

Deep Learning

Lecture 3 – Deep Neural Networks

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Robotics, Computer Vision, Deep Learning, Machine Learning, System Software



Agenda

3.1 Backpropagation with Tensors

3.2 The XOR Problem

3.3 Multi-Layer Perceptrons

3.4 Universal Approximation

3.1

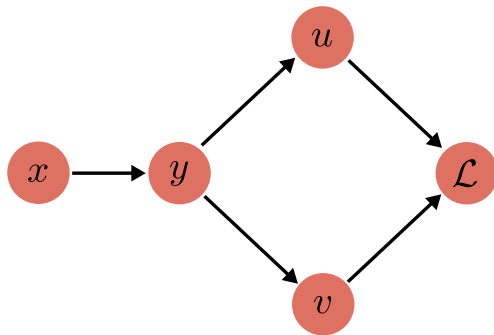
Backpropagation with Tensors

Recap: Backpropagation with Scalars

Forward Pass:

- (1) $y = y(x)$
- (2) $u = u(y)$
- (2) $v = v(y)$
- (3) $\mathcal{L} = \mathcal{L}(u, v)$

Loss: $\mathcal{L}(u(y(x)), v(y(x)))$



Recap: Backpropagation with Scalars

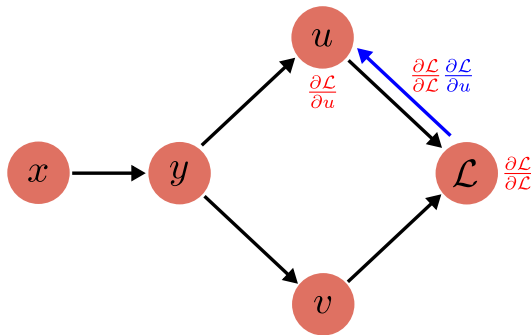
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- (1) $y = y(x)$
- (2) $u = u(y)$
- (2) $v = v(y)$
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Backward Pass:

(3) $\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial u}$

Loss: $\mathcal{L}(u(y(x)), v(y(x)))$



Recap: Backpropagation with Scalars

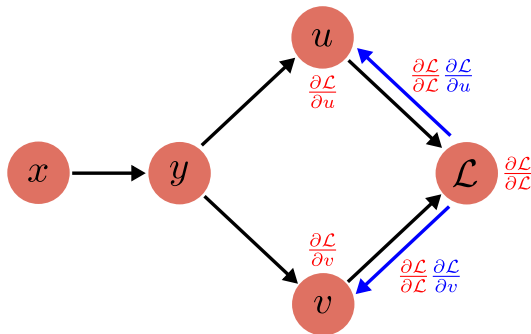
Forward Pass:

- (1) $y = y(x)$
- (2) $u = u(y)$
- (2) $v = v(y)$
- (3) $\mathcal{L} = \mathcal{L}(u, v)$

Backward Pass:

$$(3) \quad \frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial u}$$
$$(3) \quad \frac{\partial \mathcal{L}}{\partial v} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \frac{\partial \mathcal{L}}{\partial v} = \frac{\partial \mathcal{L}}{\partial v}$$

Loss: $\mathcal{L}(u(y(x)), v(y(x)))$



Recap: Backpropagation with Scalars

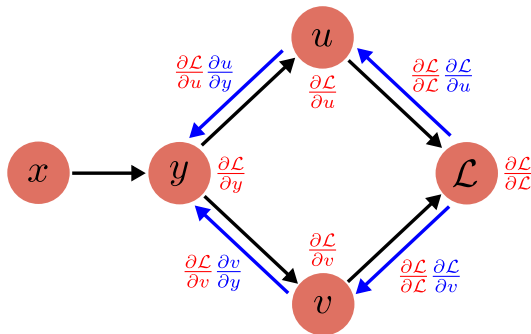
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- (2) $u = u(y)$
- (2) $v = v(y)$
- (3) $\mathcal{L} = \mathcal{L}(u, v)$

Backward Pass:

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

Loss: $\mathcal{L}(u(y(x)), v(y(x)))$



Recap: Backpropagation with Scalars

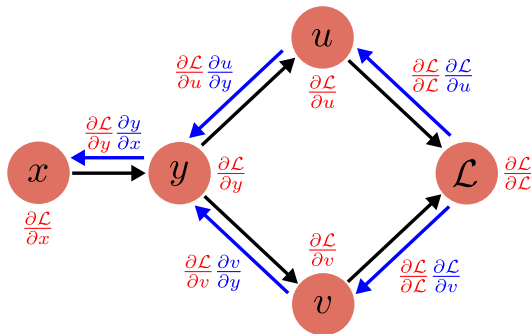
Forward Pass:

- (1) $y = y(x)$
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- (2) $v = v(y)$
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Backward Pass:

- (3) $\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial u}$
- (3) $\frac{\partial \mathcal{L}}{\partial v} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \frac{\partial \mathcal{L}}{\partial v} = \frac{\partial \mathcal{L}}{\partial v}$
- (2) $\frac{\partial \mathcal{L}}{\partial y} = \frac{\partial \mathcal{L}}{\partial u} \frac{\partial u}{\partial y} + \frac{\partial \mathcal{L}}{\partial v} \frac{\partial v}{\partial y}$
- (1) $\frac{\partial \mathcal{L}}{\partial x} = \frac{\partial \mathcal{L}}{\partial y} \frac{\partial y}{\partial x}$

Loss: $\mathcal{L}(u(y(x)), v(y(x)))$



Recap: Backpropagation with Scalars

Forward Pass:

- (1) $y = y(x)$
- (2) $u = u(y)$
- (2) $v = v(y)$
- (3) $\mathcal{L} = \mathcal{L}(u, v)$

Backward Pass:

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

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

`x.value = Input`

`y.value = y(x.value)`

`u.value = u(y.value)`

`v.value = v(y.value)`

`L.value = $\mathcal{L}(u.value, v.value)$`

Recap: Backpropagation with Scalars

Forward Pass:

- (1) $y = y(x)$
- (2) $u = u(y)$
- (2) $v = v(y)$
- (3) $\mathcal{L} = \mathcal{L}(u, v)$

Backward Pass:

- (3) $\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial u}$
- (3) $\frac{\partial \mathcal{L}}{\partial v} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \frac{\partial \mathcal{L}}{\partial v} = \frac{\partial \mathcal{L}}{\partial v}$
- (2) $\frac{\partial \mathcal{L}}{\partial y} = \frac{\partial \mathcal{L}}{\partial u} \frac{\partial u}{\partial y} + \frac{\partial \mathcal{L}}{\partial v} \frac{\partial v}{\partial y}$
- (1) $\frac{\partial \mathcal{L}}{\partial x} = \frac{\partial \mathcal{L}}{\partial y} \frac{\partial y}{\partial x}$

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

$$\textcolor{red}{x.grad} = \textcolor{red}{y.grad} = \textcolor{red}{u.grad} = \textcolor{red}{v.grad} = 0$$

$$\textcolor{red}{L.grad} = 1$$

$$\textcolor{red}{u.grad} += \textcolor{red}{L.grad} * (\partial \mathcal{L} / \partial u)(\textcolor{blue}{u.value}, \textcolor{blue}{v.value})$$

$$\textcolor{red}{v.grad} += \textcolor{red}{L.grad} * (\partial \mathcal{L} / \partial v)(\textcolor{blue}{u.value}, \textcolor{blue}{v.value})$$

$$\textcolor{red}{y.grad} += \textcolor{red}{u.grad} * (\partial u / \partial y)(\textcolor{blue}{y.value})$$

$$\textcolor{red}{y.grad} += \textcolor{red}{v.grad} * (\partial v / \partial y)(\textcolor{blue}{y.value})$$

$$\textcolor{red}{x.grad} += \textcolor{red}{y.grad} * (\partial y / \partial x)(\textcolor{blue}{x.value})$$

Scalar vs. Matrix Operations

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

$$y = \sigma(w_1x + w_0)$$

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

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

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

Backpropagation on Loops

The matrix/vector computation

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

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] =  $\sigma$ (u.value[i] + b.value[i])
```

Backpropagation on Loops

The backpropagated gradients for

```
for i  y.value[i] =  $\sigma(\mathbf{u.value[i]} + \mathbf{b.value[i]})$ 
```

are:

```
for i  u.grad[i] += y.grad[i] *  $\sigma'(\mathbf{u.value[i]} + \mathbf{b.value[i]})$ 
```

```
for i  b.grad[i] += y.grad[i] *  $\sigma'(\mathbf{u.value[i]} + \mathbf{b.value[i]})$ 
```

► **Red:** back-propagated gradients

► **Blue:** local gradients

Backpropagation on 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 on 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] =  $\sigma$ (U.value[h,i,j])
```

Backpropagation loops:

```
h,i,j  U.grad += Y.grad[h,i,j] *  $\sigma'$ (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 $\mathbf{X} \in \mathbb{R}^{N \times D}$ is a data point, bias $\mathbf{b} \in \mathbb{R}^M$ is broadcast to $\mathbf{B} \in \mathbb{R}^{N \times M}$

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] =  $\sigma$ (U.value[b,i] + B.value[i])
```

- Only inputs and outputs depend on batch index b , not the parameters (e.g., \mathbf{A} , \mathbf{B})
- By convention, the gradients are averaged over the batch

Implementation

Affine Transformation: (applied to N data points simultaneously)

$$\mathbf{Y} = \mathbf{XA} + \mathbf{B}$$

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

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

The XOR Problem

Logistic Regression Model:

$$\hat{y} = \sigma(\mathbf{w}^\top \mathbf{x}) \quad \text{with} \quad \sigma(x) = \frac{1}{1 + e^{-x}}$$

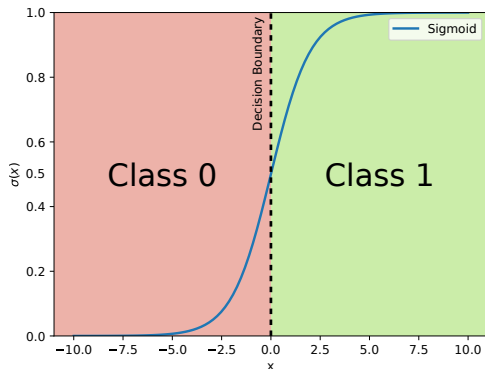
- Which problems can we solve with such a simple linear classifier?

The XOR Problem

Example: 2D Logistic Regression

$$\hat{y} = \sigma(\mathbf{w}^\top \mathbf{x} + w_0) \quad \sigma(x) = \frac{1}{1 + e^{-x}}$$

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



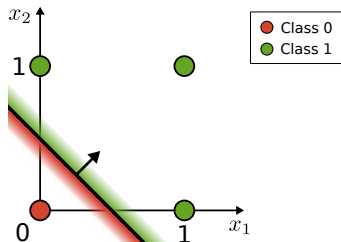
The XOR Problem

Linear Classifier:

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

$$\underbrace{\begin{pmatrix} 1 & 1 \end{pmatrix}}_{\mathbf{w}^\top} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{0.5}_{-w_0}$$

x_1	x_2	$\text{OR}(x_1, x_2)$
0	0	0
0	1	1
1	0	1
1	1	1



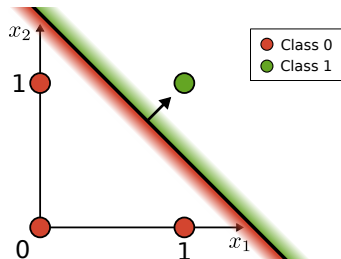
The XOR Problem

Linear Classifier:

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

x_1	x_2	$\text{AND}(x_1, x_2)$
0	0	0
0	1	0
1	0	0
1	1	1

$$\underbrace{\begin{pmatrix} 1 & 1 \end{pmatrix}}_{\mathbf{w}^\top} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{1.5}_{-w_0}$$



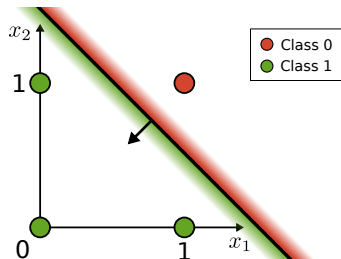
The XOR Problem

Linear Classifier:

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

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

$$\underbrace{\begin{pmatrix} -1 & -1 \end{pmatrix}}_{\mathbf{w}^\top} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{-1.5}_{-w_0}$$



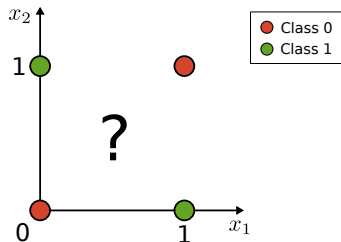
The XOR Problem

Linear Classifier:

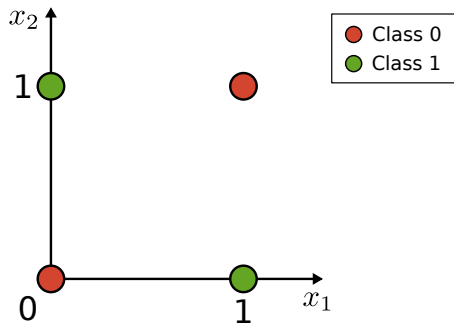
$$\text{Class 1} \Leftrightarrow \mathbf{w}^\top \mathbf{x} > -w_0$$

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

$$\underbrace{\begin{pmatrix} ? & ? \end{pmatrix}}_{\mathbf{w}^\top} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} > \underbrace{?}_{-w_0}$$

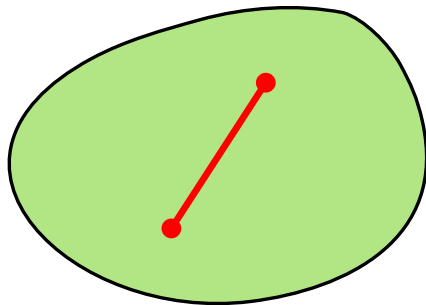
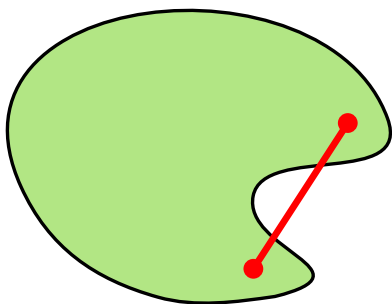


The XOR Problem



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

Convex Sets

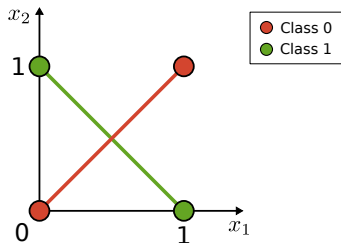


- A set \mathcal{S} is **convex** if any line segment connecting 2 points in \mathcal{S} lies entirely within \mathcal{S} :

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

The XOR Problem

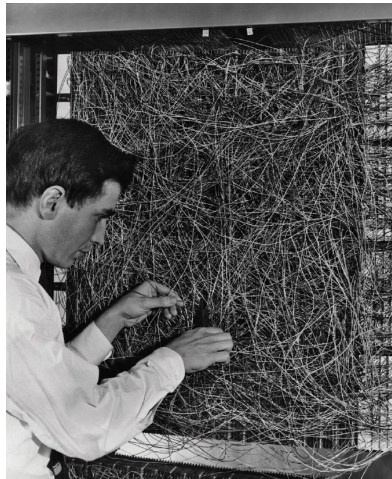
- ▶ Half-spaces (e.g., decision regions) are convex sets
- ▶ Suppose there was a feasible hypothesis. If the positive examples are in the positive half-space, then the green line segment must be as well.
- ▶ Similarly the red line must lie within the negative half-space.
- ▶ But the intersection can't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



The 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?

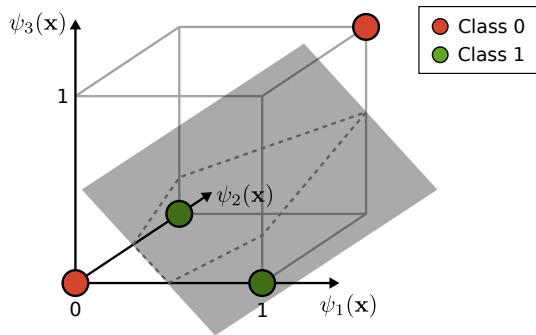


The XOR Problem

**Linear classifier with
non-linear features ψ :**

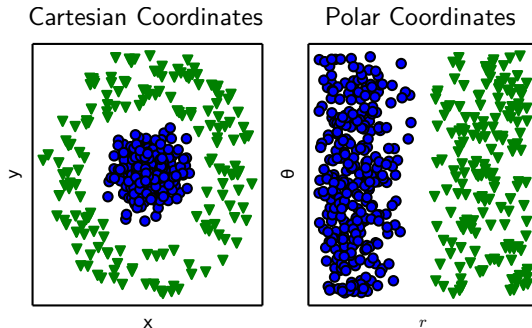
$$\mathbf{w}^\top \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix}}_{\psi(\mathbf{x})} > -w_0$$

x_1	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 \Rightarrow **Representation learning**
- ▶ Human needs to choose the right function family rather than the correct function

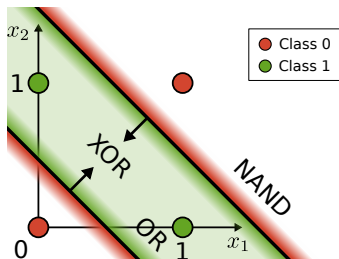
The XOR Problem

Linear Classifier:

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

x_1	x_2	$\text{XOR}(x_1, x_2)$
0	0	0
0	1	1
1	0	1
1	1	0

$$\text{XOR}(x_1, x_2) = \text{AND}(\text{OR}(x_1, x_2), \text{NAND}(x_1, x_2))$$



The XOR Problem

$$\text{XOR}(x_1, x_2) = \text{AND}(\text{OR}(x_1, x_2), \text{NAND}(x_1, x_2))$$

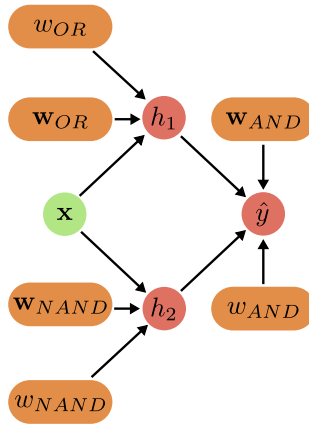
The above expression can be rewritten as a **program of logistic regressors**:

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

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

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

Note that $\mathbf{h}(\mathbf{x})$ is a non-linear feature of \mathbf{x} .
We call $\mathbf{h}(\mathbf{x})$ a **hidden** layer.

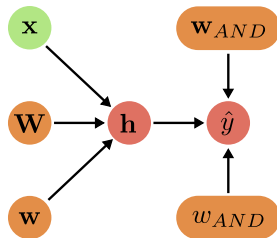


The XOR Problem

$$\text{XOR}(x_1, x_2) = \text{AND}(\text{OR}(x_1, x_2), \text{NAND}(x_1, x_2))$$

Writing the two 1D mappings $h_1(\mathbf{x})$ and $h_2(\mathbf{x})$ as a **single 2D mapping** $\mathbf{h}(\mathbf{x})$ yields:

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



Parameters can be learned using backprop. This is our first **Multi-Layer Perceptron!**

3.3

Multi-Layer Perceptrons

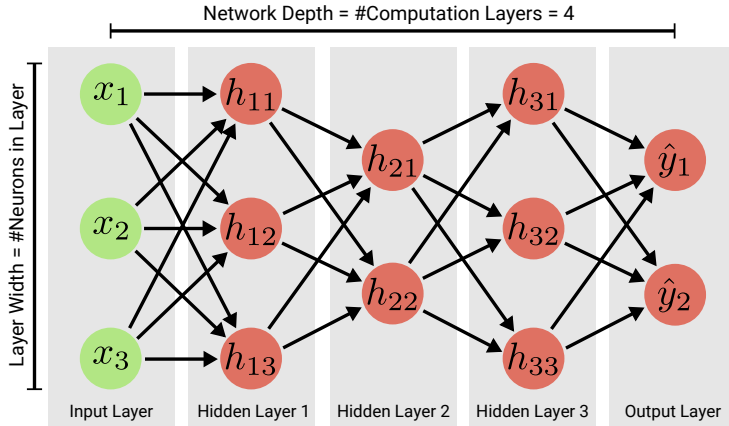
Multi-Layer Perceptrons

- ▶ MLPs are **feedforward** neural networks (no feedback connections)
- ▶ They **compose** several non-linear functions $\mathbf{f}(\mathbf{x}) = \hat{\mathbf{y}}(\mathbf{h}_3(\mathbf{h}_2(\mathbf{h}_1(\mathbf{x}))))$ 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** ($\mathbf{a}^\top \mathbf{x} + \mathbf{b}$) followed by non-linear **activation functions** (g):

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

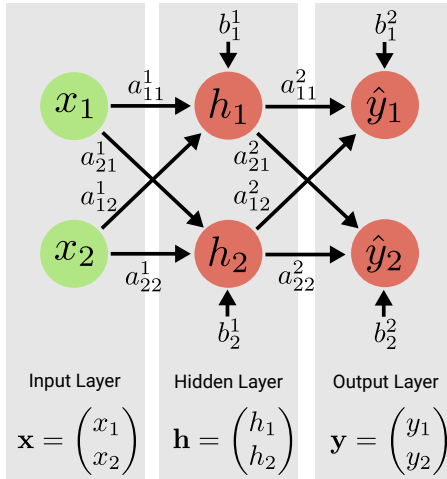
- ▶ Each neuron in each layer is **fully connected** to all neurons of the previous layer
- ▶ The overall length of the chain is the **depth** of the model \Rightarrow “Deep Learning”
- ▶ The name MLP is misleading as we don’t use threshold units as in Perceptrons

MLP Network Architecture



- Neurons are grouped into layers, each neuron **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 **activ. function** $h(\cdot)$ and weights $\mathbf{A}_L, \mathbf{b}_L$

MLP Network Architecture



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

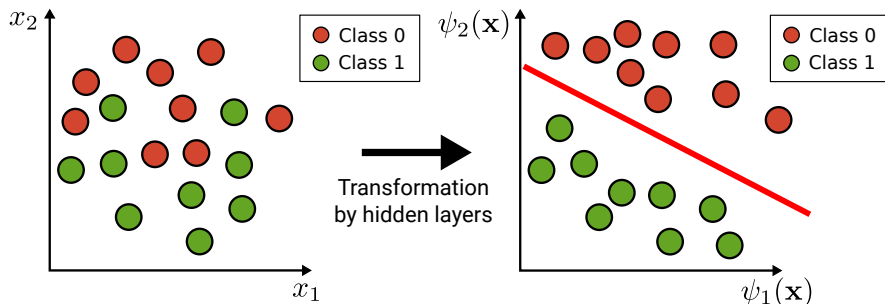
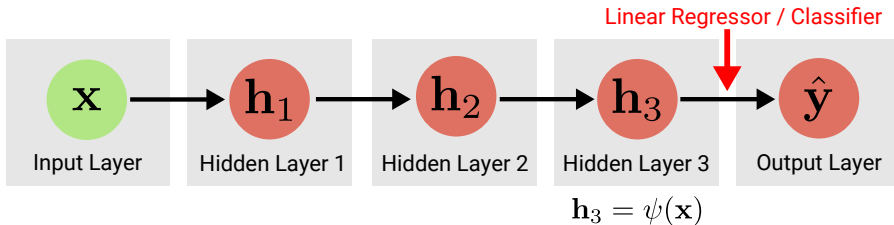
$$\mathbf{y} = h(\mathbf{A}_2 \mathbf{h} + \mathbf{b}_2)$$

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

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

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

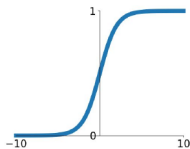
Feature Learning Perspective



Activation Functions $g(\cdot)$

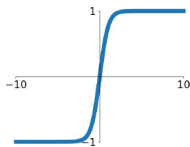
Sigmoid

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



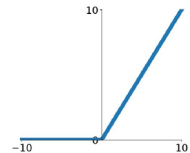
tanh

$$\tanh(x)$$



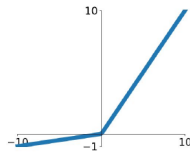
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

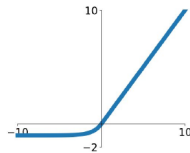


Maxout

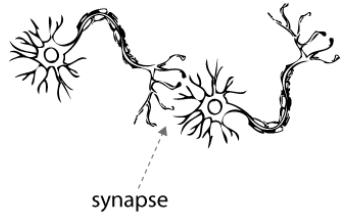
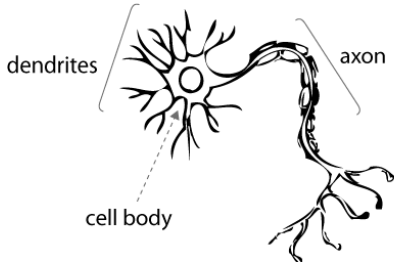
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



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

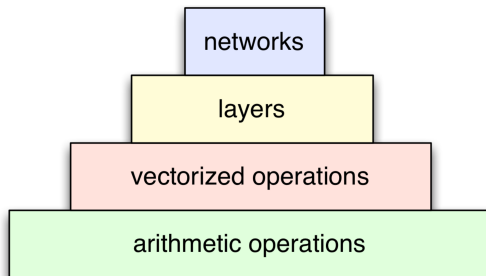
Algorithm for training an MLP using (stochastic) gradient descent:

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 $\mathbf{h}_1, \mathbf{h}_2, \dots, \hat{\mathbf{y}}$
 - 3.2 Backpropagate gradients through network to obtain $\nabla_{\mathbf{w}} \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y})$
4. Update gradients: $\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \frac{1}{|\mathcal{X}_{\text{batch}}|} \sum_{(\mathbf{x}, \mathbf{y}) \in \mathcal{X}_{\text{batch}}} \nabla_{\mathbf{w}} \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y})$
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

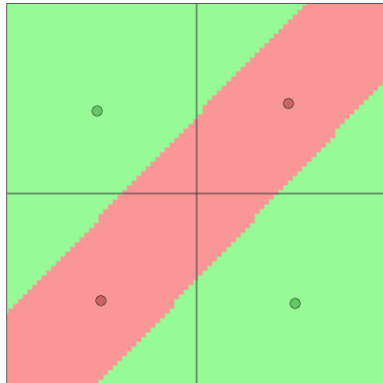


- ▶ When designing neural networks and machine learning algorithms, you'll need to simultaneously think at multiple level's of abstraction
- ▶ "The psychological profiling [of a programmer] is mostly the ability to shift levels of abstraction, from low level to high level. To see something in the small and to see something in the large." [Donald E. Knuth]

The 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

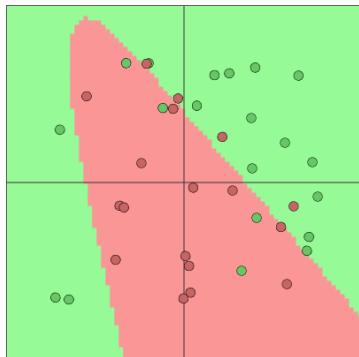


- Note that we have learned a boolean circuit! \Rightarrow differentiable programming

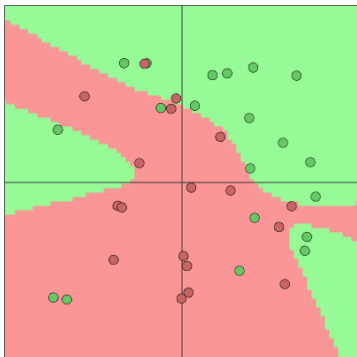
<https://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html>

A More Challenging Problem

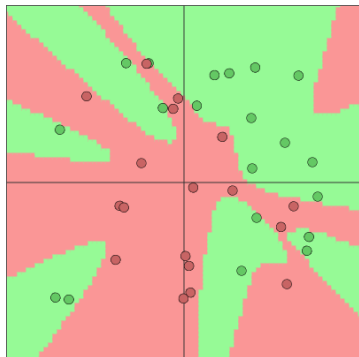
2 Hidden Neurons



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

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

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?

3.4

Universal Approximation

Universal Approximation Theorem

Theorem 1

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

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

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

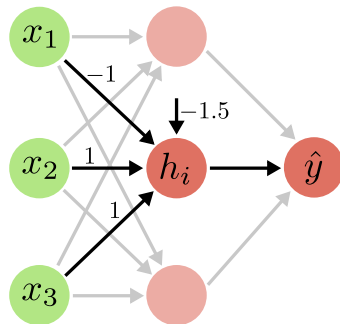
$$|G(\mathbf{x}) - f(\mathbf{x})| < \epsilon \quad \text{for all } \mathbf{x} \in I_n$$

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

Example: Binary Case

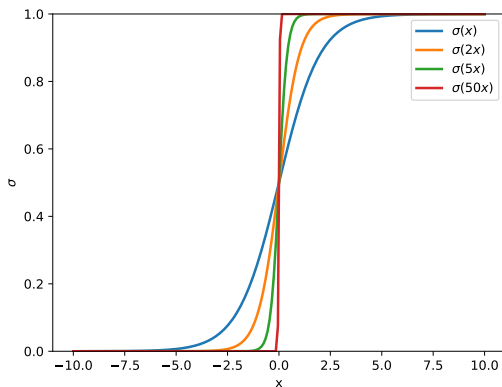
x_1	x_2	x_3	y
\vdots	\vdots	\vdots	\vdots
0	1	0	0
0	1	1	1
1	0	0	0
\vdots	\vdots	\vdots	\vdots

$$\hat{y} = \sum_i \underbrace{[\mathbf{a}_i^\top \mathbf{x} + b_i]_+}_{h_i}$$



- 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 **soft threshold** (e.g., sigmoid)
- Sigmoids approximate step functions when increasing the input weight

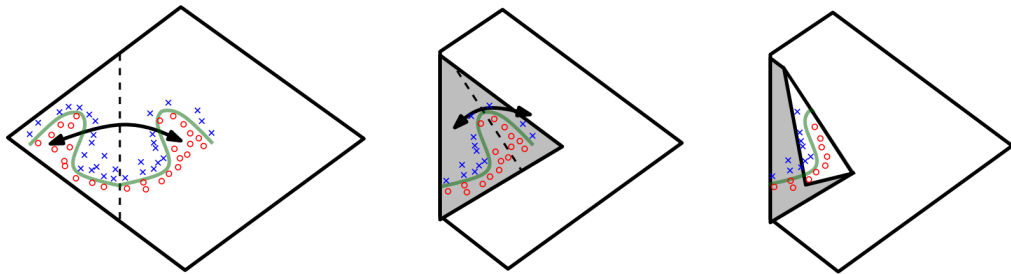
Network Width vs. Depth

- ▶ 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 \Rightarrow 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

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

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

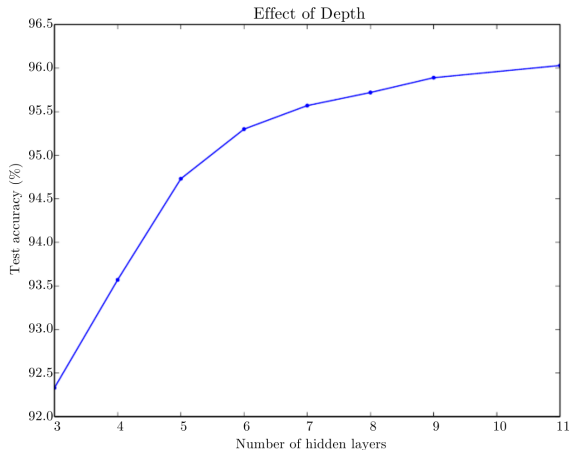
Space Folding Intuition



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

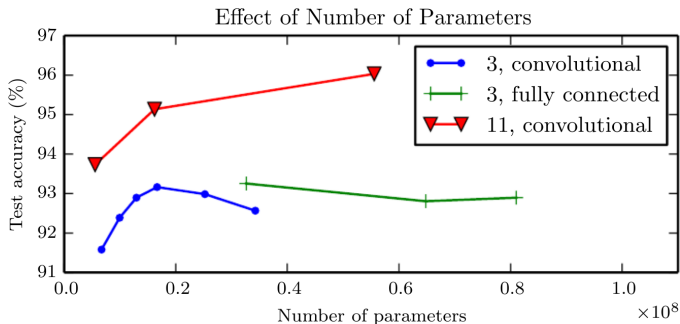
- ▶ Geometric explanation of the exponential advantage of deeper networks
- ▶ Mirror axis of symmetry given by the hyperplane (defined by weights and bias)
- ▶ Complex functions arise as mirrored images of simpler patterns

Effect of Network Depth



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

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