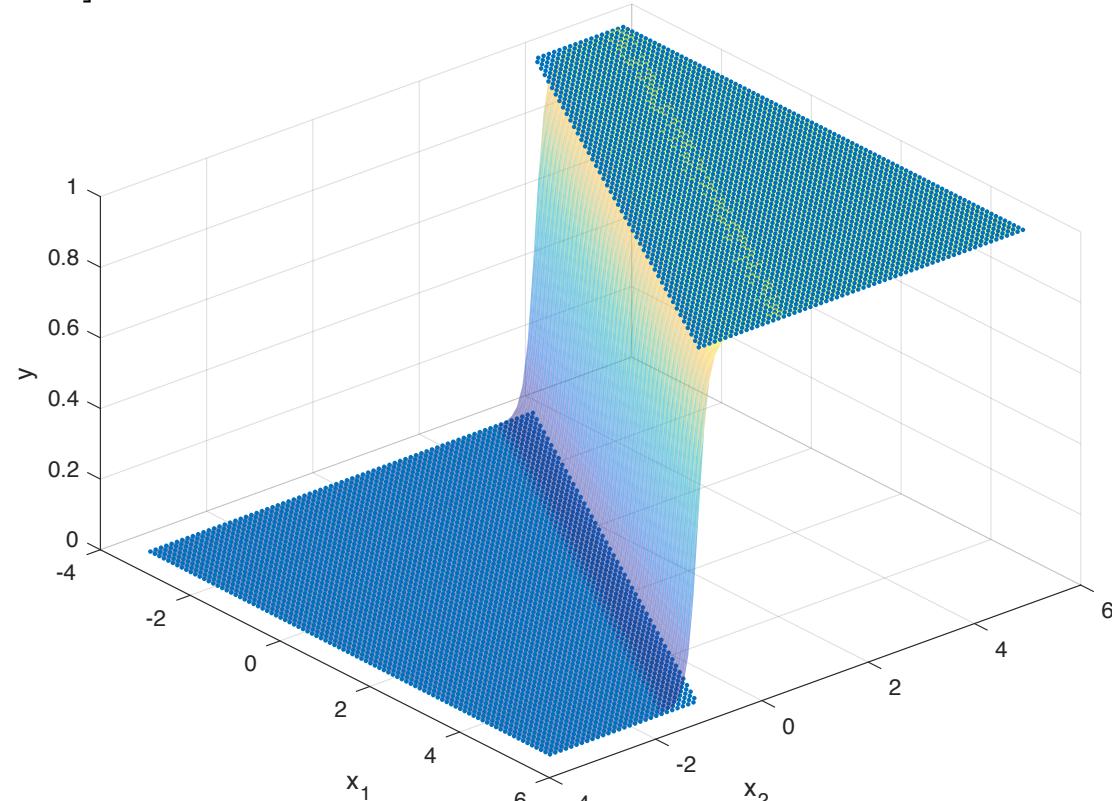
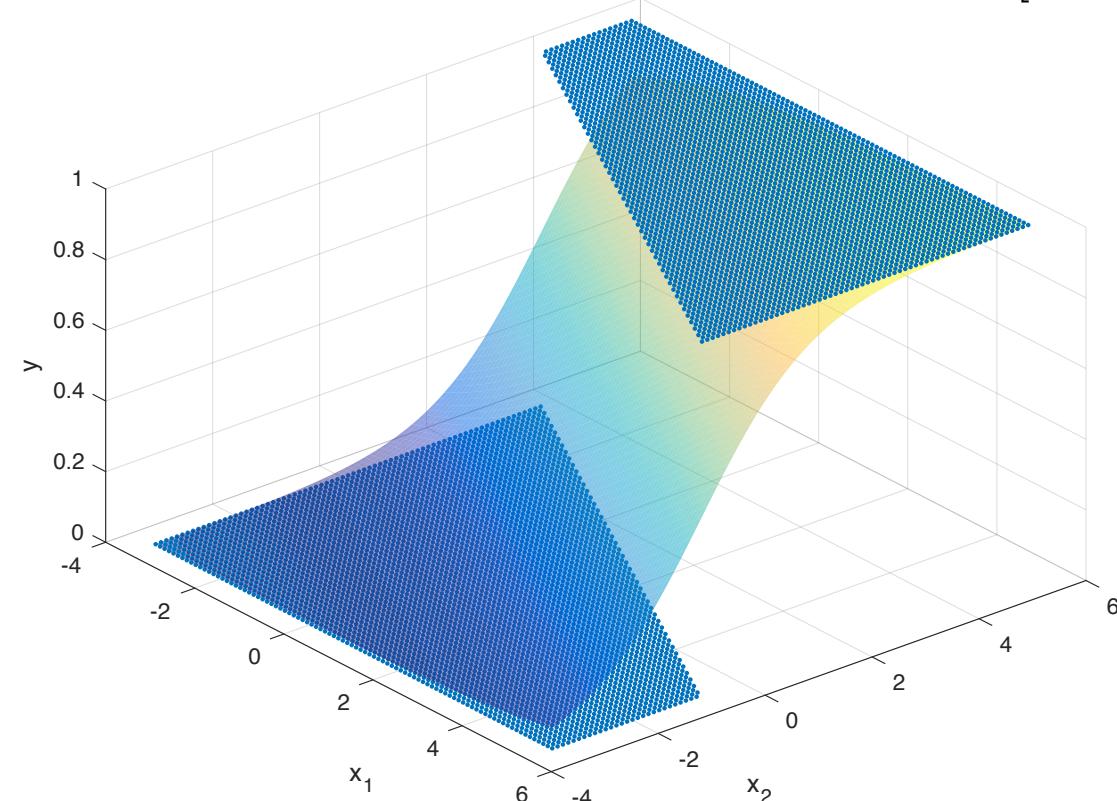
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# Logistic Regression

## - Analysis of decision boundaries

- If we actually run a learning algorithm on this data set for many iterations
  - The absolute values of the parameters in  $\mathbf{a} = [a_2, a_1, a_0]^\top$  will get larger to make the logistic slope sharper



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# Logistic Regression

- Classification process
  - The recipe for classification
    - Prepare labeled training data
    - Prepare your label vector  $y$ 
      - 0 for class A, 1 for class B
    - Estimate the parameters, e.g. by using gradient descent
      - I mean the weight vector  $a$
    - Your parameters will define the decision boundary
      - And the decision is natural thanks to the sigmoid functions
  - Are we missing something?
    - Of course we are



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# Multilayer Perceptron

- The XOR problem
- In this lecture so far we saw that
  - Many problems are just a kind of function approximation
  - Linear line fitting or linear surface fitting was very easy:  $y \approx a^\top X$
  - Binary classification can be done by using a smooth step function, e.g. the logistic function:  
$$y \approx g(a^\top X)$$
  - They all can be represented as a network
    - Input nodes: the multidimensional data samples
    - Arrows: the weights and bias
    - Output nodes: the predicted targets
- What I will show you in the next slides
  - We can solve ALL (non-linear) function approximation problems by using the same structure
    - i.e. Linear combination of the input wrapped by a step function
    - Instead of guessing a particular parametric function (e.g. a high degree polynomial)
  - By increasing the number of layers



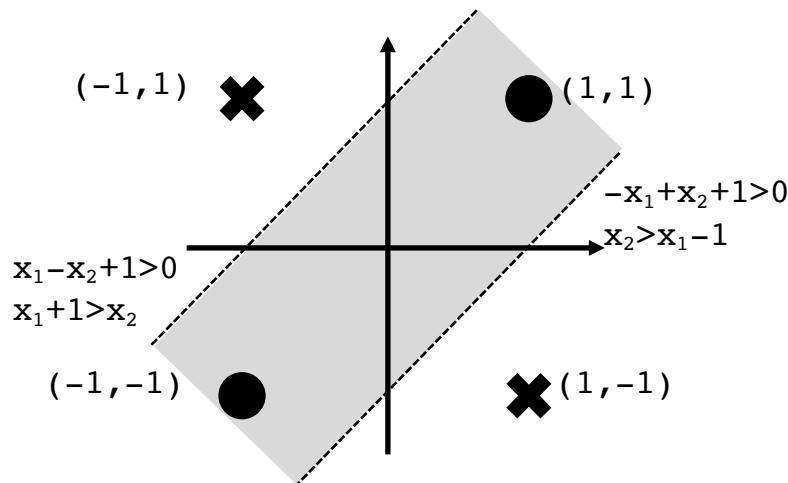
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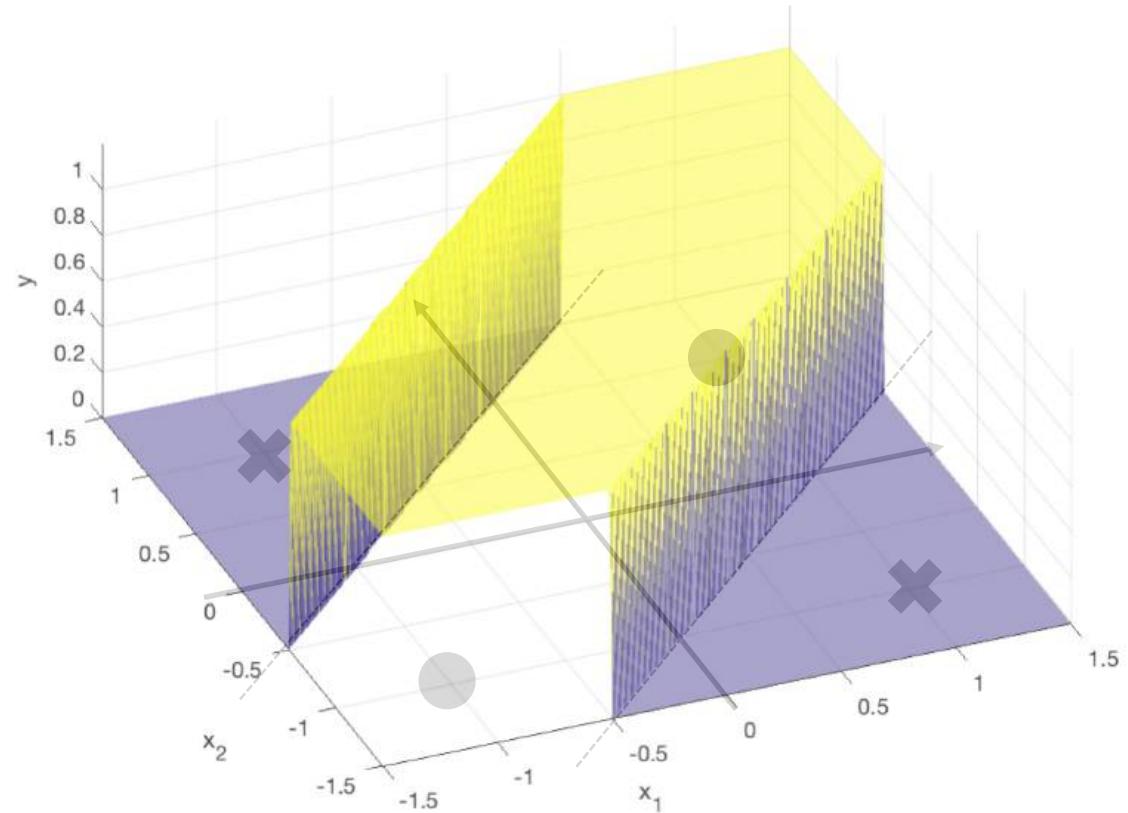
# Multilayer Perceptron

## - The XOR problem

- XOR is not linearly separable

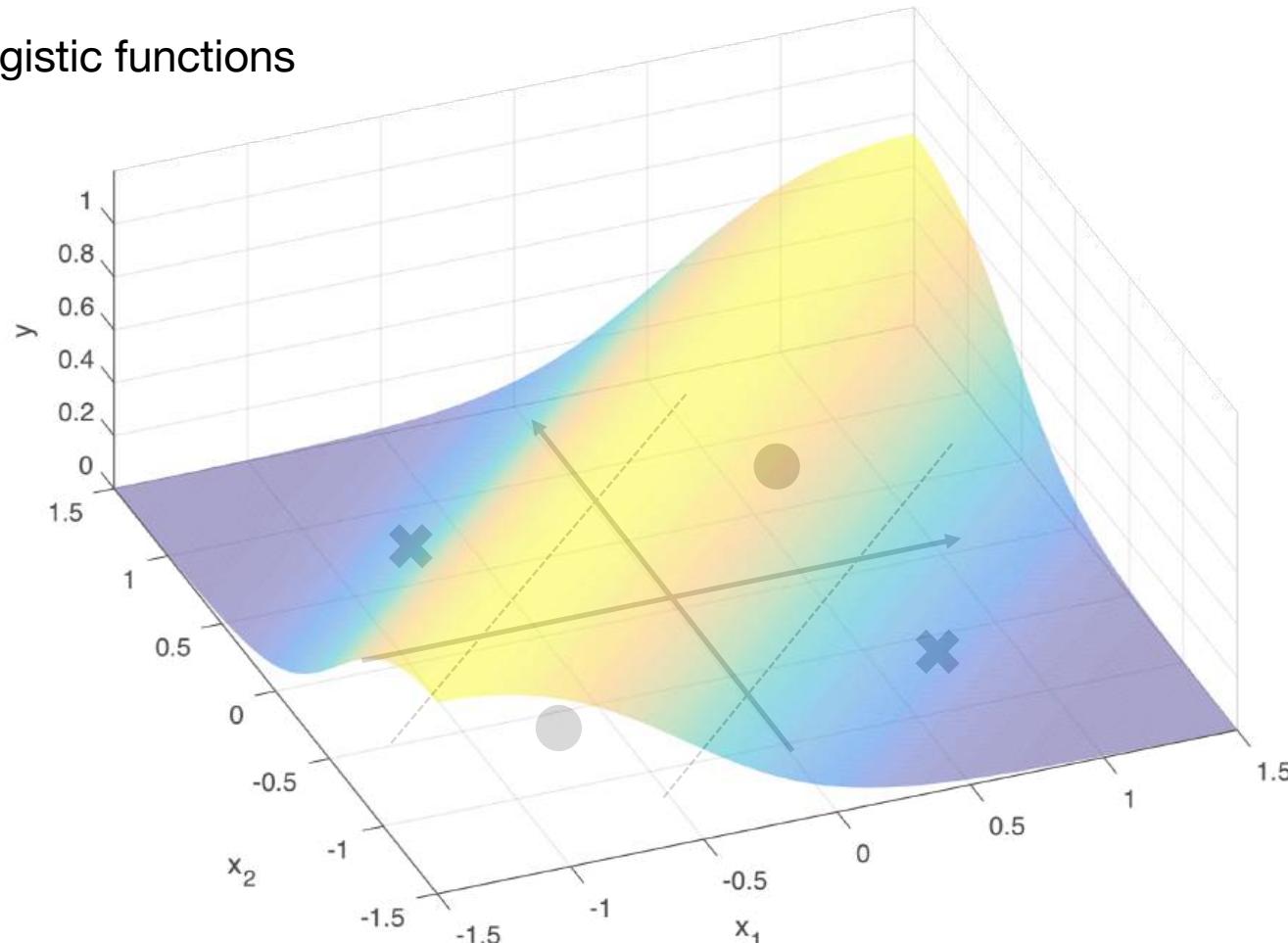


- Two hyperplanes can solve



# Multilayer Perceptron

- The XOR problem
- I may need two logistic functions

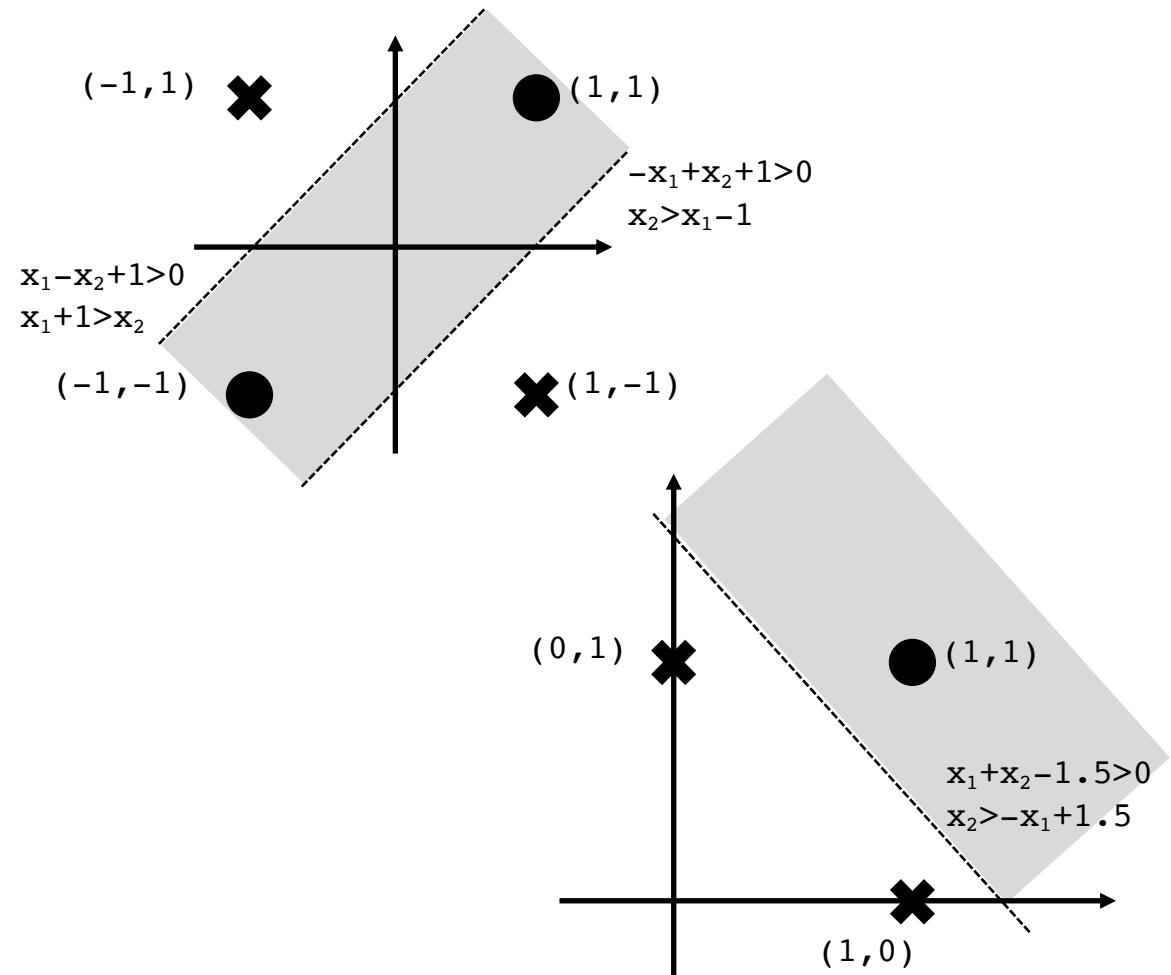
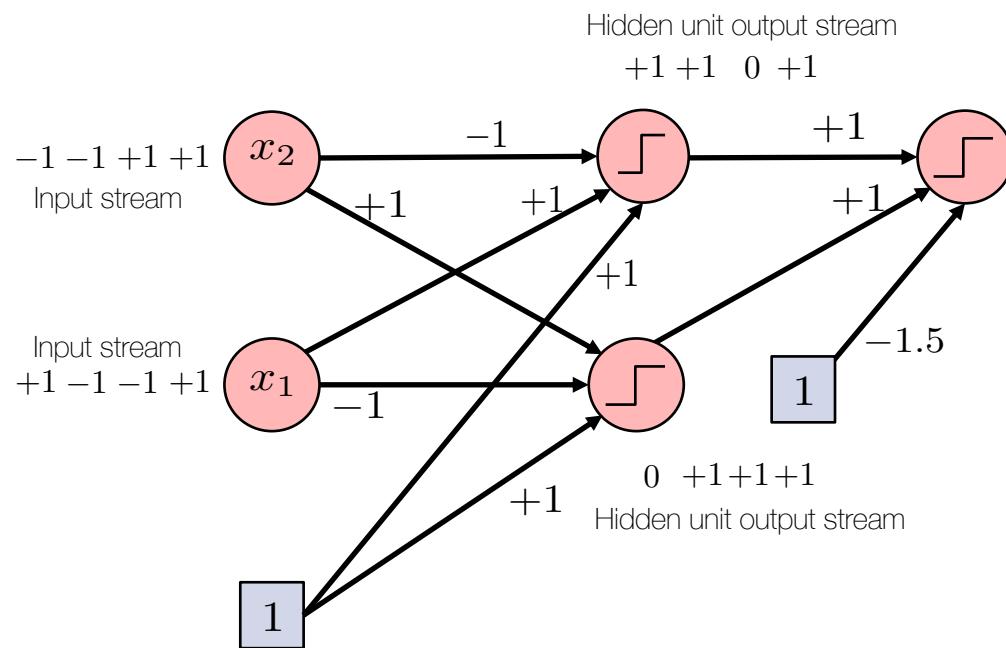


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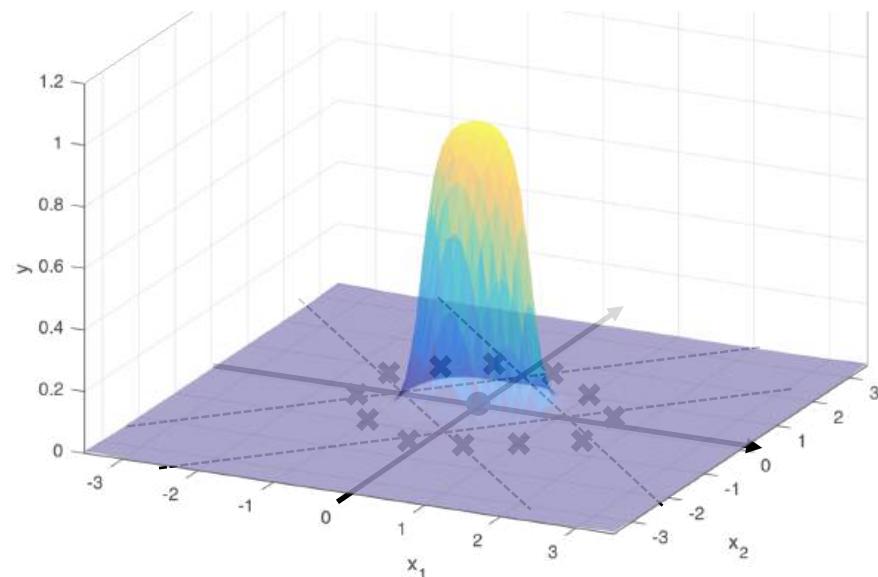
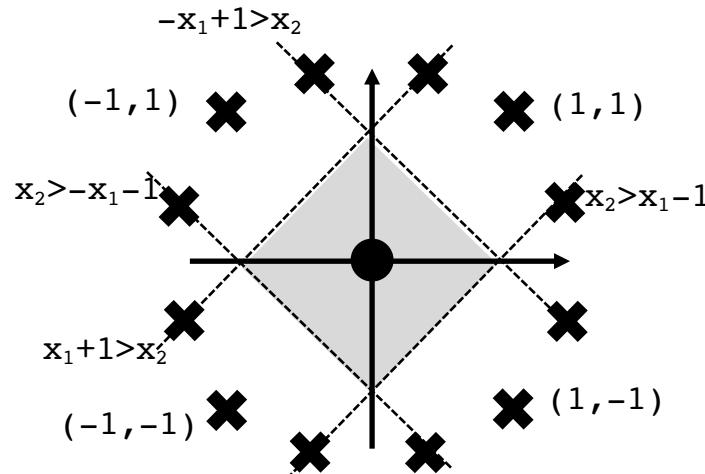
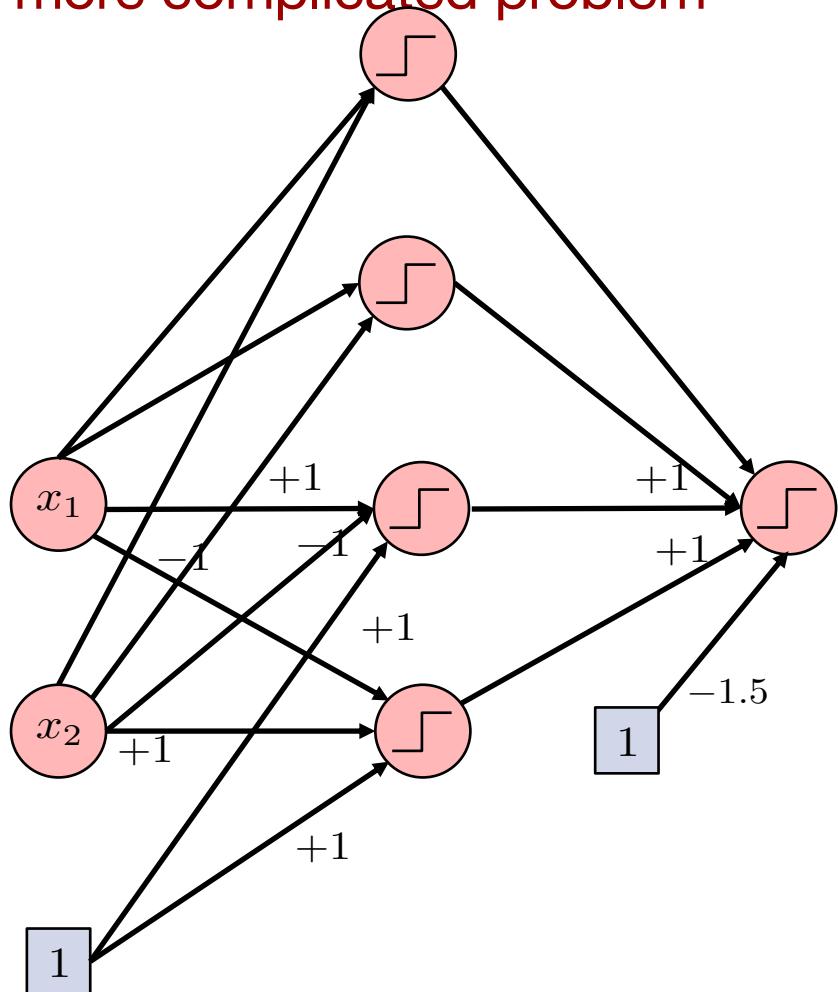
# Multilayer Perceptron

## - The XOR problem



# Multilayer Perceptron

- A more complicated problem



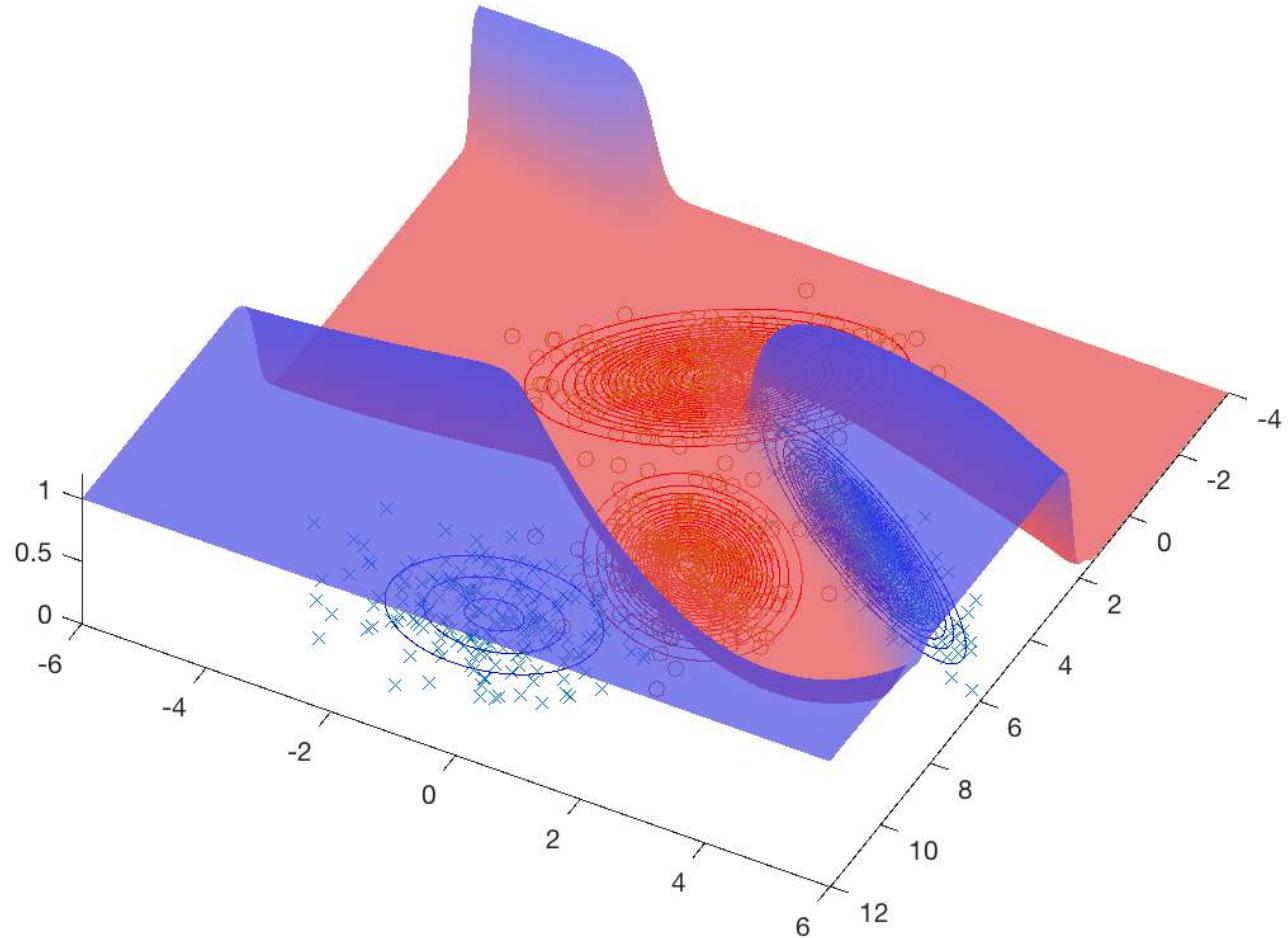
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# Multilayer Perceptron

- The universal approximation theorem

- If we're allowed to use as many hidden units as we want, we can approximate any target function
- The GMM classifier's posterior distribution



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# Multilayer Perceptron

## - Error backpropagation

- First we randomly initialize the weights and forwardpropagate

- Layer 1

$$\begin{bmatrix} z_2^{(1)} \\ z_1^{(1)} \end{bmatrix} = \begin{bmatrix} A_{22}^{(1)} & A_{21}^{(1)} & A_{20}^{(1)} \\ A_{12}^{(1)} & A_{11}^{(1)} & A_{10}^{(1)} \end{bmatrix} \cdot \begin{bmatrix} x_2^{(1)} \\ x_1^{(1)} \\ 1 \end{bmatrix} \quad \mathbf{z}^{(1)} = \mathbf{A}^{(1)} \mathbf{x}^{(1)}$$

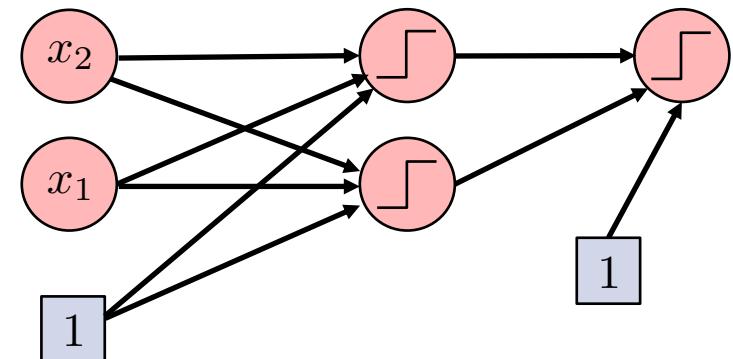
$$\begin{bmatrix} x_2^{(2)} \\ x_1^{(2)} \end{bmatrix} = g\left(\begin{bmatrix} z_2^{(1)} \\ z_1^{(1)} \end{bmatrix}\right) \quad \mathbf{x}^{(2)} = g(\mathbf{z}^{(1)})$$

- Final layer

$$z_1^{(2)} = \begin{bmatrix} A_{12}^{(2)} & A_{11}^{(2)} & A_{10}^{(2)} \end{bmatrix} \cdot \begin{bmatrix} x_2^{(2)} \\ x_1^{(2)} \\ 1 \end{bmatrix} \quad z^{(2)} = \mathbf{A}^{(2)} \mathbf{x}^{(2)}$$

$$\hat{y} = g(z^{(2)})$$

- Calculate the error  $\mathcal{E} = \frac{1}{2}(\hat{y} - y)^2$



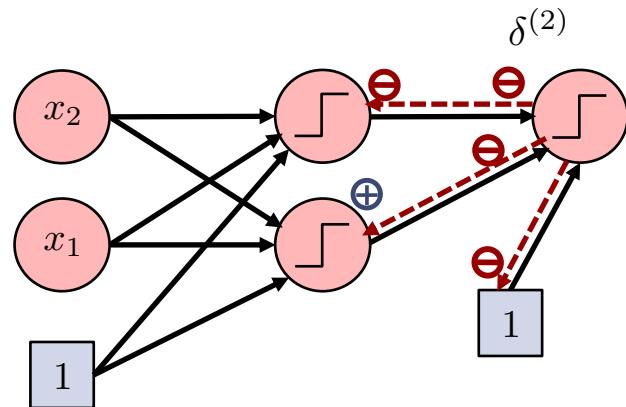
# Multilayer Perceptron

## - Error backpropagation

- If the error is zero, we're good. Move on to the next sample
- Otherwise, update  $A^{(2)} = A^{(2)} - \rho \nabla A^{(2)} = A^{(2)} - \rho \frac{\partial \mathcal{E}}{\partial A^{(2)}}$
- $$\frac{\partial \mathcal{E}}{\partial A^{(2)}} = \frac{\partial \mathcal{E}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial A^{(2)}} = \underbrace{(\hat{y} - y)g'(z^{(2)})x^{(2)\top}}_{\text{BP error} \times \text{the input of the layer}} = \delta^{(2)}x^{(2)\top}$$
  

$$\text{Error } \frac{\partial \mathcal{E}}{\partial z^{(2)}} = \delta^{(2)}$$
- Let's see why it works
  - Suppose some negative error  $\hat{y} - y = -1$  (i.e. network output not big enough)
    - Then the BP error is negative
      - Because  $g'(z^{(2)})$  is positive everywhere
    - **To fix this error we need to promote  $\hat{y} \uparrow$**
  - Given that, if the input was positive, say  $x_1^{(2)} = 1$ 
    - We need to promote the weights coming from it  $A_{11}^{(2)} \uparrow$
    - The gradient  $\nabla A_{11}^{(2)}$  must be negative  $\rightarrow -\nabla A_{11}^{(2)}$  is positive  $\rightarrow \nabla A_{11}^{(2)} = \delta_1^{(2)}x_1^{(2)} < 0$   $\leftarrow$  This is why we need negative BP error
  - If the input was negative, say  $x_2^{(2)} = -1$   
 (this doesn't happen with logistic activation though)
    - We demote  $A_{12}^{(2)} \downarrow \rightarrow -\nabla A_{12}^{(2)}$  should be negative  $\rightarrow \nabla A_{12}^{(2)} = \delta_2^{(2)}x_2^{(2)} > 0$
  - Same arguments hold for the positive error
- Negative error with positive input  $\rightarrow$  promotes weights  $A^{(2)} \uparrow$
- Negative error with negative input  $\rightarrow$  demotes weights  $A^{(2)} \downarrow$

$$\begin{aligned} z^{(1)} &= A^{(1)}x^{(1)} \\ x^{(2)} &= g(z^{(1)}) \\ z^{(2)} &= A^{(2)}x^{(2)} \\ \hat{y} &= g(z^{(2)}) \\ \mathcal{E} &= \frac{1}{2}(\hat{y} - y)^2 \end{aligned}$$



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# Multilayer Perceptron

## - Error backpropagation

- Now let's work on the first layer

- Update  $\mathbf{A}^{(1)} = \mathbf{A}^{(1)} - \rho \nabla \mathcal{E} = \mathbf{A}^{(1)} - \rho \frac{\partial \mathcal{E}}{\partial \mathbf{A}^{(1)}}$

$$\frac{\partial \mathcal{E}}{\partial \mathbf{A}^{(1)}} = \underbrace{\frac{\partial \mathcal{E}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{(2)}}}_{\text{BP Error (final layer)}} \underbrace{\frac{\partial z^{(2)}}{\partial \mathbf{x}^{(2)}} \frac{\partial \mathbf{x}^{(2)}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{A}^{(1)}}}_{\text{BP Error (hidden layer)}} = \underbrace{\left\{ \left( \mathbf{A}^{(2)\top} \delta^{(2)} \right) \odot g'(\mathbf{z}^{(1)}) \right\} \mathbf{x}^{(1)\top}}_{\{\text{BP error}\} \times \{\text{the input of the layer}\}}$$

- Error in the hidden layer

- If  $\delta^{(2)} < 0$  ( $\hat{y} - y < 0$ ) and  $A_{11}^{(2)} > 0$

- Need to promote  $x_1^{(2)}$  and, consequently,  $z_1^{(1)}$

- Promoting  $z_1^{(1)}$  means reducing the final network error only if  $\frac{\partial \mathcal{E}}{\partial z_1^{(1)}} < 0$

- Therefore,  $\delta_1^{(1)} \propto \delta^{(2)} A_{11}^{(2)} < 0$  makes sense

- If  $\delta^{(2)} < 0$  ( $\hat{y} - y < 0$ ) and  $A_{12}^{(2)} < 0$

- Need to demote  $x_2^{(2)}$  and  $z_2^{(1)}$

- $\frac{\partial \mathcal{E}}{\partial z_2^{(1)}} = \delta_2^{(1)} \propto \delta^{(2)} A_{12}^{(2)} > 0$

- Error from the final layer, weighted by the second layer weights**

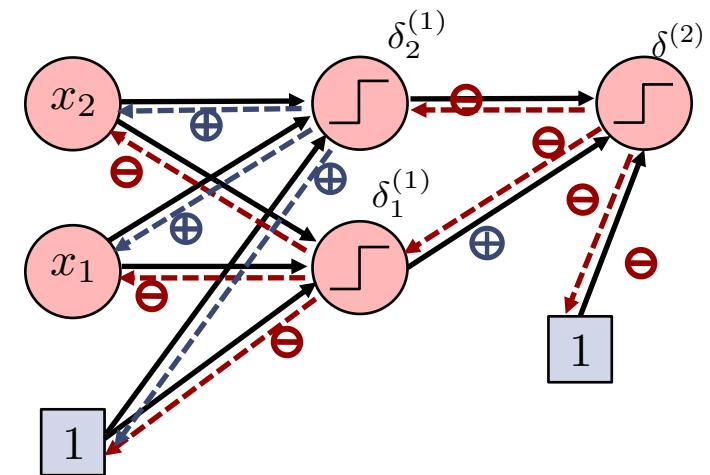
$$\mathbf{z}^{(1)} = \mathbf{A}^{(1)} \mathbf{x}^{(1)}$$

$$\mathbf{x}^{(2)} = g(\mathbf{z}^{(1)})$$

$$\mathbf{z}^{(2)} = \mathbf{A}^{(2)} \mathbf{x}^{(2)}$$

$$\hat{y} = g(\mathbf{z}^{(2)})$$

$$\mathcal{E} = \frac{1}{2} (\hat{y} - y)^2$$

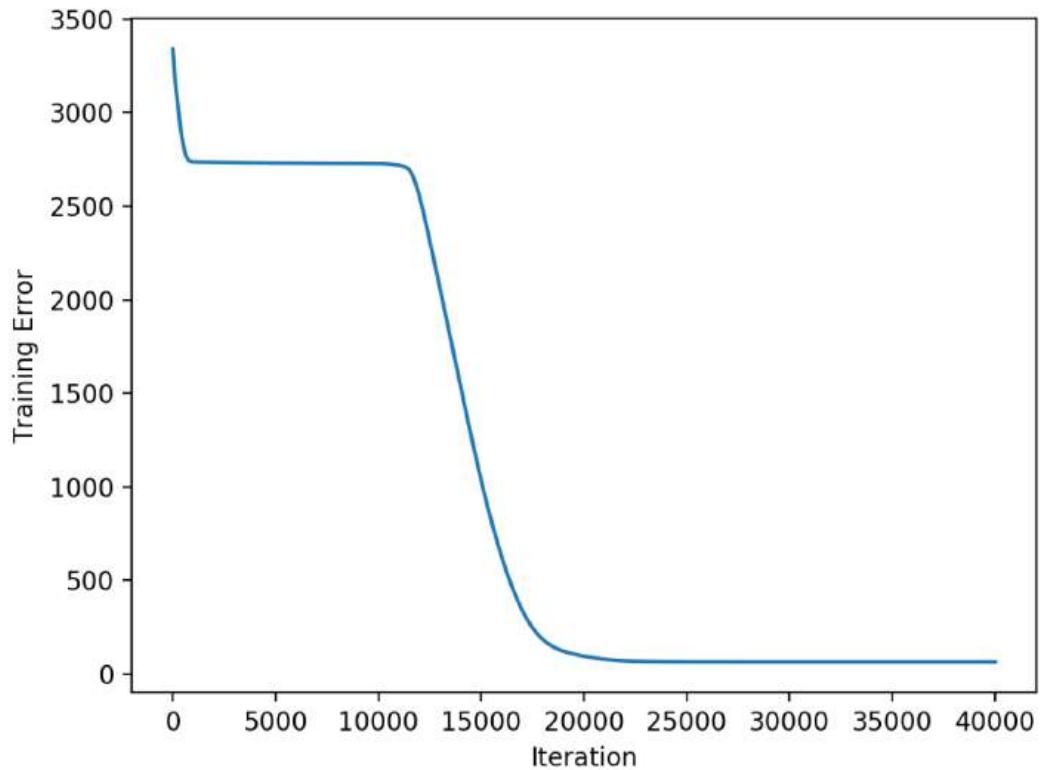
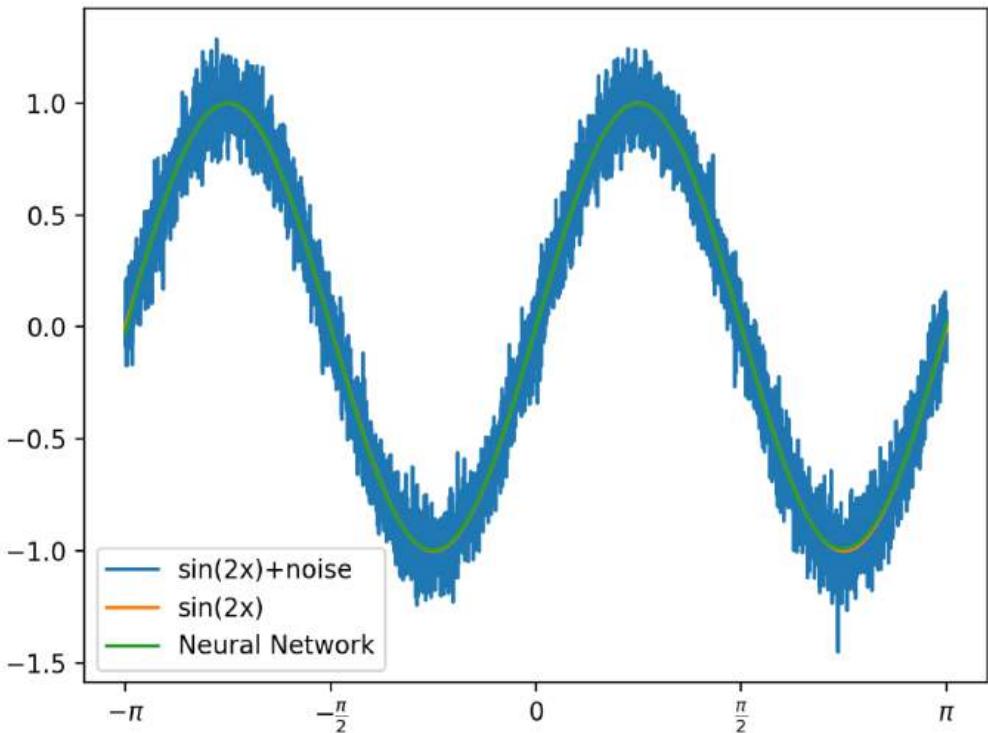


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# Multilayer Perceptron

- Does it work?
  - Sine wave denoising



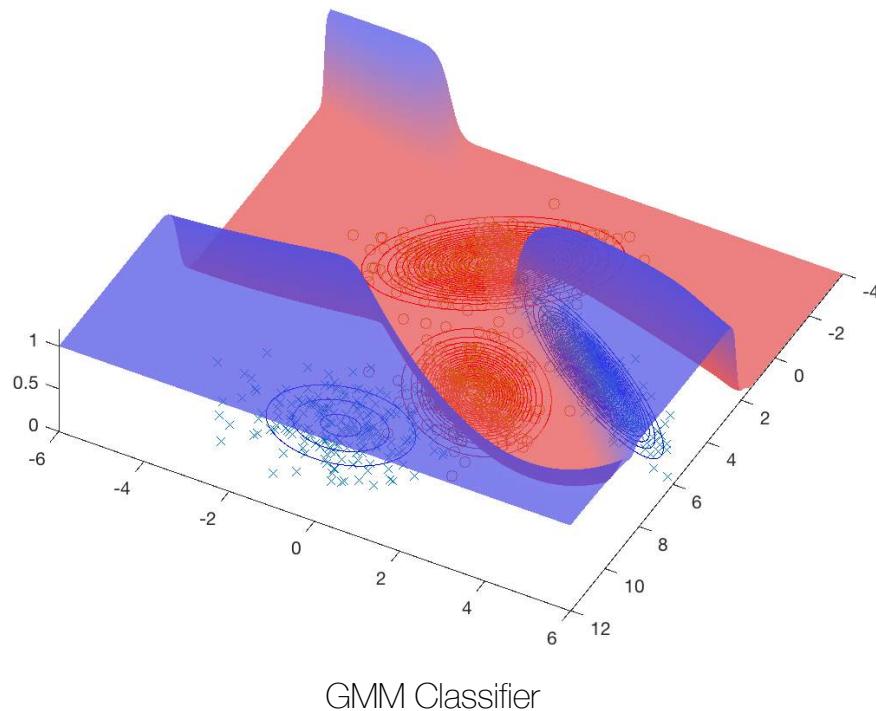
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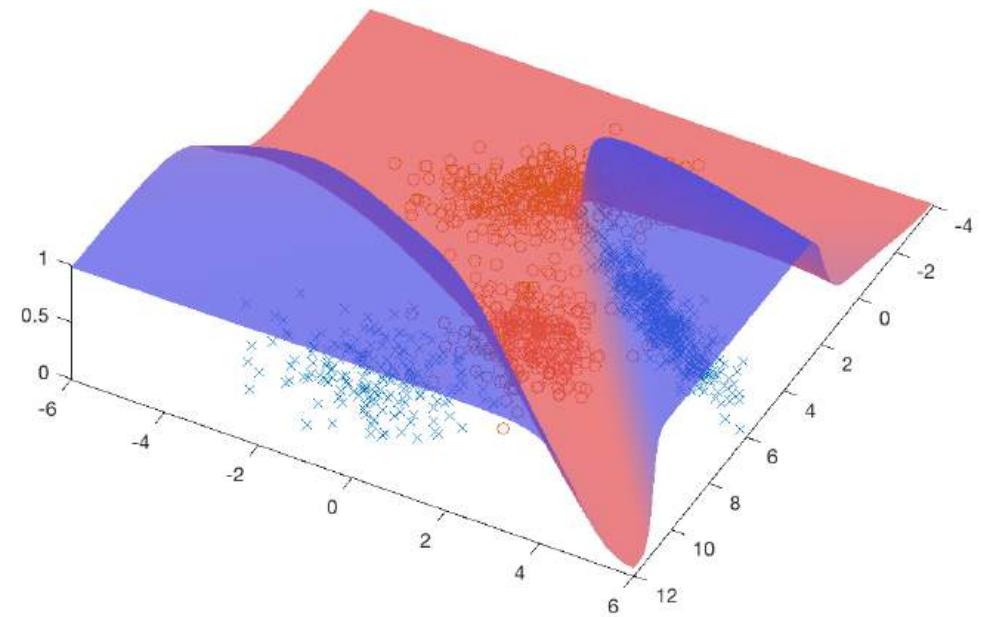
# Multilayer Perceptron

- Does it work?

- GMM classifier



GMM Classifier



Neural Network



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# Multi-class Classification

## - Logistic regression using a softmax activation

- You have 5 categories in your classification problem
  - How would you formulate your neural network output?
- Integers?
  - 1 : ★☆☆☆☆, 2 : ★★☆☆☆, ..., 5 : ★★★★★
- If the categories are not ordinal at all
  - 1 for RED, 2 for GREEN, 3 for ORANGE
  - 1 for “dog,” 2 for “lion,” 3 for “cat,” 4 for “wolf”
    - Error between “dog” and “lion” is larger than “dog” and “wolf”
- We can use something called one-hot vector
  - Different categories are equally different (Hamming distance)

$$\begin{array}{ccc} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \\ \text{RED} & \text{GREEN} & \text{ORANGE} \end{array} \quad \begin{array}{cccc} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \\ \text{dog} & \text{cat} & \text{wolf} & \text{lion} \end{array}$$



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# Multi-class Classification

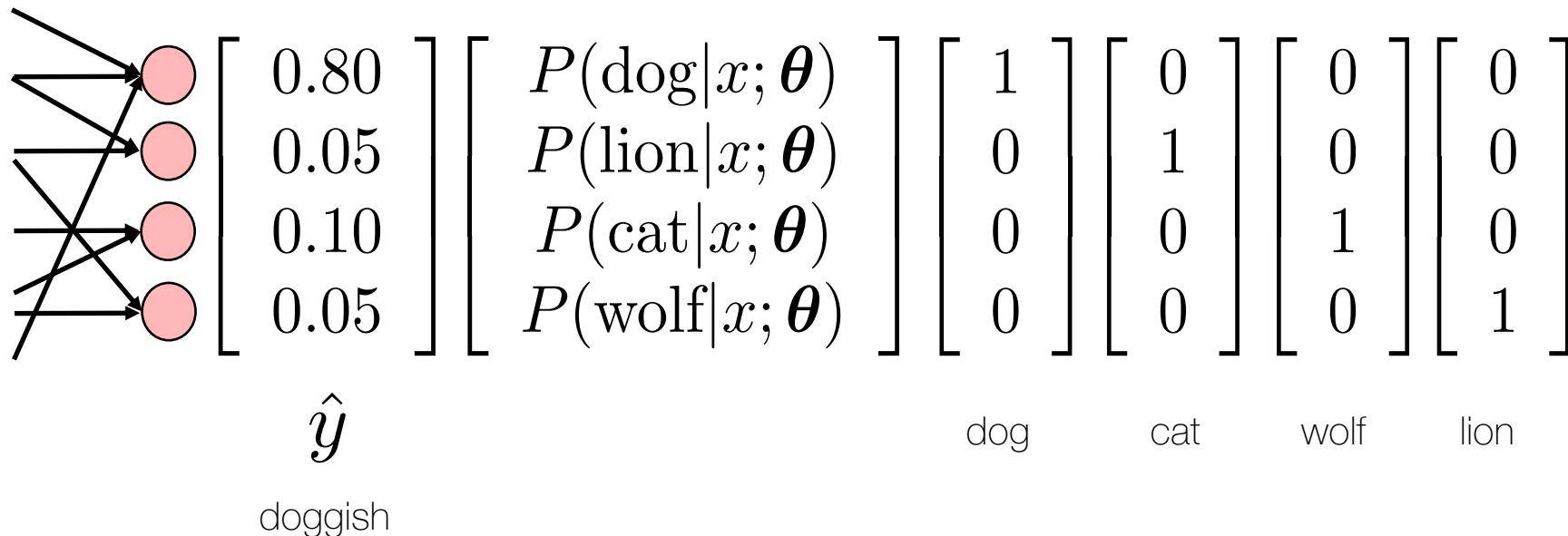
- Logistic regression using a softmax activation

- I want a smooth logistic-like function

- But, a multidimensional one this time

- Hopefully a probability vector

- What should be the final layer activation function?

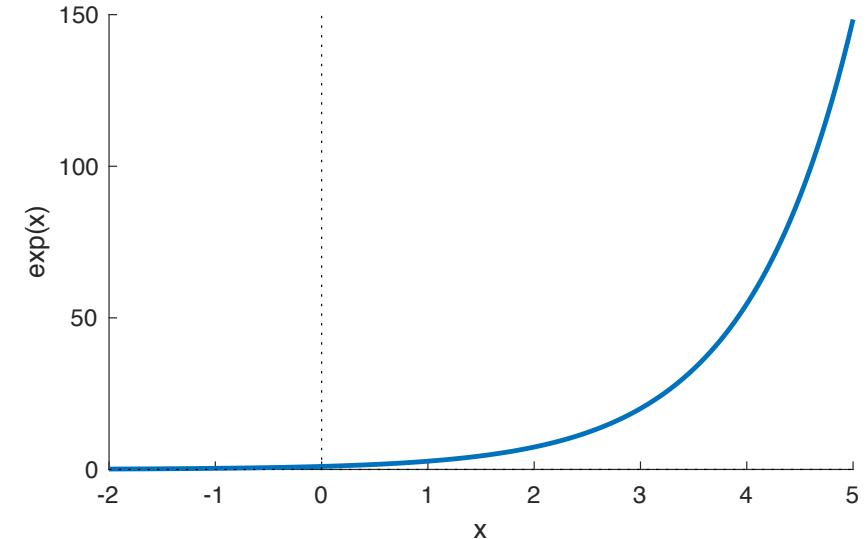
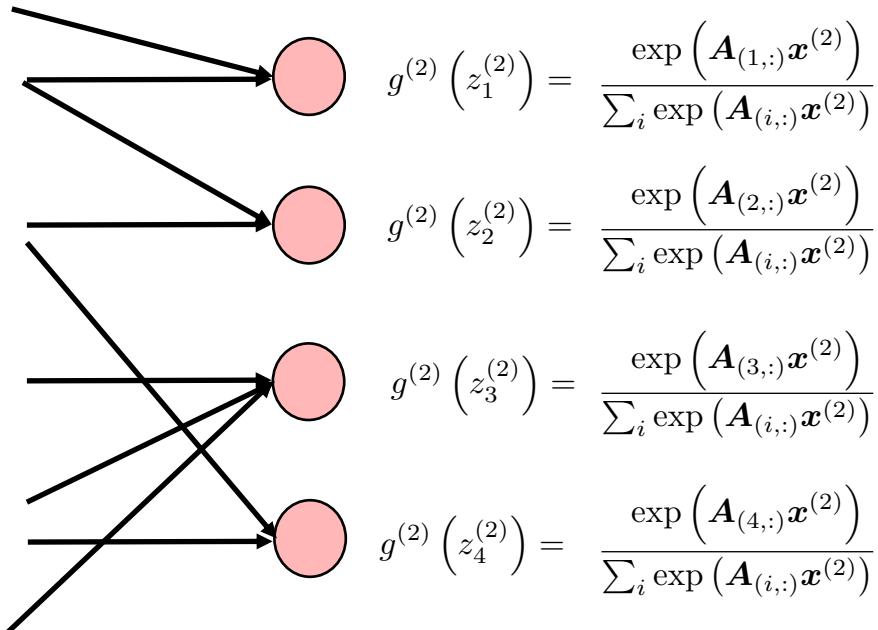


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# Multi-class Classification

- Logistic regression using a softmax activation
  - For the multi-class neural networks we use **softmax activation** function



- If you use cross entropy as your error, the BP error for the softmax regression is intuitive

$$\mathcal{E}(\mathbf{y}||\hat{\mathbf{y}}) = - \sum_i y_i \log(\hat{y}_i) \quad \frac{\partial \mathcal{E}}{\partial \mathbf{A}} = (\hat{\mathbf{y}} - \mathbf{y})\mathbf{x}^{(1)}$$



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# Recap

- Combining smooth step functions
  - Can create valleys and hills
  - Can universally approximate your objective function
- Logistic regression
  - Classification is not different from function approximation (regression)
  - Logistic function can approximate the sharp step function
    - Binary classification
  - Softmax function can approximate the one-hot vector representation
- There are a lot of choices for the hidden unit activation
- Universal approximation theorem says one hidden layer is enough
  - Why deep learning?



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# Reading

- Chapter 4
  - Feel free to skip off-topic clauses though



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# Thank You!



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