Neural Networks

CMPUT 366: Intelligent Systems

GBC §6.0-6.4.1

Lecture Outline

1. Recap
2. Nonlinear models
3. Feedforward neural networks

Recap: Calculus

- Derivatives can be used for **optimization**
  - Minimization: Increase *x* if derivative is negative & vice versa
- **Partial derivatives** are derivatives of "frozen" function:

$$\frac{\partial}{\partial x} f(x, y) = \frac{d}{dx}(f)_{y=y}(x)$$

- **Gradient** of a function is a **vector** of all its partial derivatives:

$$(\nabla f)(x, y) = \begin{bmatrix} \frac{\partial}{\partial x} f(x, y) \\ \frac{\partial}{\partial y} f(x, y) \end{bmatrix}$$

Linear Models

- Supervised models we have considered so far have been **linear:**

weights

$$y = f(\mathbf{x}; \mathbf{w}) = g(\mathbf{w}^T \mathbf{x}) = g\left(\sum_{i=1}^{n} w_i x_i \right)$$

Linear model

inputs

activation function

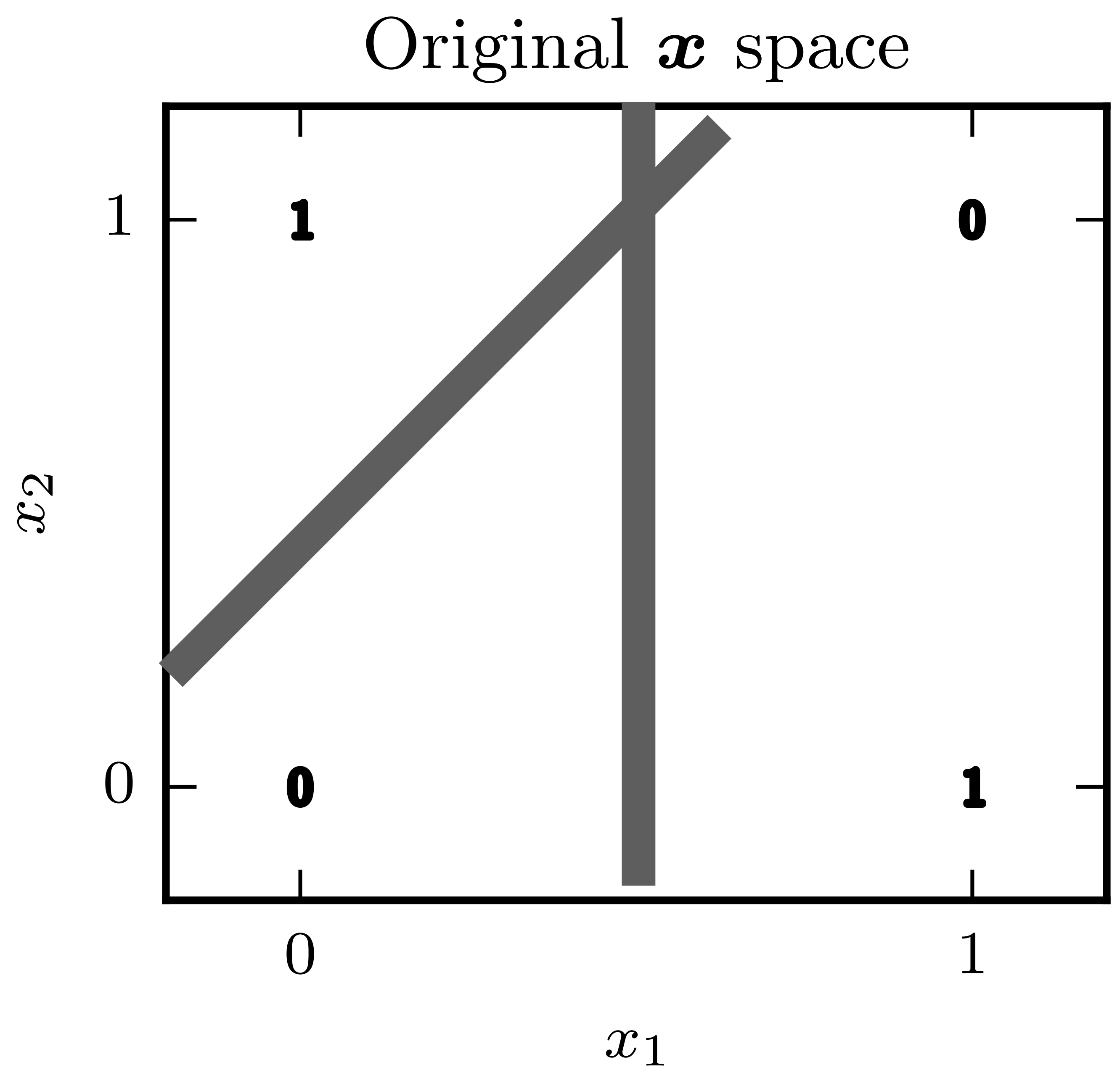
  - Linear classification / regression
  - Logistic regression

- **Advantages: Efficient** to fit (closed form sometimes!)
- **Disadvantages:** Can be really **limited**

Example: XOR

- The function f(x1, x2) = (x1 XOR x2) is not **linearly separable**
  - There is no way to draw a **straight line** with all of the 1's on one side and all of the 0's on the other
  - This means that no **linear model** can represent XOR exactly; there will always be some errors
- **Question:** What else could we do?

A: Transform inputs



(Image: Goodfellow 2017)

Nonlinear Features

$$y = f(\mathbf{x}; \mathbf{w}) = g(\mathbf{w}^T\mathbf{x}) = g\left(\sum_{i=1}^{n} w_i x_i\right)$$

- One option: Learn a linear model on **richer inputs**

1. Define a **feature mapping** $\phi(\mathbf{x})$ that returns functions of the original inputs

2. Learn a linear model of the **features** instead of the **inputs**

$$y = f(\mathbf{x}; \mathbf{w}) = g(\mathbf{w}^T\phi(\mathbf{x})) = g\left(\sum_{i=1}^{n} w_i [\phi(\mathbf{x})]_i\right)$$

Nonlinear Features for XOR

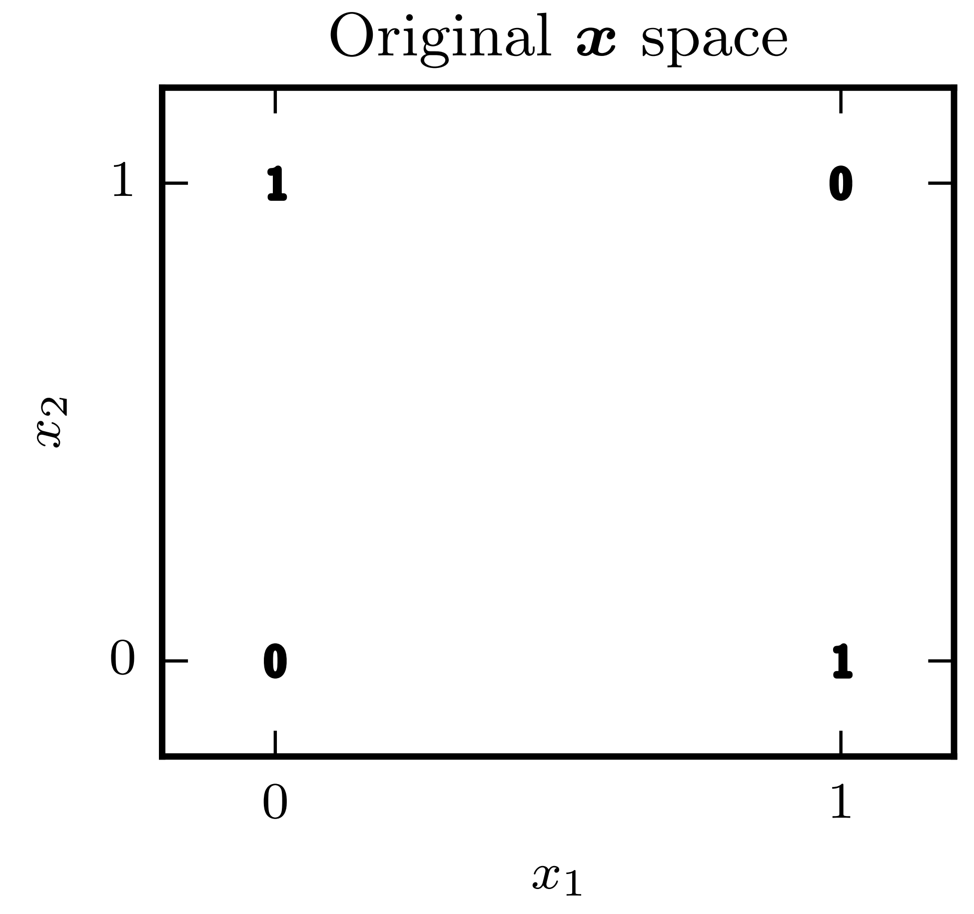
- **Question:**
  What additional features would help?

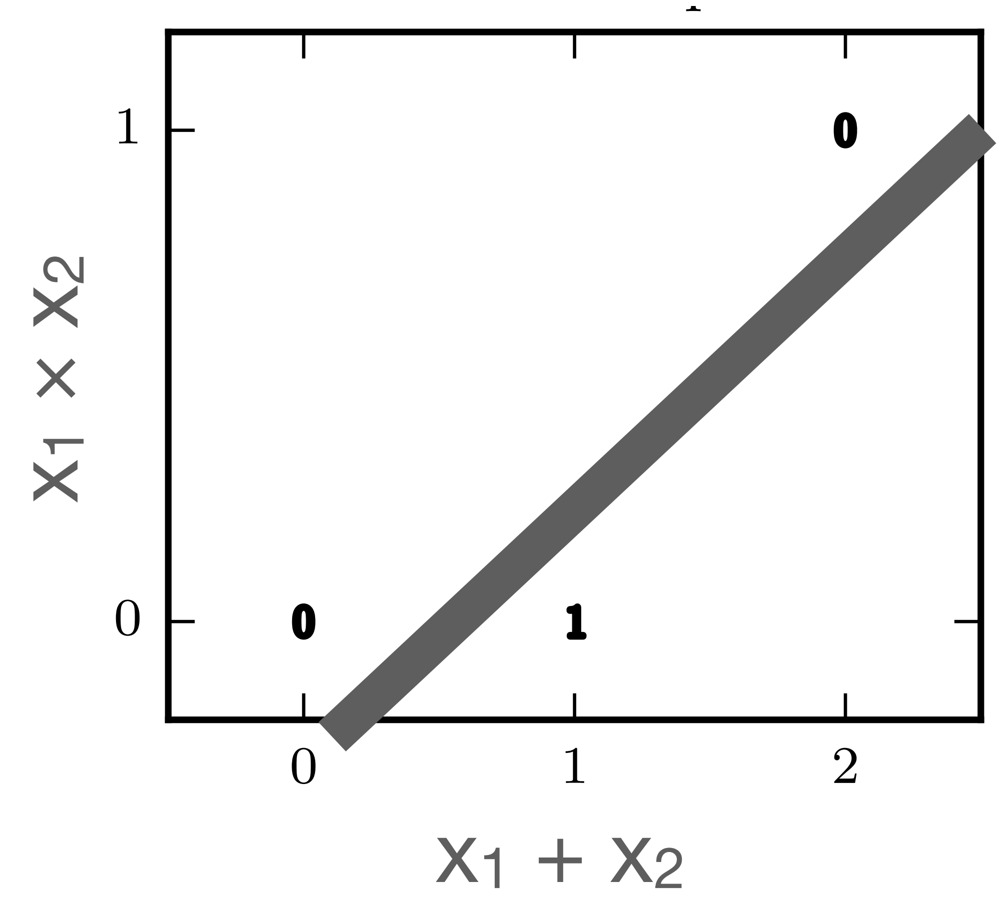
- The product of x1 and x2!

  - ϕ(x1, x2) = [1, x1, x2, x1x2]

  - **w** = [-0.2, .5, .5, -2]

- f($\mathbf{x}$; $\mathbf{w}$) = $\mathbf{w}^T\phi(\mathbf{x}) > 0$ for (0,1) and (1,0)
  f($\mathbf{x}$; $\mathbf{w}$) = $\mathbf{w}^T\phi(\mathbf{x}) < 0$ for (1,1) and (0,0)





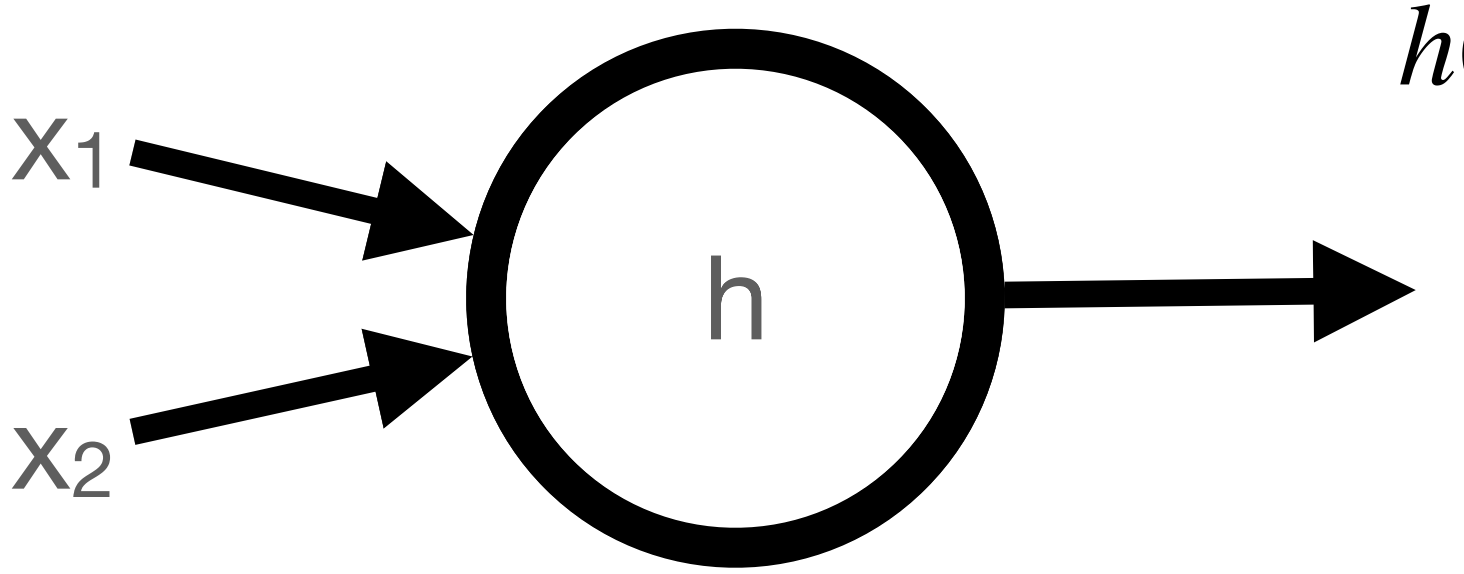
(Image: Goodfellow 2017)

Learning Nonlinear Features

- Manually constructing good features is extremely **hard**
- Manually constructed features are not **transferrable** between domains
    - e.g., SIFT features were a revolution in computer vision, but are **only** for computer vision
- Deep learning aims to learn ϕ **automatically** from the data

Neural Units

- Deep learning learns ϕ by **composing** little functions
- These function are called **units**



$$h(\mathbf{x};\mathbf{w}) = g(\mathbf{w}^T\mathbf{x}) = g\left(\sum_{i=1}^{n} w_i \mathbf{x}_i\right)$$

weights

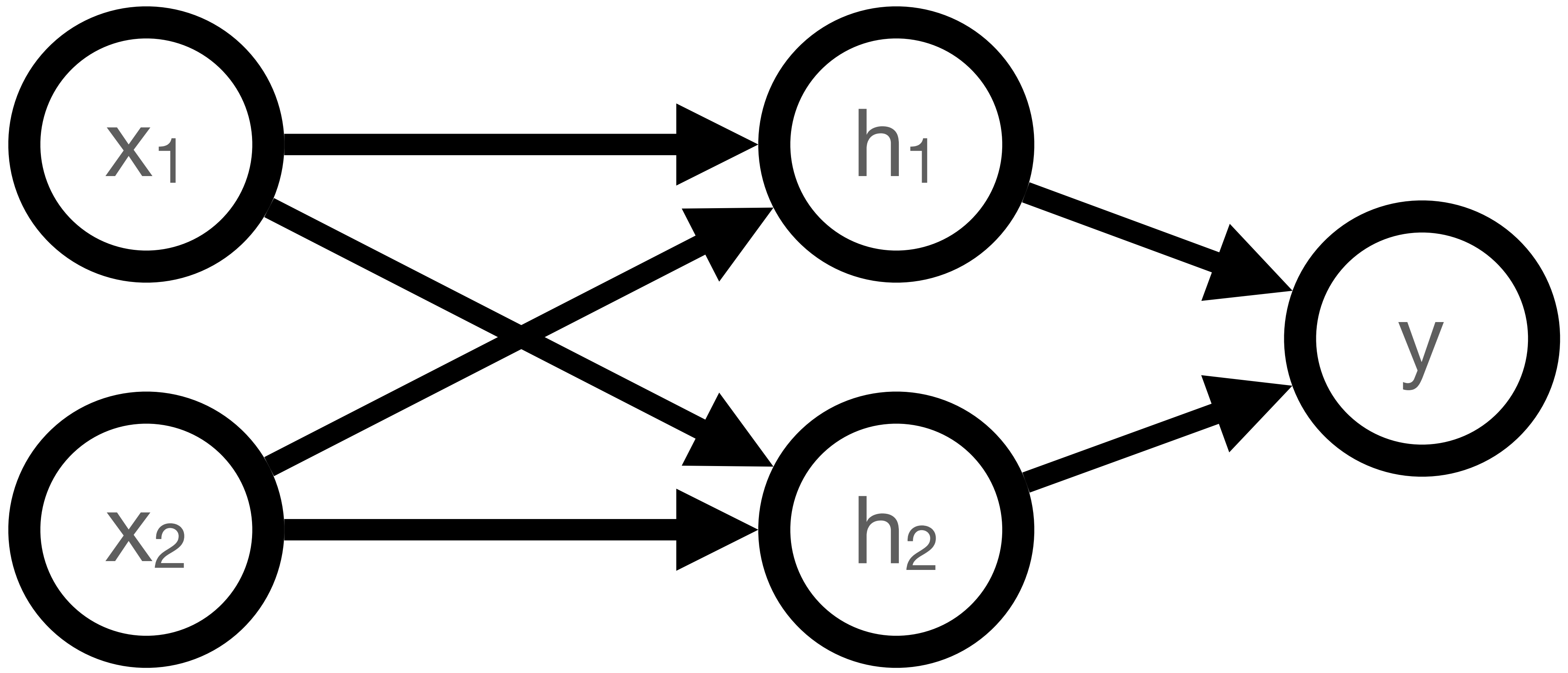
activation function

- **Question:** How is this different from a linear model?

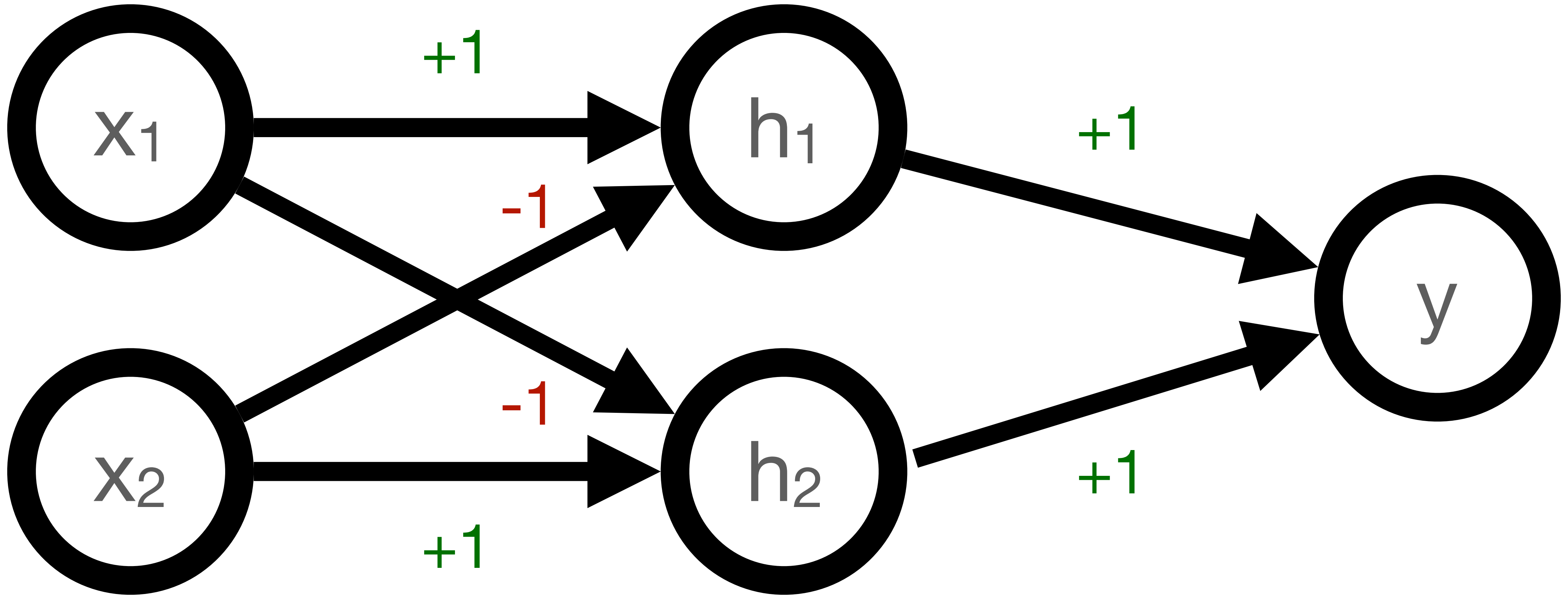
A: The activation function is non-linear, so composition of units will also be nonlinear.

Feedforward Neural Network

- A **neural network** is many units **composed** together
- **Feedforward neural network:** Units arranged into **layers**
    - Each layer takes outputs of **previous layer** as its **inputs**

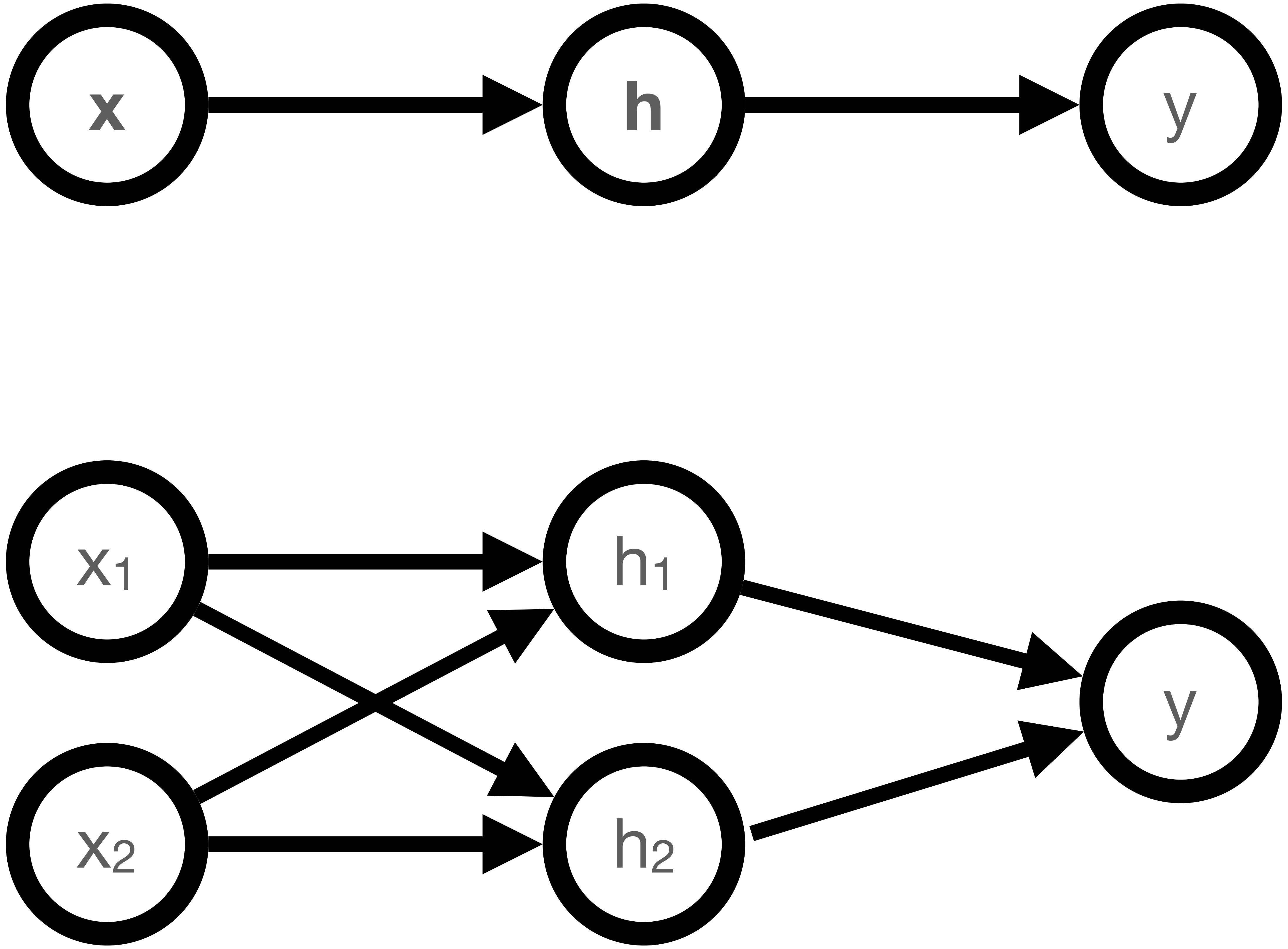


Example: XOR network



- *Activation*: g(z) = max{0, z} ("recified linear unit")
- Weights: [+1, -1] for h1; [-1, +1] for h2
  - [+1, +1] for y

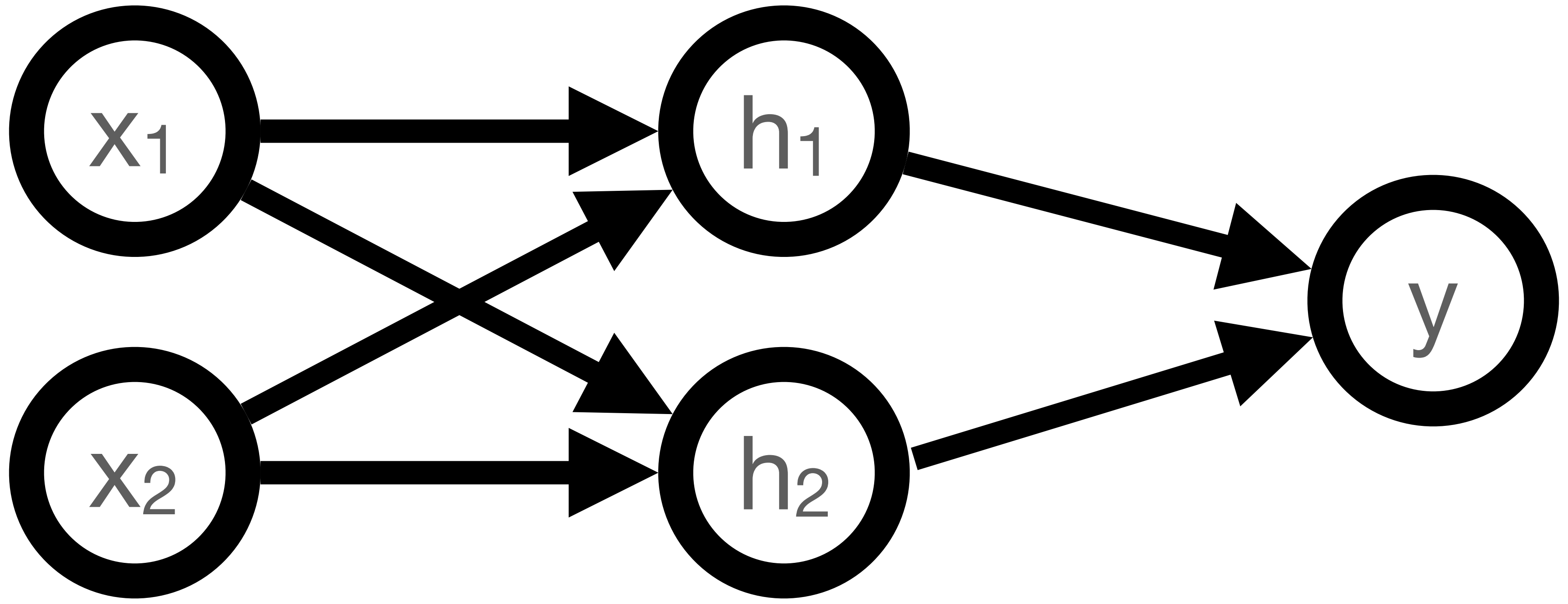
Matrix Representation



- You can think of the outputs of each **layer** as a **vector** **h**
- The **weights** from all the outputs of a previous layer to each of the units of the layer can be collected into a **matrix** **W**
- A **bias term** for each unit can be collected into a vector **b**:

$$\mathbf{h} = g\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right)$$

Architecture



Design decisions:

1. **Depth**: number of layers

2. **Width**: number of nodes in each layer

3. Fully-connected?

Universal Approximation Theorem

Theorem: (Hornik et al. 1989; Cybenko 1989; Leshno et al. 1993)
A feedforward network with at least one hidden layer with a "squashing" activation or rectified linear activation and a linear output layer can approximate **any function** to within **any given error bound**, given enough hidden units.

- So a large feedforward network can **represent** any function we're trying to learn!
- **Question:** Why bother with multiple layers?

Hidden Unit Activations

- Default choice: **Rectified linear** units (ReLU)
  g(z) = max(0, z)

- Other common types:

  - tanh(z)

  - $\dfrac{1}{1+e^{-z}}$ (sigmoid)

- Sigmoid suffers from **vanishing gradients**; relu does not

Training

- Neural networks are trained using variants of **gradient descent**
  - e.g., stochastic gradient descent
- **Back propagation** is an algorithm that allows for efficient computation of the **gradient**
- Modern frameworks can compute the gradient in other ways (e.g., **automatic differentiation**) even for complicated units)

Summary

- Generalized linear models are **insufficiently expressive**
- Composing GLMs into a network is **arbitrarily expressive**
  - A neural network with a **single hidden layer** can approximate **any function**
  - But the network might need to be impractically large, prone to overfitting, or inefficient to train
- Trained using variants of **gradient descent**
- **Architectural choices** can make a network easier to train, less prone to overfitting