Computer Vision with Deep Learning

Deep Neural Networks

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COMP411/511 - Fall 2024

PLAN

Backprop with Tensors

XOR Problem

Multi-Layer Perceptron

Universal Approximation

Quick Recap

Backpropagation with Scalars

Forward Pass:

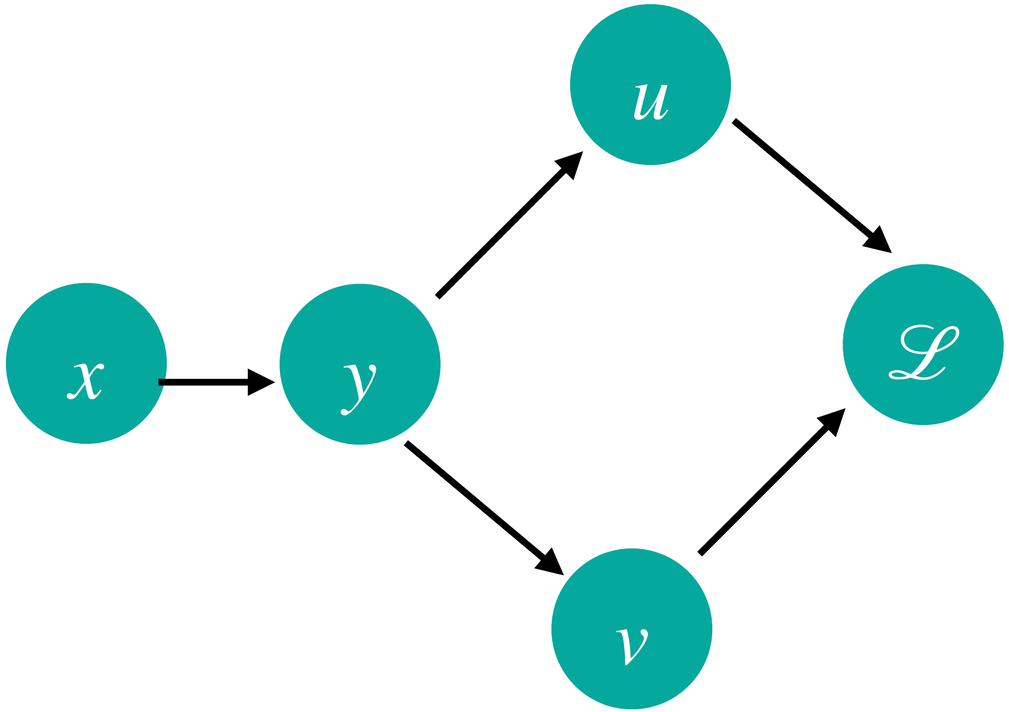
(1) $y = y(x)$

(2) $u = u(y)$

(3) $v = v(y)$

(4) $\mathscr{L} = \mathscr{L}(u, v)$

Loss: $\mathscr{L}\left(u\left(y(x)\right), v\left(y(x)\right)\right)$



Backpropagation with Scalars

Forward Pass:

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(2) $u = u(y)$

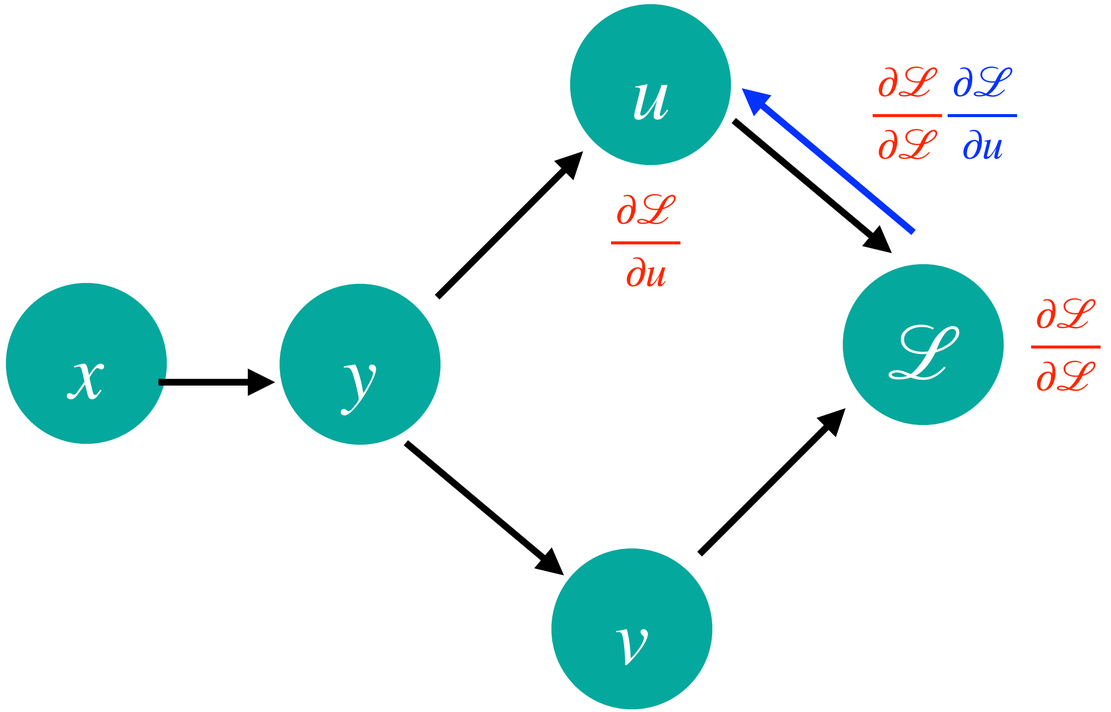
(3) $v = v(y)$

(4) $\mathscr{L} = \mathscr{L}(u, v)$

Backward Pass:

(4) $\dfrac{\partial \mathscr{L}}{\partial u} = \dfrac{\partial \mathscr{L}}{\partial \mathscr{L}} \dfrac{\partial \mathscr{L}}{\partial u} = \dfrac{\partial \mathscr{L}}{\partial u}$

Loss: $\mathscr{L}\left(u\left(y(x)\right), v\left(y(x)\right)\right)$



Backpropagation with Scalars

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(4) $\mathscr{L} = \mathscr{L}(u, v)$

Backward Pass:

(4) $$\frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}} \frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial u}$$

(3) $$\frac{\partial \mathscr{L}}{\partial v} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}} \frac{\partial \mathscr{L}}{\partial v} = \frac{\partial \mathscr{L}}{\partial v}$$

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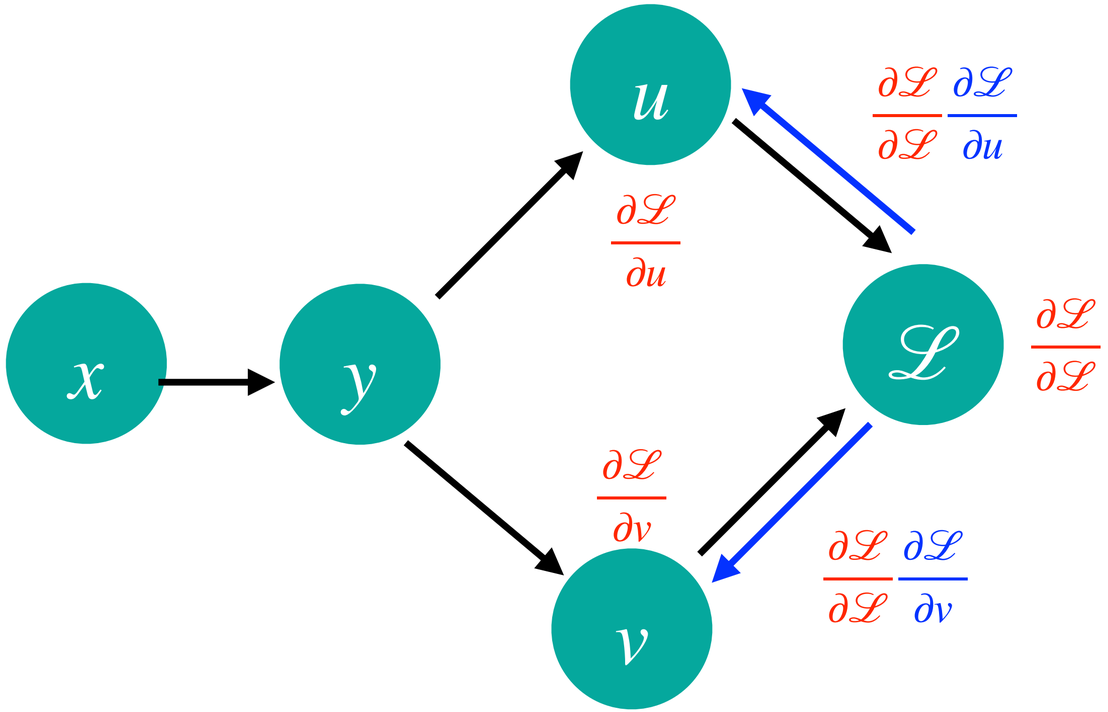

Backpropagation with Scalars

Forward Pass:

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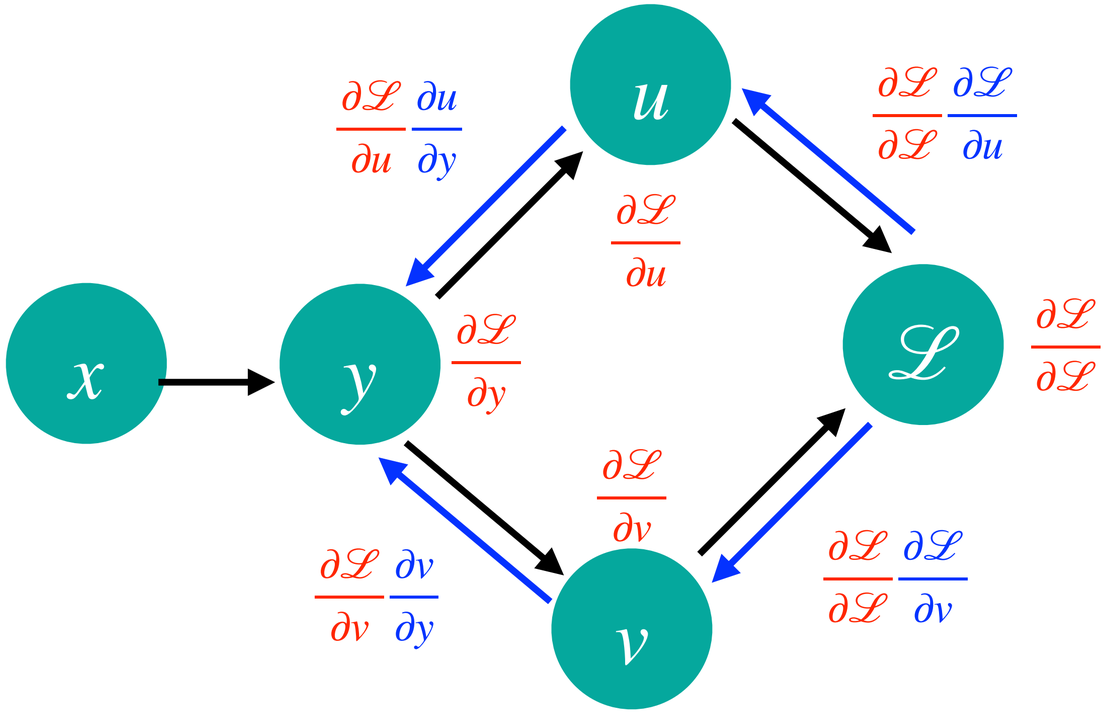


Backward Pass:

(4) $$\frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}}\frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial u}$$

(3) $$\frac{\partial \mathscr{L}}{\partial v} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}}\frac{\partial \mathscr{L}}{\partial v} = \frac{\partial \mathscr{L}}{\partial v}$$

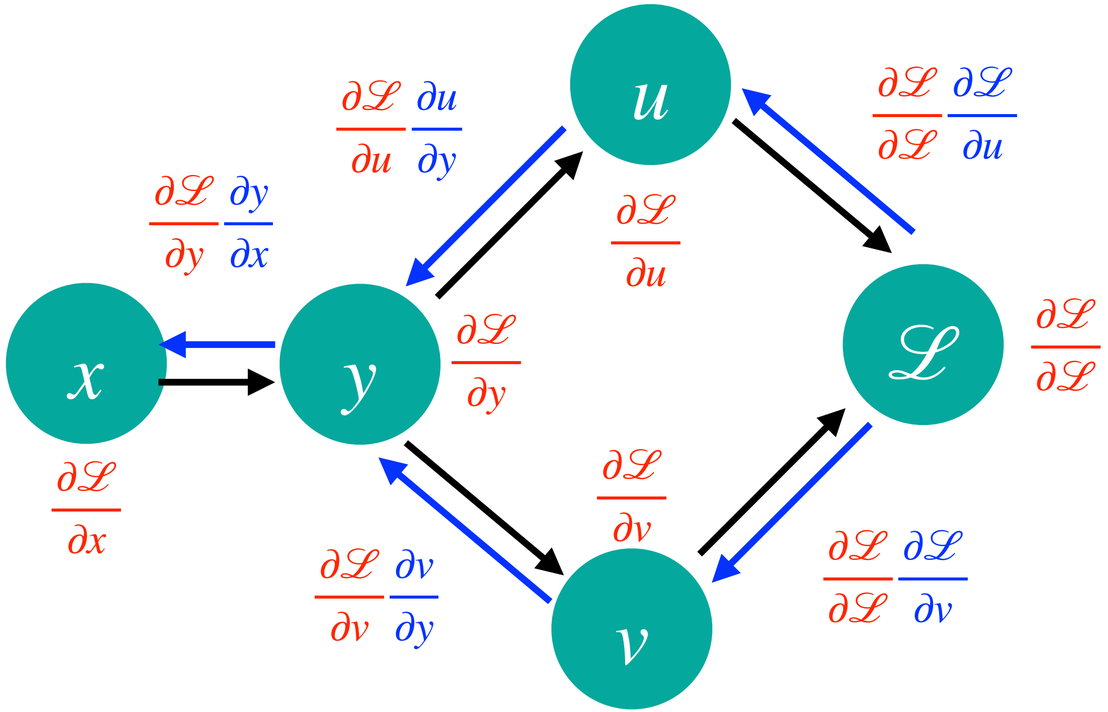
(2) $$\frac{\partial \mathscr{L}}{\partial y} = \frac{\partial \mathscr{L}}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial \mathscr{L}}{\partial v}\frac{\partial v}{\partial y}$$

Backpropagation with Scalars

Forward Pass:

$$
\begin{aligned}
&(1) \quad y = y(x) \\
&(2) \quad u = u(y) \\
&(3) \quad v = v(y) \\
&(4) \quad \mathscr{L} = \mathscr{L}(u, v)
\end{aligned}
$$

Loss: $\mathscr{L}\left(u\left(y(x)\right), v\left(y(x)\right)\right)$



Backward Pass:

$$
\begin{aligned}
&(4) \quad \frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}} \frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial u} \\
&(3) \quad \frac{\partial \mathscr{L}}{\partial v} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}} \frac{\partial \mathscr{L}}{\partial v} = \frac{\partial \mathscr{L}}{\partial v} \\
&(2) \quad \frac{\partial \mathscr{L}}{\partial y} = \frac{\partial \mathscr{L}}{\partial u} \frac{\partial u}{\partial y} + \frac{\partial \mathscr{L}}{\partial v} \frac{\partial v}{\partial y} \\
&(1) \quad \frac{\partial \mathscr{L}}{\partial x} = \frac{\partial \mathscr{L}}{\partial y} \frac{\partial y}{\partial x}
\end{aligned}
$$

Backpropagation with Scalars

Forward Pass:

$$(1) \quad y = y(x)$$

$$(2) \quad u = u(y)$$

$$(3) \quad v = v(y)$$

$$(4) \quad \mathscr{L} = \mathscr{L}(u, v)$$

Backward Pass:

$$(4) \quad \frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}} \frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial u}$$

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$$(2) \quad \frac{\partial \mathscr{L}}{\partial y} = \frac{\partial \mathscr{L}}{\partial u} \frac{\partial u}{\partial y} + \frac{\partial \mathscr{L}}{\partial v} \frac{\partial v}{\partial y}$$

$$(1) \quad \frac{\partial \mathscr{L}}{\partial x} = \frac{\partial \mathscr{L}}{\partial y} \frac{\partial y}{\partial x}$$

Implementation: Each variable/node is an object and has attributes `x.value` and `x.grad`. Values are computed **forward**:

```
x.value = Input
y.value = y(x.value)
u.value = u(y.value)
v.value = v(y.value)
L.value = ℒ(u.value, v.value)
```

Backpropagation with Scalars

Forward Pass:

(1) $y = y(x)$

(2) $u = u(y)$

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(4) $\mathscr{L} = \mathscr{L}(u, v)$

Backward Pass:

(4) $$\frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial \mathscr{L}} \frac{\partial \mathscr{L}}{\partial u} = \frac{\partial \mathscr{L}}{\partial u}$$

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(2) $$\frac{\partial \mathscr{L}}{\partial y} = \frac{\partial \mathscr{L}}{\partial u} \frac{\partial u}{\partial y} + \frac{\partial \mathscr{L}}{\partial v} \frac{\partial v}{\partial y}$$

(1) $$\frac{\partial \mathscr{L}}{\partial x} = \frac{\partial \mathscr{L}}{\partial y} \frac{\partial y}{\partial x}$$

Implementation: Each variable/node is an object and has attributes `x.value` and `x.grad`. Values are computed **forward** and gradients **backward**:

```
x.grad = y.grad = u.grad = v.grad = 0
L.grad = 1
u.grad += L.grad * (∂ℒ/∂u)(u.value, v.value)
v.grad += L.grad * (∂ℒ/∂v)(u.value, v.value)
y.grad += u.grad * (∂u/∂y)(y.value)
y.grad += v.grad * (∂v/∂y)(y.value)
x.grad += y.grad * (∂y/∂x)(x.value)
```

Backpropagation with Tensors

Scalar vs. Matrix Operations

So far we have considered computations on **scalars**:

$$y = \sigma\left(w_1 x + w_0\right)$$

We now consider computations on **vectors** and **matrices**:

$$\mathbf{y} = \sigma\left(\mathbf{A}\mathbf{x} + \mathbf{b}\right)$$

- Matrix $\mathbf{A}$ and vector $\mathbf{b}$ are objects with attributes `value` and `grad`
- `A.grad` stores $\nabla_{\mathbf{A}} \mathscr{L}$ and `b.grad` stores $\nabla_{\mathbf{b}} \mathscr{L}$
- `A.grad` has the same shape/dimensions as `A.value` (since $\mathscr{L}$ is scalar)

Backpropagation with Loops

The matrix/vector computation

$$\mathbf{y} = \sigma(\underbrace{\mathbf{A}\mathbf{x}}_{=u} + \mathbf{b})$$

can be written as **loops over scalar operations**:

for i `u.value[i] = 0`

for i,j `u.value[i] += A.value[i,j] * x.value[j]`

for i `y.value[i] = σ(u.value[i] + b.value[i])`

Backpropagation with Loops

The backpropagated gradients for

for i `y.value[i] = σ(u.value[i] + b.value[i])`

are:

for i `u.grad[i] += y.grad[i] * σ′(u.value[i] + b.value[i])`

for i `b.grad[i] += y.grad[i] * σ′(u.value[i] + b.value[i])`

- **Red**: back-propagated gradients
- **Blue**: local gradients

Backpropagation with Loops

The backpropagated gradients for

for i,j `u.value[i] += A.value[i,j] * x.value[j]`

are:

for i,j `A.grad[i,j] += u.grad[i] * x.value[j]`

for i,j `x.grad[j] += u.grad[i] * A.value[i,j]`

- **Red**: back-propagated gradients
- **Blue**: local gradients

Backpropagation with Loops

In practice, all deep learning operations can be written using loops over scalar assignments. Example for a **higher-order tensor:**

for h,i,j,k `U.value[h,i,j] += A.value[h,i,k] * B.value[h,j,k]`

for h,i,j `Y.value[h,i,j] = σ(U.value[h,i,j])`

Backpropagation loops:

h,i,j `U.grad += Y.grad[h,i,j] * σ'(U.value[h,i,j])`

h,i,j,k `A.grad += U.grad[h,i,j] * B.value[h,j,k]`

h,i,j,k `B.grad += U.grad[h,i,j] * A.value[h,i,k]`

Minibatching

Source code has two components:

- ✦ Slow part: Sequential operations (Python)
- ✦ Fast part: Vector/matrix operations (NumPy, BLAS, CUDA)

Goal:

- ✦ Fast part should dominate computation (wall clock time)
- ✦ Reduce the number of slow sequential operations (e.g., Python loops) by running the fast vector/matrix operations on several data points jointly
- ✦ This is called **minibatching** and used in stochastic gradient descent

Minibatching

Affine + Sigmoid: (applied to N data points simultaneously)

$$\mathbf{Y} = \sigma(\underbrace{\mathbf{XA}}_{=\mathbf{U}} + \mathbf{B})$$

✦ Each row in $\mathbf{X} \in \mathscr{R}^{N \times D}$ is a data point, bias $\mathbf{b} \in \mathscr{R}^{M}$ is broadcast to $\mathbf{B} \in \mathscr{R}^{N \times M}$

Loops now include **batch index** `b`:

for b,i `U.value[b,i] = 0`

for b,i,j `U.value[b,i] += X.value[b,j] * A.value[j,i]`

for b,i `Y.value[b,i] = σ(U.value[b,i] + B.value[i])`

✦ Only inputs and outputs depend on batch index `b`, not the parameters (e.g., `A, B`)

✦ By convention, the gradients are averaged over the batch

Implementation

Affine Transformation: (applied to N data points simultaneously)

$$\mathbf{Y} = \mathbf{X}\mathbf{A} + \mathbf{B}$$

- Each row in $\mathbf{X} \in \mathcal{R}^{N \times D}$ is a data point, bias $\mathbf{b} \in \mathcal{R}^{M}$ is broadcast to $\mathbf{B} \in \mathcal{R}^{N \times M}$

Implementation in EDF:

```
def forward(self):
    self.value = np.matmul(self.x.value,self.w.A.value) + self.w.b.value

def backward(self):
    self.x.addgrad(np.matmul(self.grad,self.w.A.value.transpose()))
    self.w.b.addgrad(self.grad)
    self.w.A.addgrad(self.x.value[:,:,np.newaxis] * self.grad[:,np.newaxis,:])
```

- Computation graphs are easy to understand using the loop notation
- Efficient implementation using NumPy primitives not always obvious

XOR Problem

XOR Problem

Logistic Regression Model:

$$\hat{y} = \sigma\left(\mathbf{w}^T \mathbf{x}\right) \quad \text{where} \quad \sigma(x) = \frac{1}{1 + e^{-x}}$$

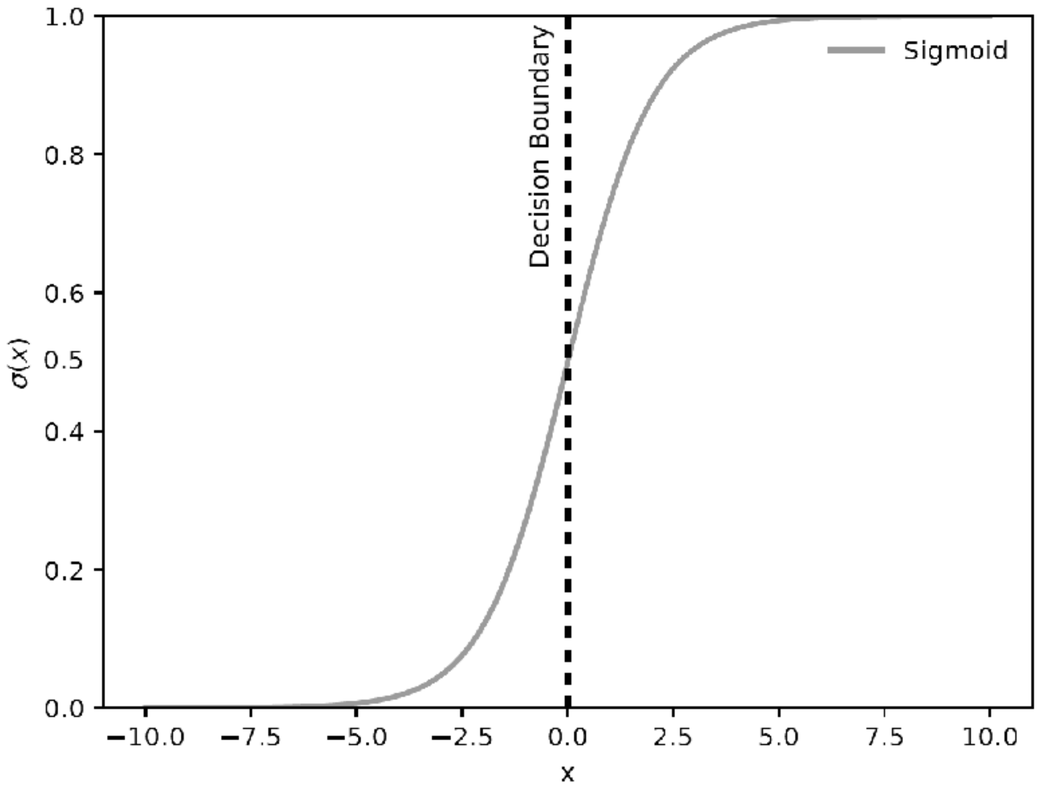
- ✦ Which problems can we solve with such a simple linear classifier?

XOR Problem

Example: 2D Logistic Regression

$$\hat{y} = \sigma\left(\mathbf{w}^T\mathbf{x} + w_0\right) \quad \text{where} \quad \sigma(x) = \frac{1}{1 + e^{\cdot}}$$

- Let $\mathbf{x} \in \mathscr{R}^2$
- Decision boundary: $\mathbf{w}^T\mathbf{x} + w_0 = 0$

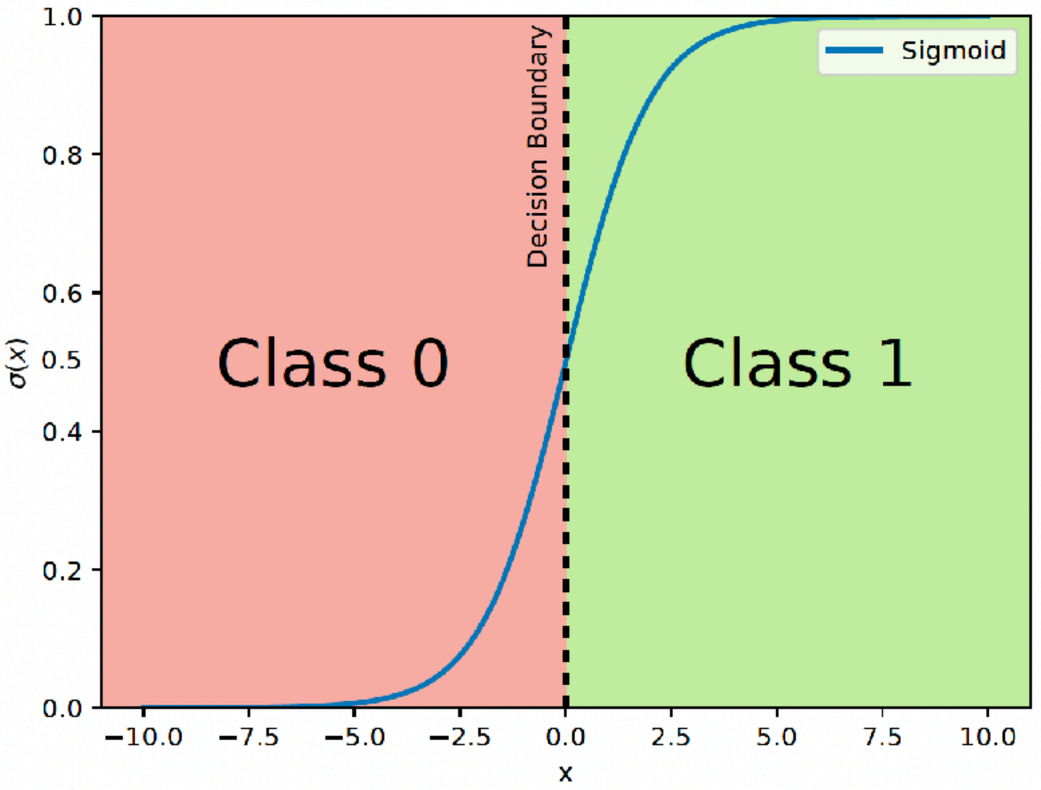


XOR Problem

Example: 2D Logistic Regression

$$\hat{y} = \sigma\left(\mathbf{w}^T\mathbf{x} + w_0\right) \quad \text{where} \quad \sigma(x) = \frac{1}{1 + e^{\cdot}}$$

- Let $\mathbf{x} \in \mathscr{R}^2$
- Decision boundary: $\mathbf{w}^T\mathbf{x} + w_0 = 0$
- Decide for class $1 \Leftrightarrow \mathbf{w}^T\mathbf{x} > -w_0$
- Decide for class $0 \Leftrightarrow \mathbf{w}^T\mathbf{x} < -w_0$



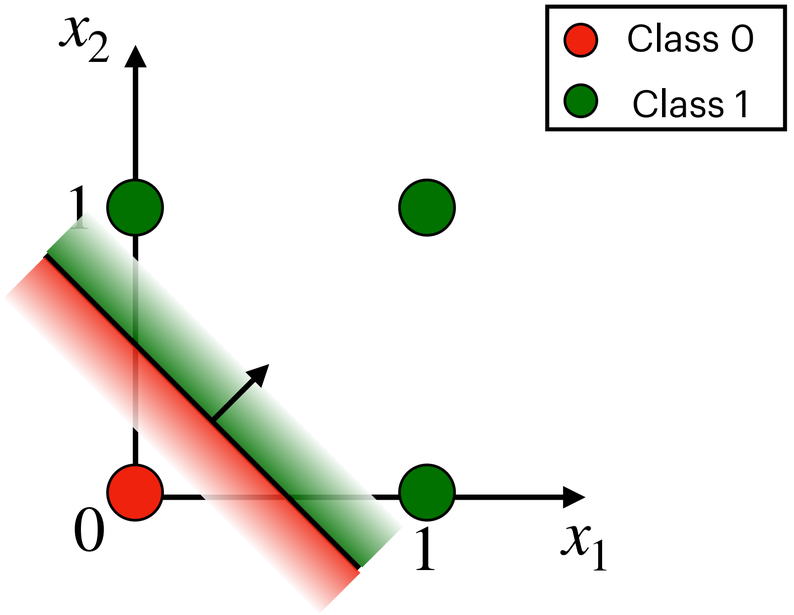
XOR Problem

Linear Classifier:

$$\text{Class } 1 \Leftrightarrow \mathbf{w}^T\mathbf{x} > -w_0$$

$$\underbrace{(\quad)}_{\mathbf{w}^T}\underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{\quad}_{-w_0}$$

x_1	x_2	OR(x_1, x_2)
0	0	0
0	1	1
1	0	1
1	1	1



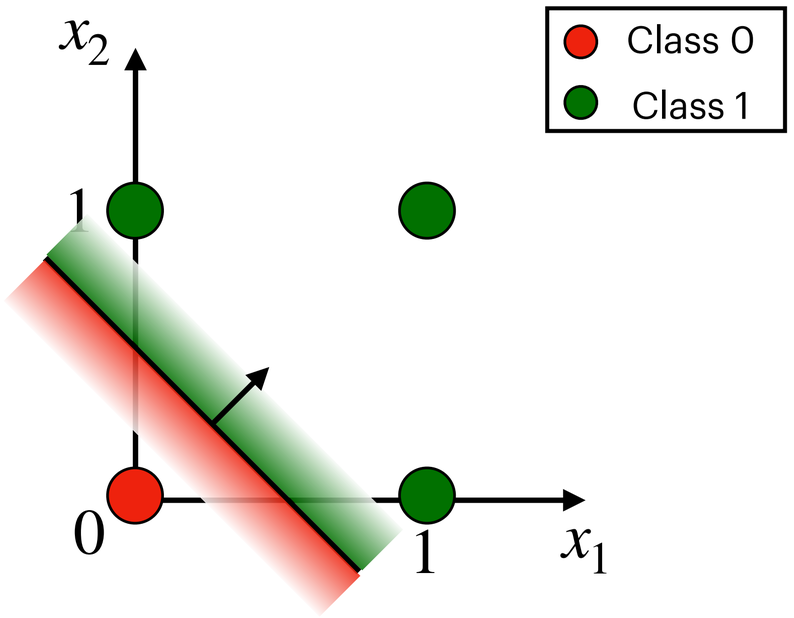
XOR Problem

Linear Classifier:

$$\text{Class } 1 \Leftrightarrow \mathbf{w}^T\mathbf{x} > -w_0$$

$$\underbrace{(1 \quad 1)}_{\mathbf{w}^T} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{0.5}_{-w_0}$$

x_1	x_2	OR(x_1, x_2)
0	0	0
0	1	1
1	0	1
1	1	1



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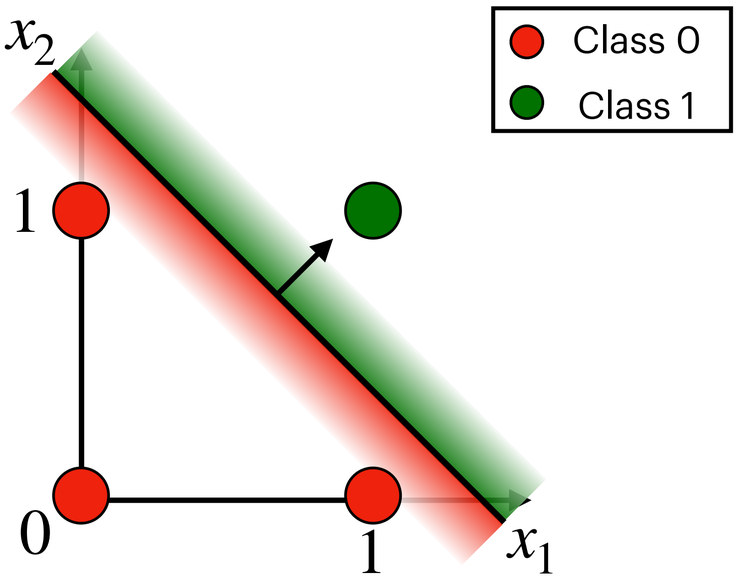
$$\underbrace{(\quad)}_{\mathbf{w}^T}\underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{\quad}_{-w_0}$$

x_1	x_2	AND(x_1, x_2)
0	0	0
0	1	0
1	0	0
1	1	1



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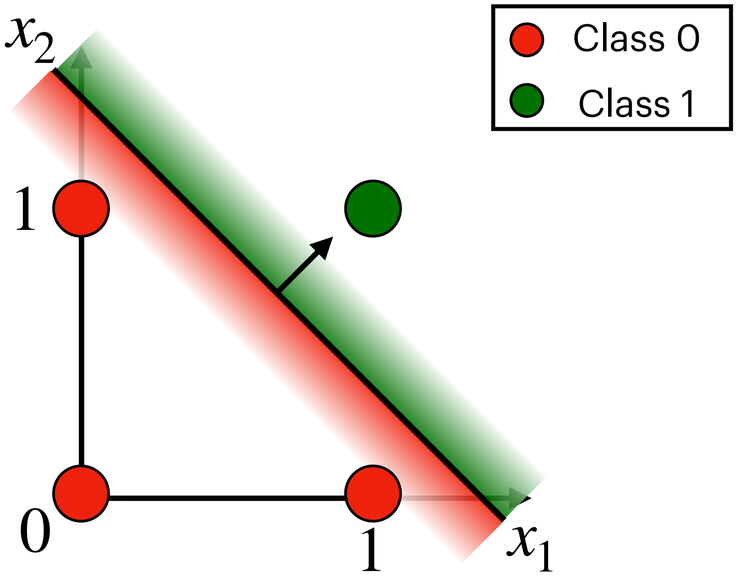
$$\underbrace{(1 \quad 1)}_{\mathbf{w}^T} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{1.5}_{-w_0}$$

x_1	x_2	AND(x_1, x_2)
0	0	0
0	1	0
1	0	0
1	1	1



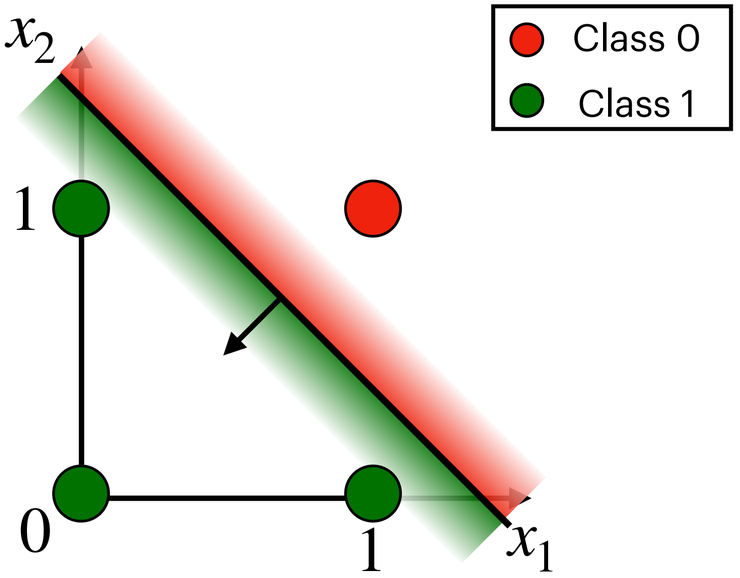
XOR Problem

Linear Classifier:

$$\text{Class } 1 \Leftrightarrow \mathbf{w}^T\mathbf{x} > -w_0$$

$$\underbrace{(\quad)}_{\mathbf{w}^T}\underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{\quad}_{-w_0}$$

x_1	x_2	NAND(x_1, x_2)
0	0	1
0	1	1
1	0	1
1	1	0



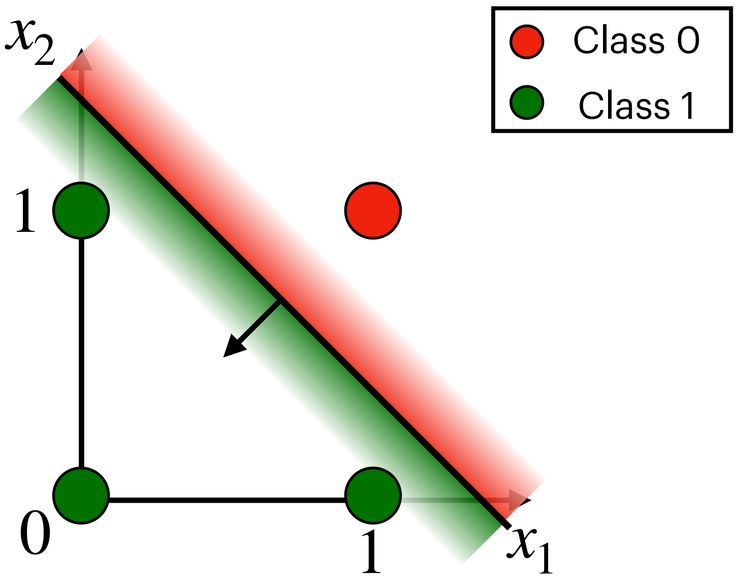
XOR Problem

Linear Classifier:

$$\text{Class } 1 \Leftrightarrow \mathbf{w}^T\mathbf{x} > -w_0$$

$$\underbrace{(-1 \quad -1)}_{\mathbf{w}^T} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{-1.5}_{-w_0}$$

x_1	x_2	NAND(x_1, x_2)
0	0	1
0	1	1
1	0	1
1	1	0



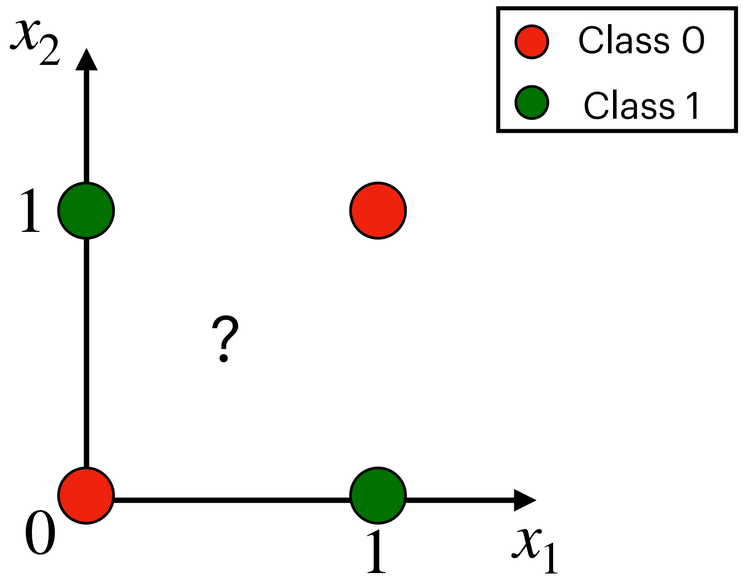
XOR Problem

Linear Classifier:

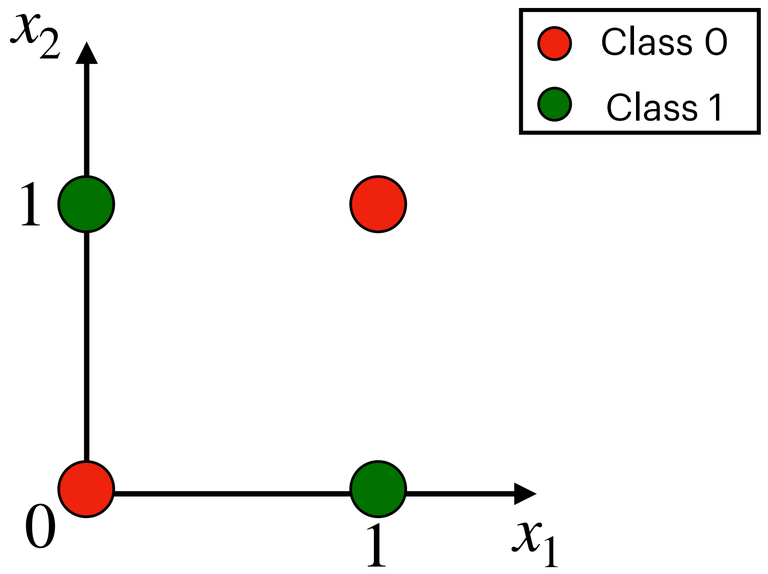
$$\text{Class } 1 \Leftrightarrow \mathbf{w}^T\mathbf{x} > -w_0$$

$$\underbrace{(?\quad ?)}_{\mathbf{w}^T}\underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{?}_{-w_0}$$

x_1	x_2	XOR(x_1, x_2)
0	0	0
0	1	1
1	0	1
1	1	0

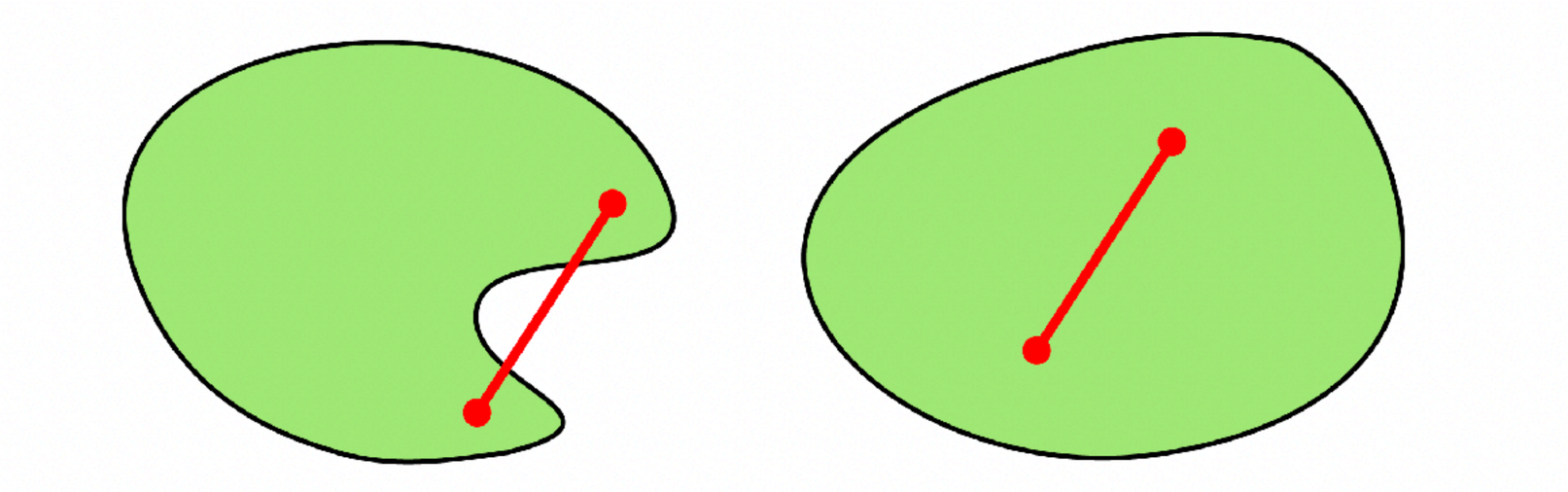


XOR Problem



- Visually it is obvious that XOR is not linearly separable
- How can we formally prove this?

Convex Sets

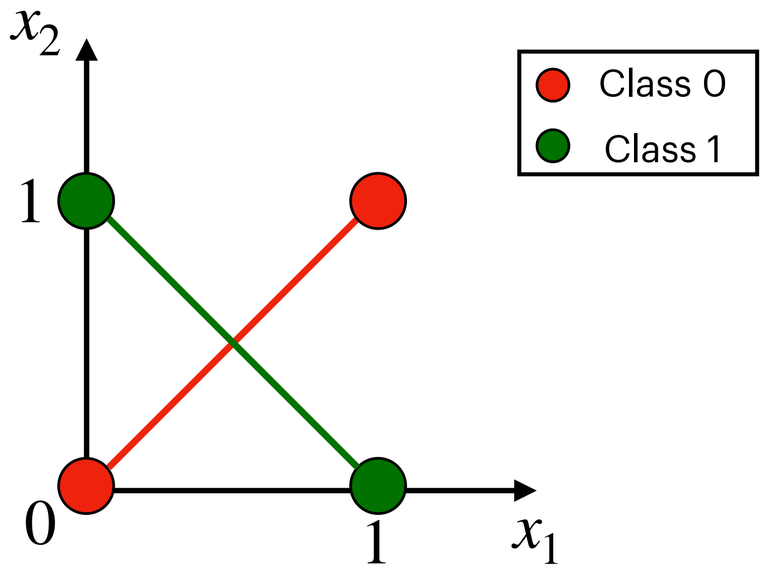


- A set $\mathcal{S}$ is **convex** if any line segment connecting 2 points in $\mathcal{S}$ lies entirely within $\mathcal{S}$:

$$\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{S} \Rightarrow \lambda \mathbf{x}_1 + (1 - \lambda)\mathbf{x}_2 \in \mathcal{S} \text{ for } \lambda \in [0,1]$$

XOR Problem

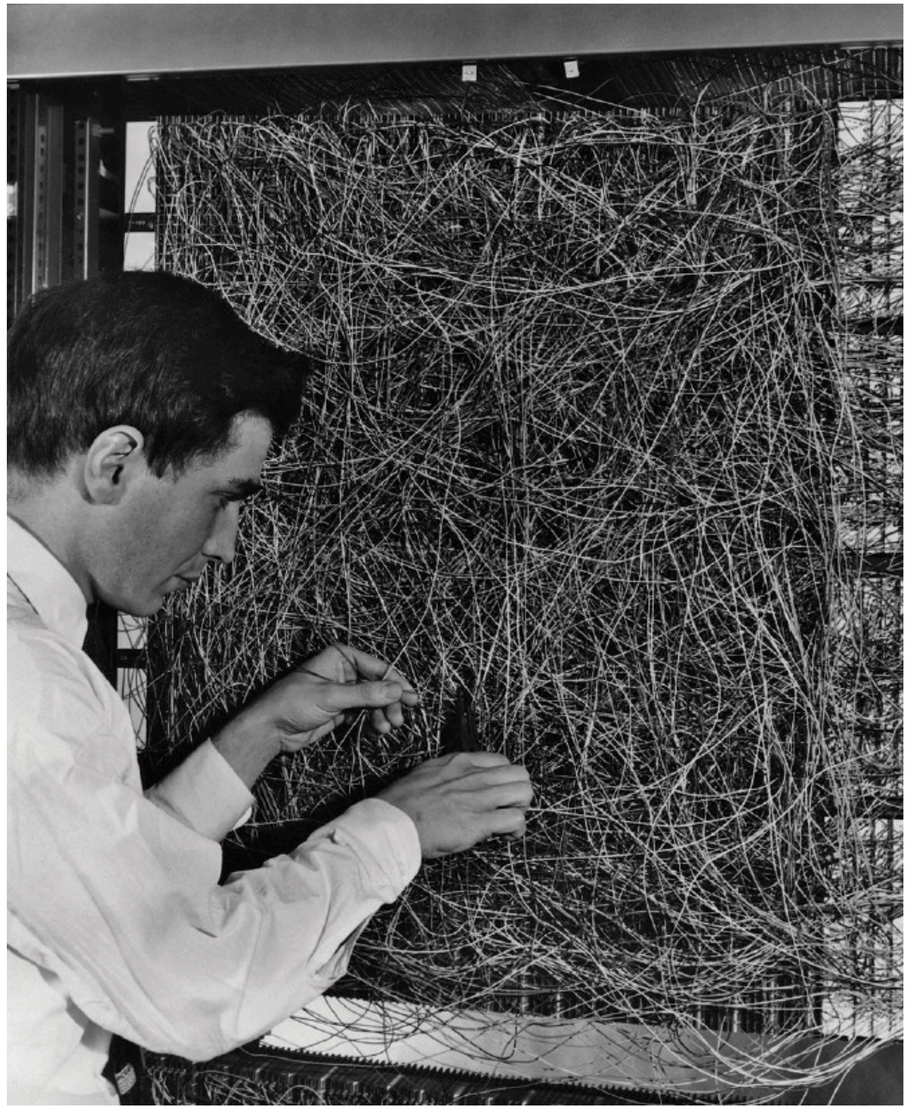
- Half-spaces (e.g., decision regions) are convex sets
- Suppose there was a feasible hypothesis. If the positive examples are in the positive half-space, then the green line segment must be as well.
- Similarly the red line must lie within the negative half-space.
- But the intersection can’t lie in both half-spaces. Contradiction!



XOR Problem

Some Historical Remarks:

- While linear classification showed some promising results in the 50s and 60s on simple image classification problems (Perceptron)
- But limitations became clear very soon (e.g., Minsky and Papert book “Perceptrons”, 1969)
- **XOR problem** is simple but cannot be solved as model capacity limited to linear decisions
- Led to decline in neural net research in the 70s
- How can we solve non-linear problems?

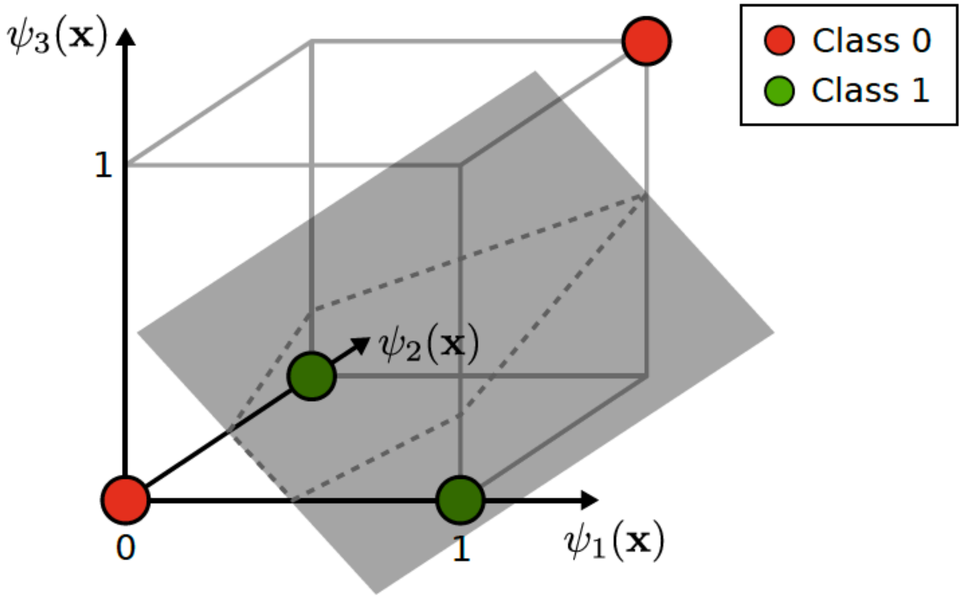


XOR Problem

Linear classifier with non-linear features ψ:

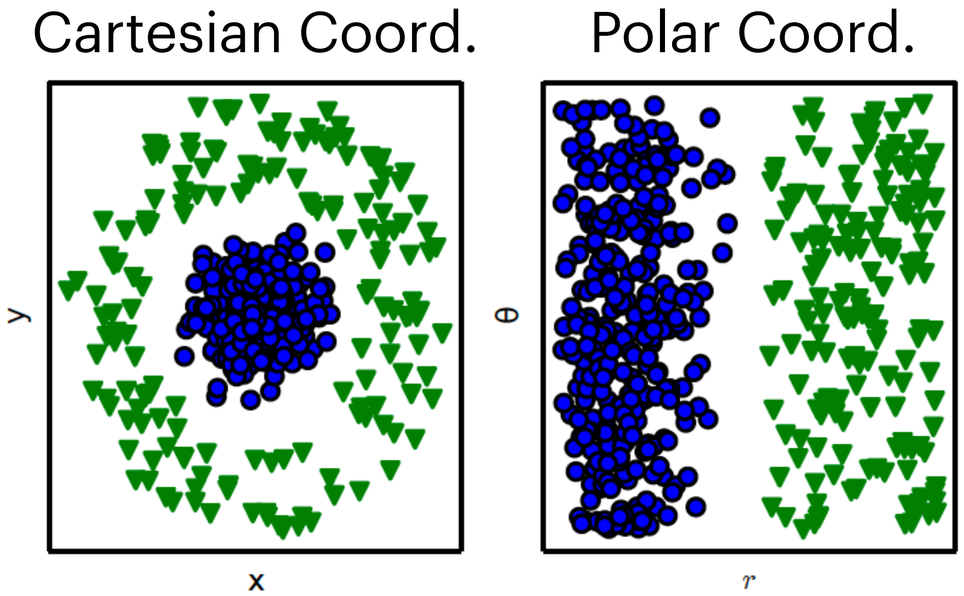
$$\mathbf{w}^T \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix}}_{\psi(\mathbf{x})} > -w_0$$

$\mathbf{x}_1$	$\mathbf{x}_2$	$\psi_1(\mathbf{x})$	$\psi_2(\mathbf{x})$	$\psi_3(\mathbf{x})$	XOR
0	0	0	0	0	0
0	1	0	1	0	1
1	0	1	0	0	1
1	1	1	1	1	0



- Non-linear features allow linear classifier to solve non-linear classification problems!
- Analogous to polynomial curve fitting

Representation Matters



- But how to choose the transformation? Can be very hard in practice.
- Yet, this was the dominant approach until the 2000s (vision, speech, ...)
- In this class we want to learn them ⇒ **Representation learning**
- Human needs to choose the right function family rather than the correct function

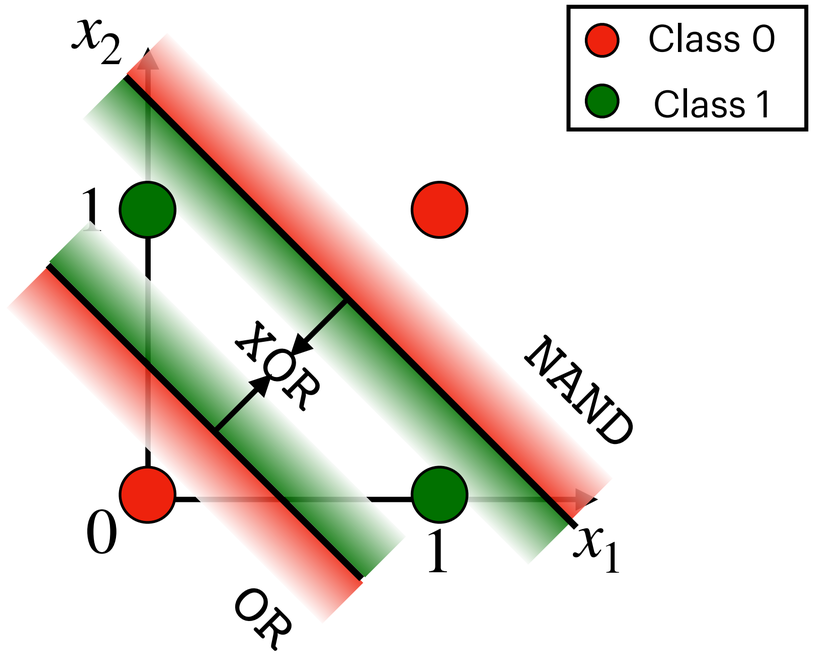
XOR Problem

Linear Classifier:

$$\text{Class } 1 \Leftrightarrow \mathbf{w}^T\mathbf{x} > -w_0$$

x_1	x_2	XOR(x_1, x_2)
0	0	0
0	1	1
1	0	1
1	1	0

XOR(x_1, x_2) = AND(OR(x_1, x_2), NAND(x_1, x_2))



XOR Problem

`XOR(x1, x2) = AND(OR(x1, x2), NAND(x1, x2))`

This expression can be rewritten as a **program of logistic regressors**:

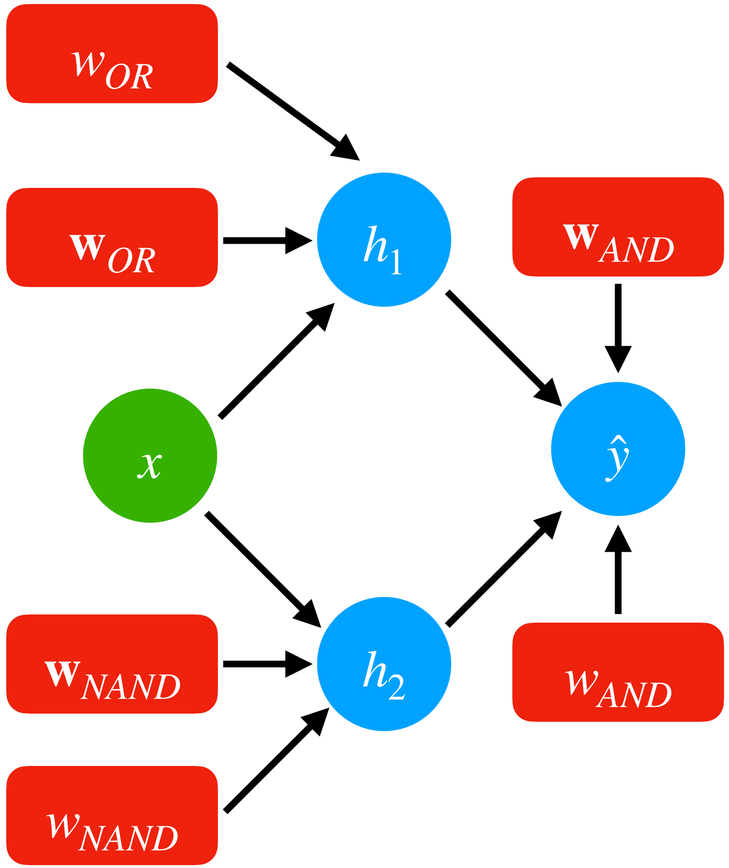
$$h_1 = \sigma\left(\mathbf{w}_{OR}^T \mathbf{x} + w_{OR}\right)$$

$$h_2 = \sigma\left(\mathbf{w}_{NAND}^T \mathbf{x} + w_{NAND}\right)$$

$$\hat{y} = \sigma\left(\mathbf{w}_{AND}^T \mathbf{h} + w_{AND}\right)$$

Note that $\mathbf{h}(\mathbf{x})$ is a non-linear feature of $\mathbf{x}$.

We call $\mathbf{h}(\mathbf{x})$ a hidden layer.



XOR Problem

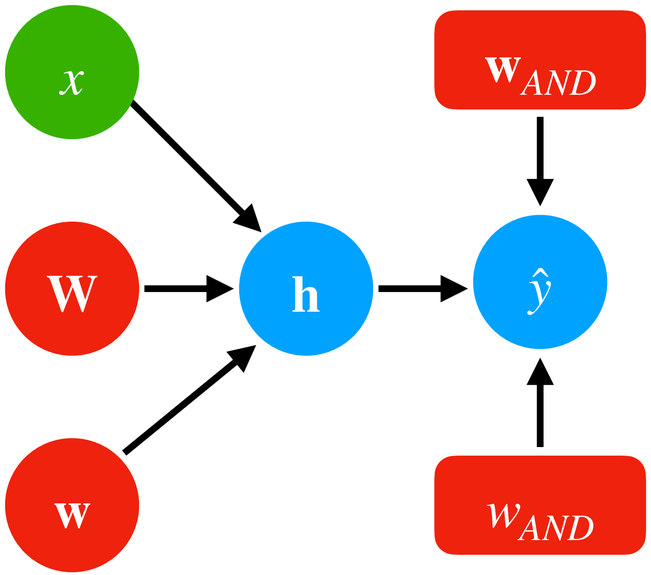
`XOR(x1, x2) = AND(OR(x1, x2), NAND(x1, x2))`

Writing the two 1D mappings $h_1(\mathbf{x})$ and $h_2(\mathbf{x})$

as a **single 2D mapping** $\mathbf{h}(\mathbf{x})$ yields:

$$\mathbf{h} = \sigma\left(\underbrace{\begin{pmatrix}\mathbf{w}_{OR}^T \\ \mathbf{w}_{NAND}^T\end{pmatrix}}_{\mathbf{W}}\mathbf{x} + \underbrace{\begin{pmatrix}w_{OR} \\ w_{NAND}\end{pmatrix}}_{\mathbf{w}}\right)$$

$$\hat{y} = \sigma\left(\mathbf{w}_{AND}^T\mathbf{h} + w_{AND}\right)$$



Parameters can be learned using backprop.

This is our first **Multi-Layer Perceptron**!

Multi-Layer Perceptron (MLP)

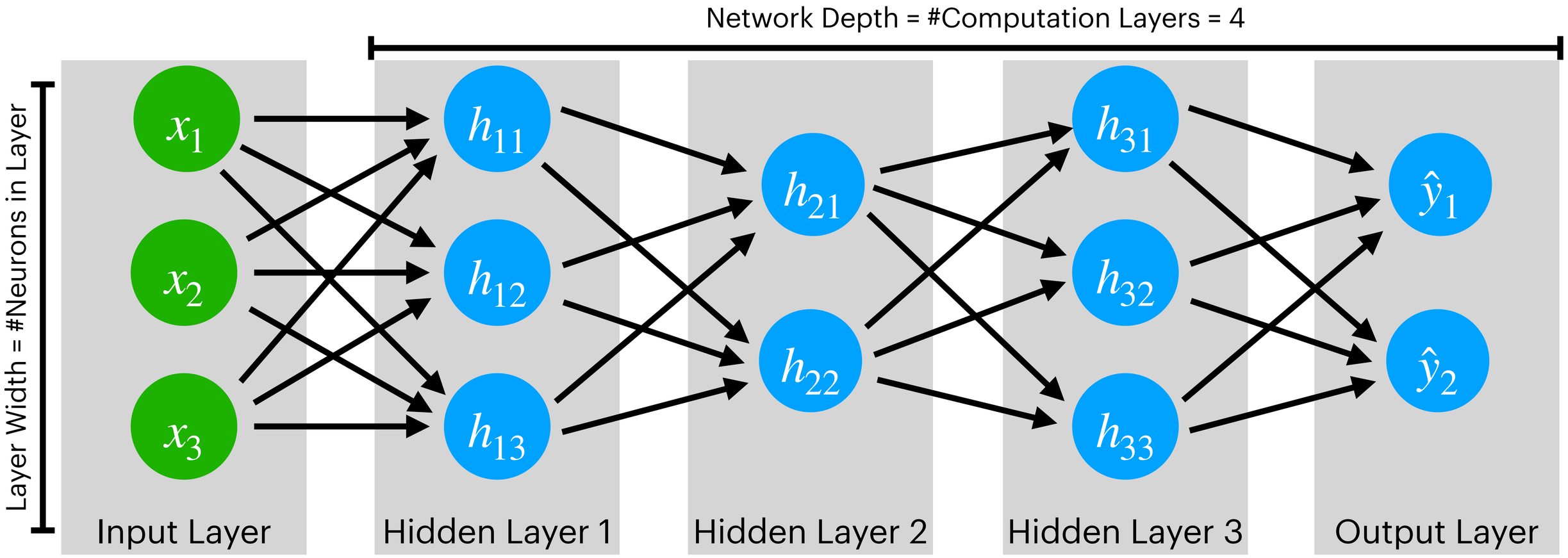
Multi-Layer Perceptron (MLP)

- MLPs are **feedforward** neural networks (no feedback connections)
- They are composed of several non-linear functions $\mathbf{f}(x) = \hat{\mathbf{y}}(\mathbf{h}_3(\mathbf{h}_2(\mathbf{h}_1(\mathbf{x}))))$ where $\mathbf{h}_i(\cdot)$ are called **hidden layers** and $\hat{\mathbf{y}}(\cdot)$ is the output layer
- The data specifies only the behavior of the output layer (thus the name “hidden”)
- Each layer i comprises multiple **neurons** j which are implemented as **affine transformations** $(\mathbf{a}^T\mathbf{x} + \mathbf{b})$ followed by non-linear **activation functions** (g):

$$h_{ij} = g(\mathbf{a}_{ij}^T\mathbf{h}_{i-1} + \mathbf{b}_{ij})$$

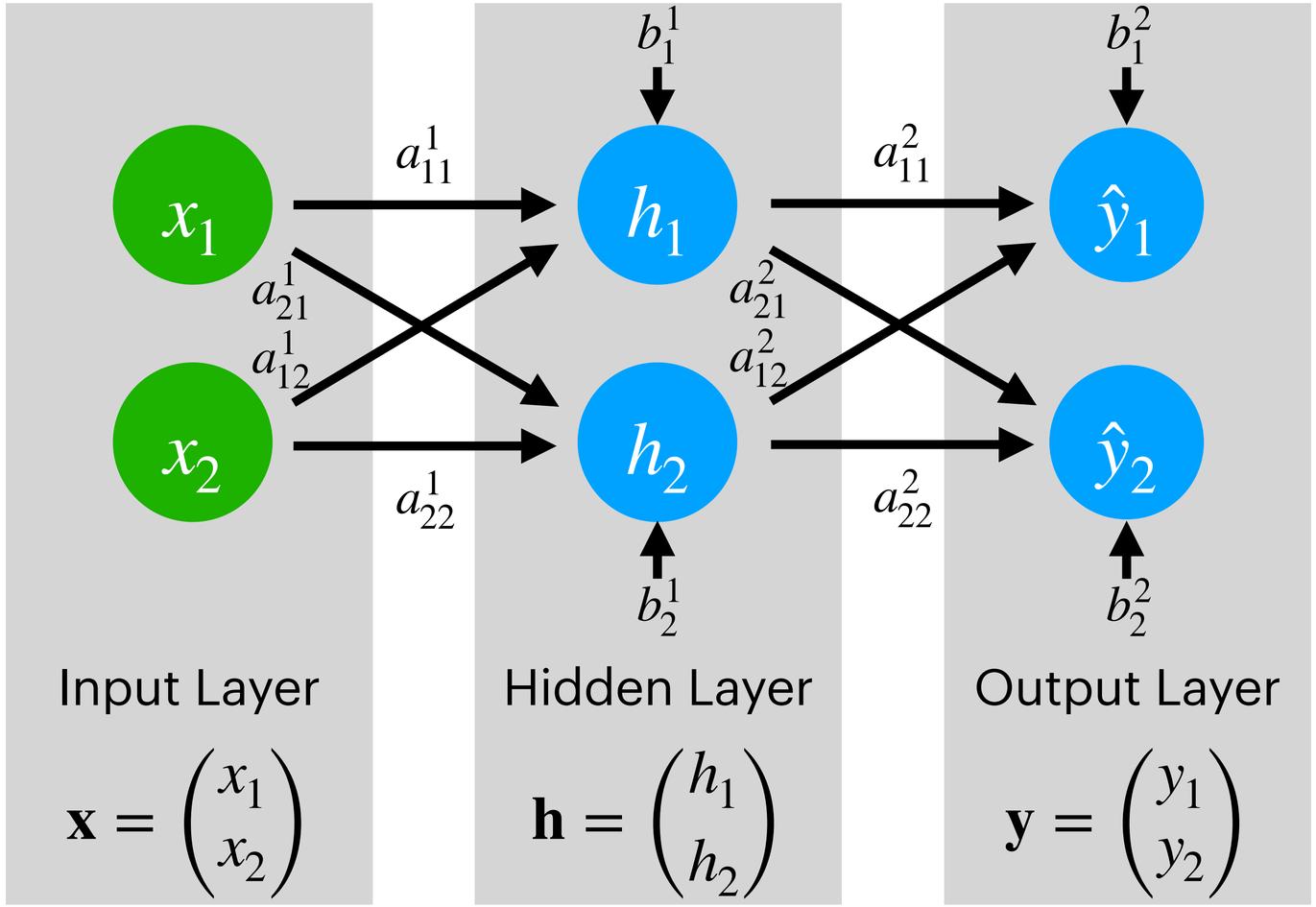
- Each neuron in each layer is **fully connected** to all neurons of the previous layer
- The overall length of the chain is the **depth** of the model ⇒ “Deep Learning”

MLP Network Architecture



- Neurons are grouped into layers, each neuron is **fully connected** to all prev. ones
- **Hidden layer** $\mathbf{h}_i = g(\mathbf{A}_i\mathbf{h}_{i-1} + \mathbf{b}_i)$ with **activation function** $g(\cdot)$ and weights $\mathbf{A}_i, \mathbf{b}_i$
- **Output layer** $\mathbf{y} = h(\mathbf{A}_L\mathbf{h}_{L-1} + \mathbf{b}_L)$ with **activation function** $h(\cdot)$ and weights $\mathbf{A}_L, \mathbf{b}_L$

MLP Network Architecture



$$\mathbf{h} = g(\mathbf{A}_1\mathbf{x} + \mathbf{b}_1)$$

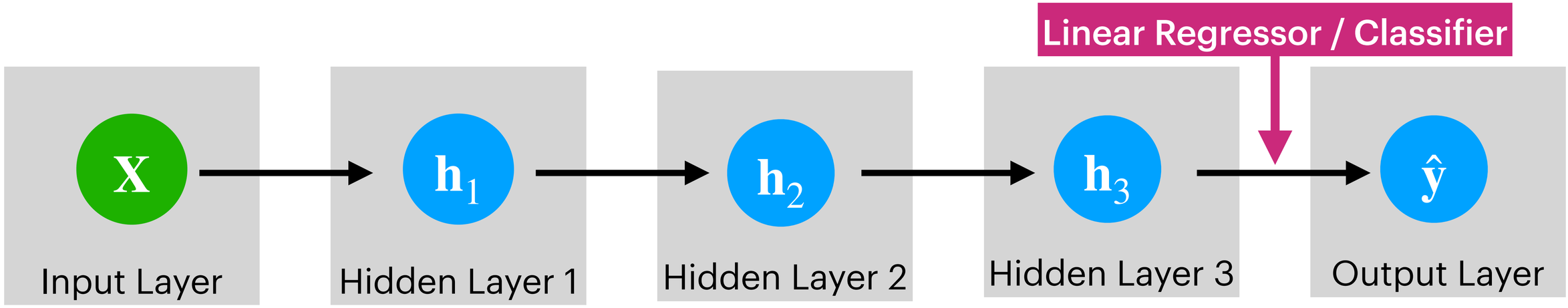
$$\mathbf{y} = h(\mathbf{A}_2\mathbf{h} + \mathbf{b}_2)$$

$$\mathbf{A}_l = \begin{pmatrix} a_{11}^l & a_{12}^l \\ a_{21}^l & a_{22}^l \end{pmatrix}$$

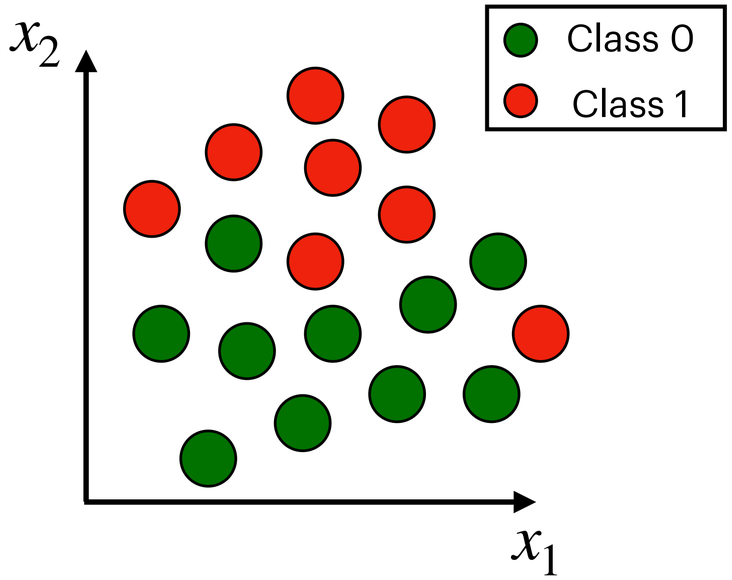
$$\mathbf{b}_l = \begin{pmatrix} b_1^l \\ b_2^l \end{pmatrix}$$

✦ Example MLP with $L = 2$ layers of width 2 and parameters $\{\mathbf{A}_1, \mathbf{A}_2, \mathbf{b}_1, \mathbf{b}_2\}$

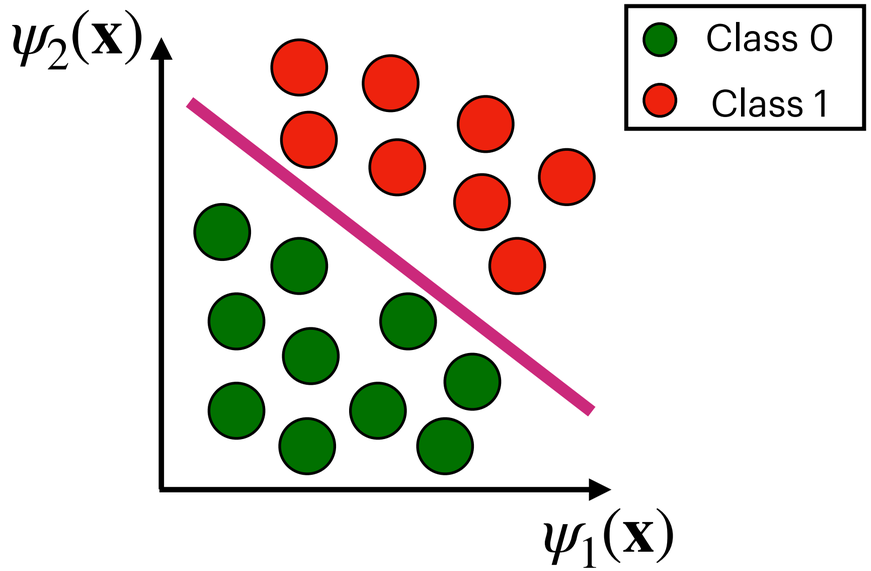
Feature Learning Perspective



$$\mathbf{h}_3 = \psi(\mathbf{x})$$



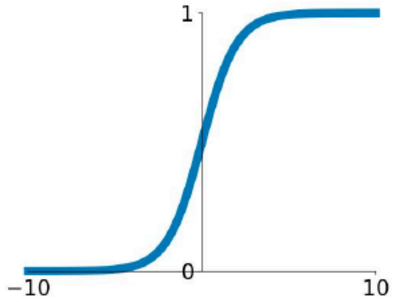
Transformation
by hidden layers



Activation Functions $g(\cdot)$

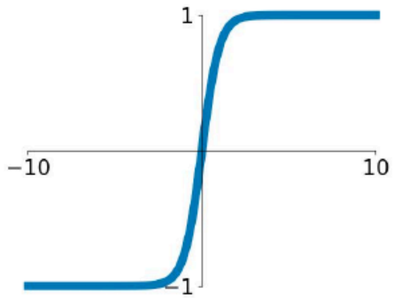
Sigmoid

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



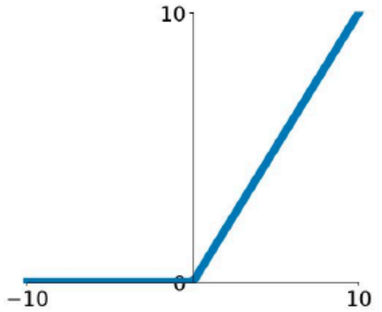
tanh

$\tanh(x)$

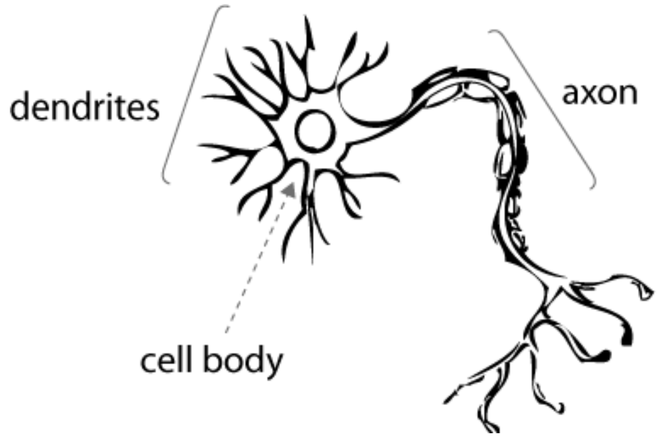


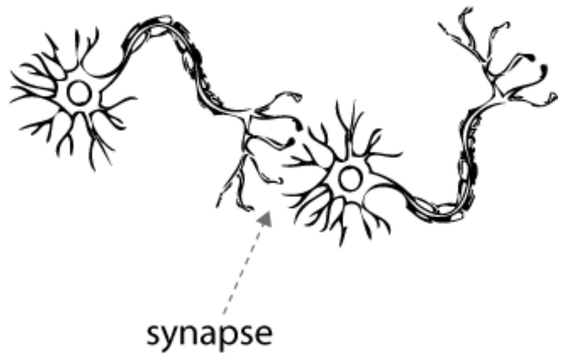
ReLU

$\max(0,x)$



Neural Motivation





- Neurons in the brain are structured in layers
- They receive input from many other units and compute their own activation
- The sigmoid activation function is guided by neuroscientific observations
- However, the architecture and training of modern networks differs radically
- Our main goal is not to model the brain, but to achieve statistical generalization

Training

Algorithm for training an MLP using (stochastic) gradient descent:

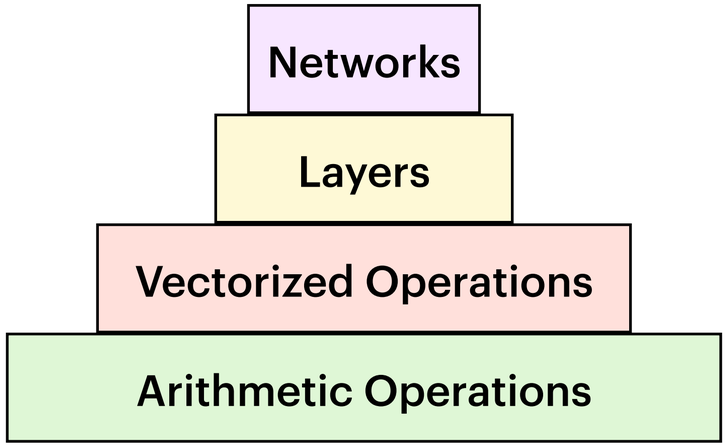
1. Initialize weights $\mathbf{w}$, pick learning rate η and minibatch size $|\mathcal{X}_{\text{batch}}|$
2. Draw (random) minibatch $\mathcal{X}_{\text{batch}} \subseteq \mathcal{X}$
3. For all elements $(\mathbf{x}, \mathbf{y}) \in \mathcal{X}_{\text{batch}}$ of minibatch (in parallel) do:
    3.1. Forward propagate $\mathbf{x}$ through network to calculate $\mathbf{h}_1, \mathbf{h}_2, \ldots, \hat{\mathbf{y}}$
    3.2. Backpropagate gradients through network to obtain $\nabla_{\mathbf{w}} \mathscr{L}(\hat{\mathbf{y}}, \mathbf{y})$
4. Update gradients: $\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \frac{1}{|\mathcal{X}_{\text{batch}}|} \sum_{(\mathbf{x},\mathbf{y}) \in \mathcal{X}_{\text{batch}}} \nabla_{\mathbf{w}} \mathscr{L}(\hat{\mathbf{y}}, \mathbf{y})$
5. If validation error decreases, go to step 2, otherwise stop

Remarks:

✦ Large datasets typically do not fit into GPU memory $\Rightarrow |\mathcal{X}_{\text{batch}}| < |\mathcal{X}|$

✦ Our examples on the next slides are small $\Rightarrow |\mathcal{X}_{\text{batch}}| = |\mathcal{X}|$

Levels of Abstraction



- When designing neural networks and machine learning algorithms, you'll need to simultaneously think at multiple levels of abstraction

  "The psychological profiling [of a programmer] is mostly the ability to shift levels of abstraction, from low level to high level. To see something in the small and to see something in the large." [Donald E. Knuth]

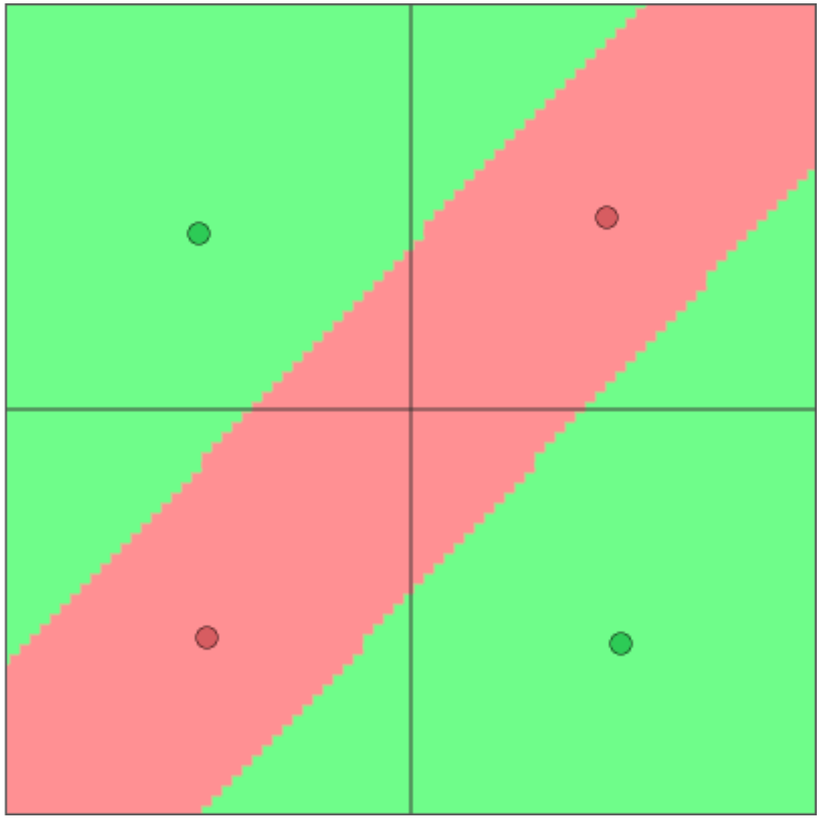
XOR Problem

```
layer_defs = [];
layer_defs.push({type:'input', out_sx:1, out_sy:1, out_depth:2});
layer_defs.push({type:'fc', num_neurons:2, activation: 'tanh'});
layer_defs.push({type:'fc', num_neurons:1, activation: 'tanh'});
layer_defs.push({type:'softmax', num_classes:2});

net = new convnetjs.Net();
net.makeLayers(layer_defs);

trainer = new convnetjs.SGDTrainer(net, {learning_rate:0.01,
momentum:0.1, batch_size:10, l2_decay:0.001});
```

change network

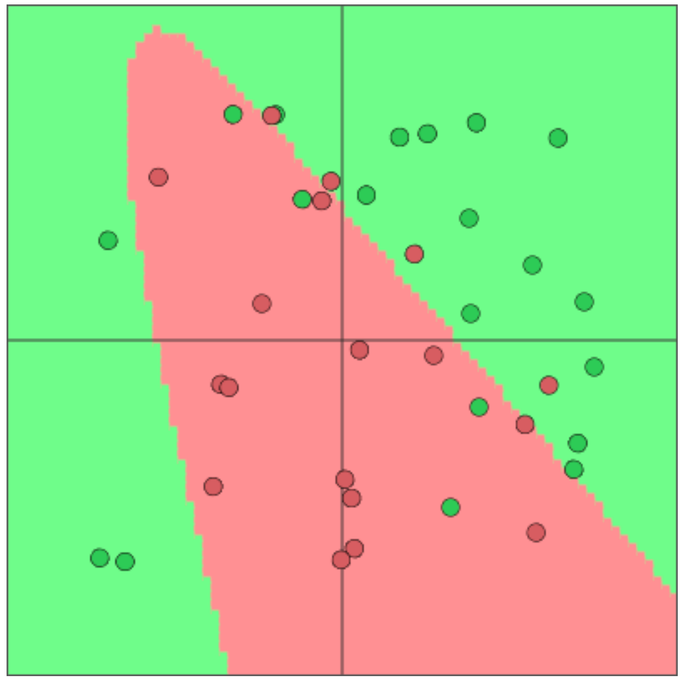


- Note that we have learned a boolean circuit! ⇒ differentiable programming

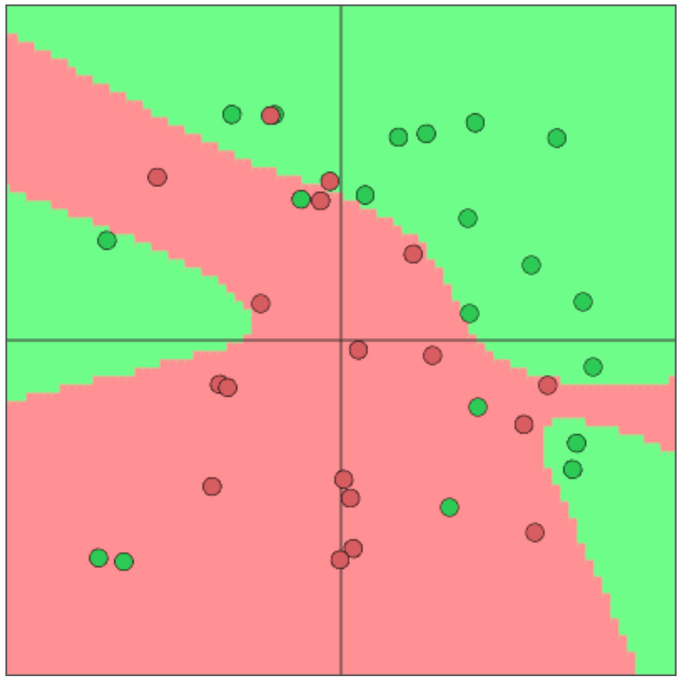
https://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html

A More Challenging Problem

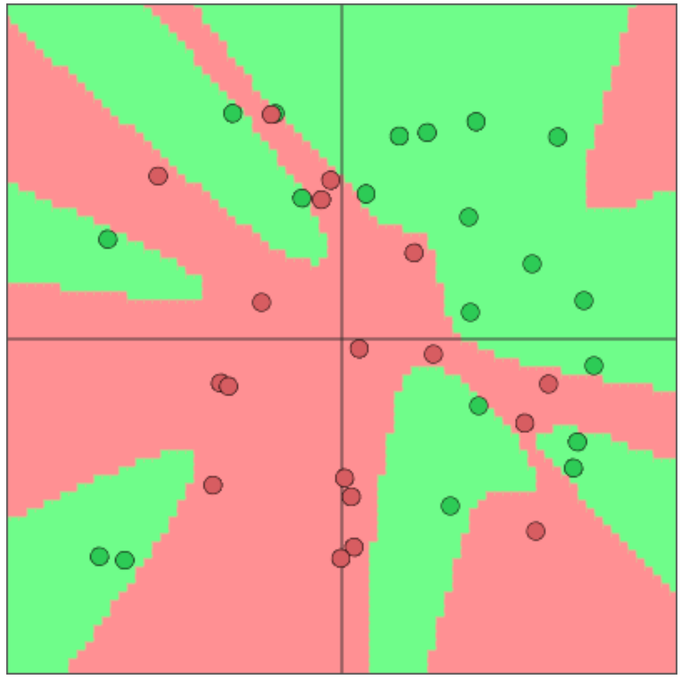
2 Hidden Neurons



5 Hidden Neurons



15 Hidden Neurons



https://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html

Expressiveness

This following two-layer MLP

$$\mathbf{h} = g(\mathbf{A}_1\mathbf{x} + \mathbf{b}_1)$$

$$\mathbf{y} = g(\mathbf{A}_2\mathbf{h} + \mathbf{b}_2)$$

can be written as

$$\mathbf{y} = g\left(\mathbf{A}_2 g(\mathbf{A}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2\right)$$

What if we would be using a linear activation function $g(\mathbf{x}) = \mathbf{x}$?

$$\mathbf{y} = \mathbf{A}_2(\mathbf{A}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 = \mathbf{A}_2\mathbf{A}_1\mathbf{x} + \mathbf{A}_2\mathbf{b}_1 + \mathbf{b}_2 = \mathbf{A}\mathbf{x} + \mathbf{b}$$

- ✦ With linear activations, a multi-layer network can only express linear functions
- ✦ What is the model capacity of MLPs with non-linear activation functions?

Universal Approximation

Universal Approximation Theorem

Theorem 1

Let σ be any continuous discriminatory function. Then finite sums of the form

$$G(\mathbf{x}) = \sum_{j=1}^{N} \alpha_j \sigma(\mathbf{a}_j^T \mathbf{x} + b_j)$$

are dense in the space of continuous functions $C(I_n)$ on the n-dimensional unit cube I_n.
In other words, given any $f \in C(I_n)$ and $\epsilon > 0$, there is a sum, $G(\mathbf{x})$ for which

$$|\, G(\mathbf{x}) - f(\mathbf{x}) \,| < \epsilon \quad \text{for all} \quad \mathbf{x} \in I_n$$

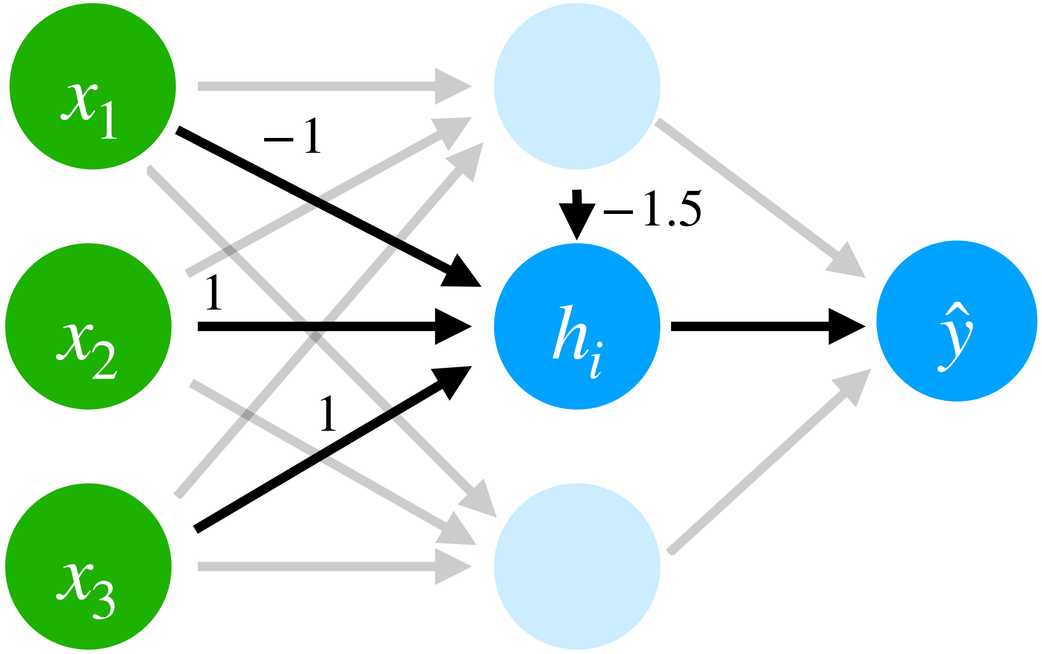
Remark: Has been proven for various activation functions (e.g., Sigmoid, ReLU).

Cybenko: Approximation by superposition of a sigmoidal function. Mathematics of Control, Signals, and Systems, 1989.

Example: Binary Case

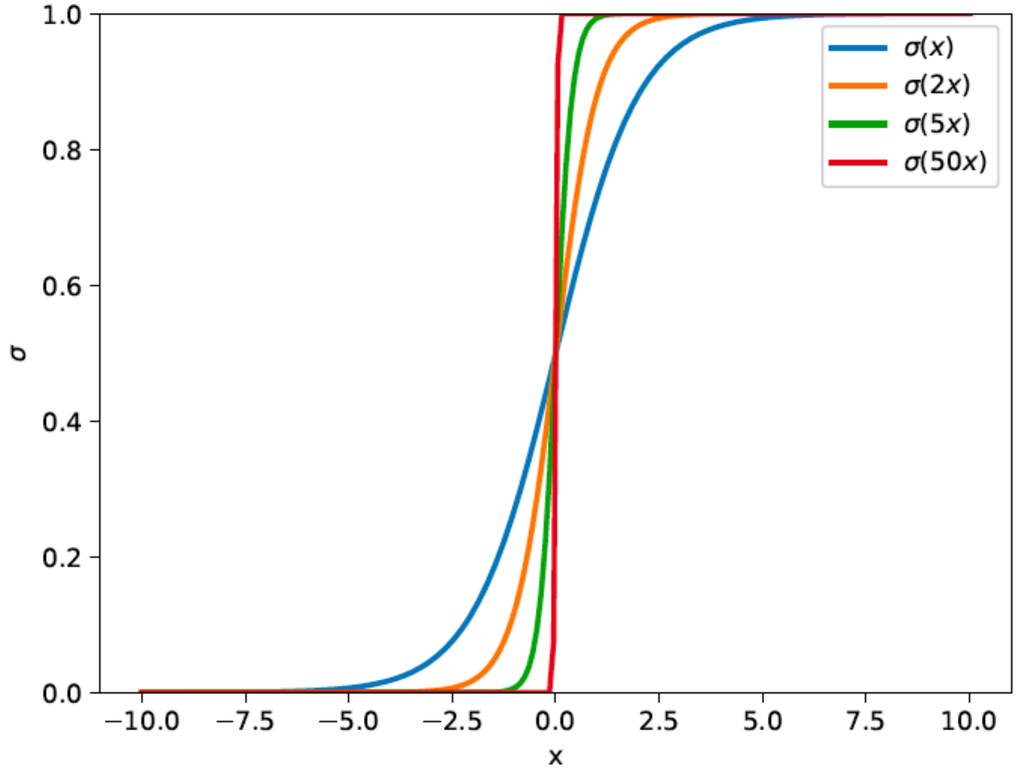
x_1	x_2	x3	y
⋮	⋮	⋮	⋮
0	1	0	0
0	**1**	**1**	**1**
1	0	0	0
⋮	⋮	⋮	⋮

$$\hat{y} = \sum_i \underbrace{\left[\mathbf{a}_i^T \mathbf{x} + b_i > 0\right]}_{h_i}$$



- Each hidden **linear threshold unit** h_i recognizes one possible input vector
- We need 2^D hidden units to **recognize** all 2^D possible inputs in the binary case

Soft Thresholds



Learning **linear threshold units** is hard as their gradient is 0 almost everywhere

- ✦ Solution: Replace hard threshold with a **soft threshold** (e.g., sigmoid)
- ✦ Sigmoids approximate step functions when increasing the input weight

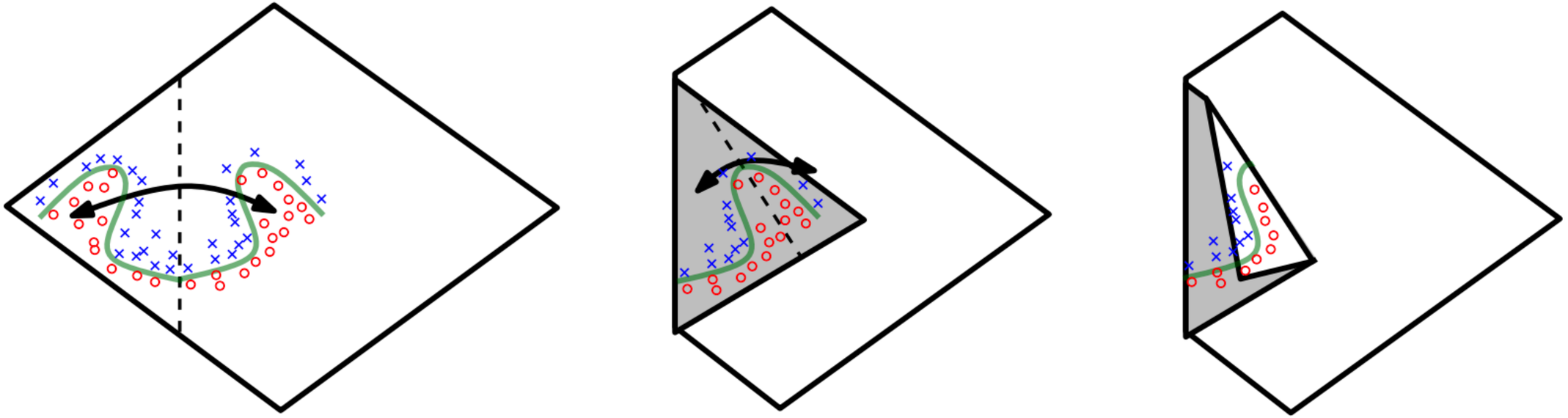
Network Width vs. Depth

- Universality of 2 layer networks is appealing but requires **exponential width**
- This leads to an exponential increase in memory and computation time
- Moreover, it doesn't lead to generalization ⇒ network simply **memorizes inputs**
- **Deep networks** can represent functions more compactly (with less parameters)
- Inductive bias: Complex functions modeled as **composition of simple functions**
- This leads to **more compact** models and **better generalization** performance
- Example: The parity function

$$f(x_1, \ldots, x_D) = \begin{cases} 1 & \text{if } \sum_i x_i \text{ is odd} \\ 0 & \text{otherwise} \end{cases}$$

requires an exponentially large shallow network but can be computed using a deep network whose size is linear in the number of inputs D.

Space Folding Intuition

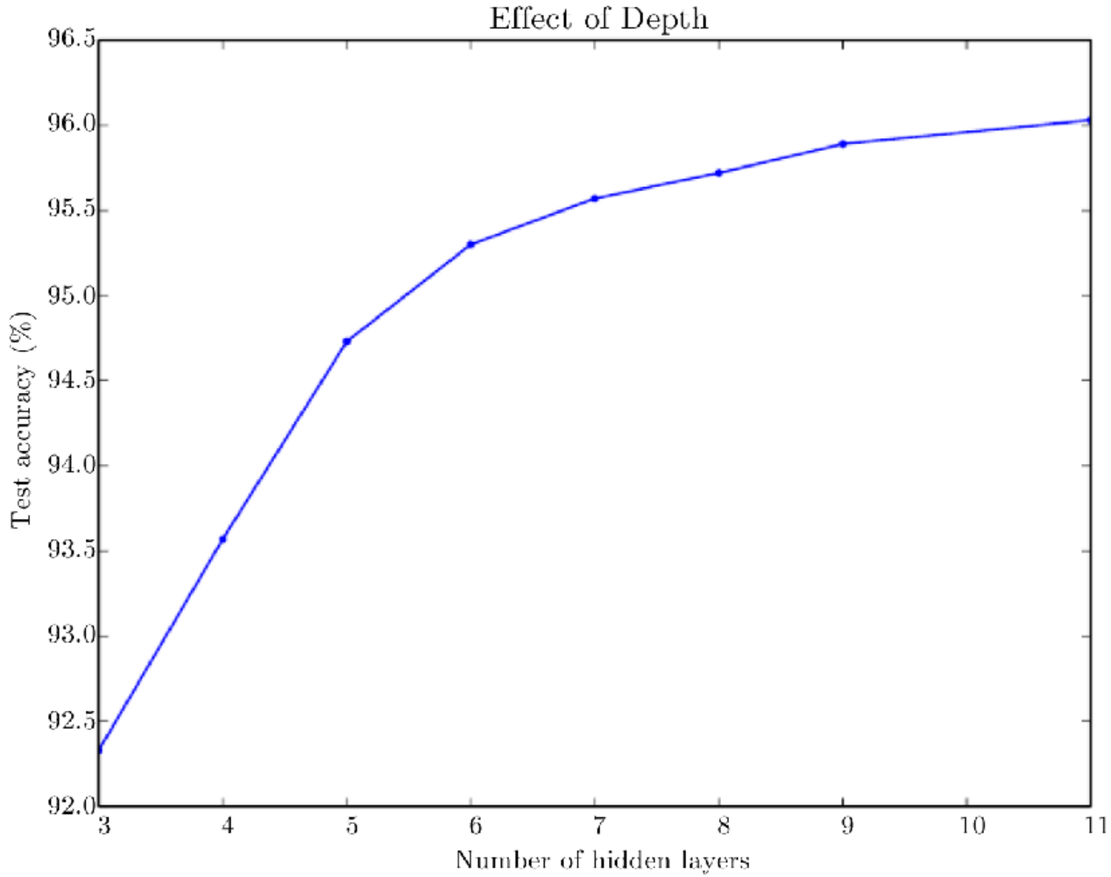


Space folding intuition for the case of **absolute value rectification units**:

- ✦ Geometric explanation of the exponential advantage of deeper networks
- ✦ Mirror axis of symmetry given by the hyperplane (de.ned by weights and bias)
- ✦ Complex functions arise as mirrored images of simpler patterns

Montufar, Pascanu, Cho and Bengio: On the Number of Linear Regions of Deep Neural Networks. NIPS, 2014.

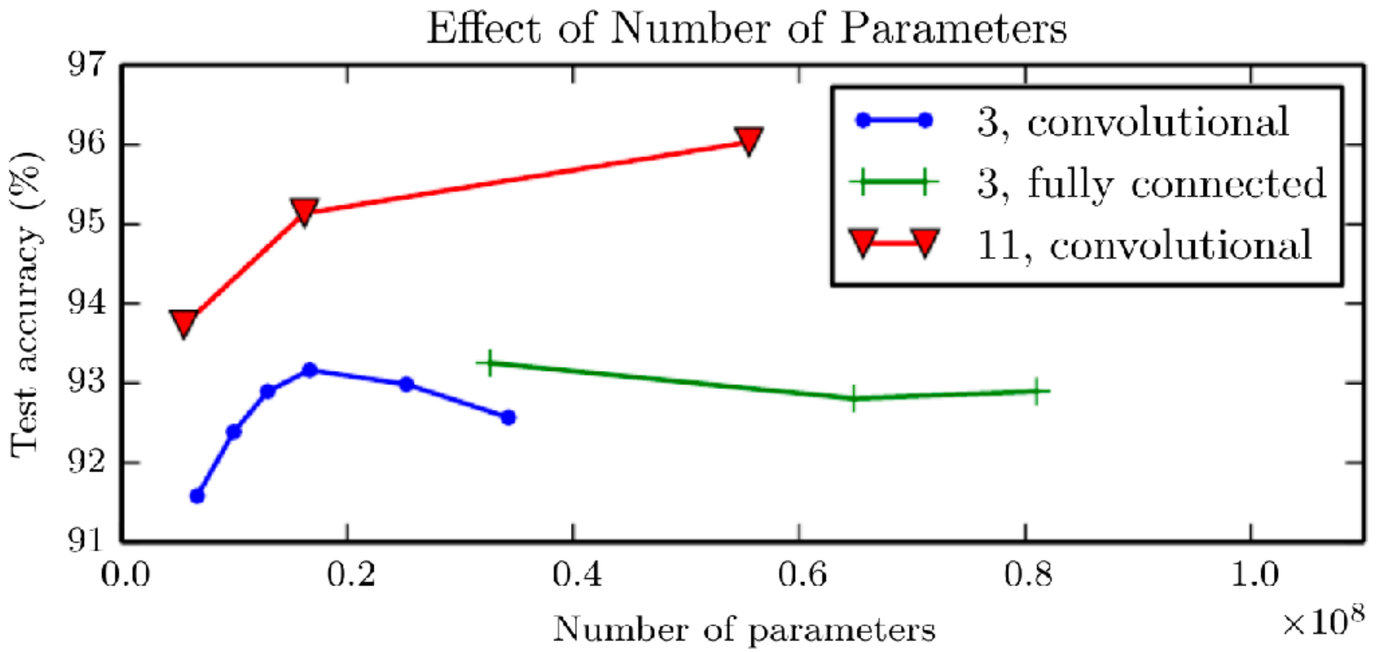
Effect of Network Depth



- ✦ Deeper networks generalize better (task: multi-digit number classification)

Goodfellow, Bulatov, Ibarz, Arnoud and Shet: Multi-digit number recognition from Street View imagery using deep convolutional neural networks. ICLR, 2014.

Effect of Network Depth



- Increasing the number of parameters is not as effective as increasing depth
- Shallow models even overfit at around 20 million parameters in this example
- Compositionality is a useful prior over the space of functions the model can learn

Goodfellow, Bulatov, Ibarz, Arnoud and Shet: Multi-digit number recognition from Street View imagery using deep convolutional neural networks. ICLR, 2014.