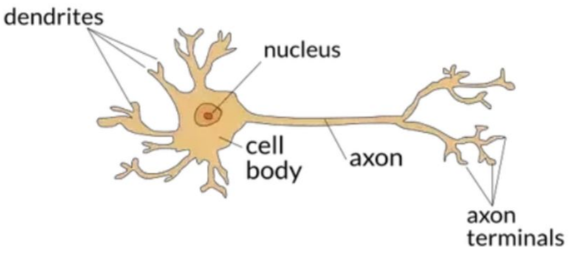
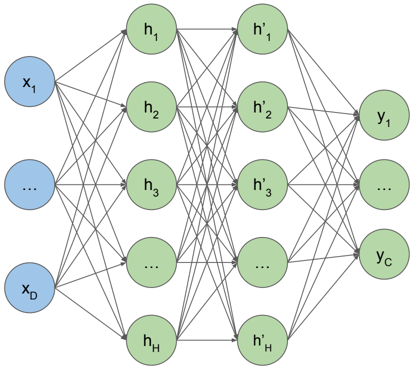
NYU CS-GY 6923
Machine Learning

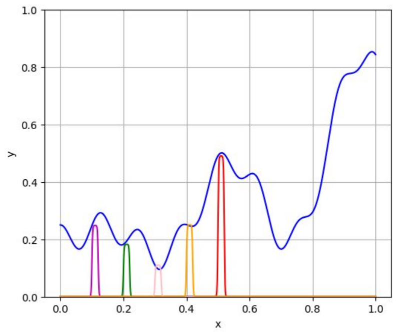
Prof. Pavel Izmailov

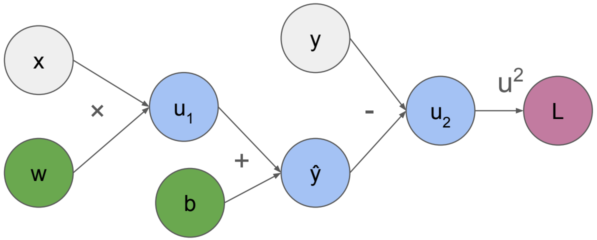
Today

- Neural Networks
- Universal Approximation
- Backpropagation
- Autograd
- Demo

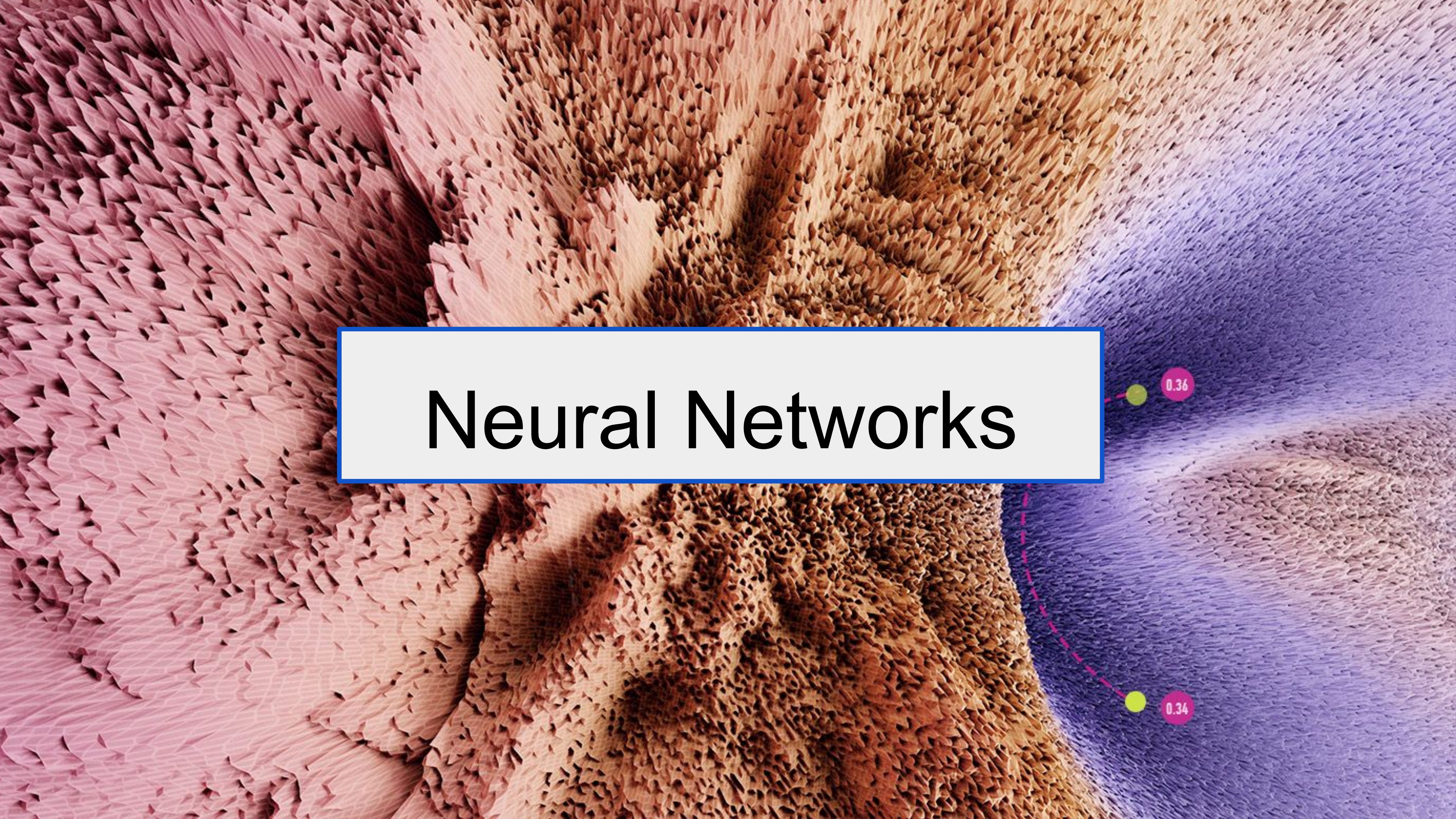




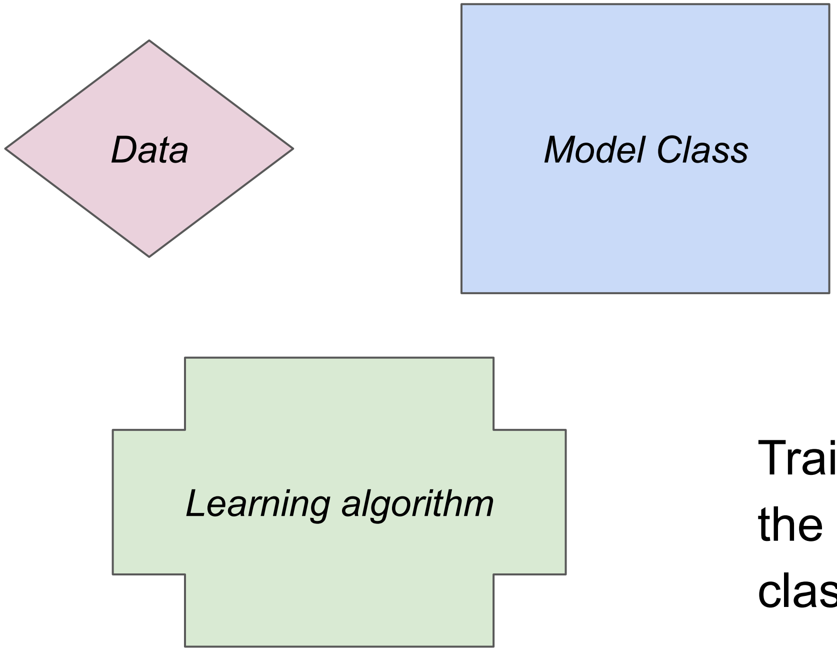




Neural Networks



General Picture of ML

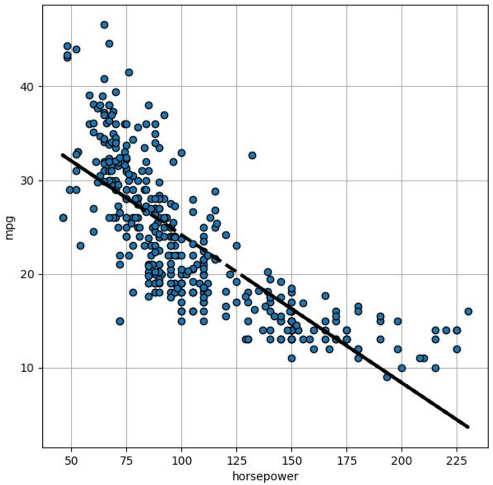


Training algorithm selects the model from a model class using data.

Example: Linear Regression

Data

Model Class:
Ridge Regression



Learning algorithm:
Exact Formula

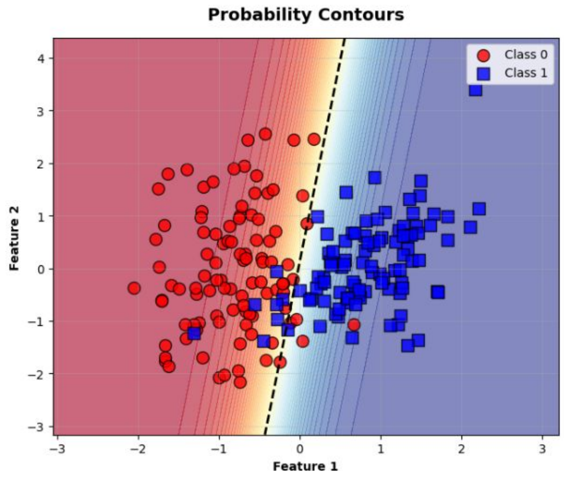
Training algorithm selects the model from a model class using data.

Example: Logistic Regression

Data

Model Class:
Logistic Regression

Learning algorithm:
Gradient Descent

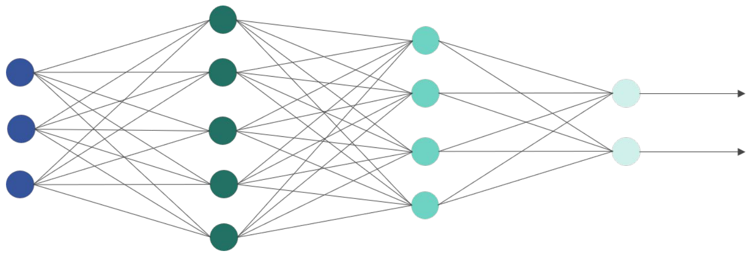


Training algorithm selects the model from a model class using data.

GD-Based Learning

Data

Model Class:
Any Model Differentiable wrt Parameters



Learning algorithm:
Gradient Descent

Training algorithm selects the model from a model class using data.

Gradient Descent is an extremely powerful learning algorithm

GD-Based Learning

Gradient-based learning:

- Define a model: $M(X_i, w)$ producing predictions based on data
  - w represents parameters of the model
  - $M(X_i, w)$ typically needs to be differentiable with respect to *w*
- Define a loss function $L(w)$
  - Typically, $L(w) = \sum_i L(M(X_i, w), y_i)$
- Minimize using gradient descent to find optimal w

GD-Based Learning

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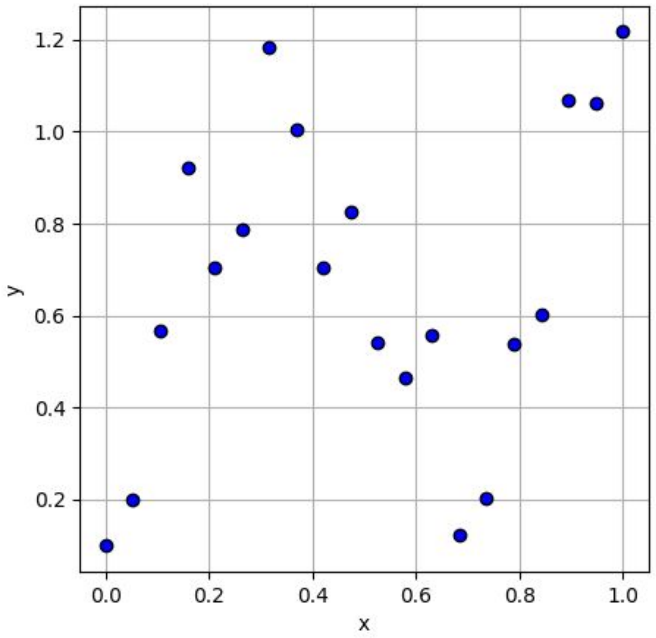
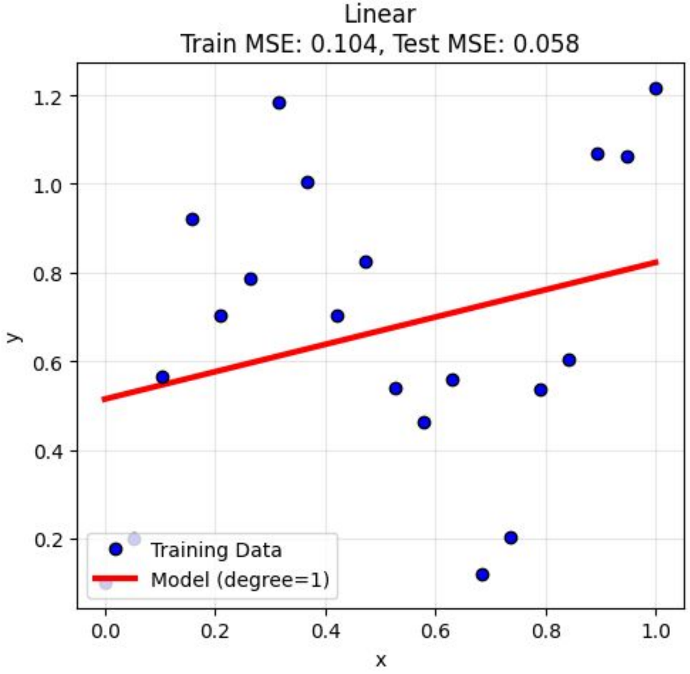
Neural Networks: Motivation

- Non-linear data



Neural Networks: Motivation

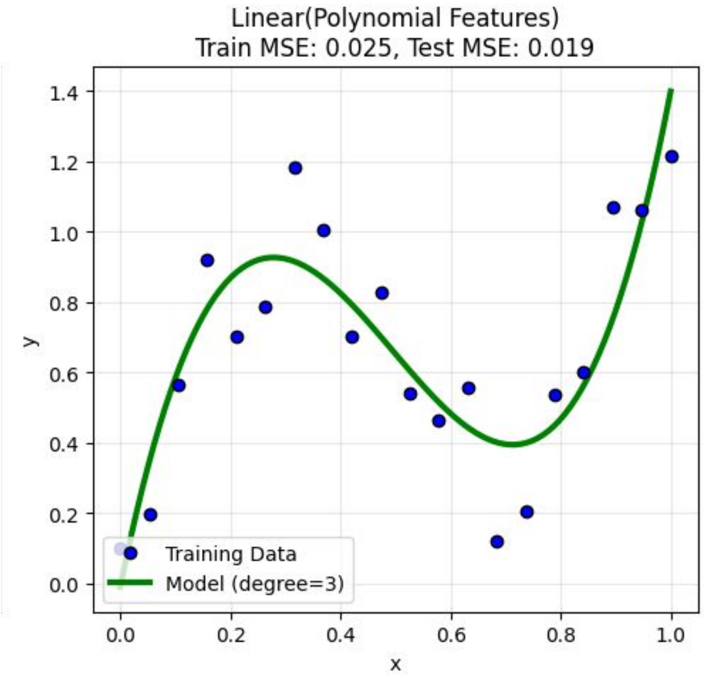
- Non-linear data
- Linear fit doesn’t work



Neural Networks: Motivation

- Non-linear data
- Linear fit doesn't work
- Old solution: use polynomial features

$$(1, x, x^2, \ldots, x^d)$$



Neural Networks: Motivation

- Non-linear data
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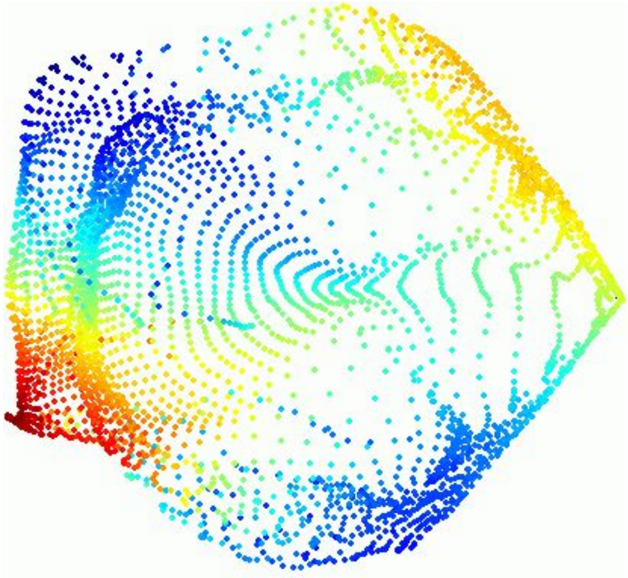
- But what if our data is very high-dimensional and we don’t know what features to use?



Feature Engineering → Feature Learning

- Let's *learn* the features!

$$h = W_1 x + b_1 \longleftarrow \text{Hidden features}$$

$$\hat{y} = W_2 h + b_2 \longleftarrow \text{Output}$$

$$h \in \mathbb{R}^H, x \in \mathbb{R}^D, \hat{y} \in \mathbb{R}$$

- Will this model be able to learn features?

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  - No, it is equivalent to a linear model!

$$W_2(W_1 x + b_1) + b_2 = (W_2 W_1)x + (b_2 + W_2 b_1) = W' x + b'$$

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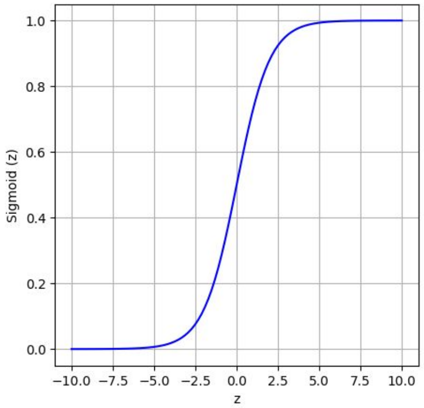
$$\boxed{h = \sigma(W_1 x + b_1)}$$



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- We need a non-linearity!

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- What loss can we use? MSE

$$L(W_1, b_1, W_2, b_2) = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Feature Engineering → Feature Learning

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- How many parameters?

- Train: minimize loss with Adam / SGD

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DH + H + H + 1

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Feature Engineering → Feature Learning

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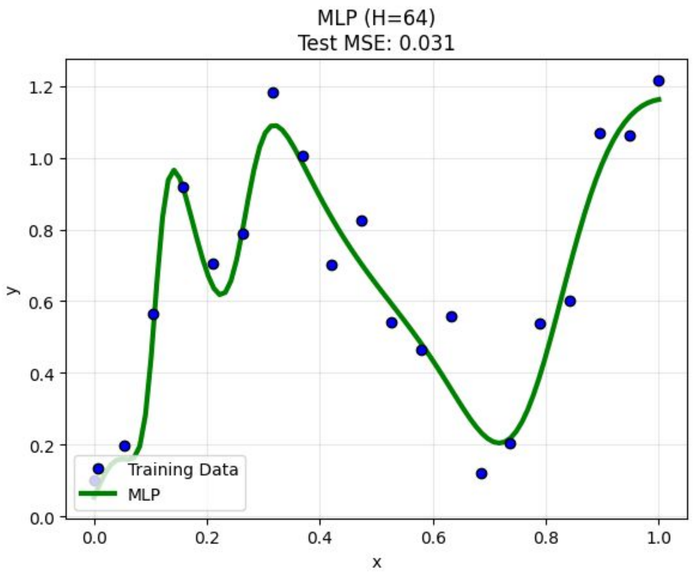

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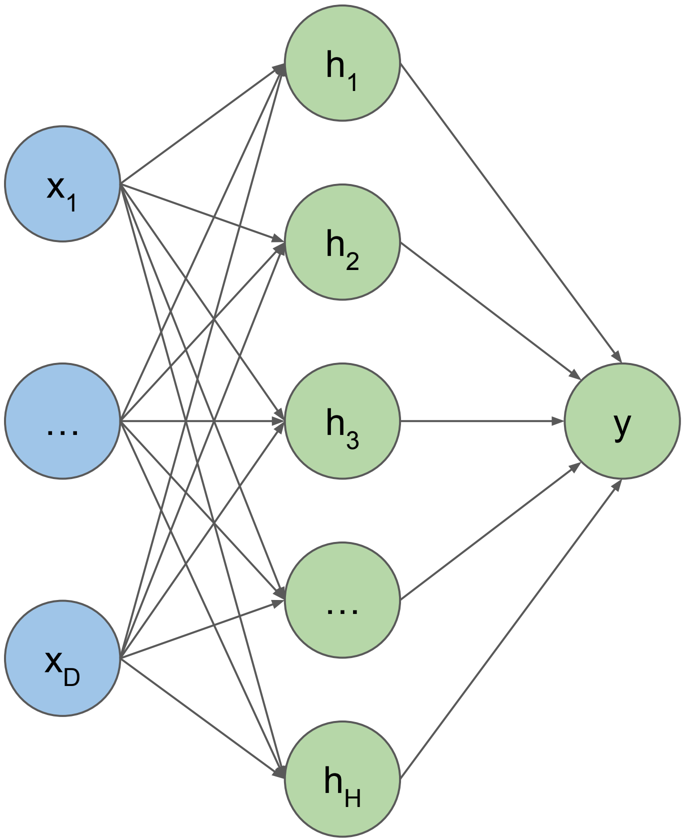
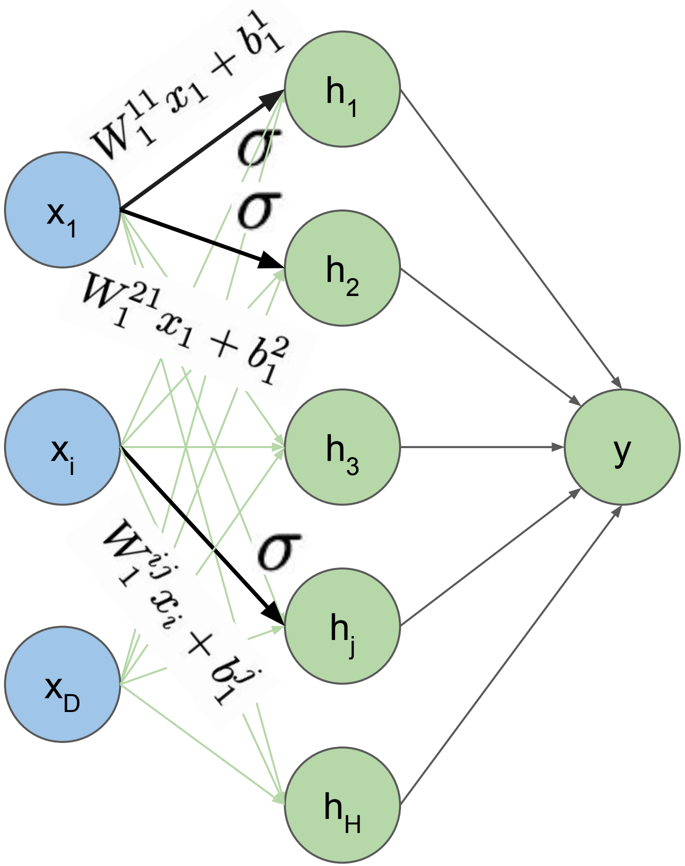
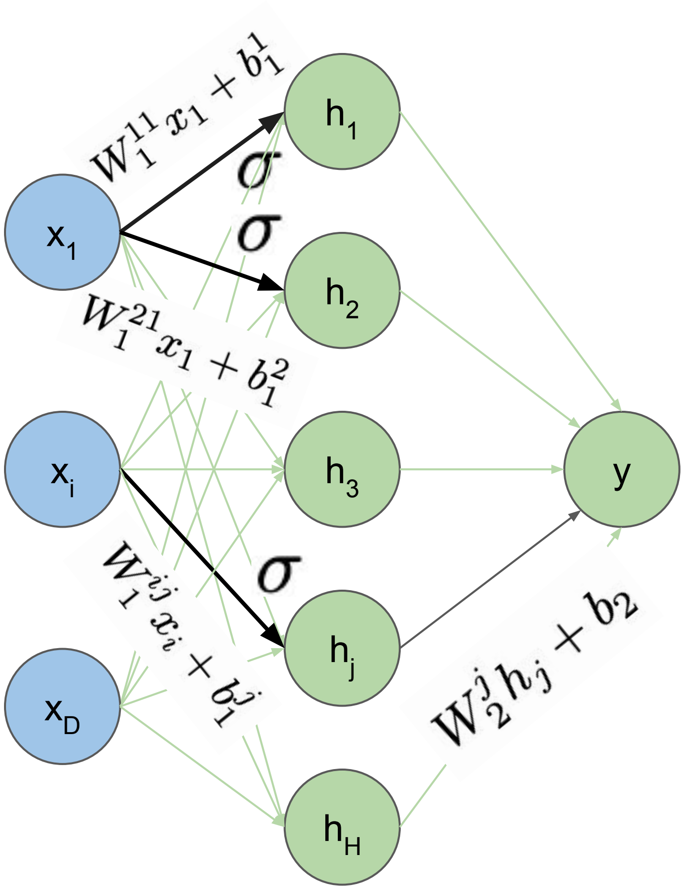
Neural Networks



Neural Networks



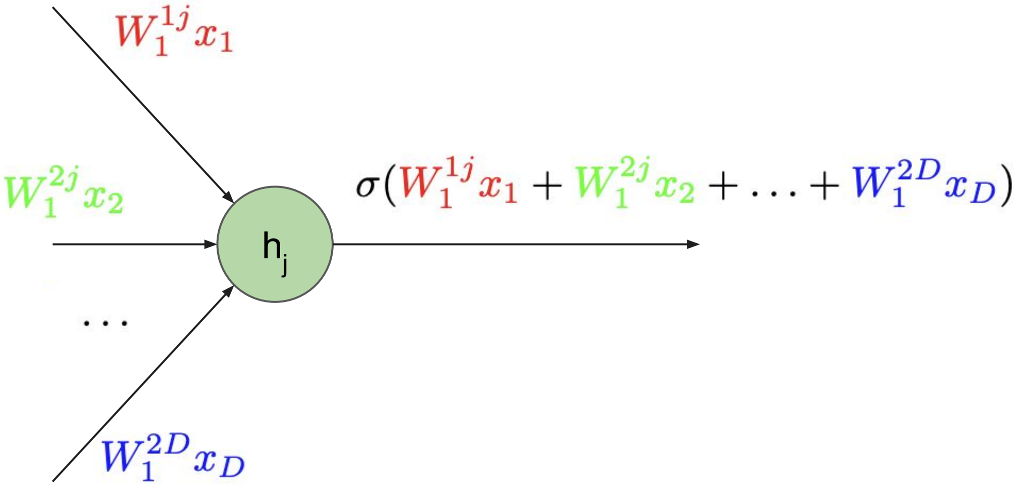
Neural Networks



$$\hat{y} = W_2\sigma(W_1x + b_1) + b_2$$

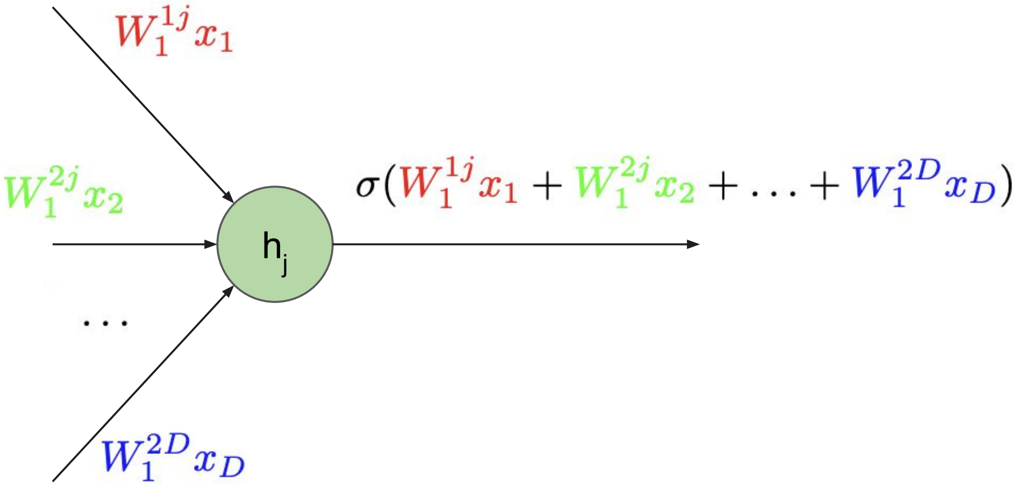
- Linear model on top of learned *hidden features **h***
- Hidden features are computed from input as a linear transform followed by element-wise non-linearity

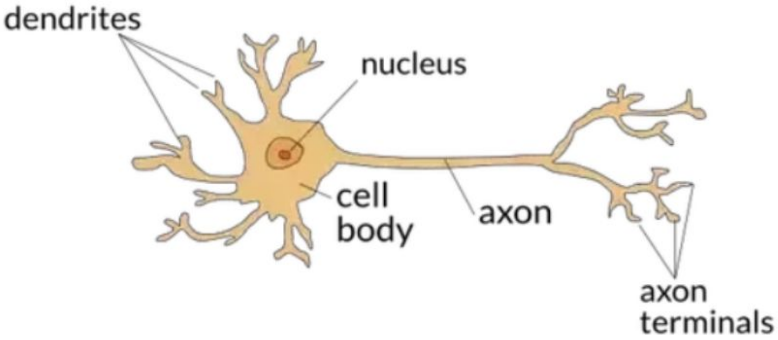
Neurons



- Each node in the network is called a neuron
- Neurons aggregate their inputs and output an *activation*

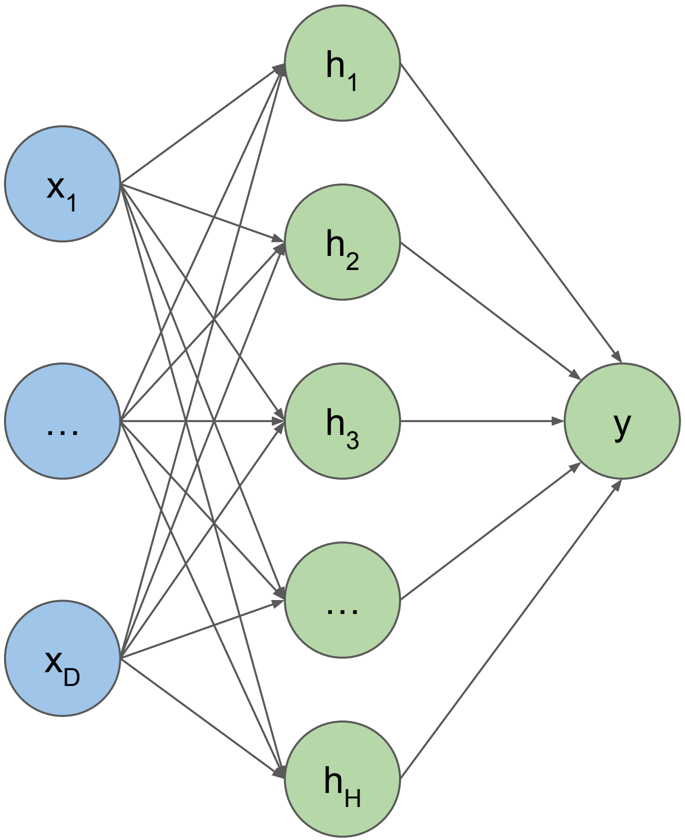
Neurons



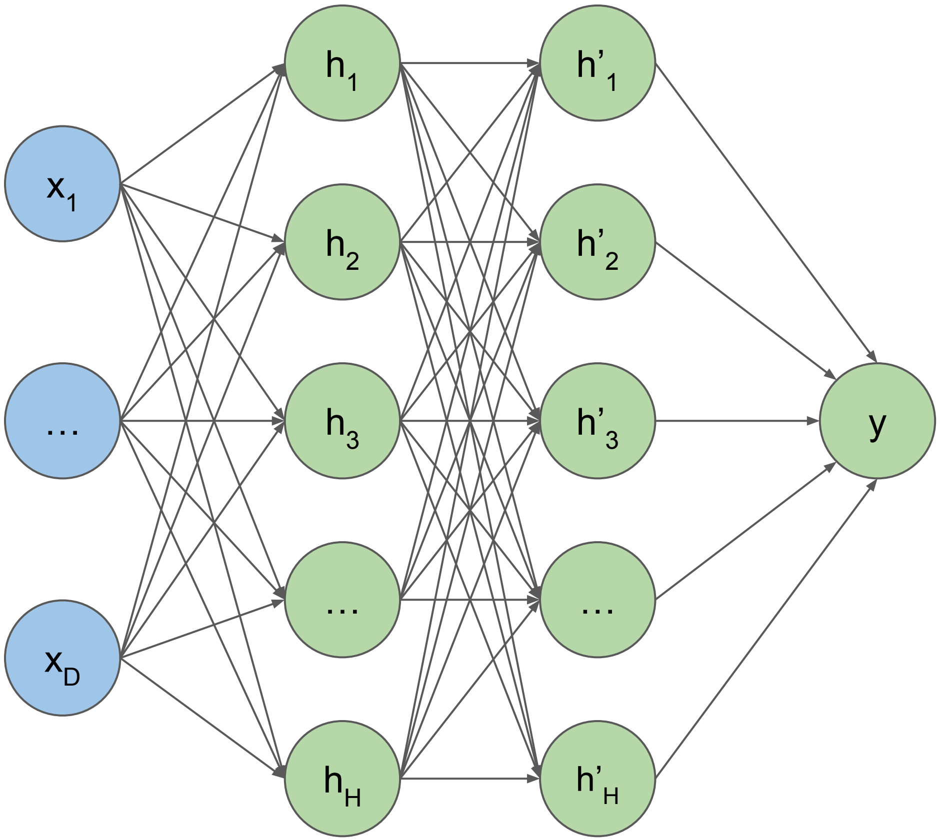


- Each node in the network is called a neuron
- Neurons aggregate their inputs and output an *activation*
- Rough analogy with a biological neuron

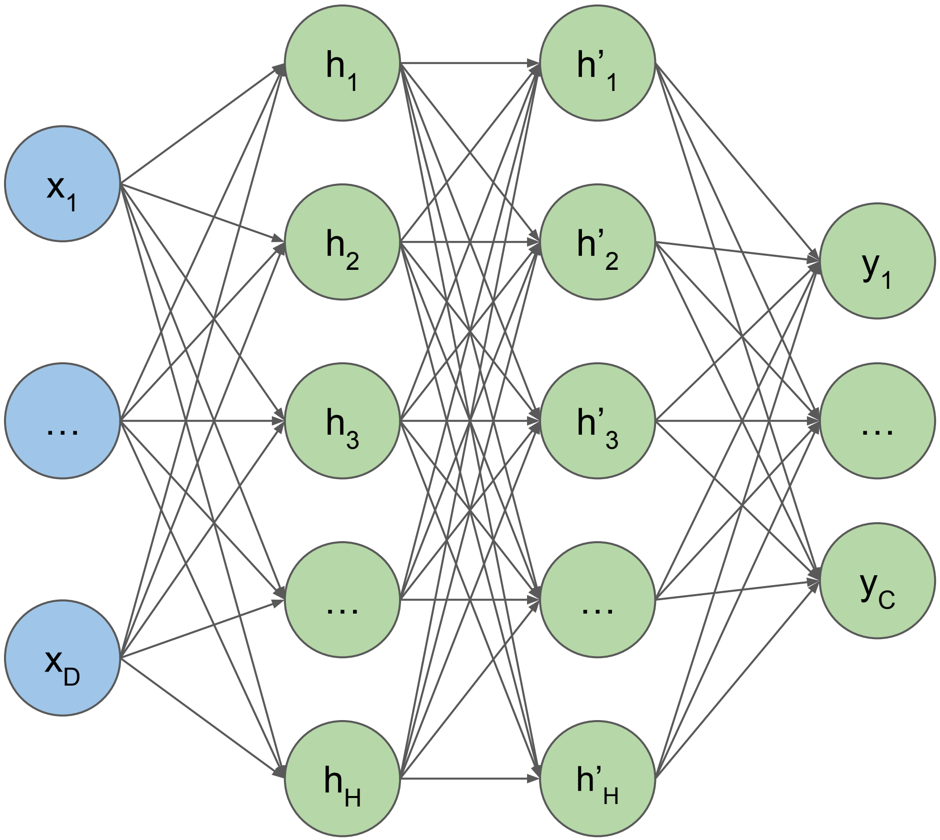
Neural Networks



Neural Networks: 2 hidden layers

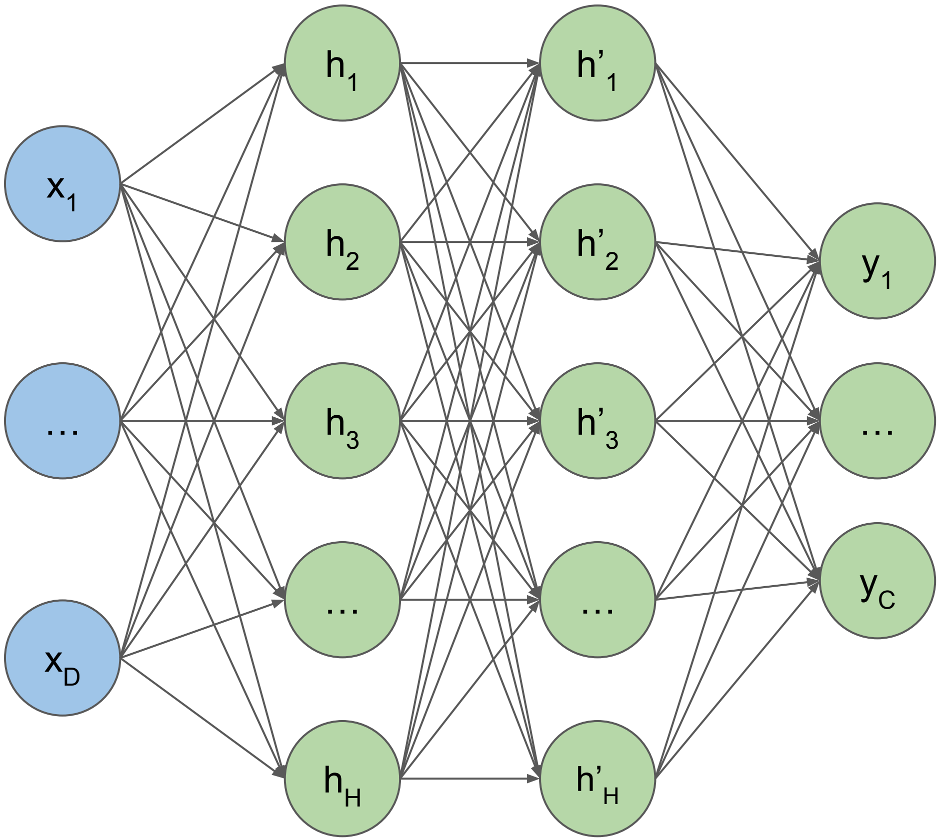


Neural Networks: multiple outputs



- How many parameters does this model have as a function of ***D, H, C***?

Neural Networks: multiple outputs



- How many parameters does this model have as a function of ***D, H, C***?

DH + H + H H + H + H C + C

Universal Approximation Theorem

See http://neuralnetworksanddeeplearning.com/, chapter 4

Universal Approximation Theorem

Universal approximation theorem—Let $C(X, \mathbb{R}^m)$ denote the set of continuous functions from a subset X of a Euclidean $\mathbb{R}^n$ space to a Euclidean space $\mathbb{R}^m$. Let $\sigma \in C(\mathbb{R}, \mathbb{R})$. Note that $(\sigma \circ x)_i = \sigma(x_i)$, so $\sigma \circ x$ denotes σ applied to each component of x.

Then σ is not polynomial if and only if for every $n \in \mathbb{N}$, $m \in \mathbb{N}$, compact $K \subseteq \mathbb{R}^n$, $f \in C(K, \mathbb{R}^m), \varepsilon > 0$ there exist $k \in \mathbb{N}$, $A \in \mathbb{R}^{k \times n}$, $b \in \mathbb{R}^k$, $C \in \mathbb{R}^{m \times k}$ such that

$$\sup_{x \in K} \|f(x) - g(x)\| < \varepsilon$$

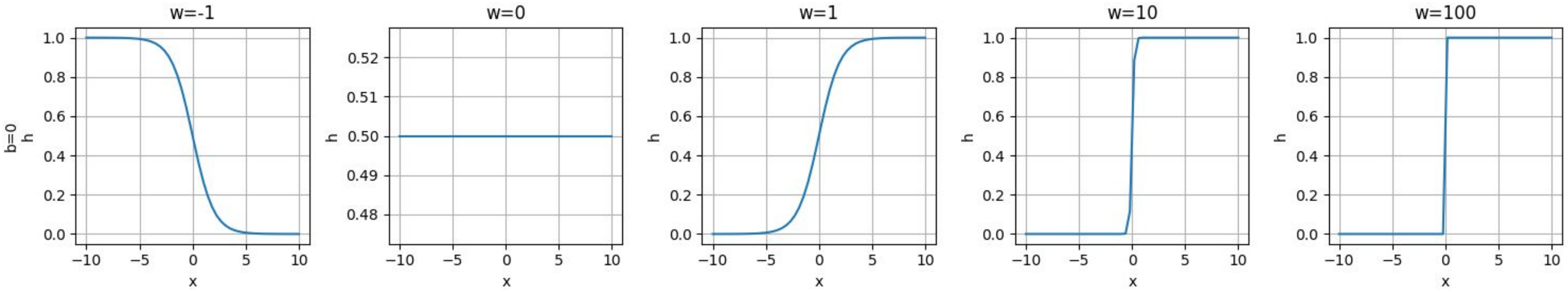
where $g(x) = C \cdot (\sigma \circ (A \cdot x + b))$

Informal version: a neural network with sufficient width with a single hidden layer can approximate any continuous function up to arbitrary precision.

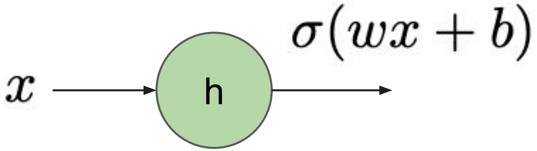
Universal Approximation Theorem

Intuitive proof sketch following Michael Nielsen's book:

$$h = \sigma(wx + b)$$



Let's look at the activations of a single neuron and change **w**



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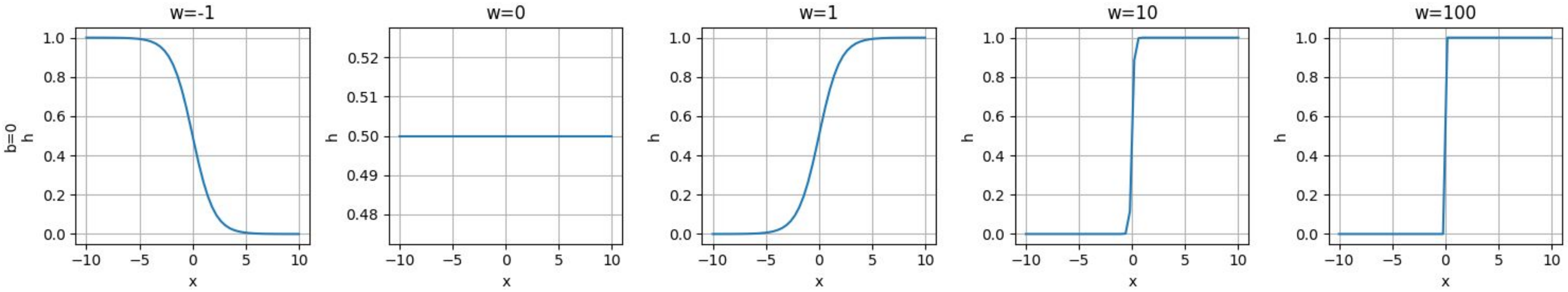
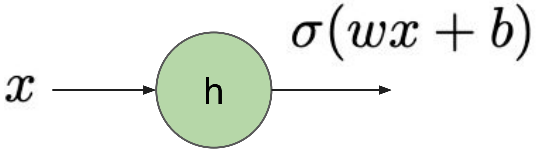


Let's look at the activations of a single neuron and change **w**

- Larger w ⇒ closer to step function



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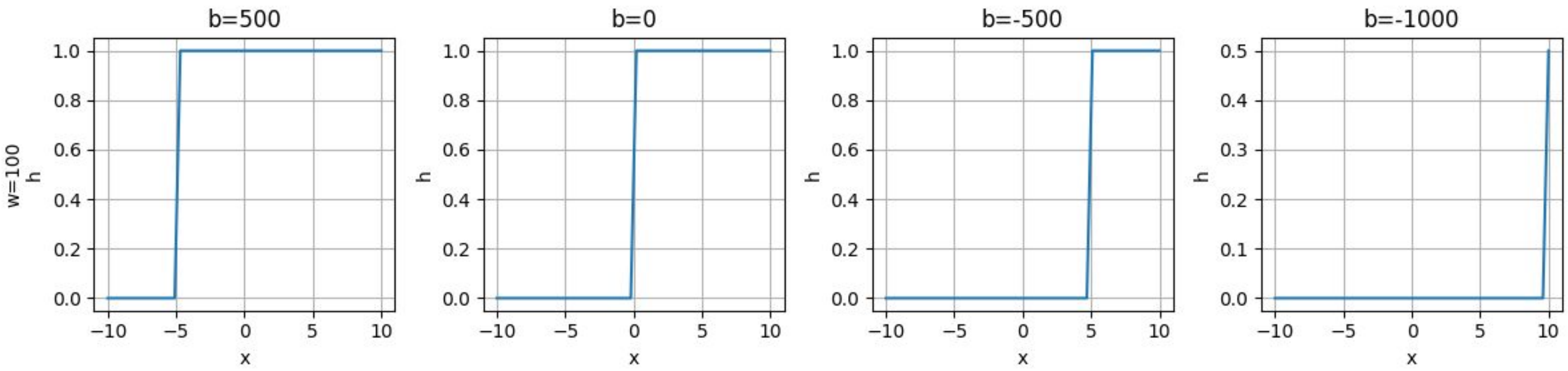
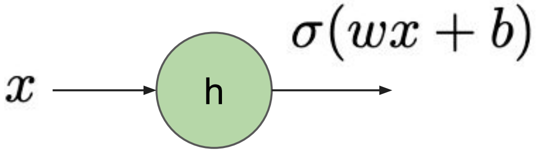


Now, let's fix **w** and change **b**.

$$\sigma(w\hat{x} + b) = 0.5 \Leftrightarrow b = -w\hat{x}.$$

- **b** shifts the curve horizontally



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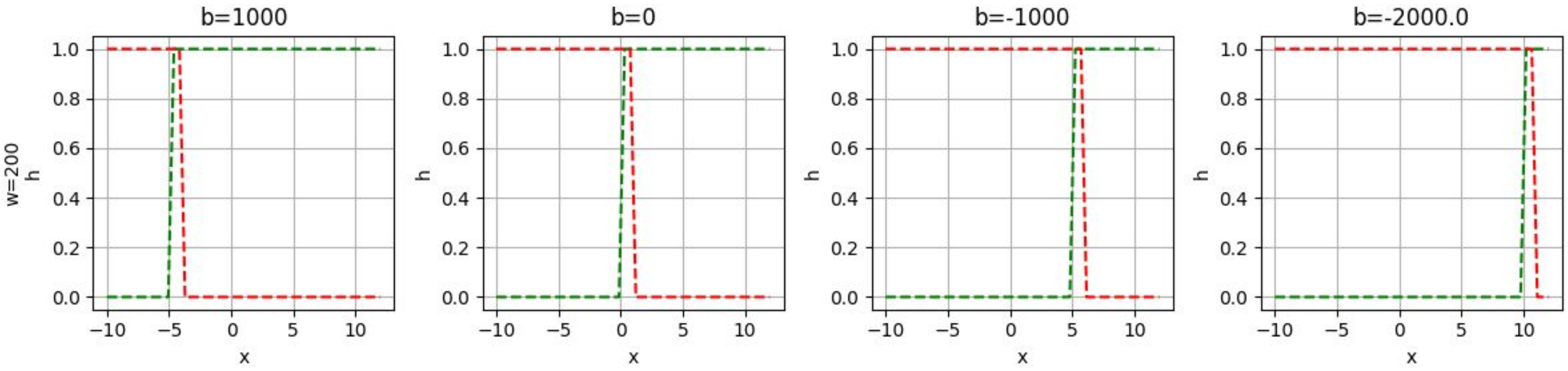


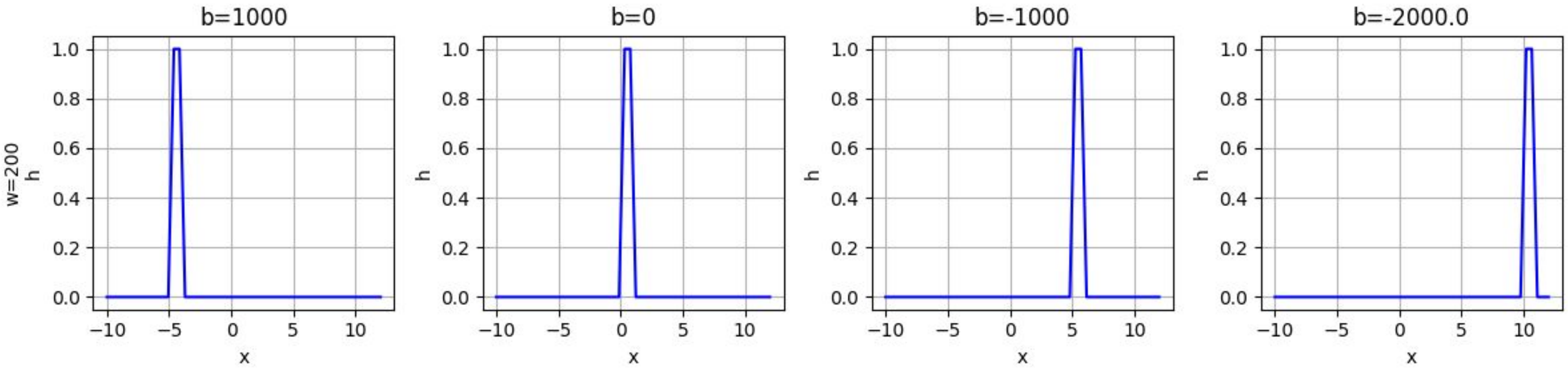
Now, let's put two of these together, but pointing in the opposite directions!

$$\sigma(wx - w\hat{x}) + \sigma(-wx + w(\hat{x} + \epsilon)) - 1$$

- We get at bump at a desired position!

Universal Approximation Theorem

Intuitive proof sketch following Michael Nielsen's book:



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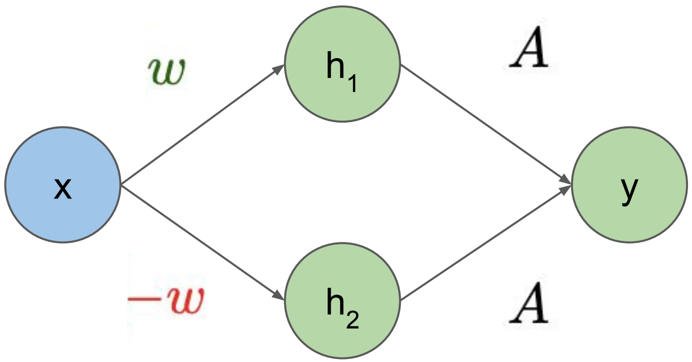
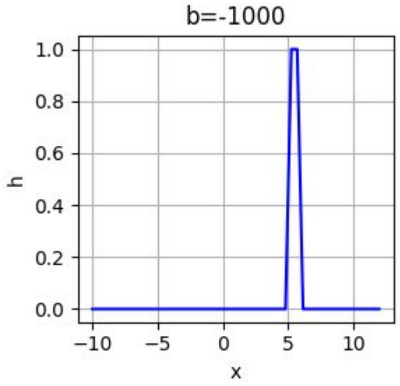
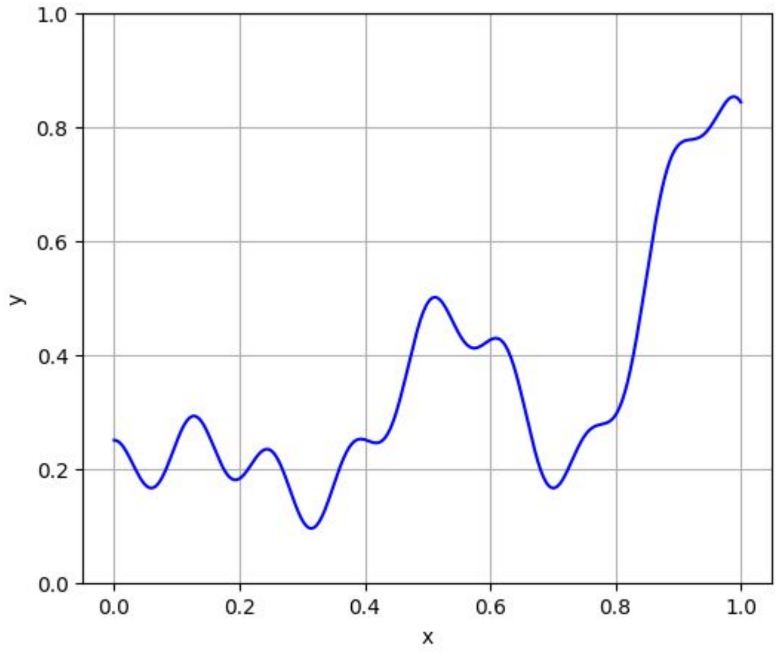




- We can create a bump with a neural net with two hidden units

$$A \cdot (\sigma(wx - w\hat{x}) + \sigma(-wx + w(\hat{x} + \epsilon)) - 1)$$

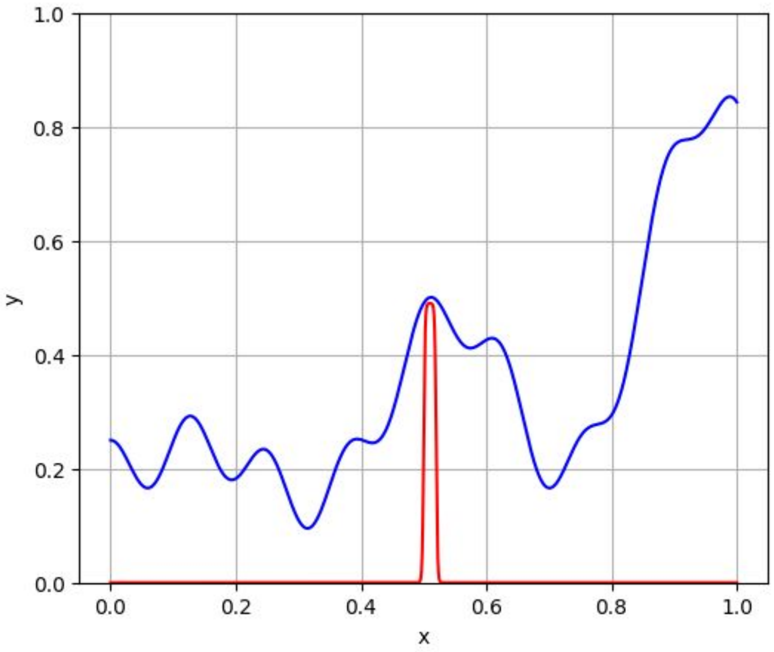
Universal Approximation Theorem



Let's approximate a function *f* with a collection of bumps.

$$\sum_{j=1}^{M} f(\hat{x}_j) \cdot (\sigma(wx - w\hat{x}_j) + \sigma(-wx + w(\hat{x}_j + \epsilon)) - 1)$$

Universal Approximation Theorem



Let's approximate a function *f* with a collection of bumps.

- Start with a bump at 0.5

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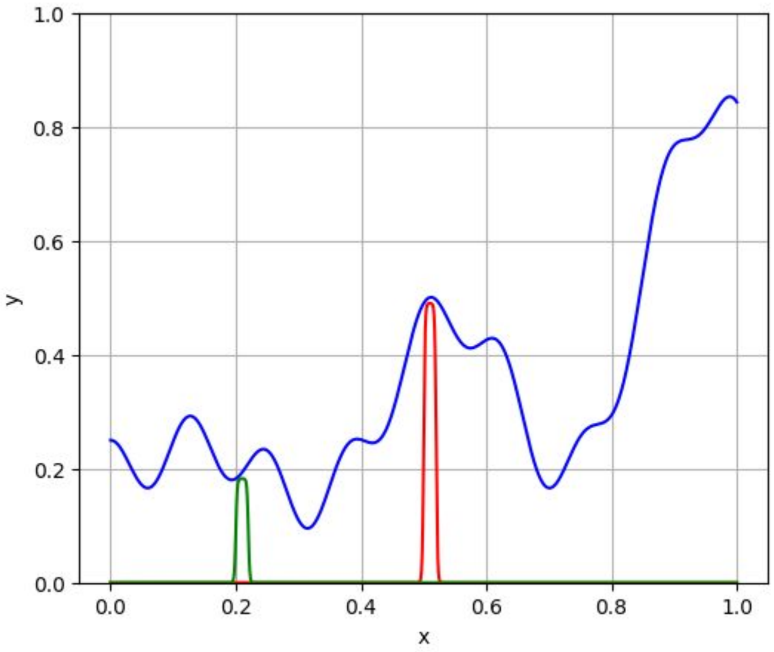
Universal Approximation Theorem

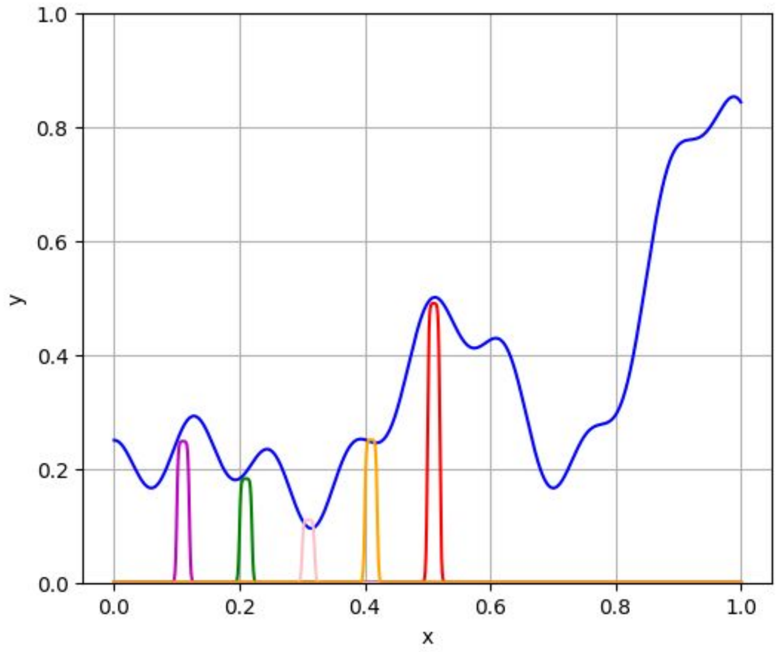


Let's approximate a function *f* with a collection of bumps.

- Start with a bump at 0.5
- Add another one at 0.2
-

$$\sum_{j=1}^{M} f(\hat{x}_j) \cdot \left(\sigma(wx - w\hat{x}_j) + \sigma(-wx + w(\hat{x}_j + \epsilon)) - 1\right)$$

Universal Approximation Theorem

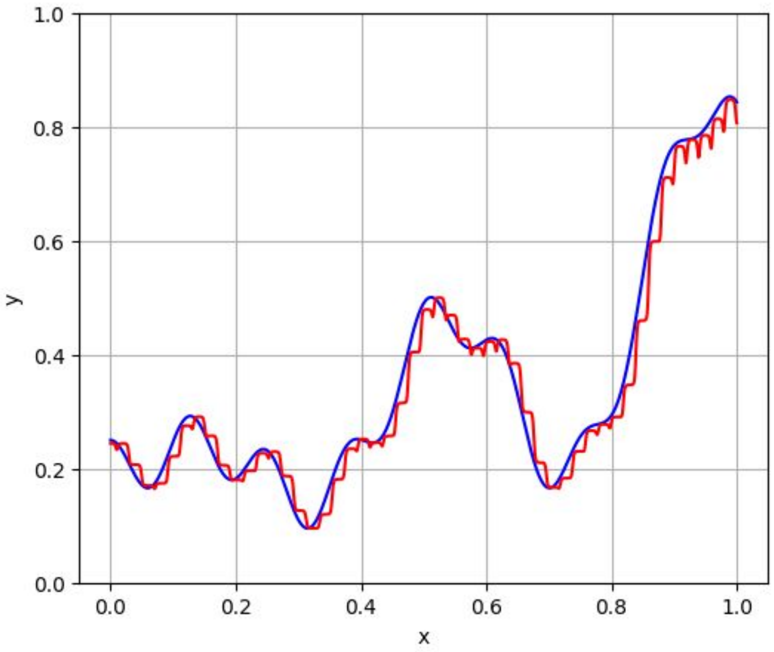


Let's approximate a function *f* with a collection of bumps.

- Start with a bump at 0.5
- Add another one at 0.2
- Keep going…

$$\sum_{j=1}^{M} f(\hat{x}_j) \cdot \left(\sigma(wx - w\hat{x}_j) + \sigma(-wx + w(\hat{x}_j + \epsilon)) - 1\right)$$

Universal Approximation Theorem

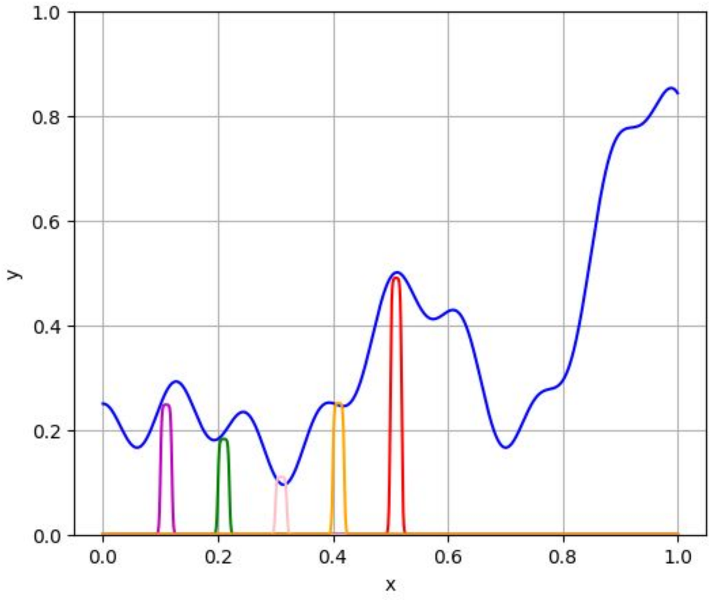


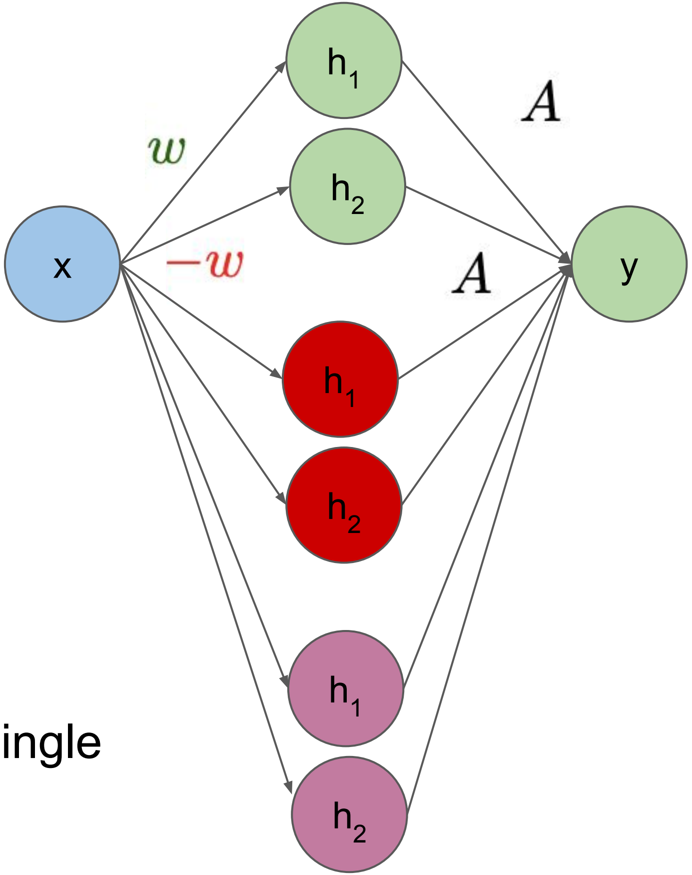
Let's approximate a function *f* with a collection of bumps.

- Start with a bump at 0.5
- Add another one at 0.2
- Keep going…
- 100 sigmoid pairs!

$$\sum_{j=1}^{M} f(\hat{x}_j) \cdot (\sigma(wx - w\hat{x}_j) + \sigma(-wx + w(\hat{x}_j + \epsilon)) - 1)$$

Universal Approximation Theorem



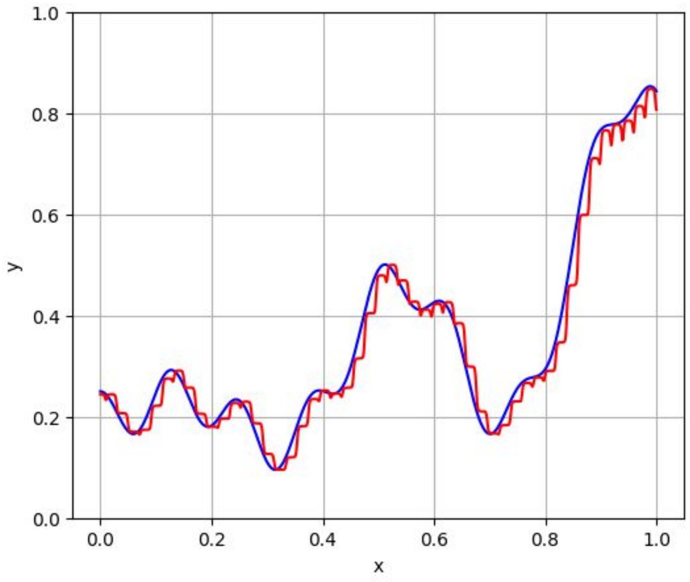


Putting the bumps together, we still get a single layer network.

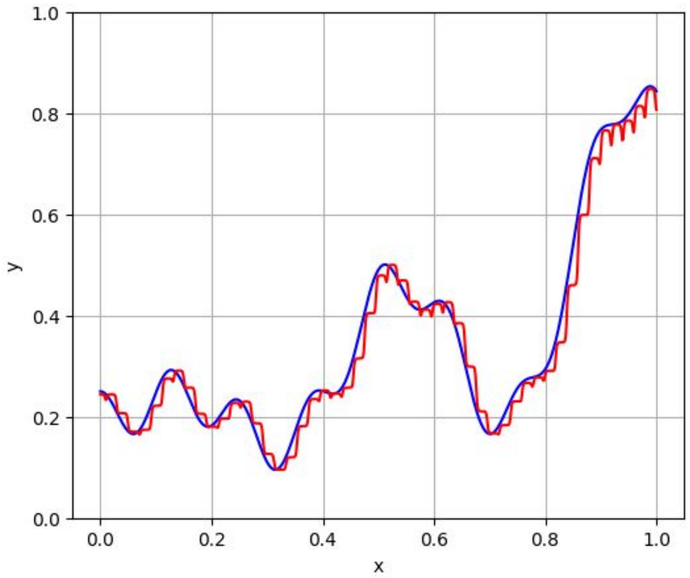
Universal Approximation Theorem

The theorem is still true if

- Multiple inputs
- Multiple outputs
- Almost arbitrary non-linearity



Universal Approximation Theorem



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- Multiple outputs
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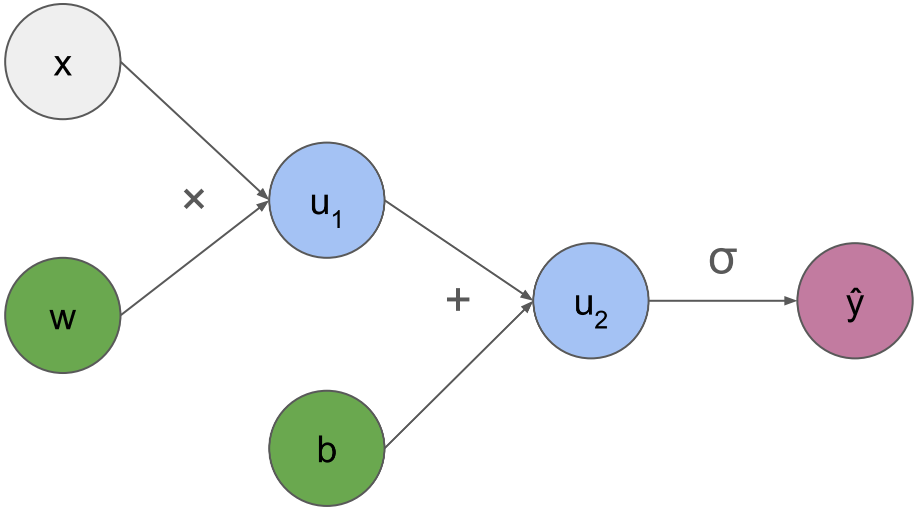
Is this how neural networks approximate functions?

- No, this is a theoretical construction; models are more parameter-efficient
- In practice, depth makes a difference

Backpropagation

See https://www.deeplearningbook.org/, chapter 6.5

Computation Graphs

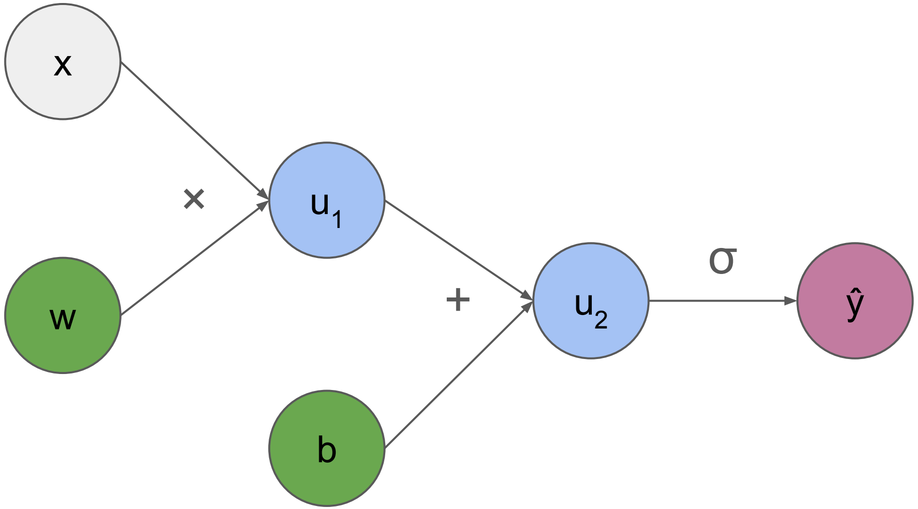


We will represent computations as graphs

- Each nodes represents a variable: input, output or intermediate
- All non-input variables are results of atomic operations on other variables
- What could the computational graph on the left do?

See https://www.deeplearningbook.org/, chapter 6.5

Computation Graphs



Notice that we introduced auxiliary variables that we don't normally have.

We will represent computations as graphs

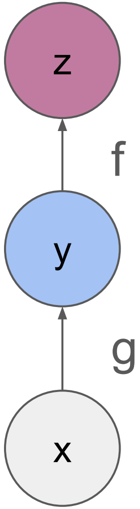
- Each nodes represents a variable: input, output or intermediate
- All non-input variables are results of atomic operations on other variables
- What could the computational graph on the left do?
  Logistic regression prediction

Chain Rule

$$z = f(g(x))$$
$$y = g(x)$$
$$z = f(y)$$

$$\frac{dz}{dx} =$$

All variables are scalars



Chain Rule

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$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$$

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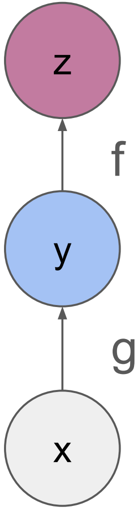

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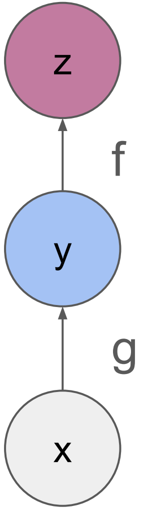

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \cdot \frac{\partial y_j}{\partial x_i}$$

If y and x are vectors

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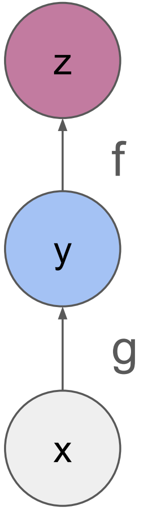

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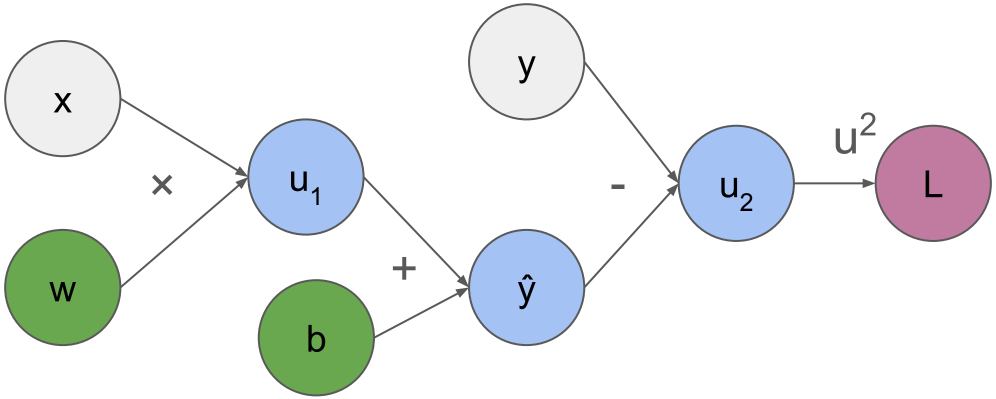
If y and x are vectors

Jacobian matrix

$$\nabla_x z = \left(\frac{\partial y}{\partial x}\right)^T \nabla_y z$$

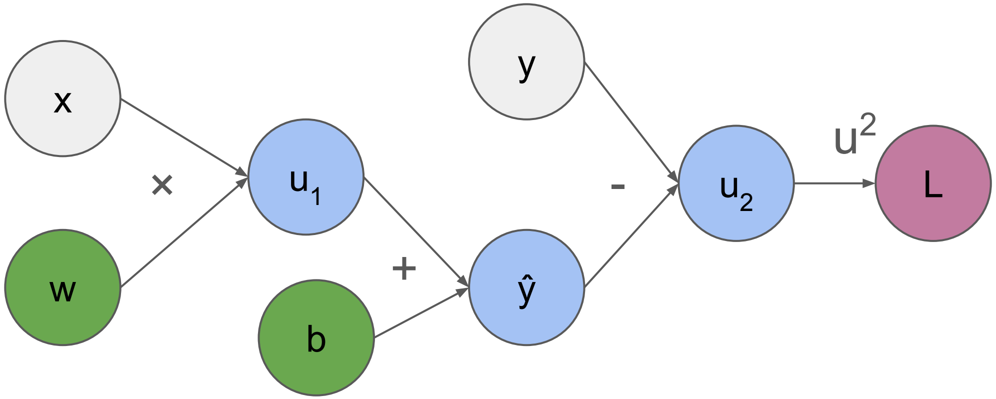
Backpropagation example: linear regression



Forward pass: evaluate the computation graph

$$u_1 = xw$$
$$\hat{y} = u_1 + b$$
$$u_2 = y - \hat{y}$$
$$L = u_2^2$$

Backpropagation example: linear regression



Backward pass: reverse the order of computation

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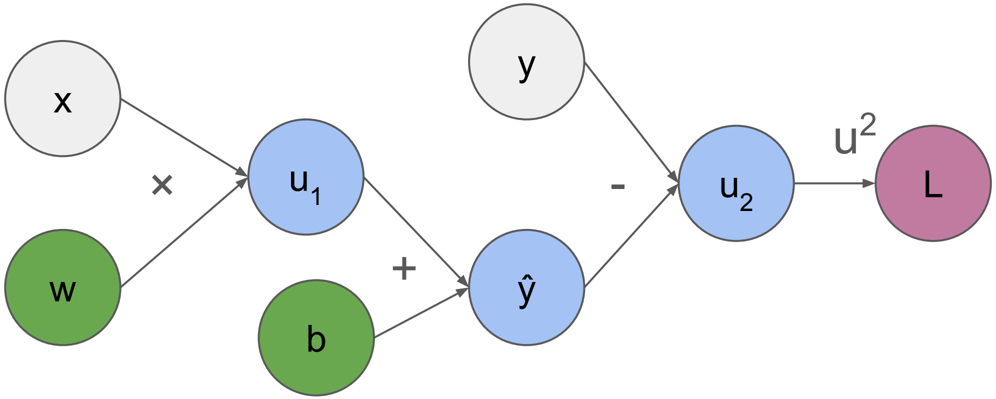

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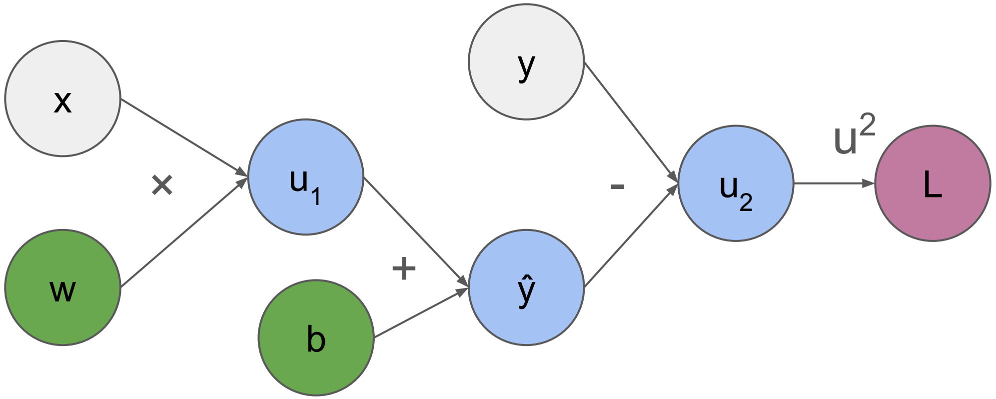

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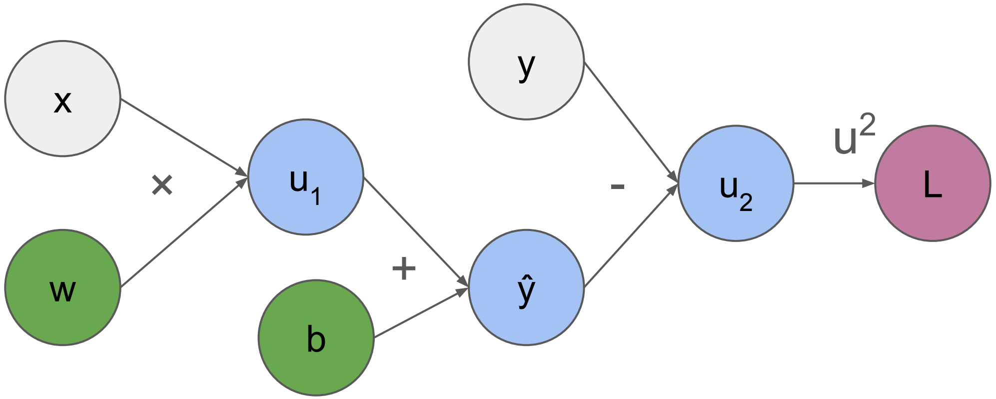

Backward pass: reverse the order of computation

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial u_1} \cdot \frac{\partial u_1}{\partial w} = -2u_2 \cdot x$$

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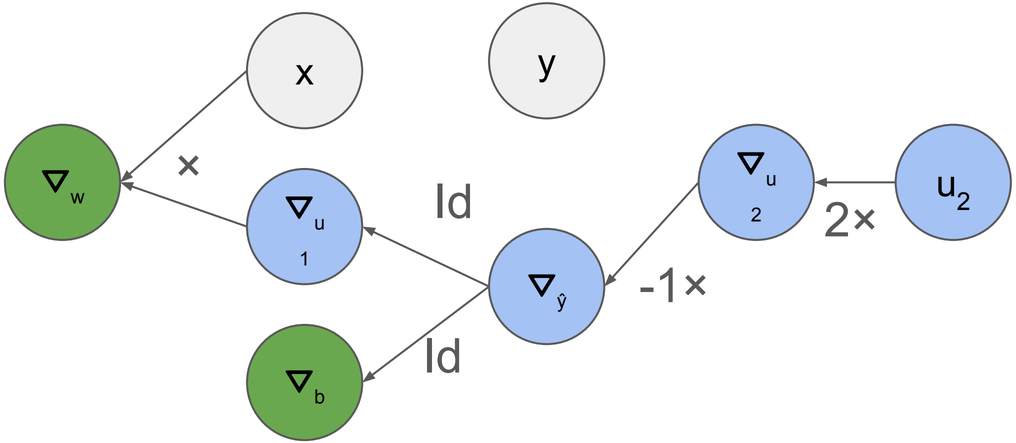

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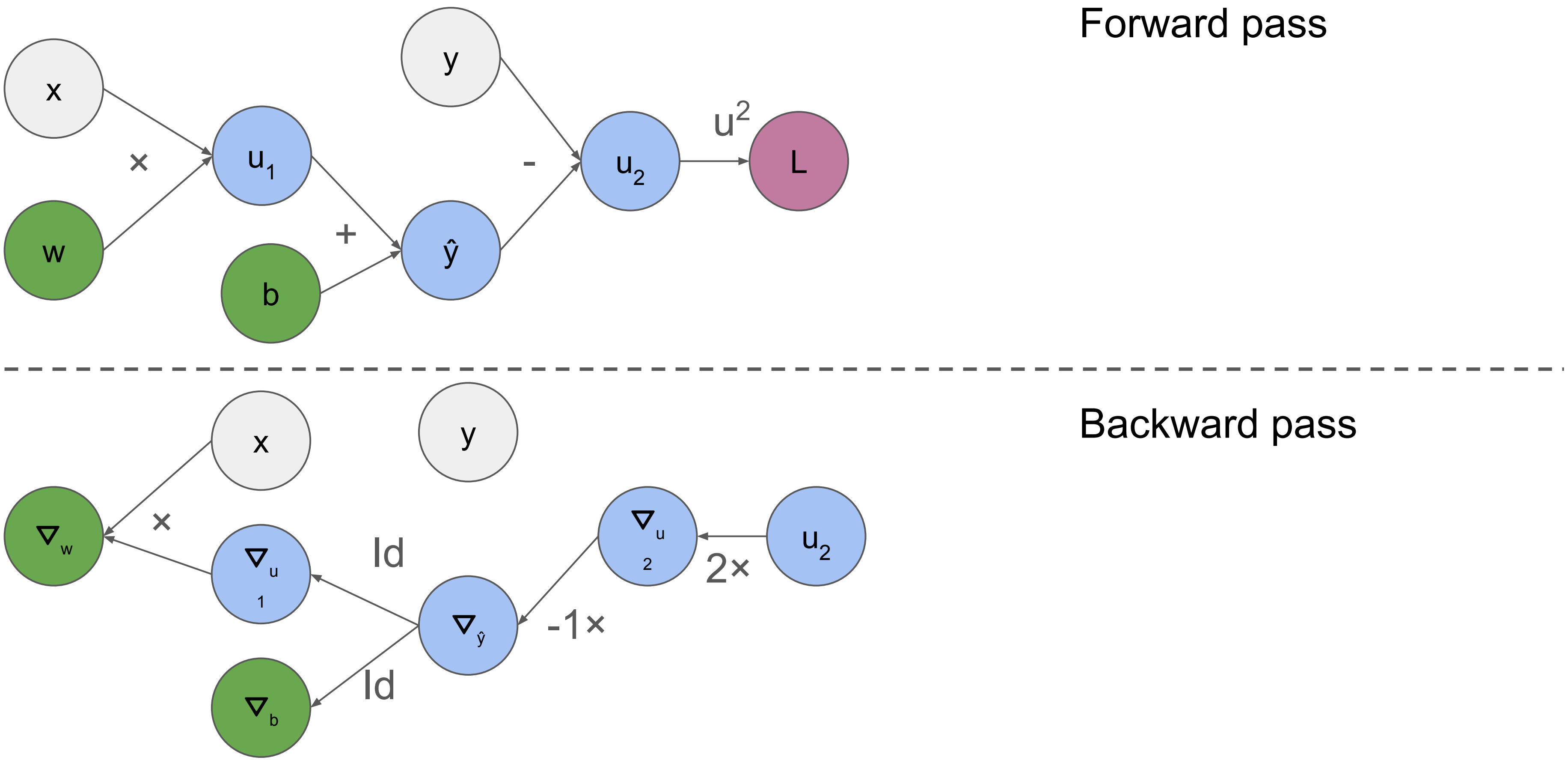
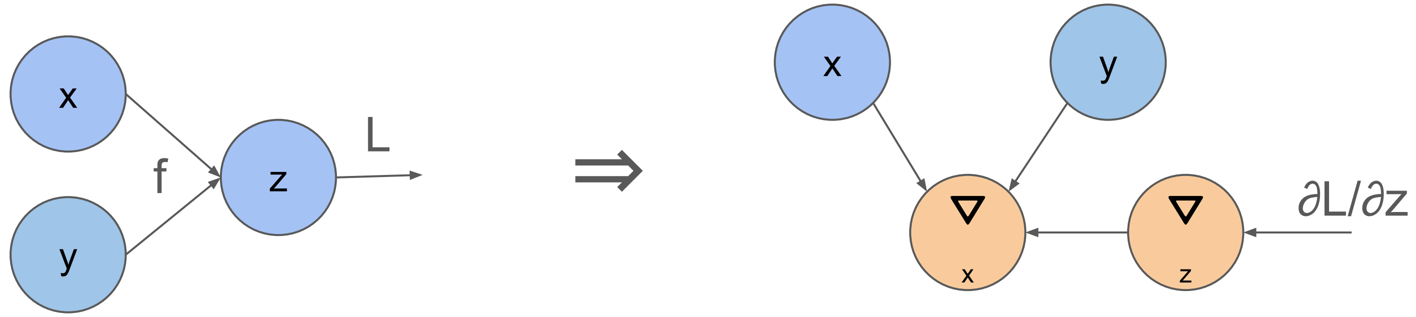


Backward computation graph

We can always construct the backward graph algorithmically

- Nodes:
  - Keep all the nodes from the forward pass
  - Add a gradient node for each of the forward nodes
- Edges:
  - Backward of the original edges + a few rules



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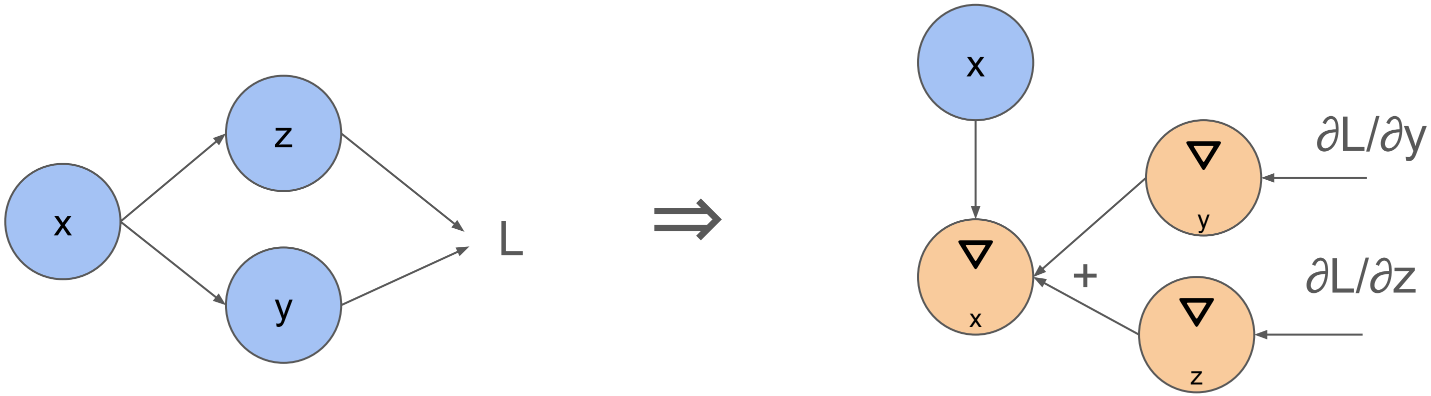

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- Nodes:
  - Keep all the nodes from the forward pass
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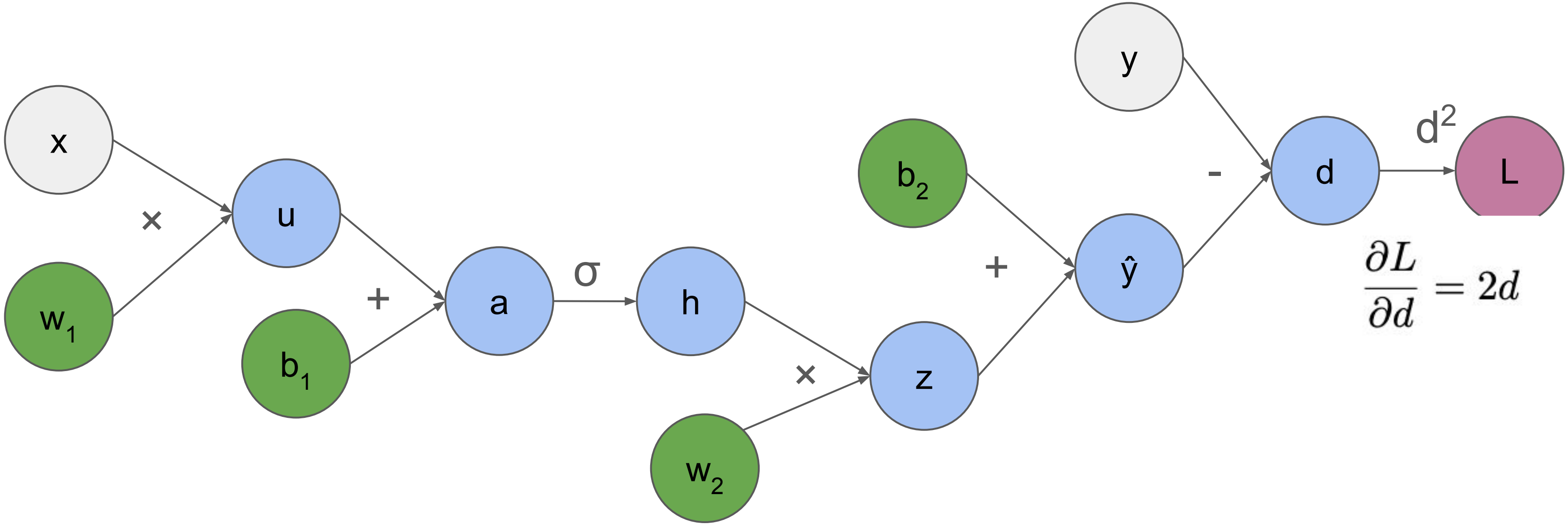
- Edges:
  - Backward of the original edges + a few rules

In general, backward pass:

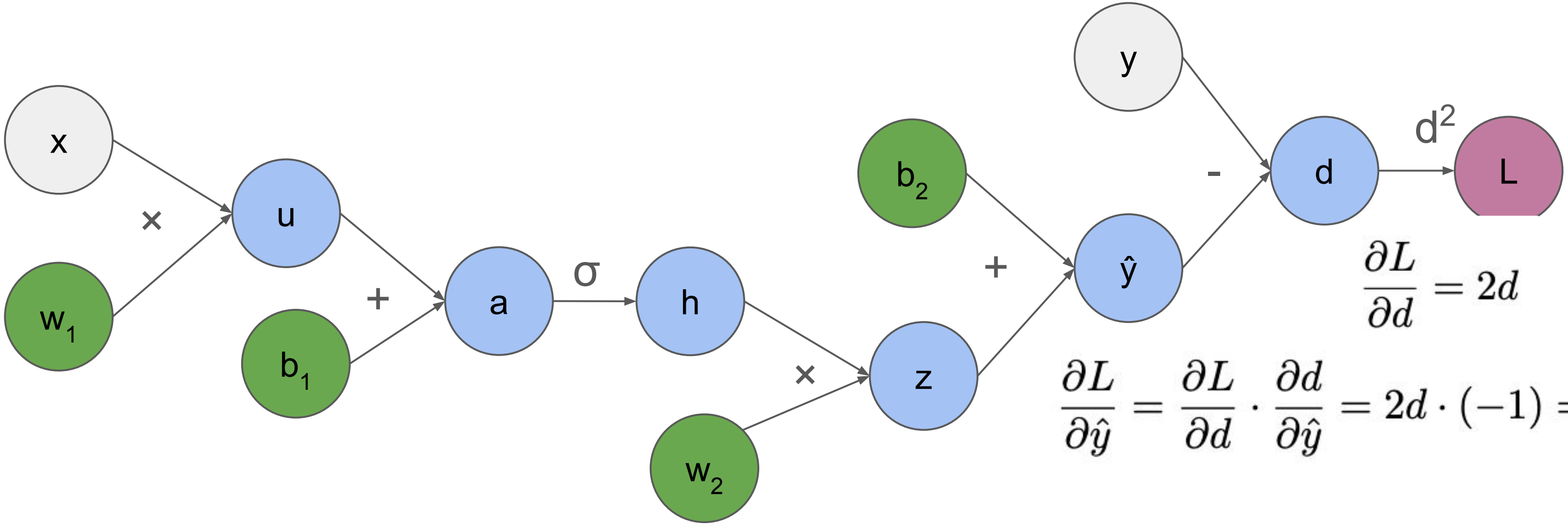
- 2x the nodes, 2x memory
- Need to keep around all intermediate values
- Backward cost ≤ c * forward cost, c is 2-4 for NNs

Backprop: MLP (scalar)



$$\frac{\partial L}{\partial d} = 2d$$

Backprop: MLP (scalar)

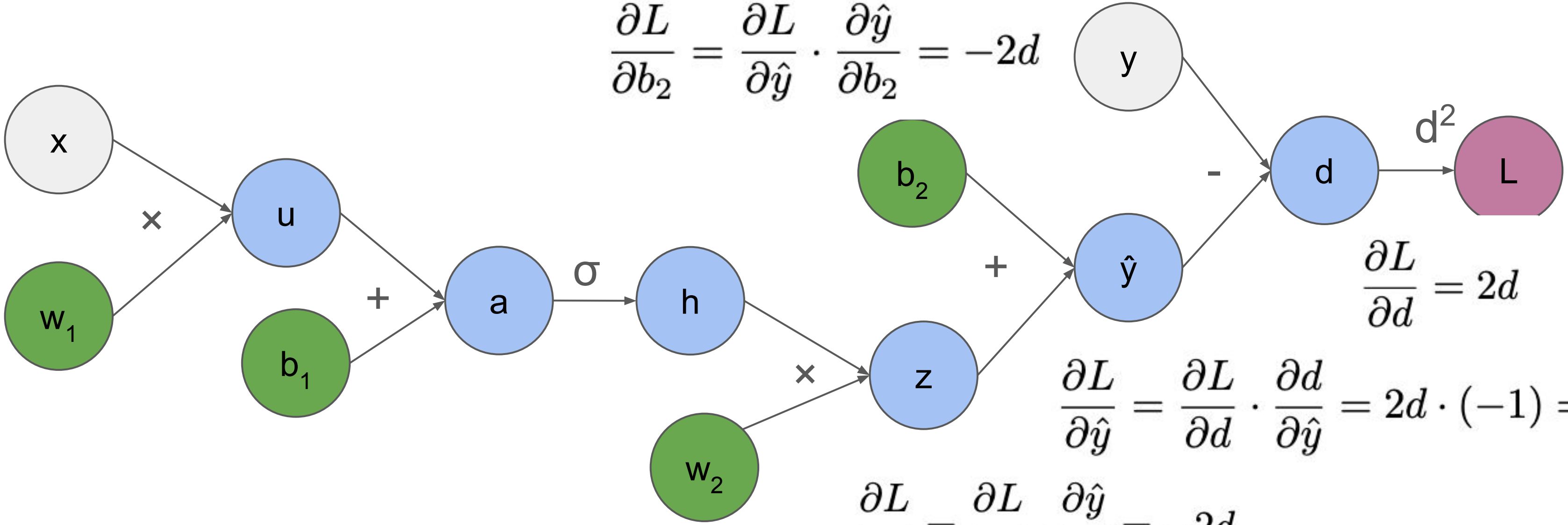


$$\frac{\partial L}{\partial d} = 2d$$

$$\frac{\partial L}{\partial \hat{y}} = \frac{\partial L}{\partial d} \cdot \frac{\partial d}{\partial \hat{y}} = 2d \cdot (-1) = -2d$$

Backprop: MLP (scalar)

$$\frac{\partial L}{\partial b_2} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial b_2} = -2d$$



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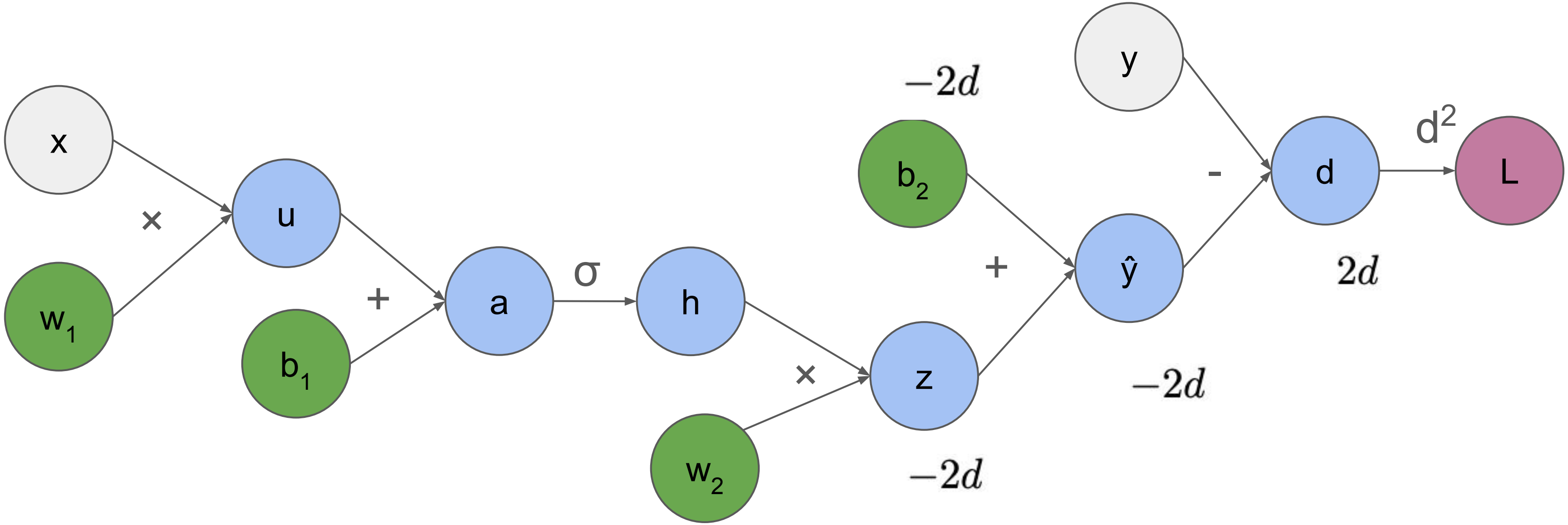
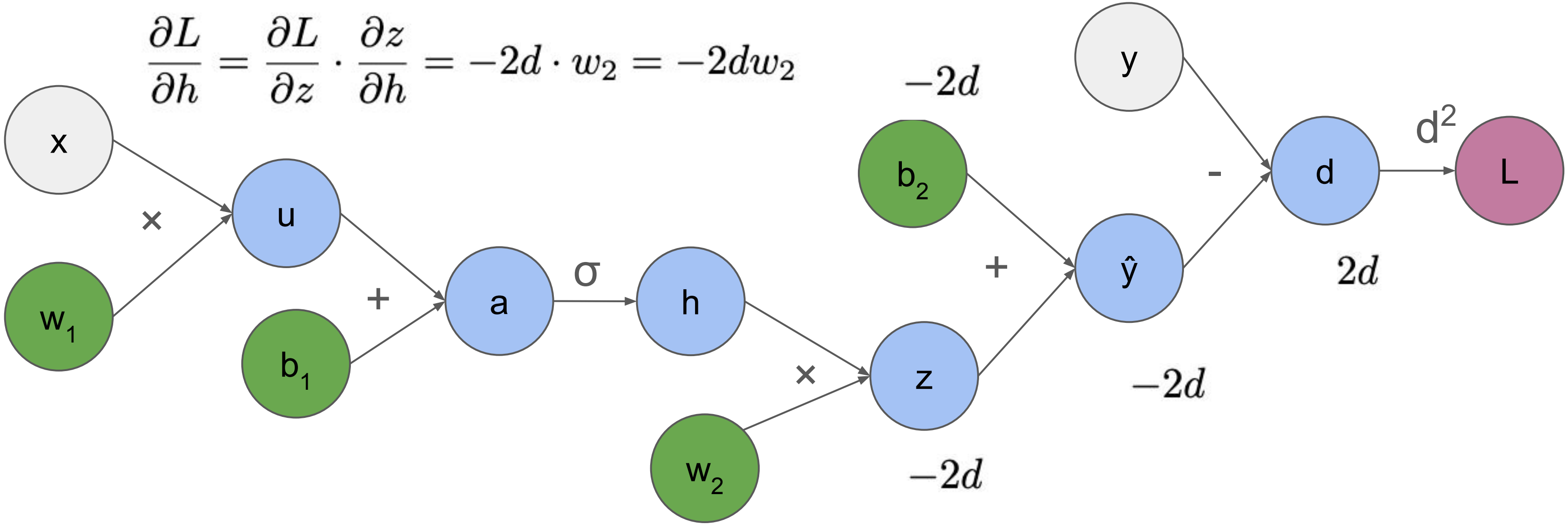


Backprop: MLP (scalar)

$$\frac{\partial L}{\partial h} = \frac{\partial L}{\partial z} \cdot \frac{\partial z}{\partial h} = -2d \cdot w_2 = -2dw_2$$



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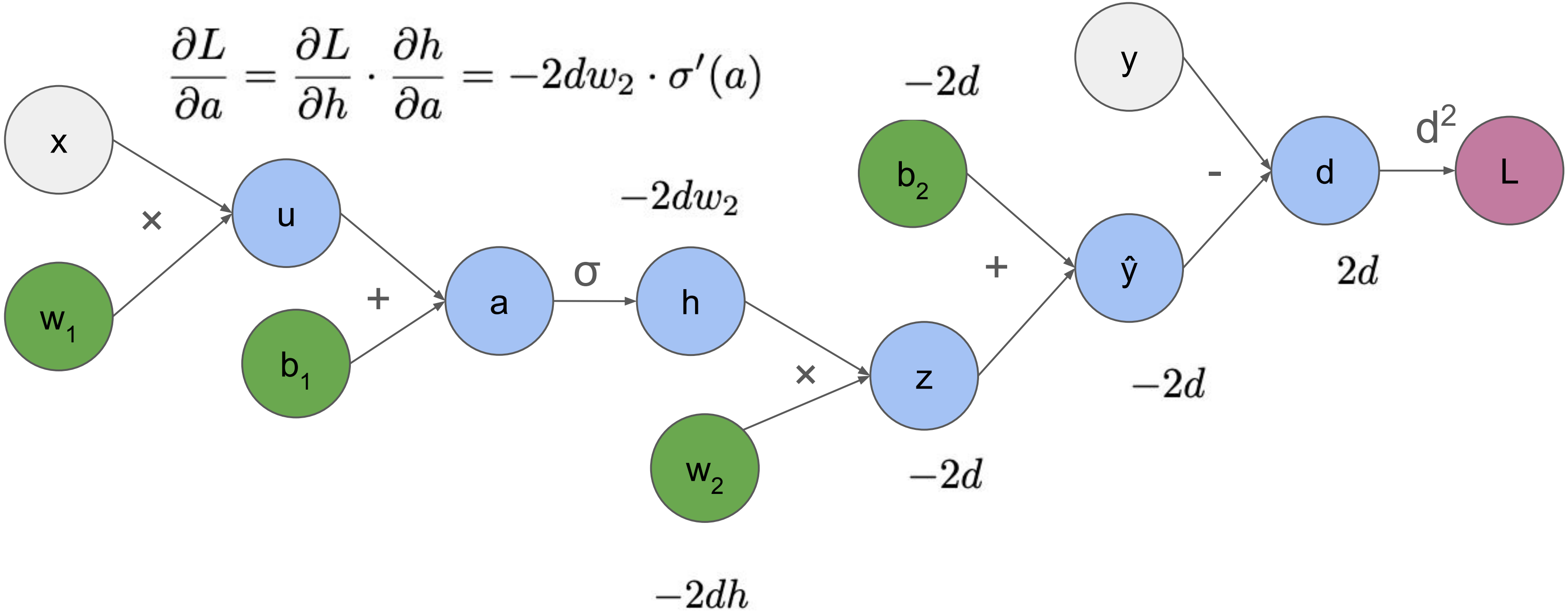
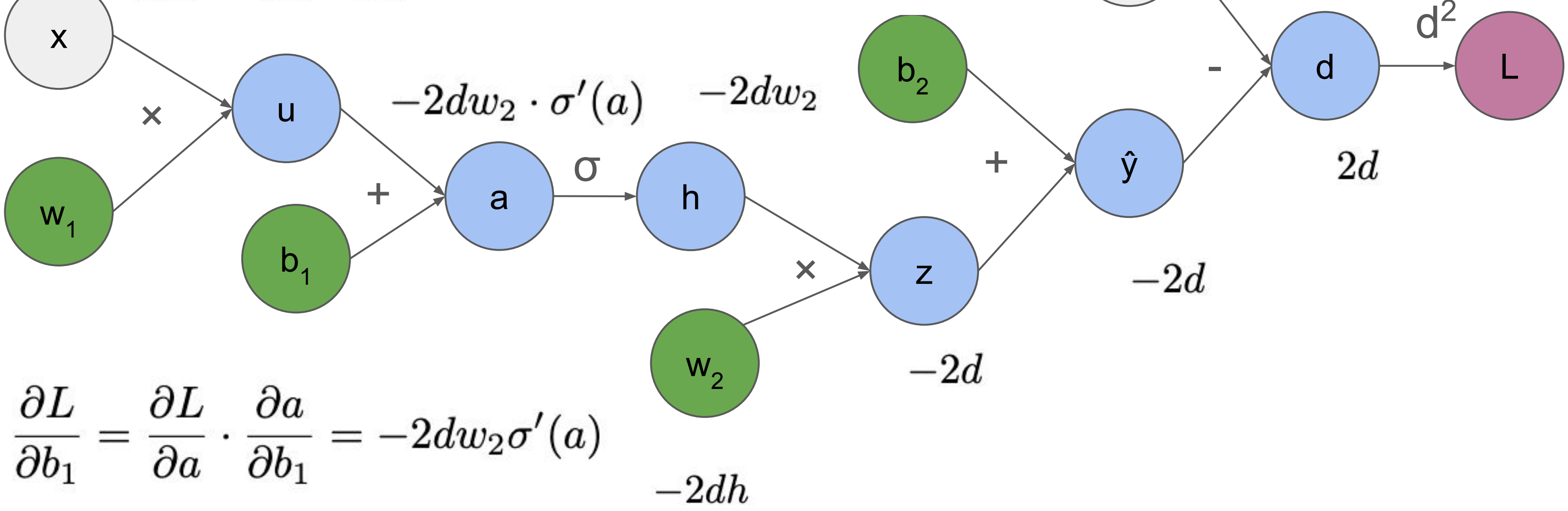
Backprop: MLP (scalar)

$$\frac{\partial L}{\partial a} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial a} = -2dw_2 \cdot \sigma'(a)$$



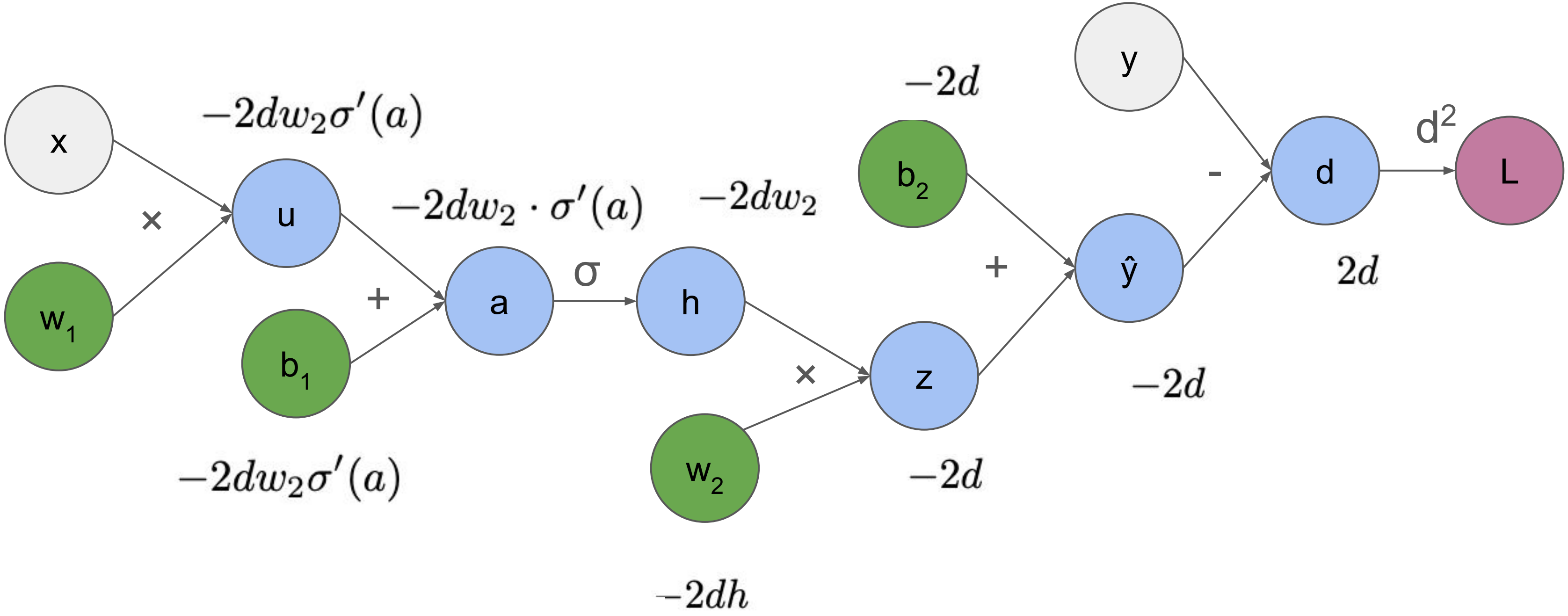
Backprop: MLP (scalar)

$$\frac{\partial L}{\partial u} = \frac{\partial L}{\partial a} \cdot \frac{\partial a}{\partial u} = -2dw_2\sigma'(a)$$



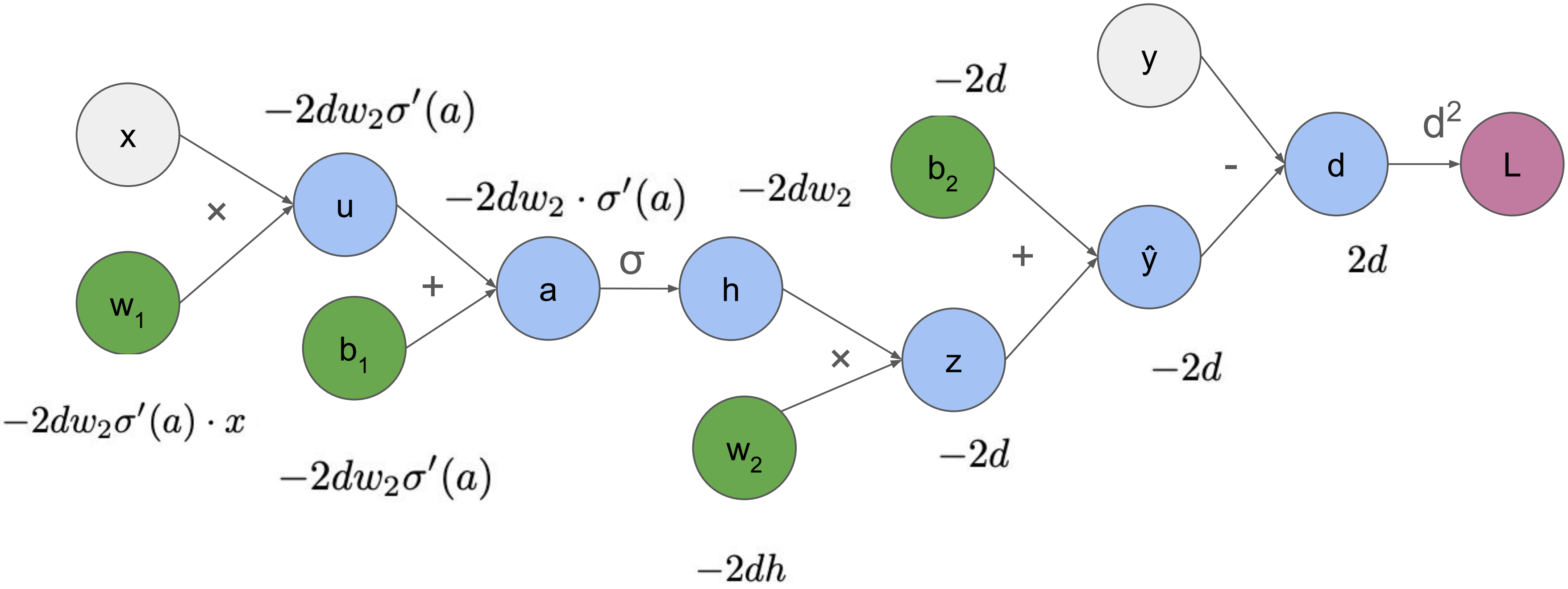
$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a} \cdot \frac{\partial a}{\partial b_1} = -2dw_2\sigma'(a)$$

Backprop: MLP (scalar)



$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial u} \cdot \frac{\partial u}{\partial w_1} = -2dw_2\sigma'(a) \cdot x$$

Backprop: MLP (scalar)



We computed the gradients with respect to all the parameters

- We can now update all the parameters with gradient descent

Backprop: MLP general case

$$x \in \mathbb{R}^{n_{in}},\ W_1 \in \mathbb{R}^{n_h \times n_{in}},\ b_1 \in \mathbb{R}^{n_h}$$
$$h \in \mathbb{R}^{n_h},\ W_2 \in \mathbb{R}^{n_{out} \times n_h},\ b_2 \in \mathbb{R}^{n_{out}}$$
$$y, \hat{y}, d \in \mathbb{R}^{n_{out}},\ L \in \mathbb{R}$$

$$u = W_1 x$$
$$a = u + b_1$$
$$h = \sigma(a)$$
$$z = W_2 h$$
$$\hat{y} = z + b_2$$
$$d = \hat{y} - y$$
$$L = d^T d = \|d\|^2$$

Forward pass

$$\frac{\partial L}{\partial L} = 1$$
$$\frac{\partial L}{\partial d} = 2d$$
$$\frac{\partial L}{\partial \hat{y}} = 2d$$
$$\frac{\partial L}{\partial b_2} = 2d$$
$$\frac{\partial L}{\partial z} = 2d$$

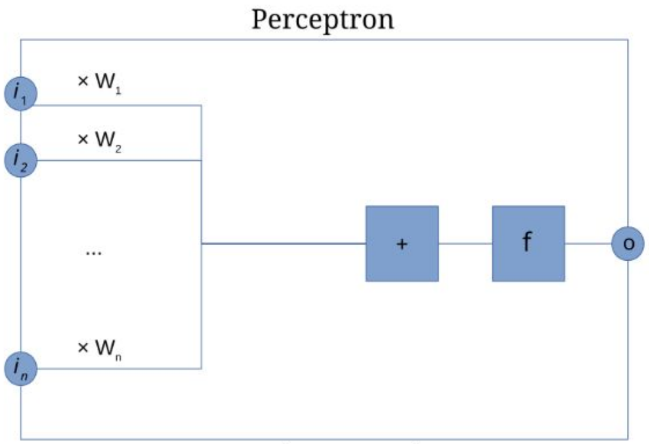
$$\frac{\partial L}{\partial W_2} = 2d\, h^T$$
$$\frac{\partial L}{\partial h} = W_2^T (2d)$$
$$\frac{\partial L}{\partial a} = \frac{\partial L}{\partial h} \odot \sigma'(a)$$

$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial a}$$
$$\frac{\partial L}{\partial u} = \frac{\partial L}{\partial a}$$
$$\frac{\partial L}{\partial W_1} = \frac{\partial L}{\partial u} x^T$$

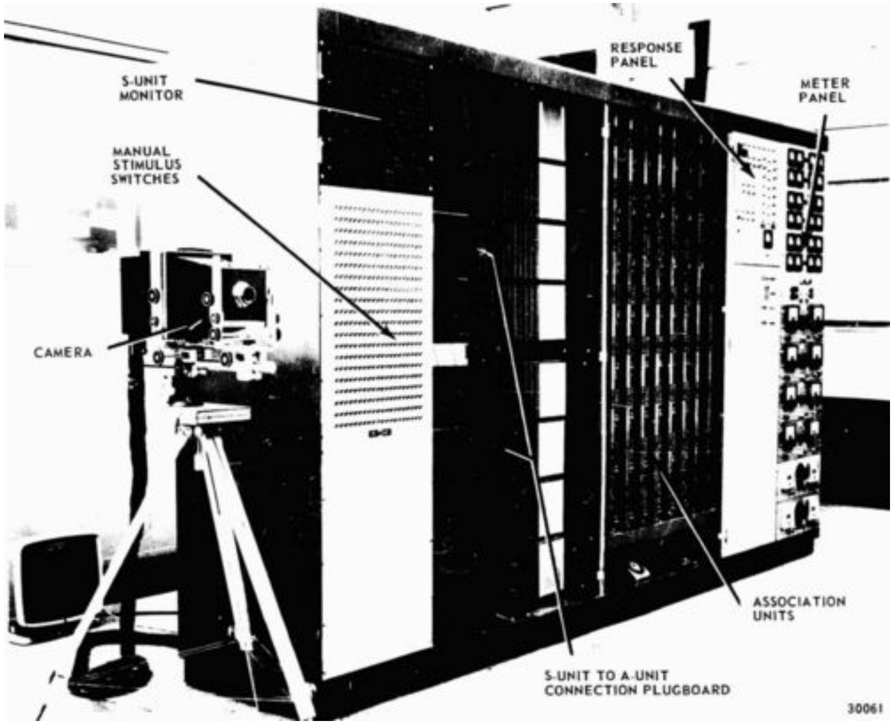
Backward pass

History

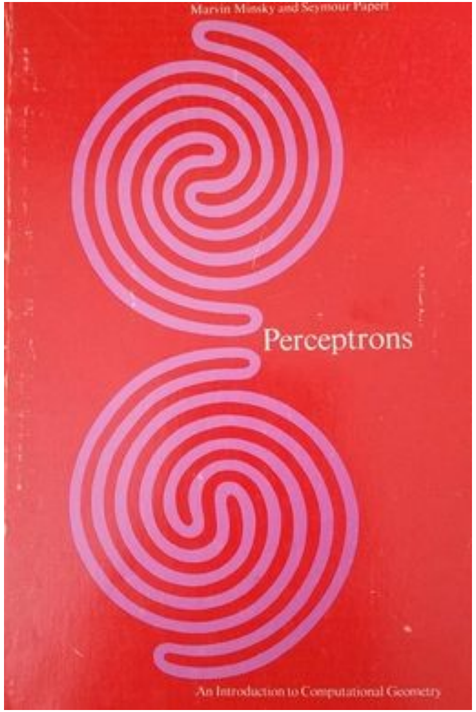
Rosenblatt Perceptron (1957)



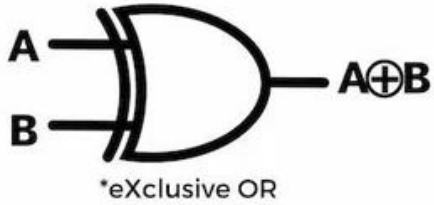
$$o = f\left(\sum_{k=1}^{n} i_k \cdot W_k\right)$$



Marvin Minsky, Seymour Papert (1969)



Showed that perceptrons cannot represent XOR

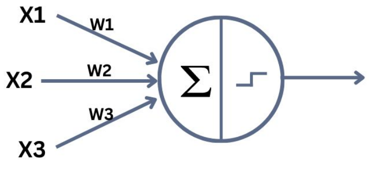


A	B	A⊕B
0	0	0
0	1	1
1	0	1
1	1	0

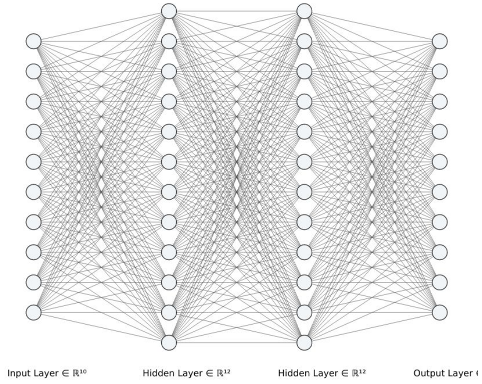
Caused AI winter

Hinton et al: Backpropagation (1986)

Showed how to train Multi-Layer Perceptrons



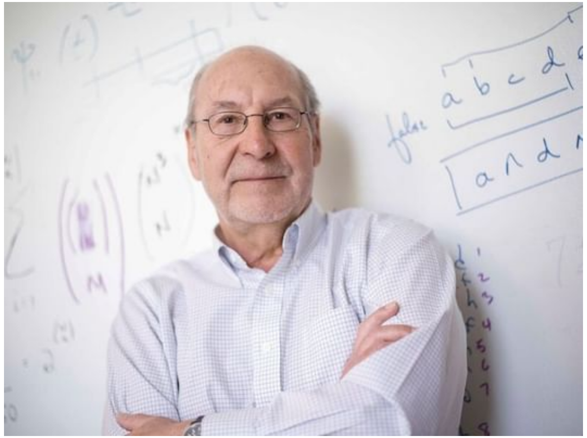
Single-layer perceptron

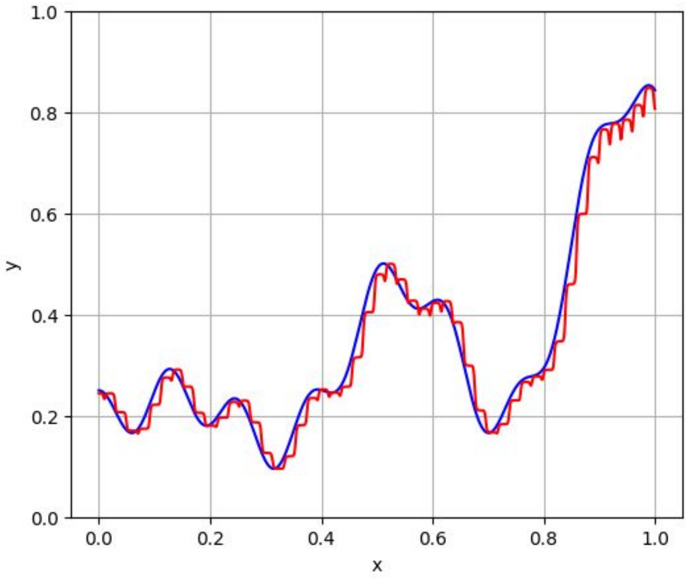


Multi-layer perceptron

Universal approximation theorem: Cybenko (1989)

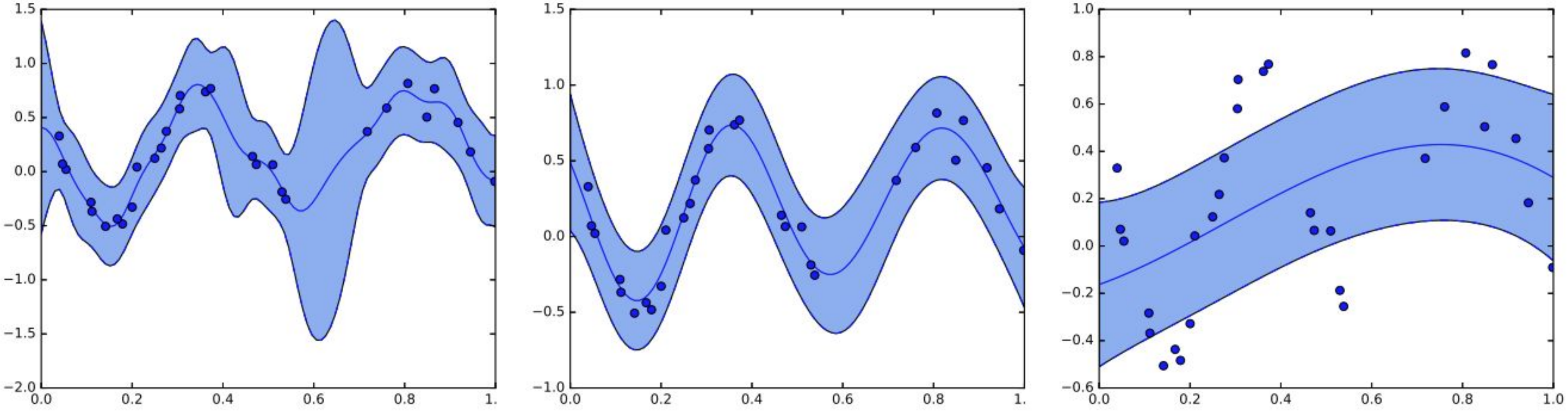
Showed MLPs can approximate arbitrary functions





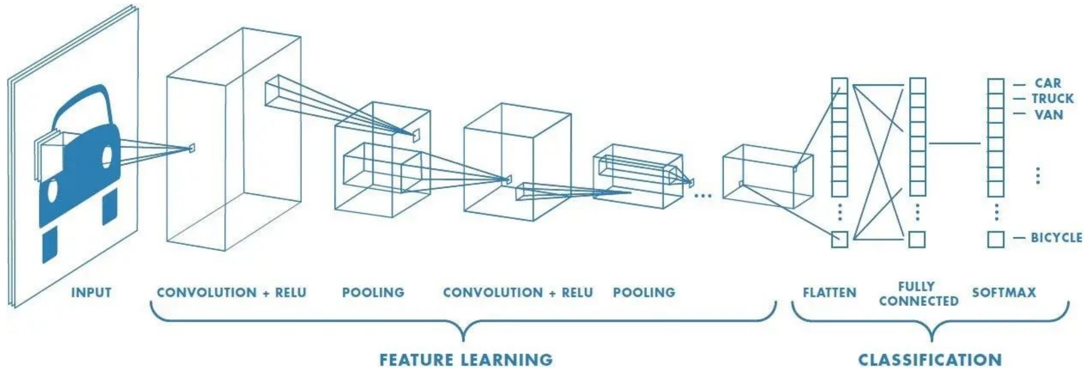
Kernel Methods (1990-2000)

Another winter: kernel methods work better and are more interpretable



ConvNets: Yann Lecun (1989)

Yann invented CNNs which eventually became state-of-the art for image processing



ImageNet Moment (2012)

Ilya Sutskever

Start of the current era, neural nets outcompete all other methods on an image processing problem.

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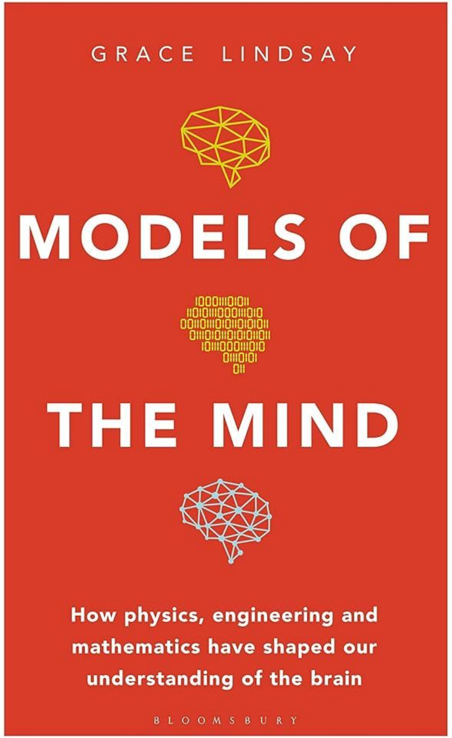
More history



Great book if you want to learn more about the history of neural networks.