17. Neural Networks

STA3142 Statistical Machine Learning

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** Slides adapted from EECS498/598 @ Univ. of Michigan by Justin Johnson*

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Assignment 4

- Due **Friday 5/17, 11:59pm**
- Topics
  - K-Means and Gaussian Mixture Models
  - Principal Component Analysis
- Please read the instruction carefully!
  - Submit one pdf and one zip file separately
  - Write your code only in the designated spaces
  - Do not import additional libraries
  - …
- If you feel difficult, consider to take option 2.

Midterm Questions

- Questions got >= 3 votes:
  - 1.1~1.4, 1.8, 1.12, 2.1, 3~

Recap: Rough Plan

- We have **13 weeks (39 hours)** of lectures.

- **6 hours** for intro & math/python review
- **15 hours** for basic ML & supervised learning
  - Regression, classification, kernel methods, validation, …
- **3 hours** for unsupervised learning
- **12 hours** for neural networks
- **3 hours** for others
  - Reinforcement learning, summary
  - Note: You can take **STA3145** for RL

Note: Other Useful ML Topics

- **Probabilistic graphical model (PGM)**
  - Bayesian networks, Markov random fields, conditional random fields, (restricted) Boltzmann machine
  - **Gradient-based neural networks are preferred these days**
- **Hidden Markov model (HMM)**
  - For sequential data; **RNNs and Transformers are good replacements**
- **Tree-based models (useful for tabular data)**
  - Decision tree and random forest
  - Bootstrapping, bagging, and boosting
- **Statistical learning theory (for theoretical ML)**
  - Probably approximately correct (PAC) learning and VC dimension

Data Representations

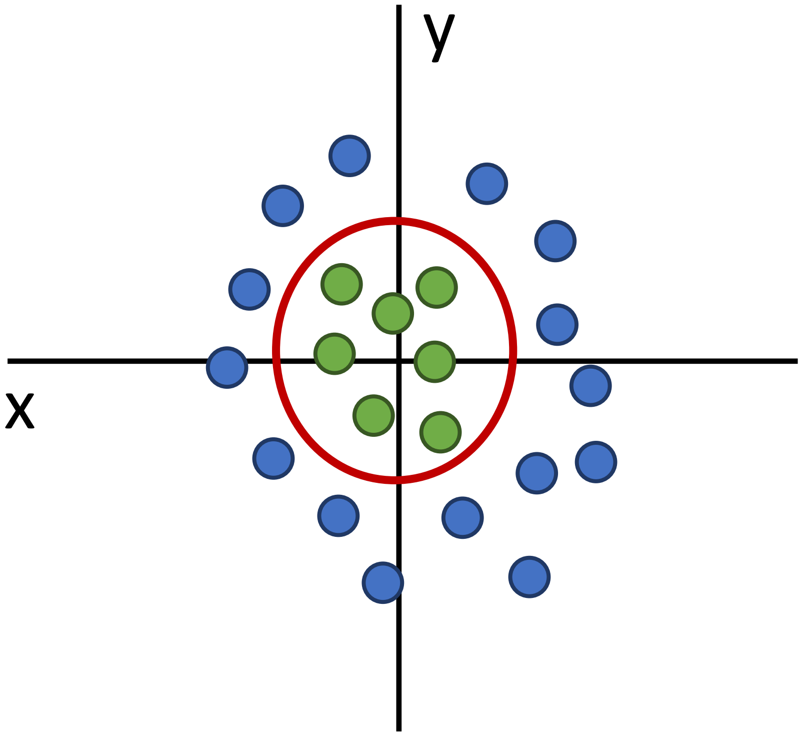
- The success of ML applications relies on having a **good representation** of the data.
  - Such that linear models perform well on top of the representation

- ML practitioners have put lots of efforts in **feature engineering**.
  - Based on domain expert's knowledge
    - E.g., Computer vision: color histogram, HoG, BoW, …
  - Time-consuming hand-tuning
  - (Arguably) a key limiting factor in advancing the state-of-the-arts

- Can we develop good representations **with less human effort**?

Beyond Linear Models: **Kernel Methods**

Original space

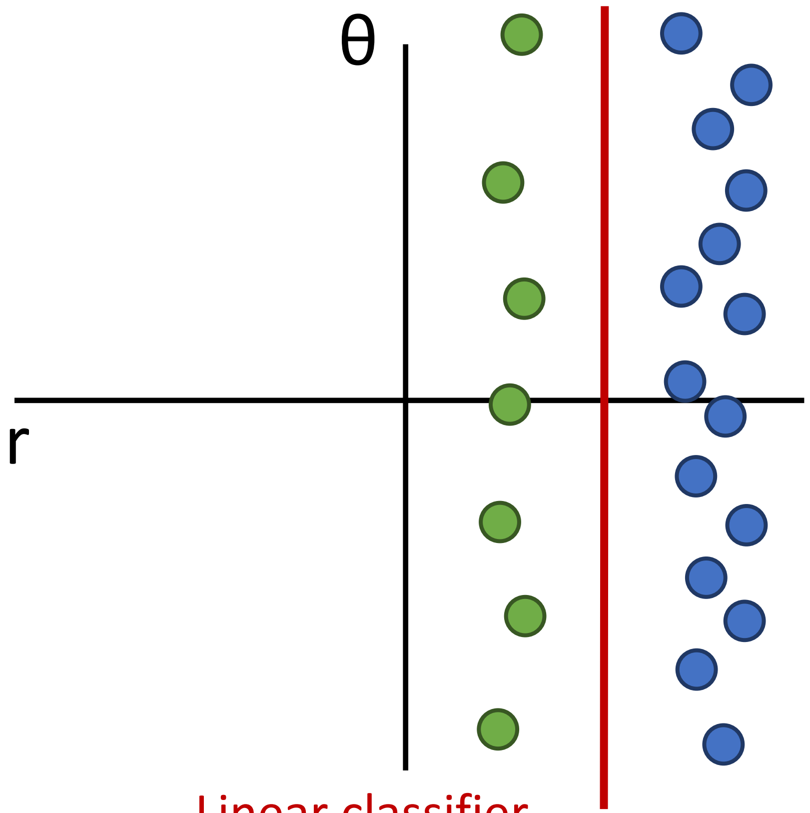


Nonlinear classifier
in original space!

$$r = (x^2 + y^2)^{1/2}$$
$$\theta = \tan^{-1}(y/x)$$

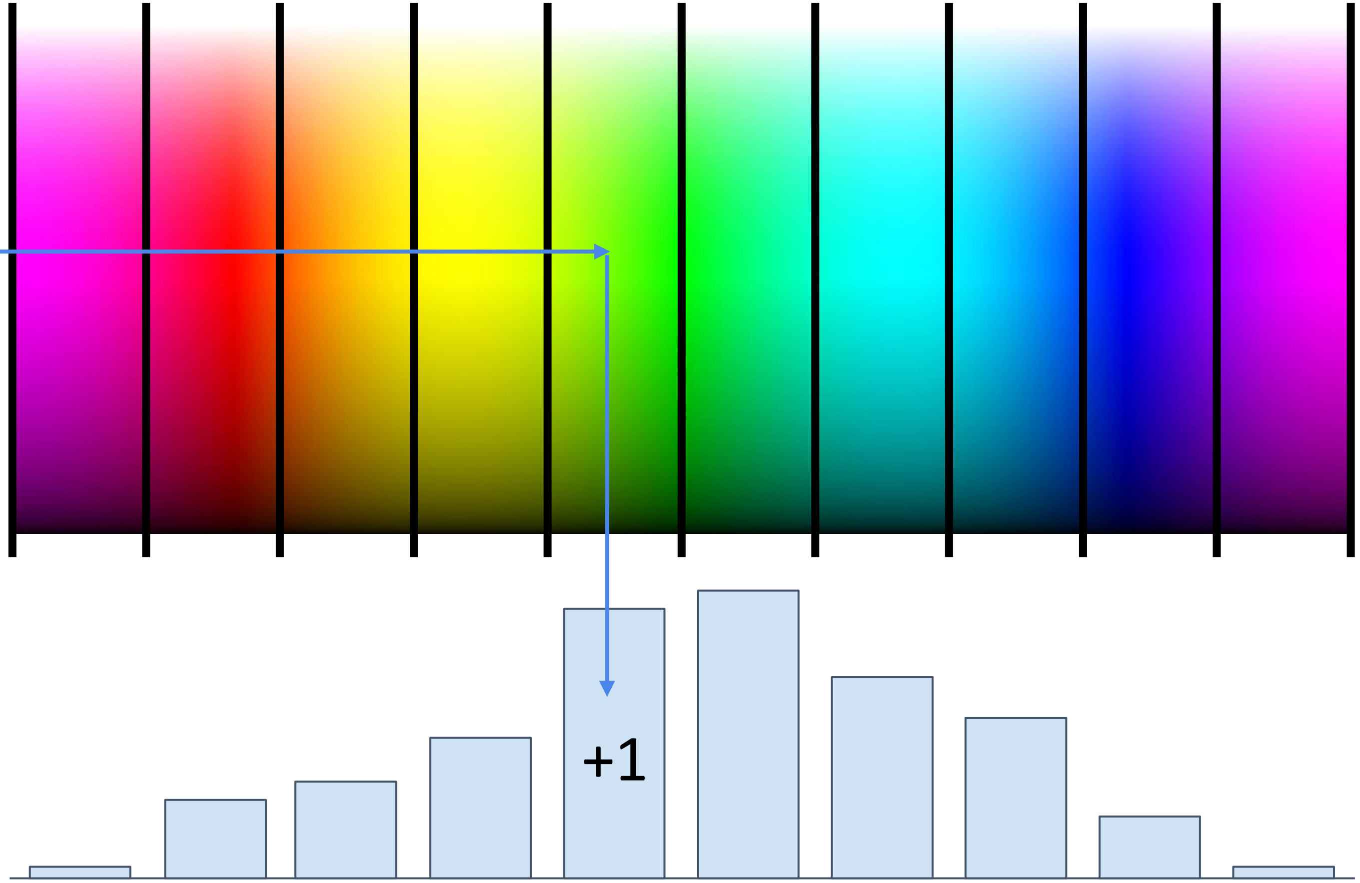
Feature transform

Feature space



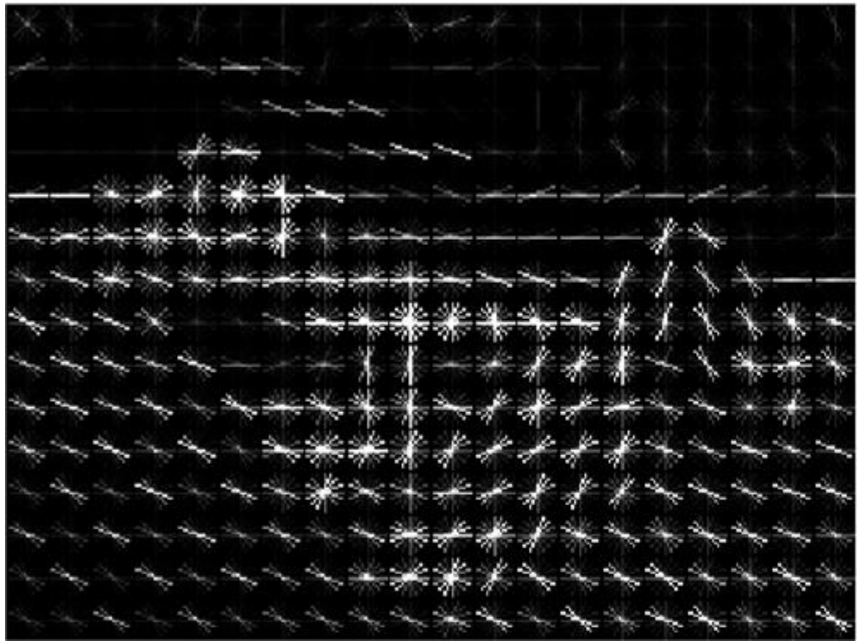
Linear classifier
in feature space

Image Features: Color Histogram



Ignores texture,
spatial positions

Image Features: Histogram of Oriented Gradients (HoG)

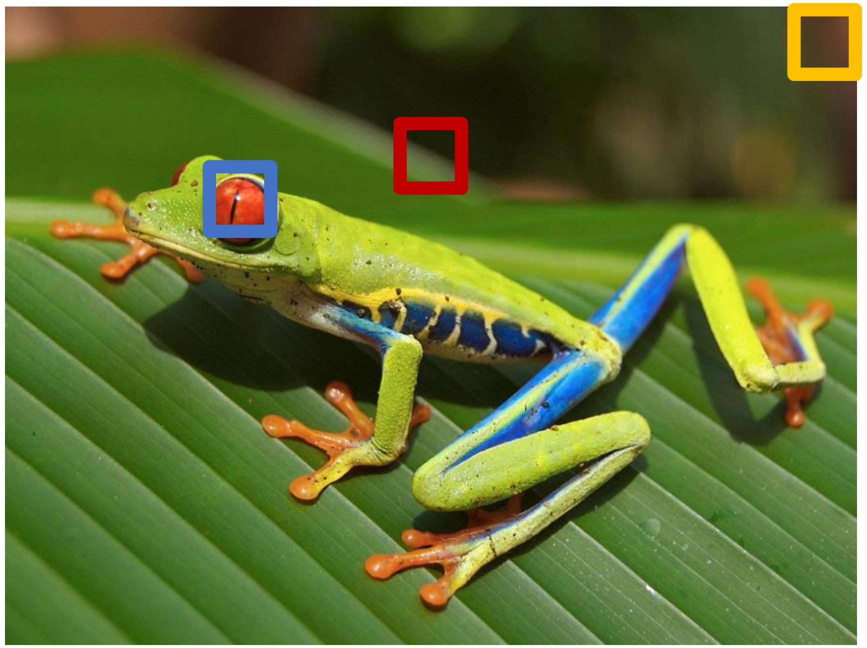


1. Compute edge direction / strength at each pixel
2. Divide image into 8x8 regions
3. Within each region compute a histogram of edge directions weighted by edge strength

Example: 320x240 image gets divided into 40x30 bins; 8 directions per bin; feature vector has 30*40*9 = 10,800 numbers

Lowe, "Object recognition from local scale-invariant features", ICCV 1999
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

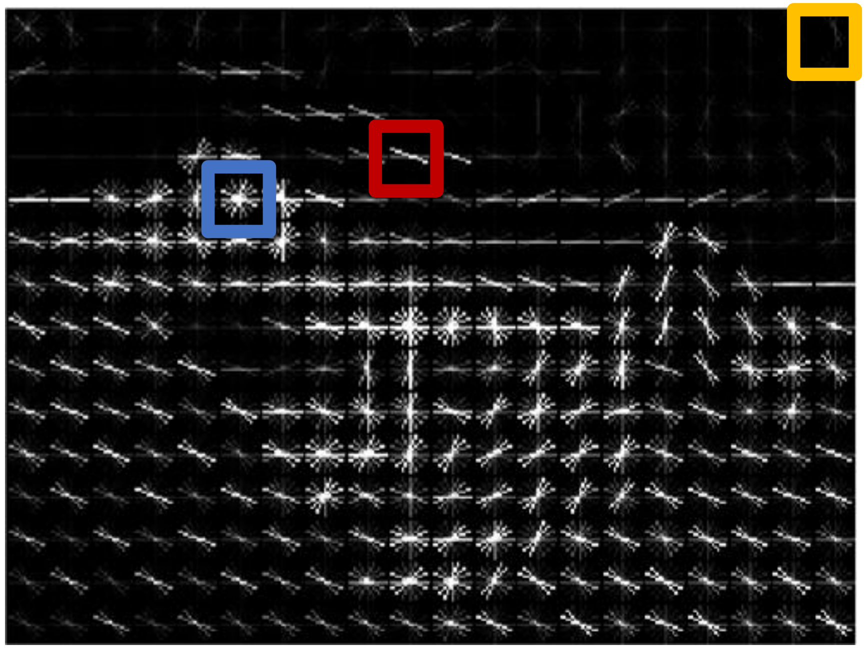
Image Features: Histogram of Oriented Gradients (HoG)



Weak edges

Strong diagonal edges

Edges in all directions



1. Compute edge direction / strength at each pixel
2. Divide image into 8x8 regions
3. Within each region compute a histogram of edge directions weighted by edge strength

Captures texture and position, robust to small image changes

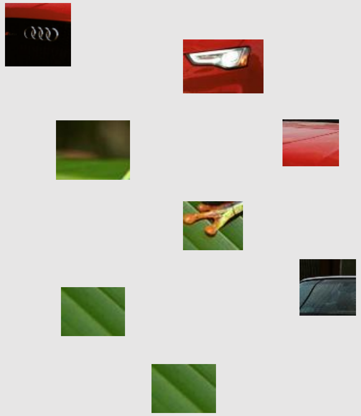
Example: 320x240 image gets divided into 40x30 bins; 8 directions per bin; feature vector has 30*40*9 = 10,800 numbers

Lowe, "Object recognition from local scale-invariant features", ICCV 1999
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

Image Features: Bag of Words (Data-Driven!)

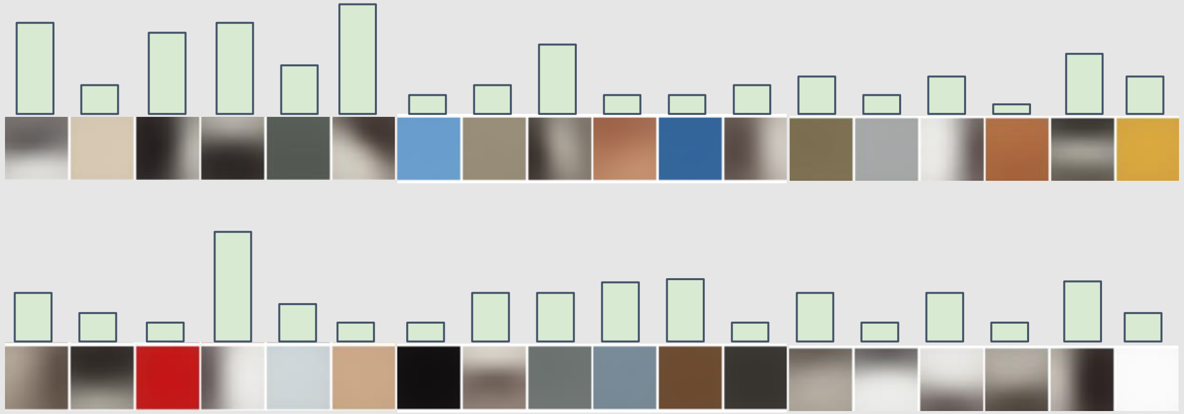
Step 1: Build codebook

Extract random patches



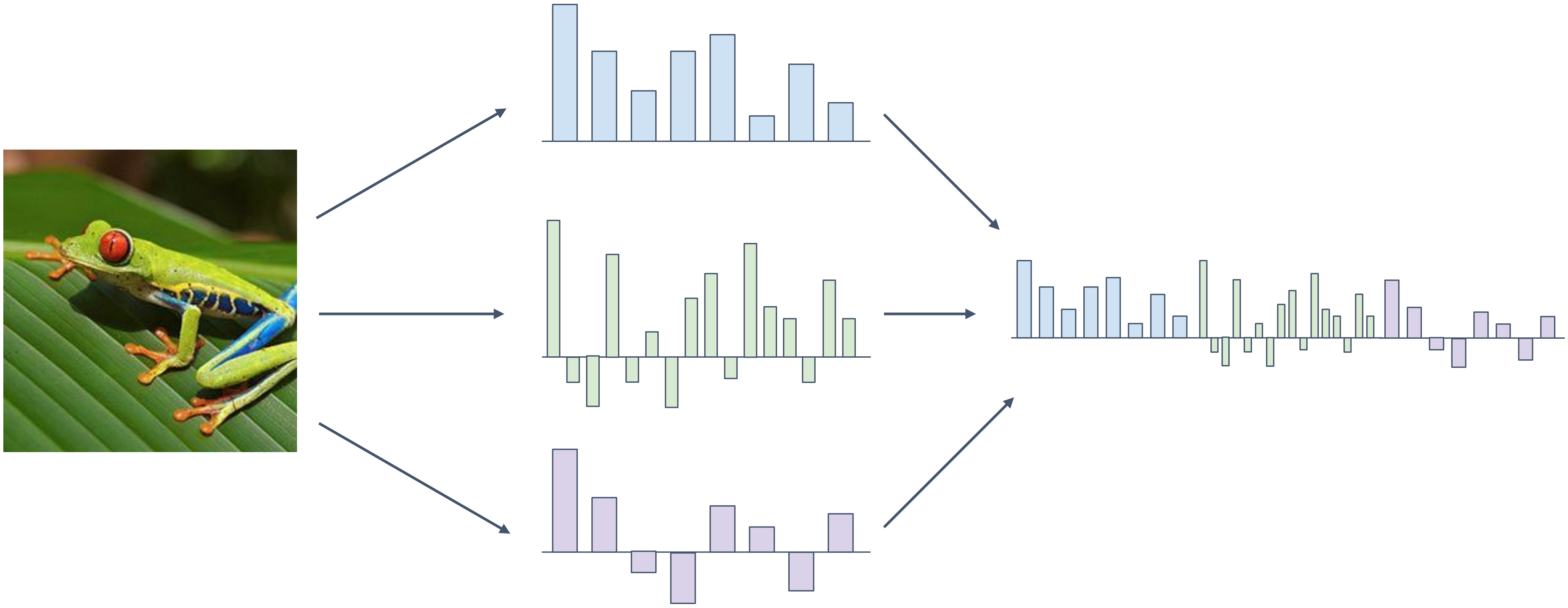
Cluster patches to form "codebook" of "visual words"

Step 2: Encode images



Fei-Fei and Perona, "A bayesian hierarchical model for learning natural scene categories", CVPR 2005

Image Features



Example: Winner of 2011 ImageNet challenge

Low-level feature extraction ≈ 10k patches per image

- SIFT: 128-dim
- color: 96-dim

$\Big\}$ reduced to 64-dim with PCA

FV extraction and compression:

- N=1,024 Gaussians, R=4 regions ⇨ 520K dim x 2
- compression: G=8, b=1 bit per dimension

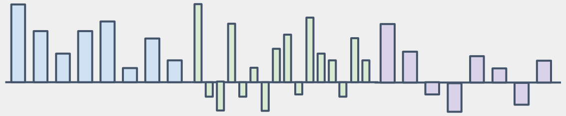
One-vs-all SVM learning with SGD

Late fusion of SIFT and color systems

F. Perronnin, J. Sánchez, “Compressed Fisher vectors for LSVRC”, PASCAL VOC / ImageNet workshop, ICCV, 2011.

Image Features

Feature Extraction



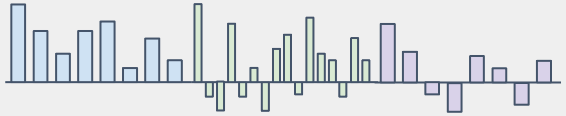
f

training

10 numbers giving scores for classes

Image Features vs. Neural Networks

Feature Extraction



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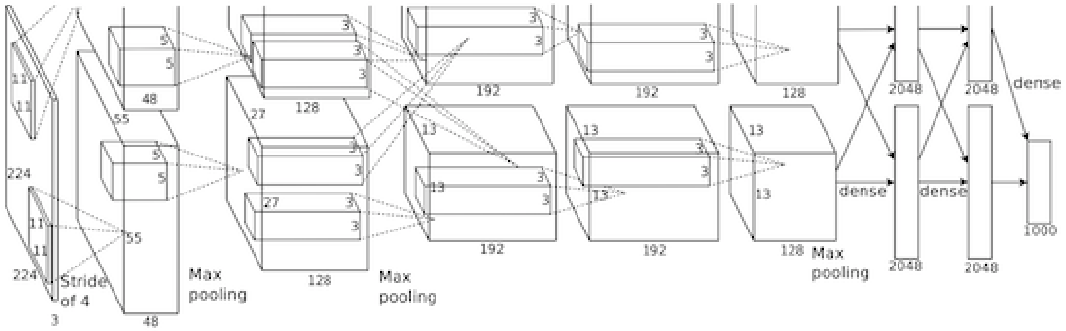
10 numbers giving scores for classes

training



Krizhevsky, Sutskever, and Hinton, “Imagenet classification with deep convolutional neural networks”, NIPS 2012.

10 numbers giving scores for classes

training

Neural Networks

Linear classifiers

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Neural Networks

Input: $x \in \mathbb{R}^D$ **Output**: $f(x) \in \mathbb{R}^C$ **Activation function**: g

Before: Linear Classifier: $f(x) = Wx + b$

Learnable parameters: $W \in \mathbb{R}^{C \times D}, b \in \mathbb{R}^C$

Now: Two-Layer Neural Network: $f(x) = W_2\, g(W_1 x + b_1) + b_2$

Learnable parameters: $W_1 \in \mathbb{R}^{H \times D}, b_1 \in \mathbb{R}^H, W_2 \in \mathbb{R}^{C \times H}, b_2 \in \mathbb{R}^C$

Neural Networks

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Feature Extraction
Linear Classifier

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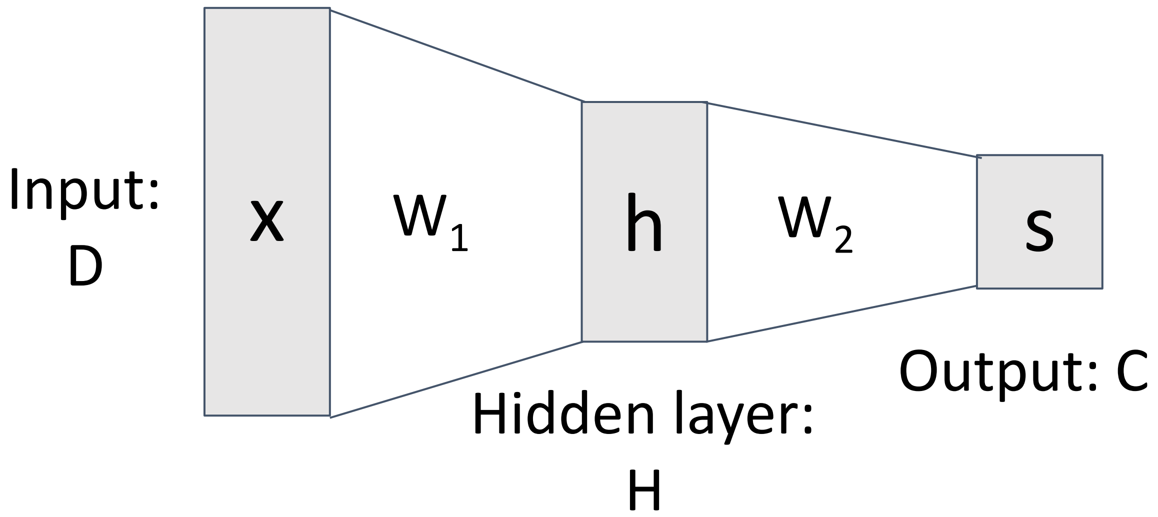
Or Three-Layer Neural Network:
$f(x) = W_3\, g(\, W_2\, g(W_1 x + b_1) + b_2) + b_3$

Neural Networks

Before: Linear classifier $f(x) = Wx + b$

Now: 2-layer Neural Network $f(x) = W_2\, g(W_1 x + b_1) + b_2$



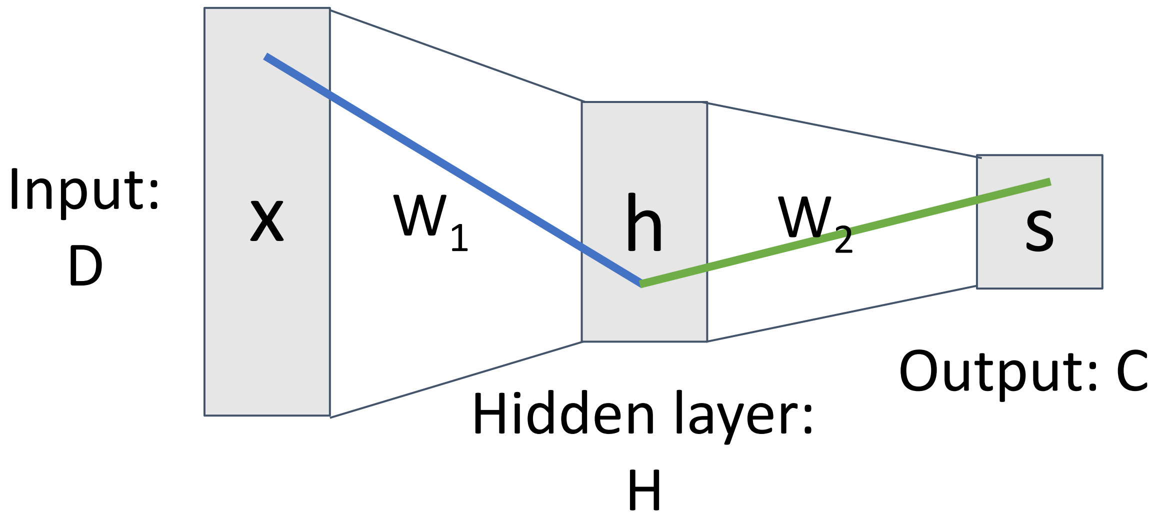
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural Networks

Before: Linear classifier $f(x) = Wx + b$

Now: 2-layer Neural Network $f(x) = W_2\, g(W_1 x + b_1) + b_2$

Element (i, j) of W_1 gives the effect on h_i from x_j



Element (i, j) of W_2 gives the effect on s_i from h_j

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

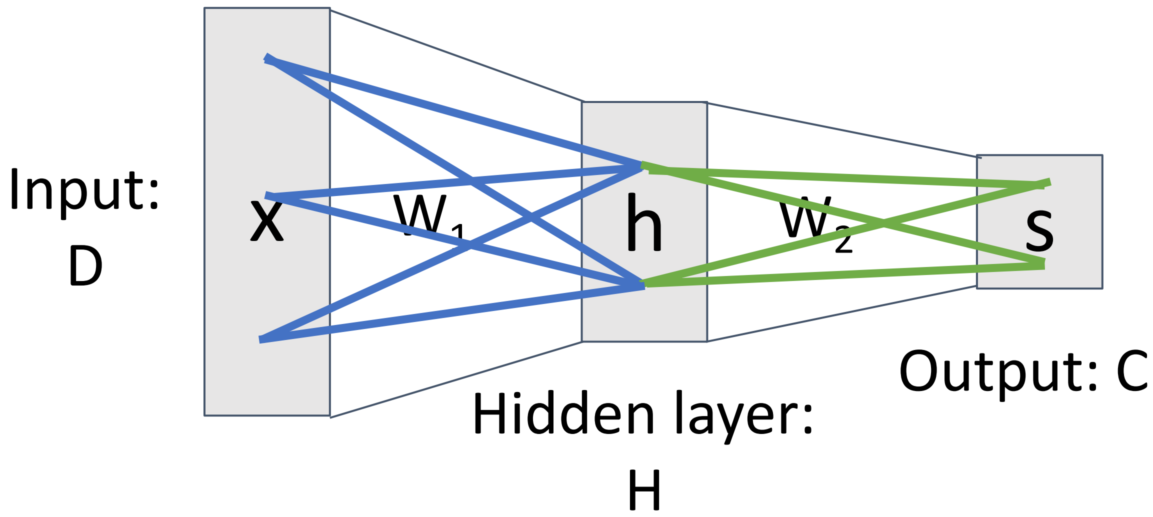
Neural Networks

Before: Linear classifier $f(x) = Wx + b$

Now: 2-layer Neural Network $f(x) = W_2\, g(W_1 x + b_1) + b_2$

Element (i, j) of W_1 gives the effect on h_i from x_j

All elements of x affect all elements of h

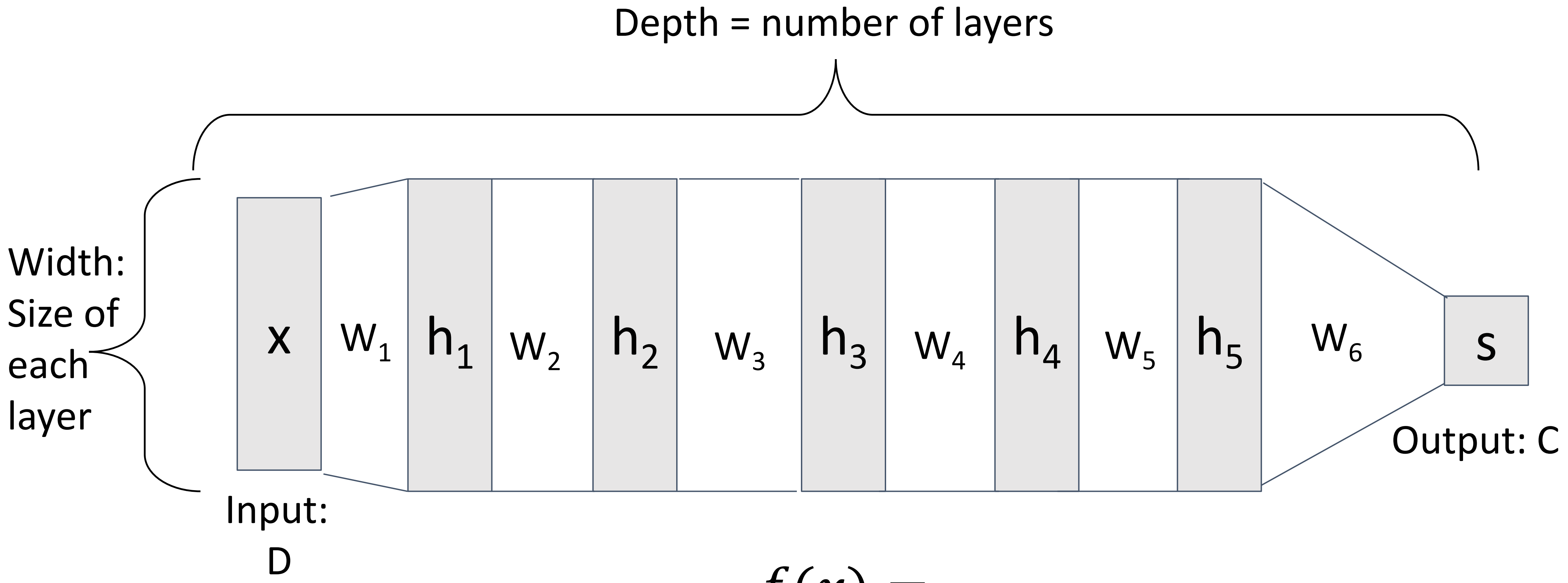


Element (i, j) of W_2 gives the effect on s_i from h_j

All elements of h affect all elements of s

Fully-connected neural network
a.k.a. "Multi-Layer Perceptron" (MLP)

Deep Neural Networks



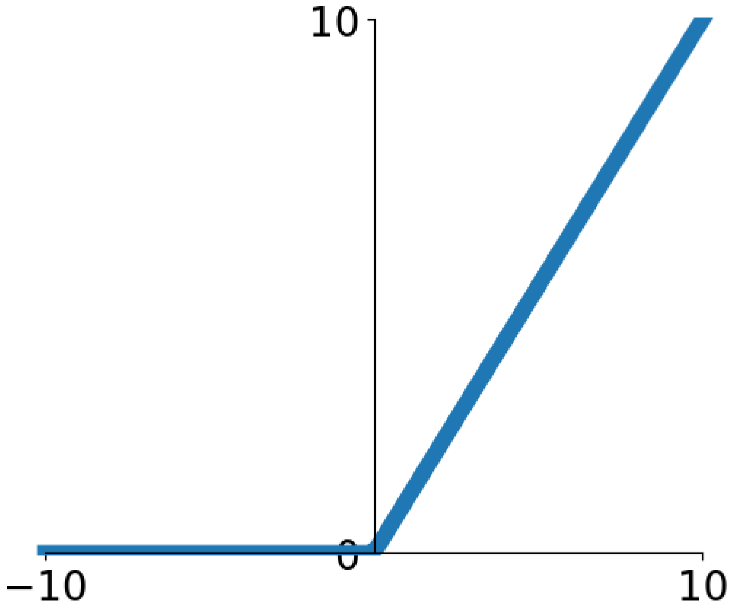
$$f(x) =$$
$$W_6\, g(W_5\, g(W_4\, g(W_3\, g(W_2\, g(W_1 x + b_1) + b_2) + b_3) + b_4) + b_5) + b_6$$

Activation Functions

2-layer Neural Network

$$f(x) = W_2 \boxed{g}(W_1 x + b_1) + b_2$$

The function $ReLU(z) = \max(0, z)$ is called "Rectified Linear Unit"



This is called the **activation function** of the neural network

Q: What happens if we build a neural network with no activation function?

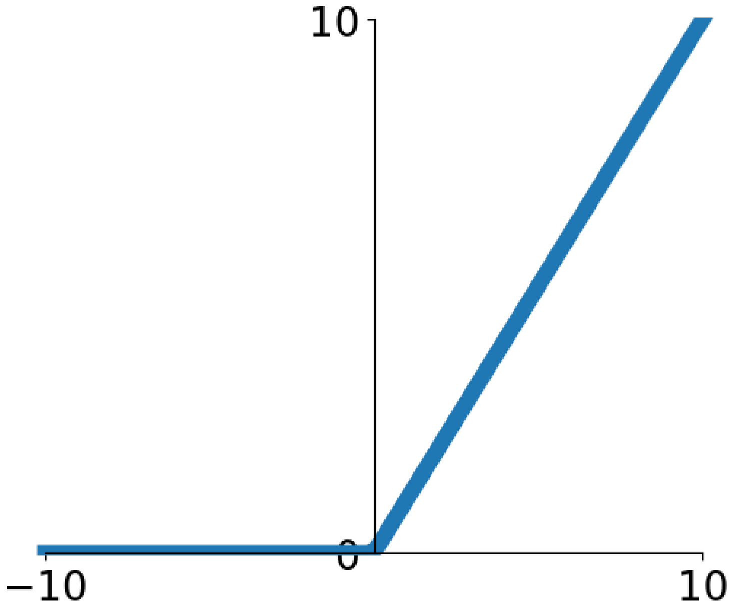
$$f(x) = W_2(W_1 x + b_1) + b_2$$

Activation Functions

2-layer Neural Network

$$f(x) = W_2 \boxed{g}(W_1 x + b_1) + b_2$$

The function $ReLU(z) = \max(0, z)$ is called "Rectified Linear Unit"



This is called the **activation function** of the neural network

Q: What happens if we build a neural network with no activation function?

$$\begin{aligned} f(x) &= W_2(W_1 x + b_1) + b_2 \\ &= (W_1 W_2)x + (W_2 b_1 + b_2) \end{aligned}$$

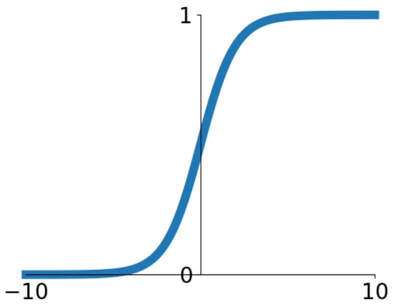
A: We end up with a linear classifier!

Activation Functions

ReLU is a good default choice for most problems

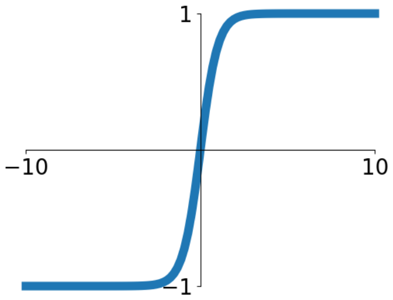
Sigmoid

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



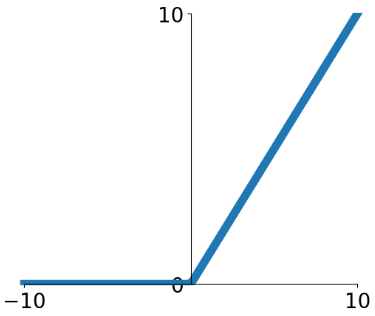
tanh

$$\tanh(x) = \frac{e^{2x} - 1}{e^{2x} + 1}$$



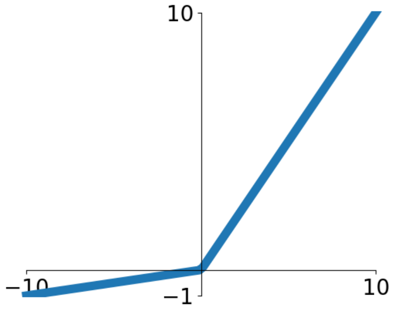
ReLU

$$\max(0, x)$$



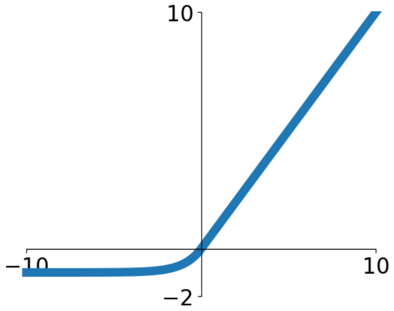
Leaky ReLU

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



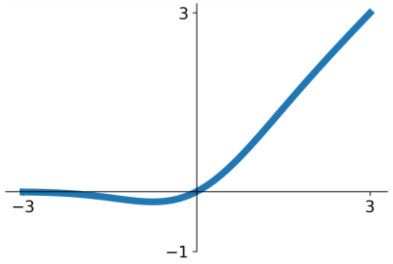
ELU

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



GELU

$$= 0.5x\left[1 + \mathrm{erf}(x/\sqrt{2})\right]$$
$$\approx x\sigma(1.702x)$$



Recap: Cross-Entropy Loss (Softmax Regression)

Input: $x \in \mathbb{R}^D$ **Output**: $f(x) \in \mathbb{R}^C$

Softmax probability vector: $p(y|x) \in [0,1]^C$

$\boldsymbol{k}$**-th class probability**: $p(y = k|x) = \frac{\exp(s_k)}{\sum_j \exp(s_j)} \in [0,1]$

Cross-Entropy Loss for a training data $\left(x^{(i)}, y^{(i)}\right)$:

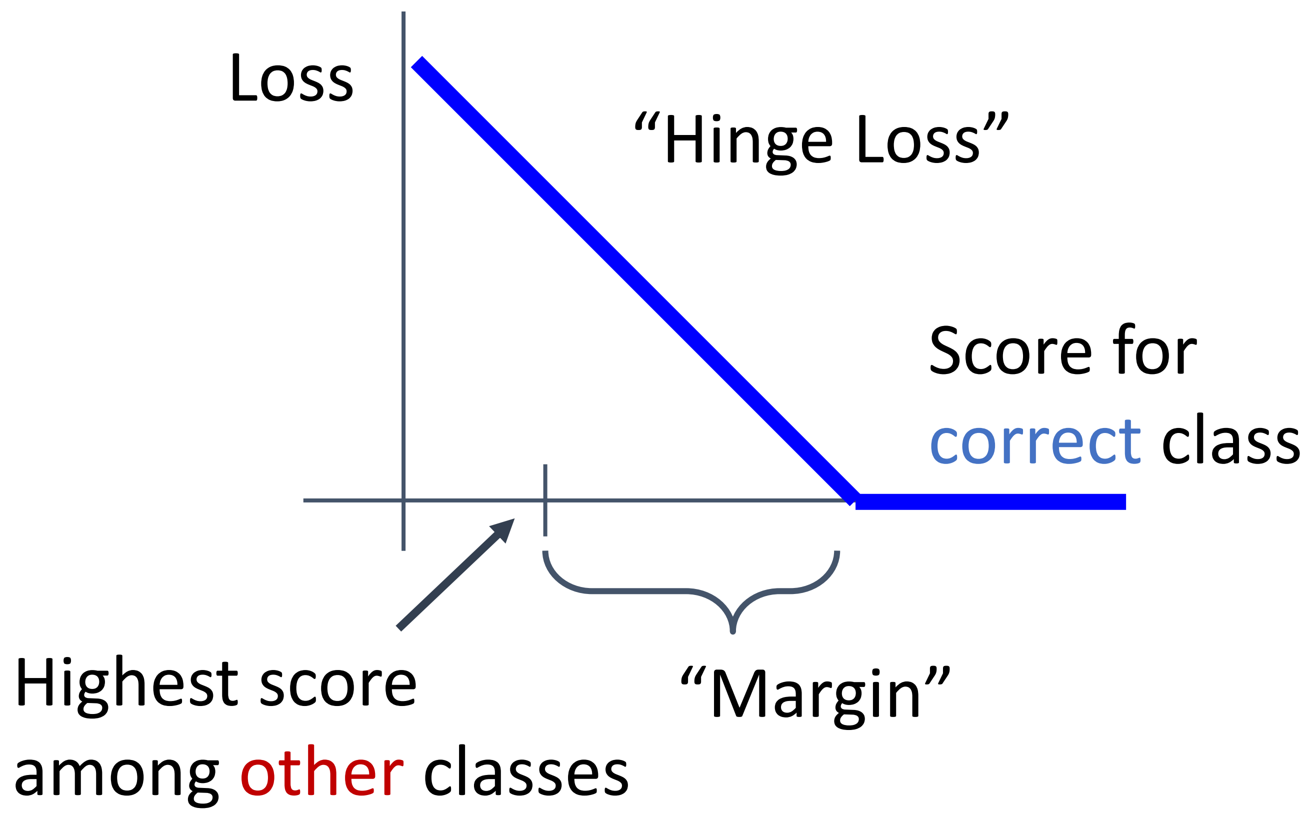
$$L_i = -\log p\left(y = y^{(i)}|x^{(i)}\right) = -\log \frac{\exp\left(s_{y^{(i)}}\right)}{\sum_j \exp\left(s_j\right)}$$

Note: we don't need softmax at test time; simply take

$$y = \underset{k}{\operatorname{argmax}}\, f_k(x)$$

Recap: Multiclass SVM Loss (Hinge Loss)

"The score of the correct class should be higher than all the other scores"



Given a training data $\left(x^{(i)}, y^{(i)}\right)$

Let $s^{(i)} = f\left(x^{(i)}\right)$ be scores.

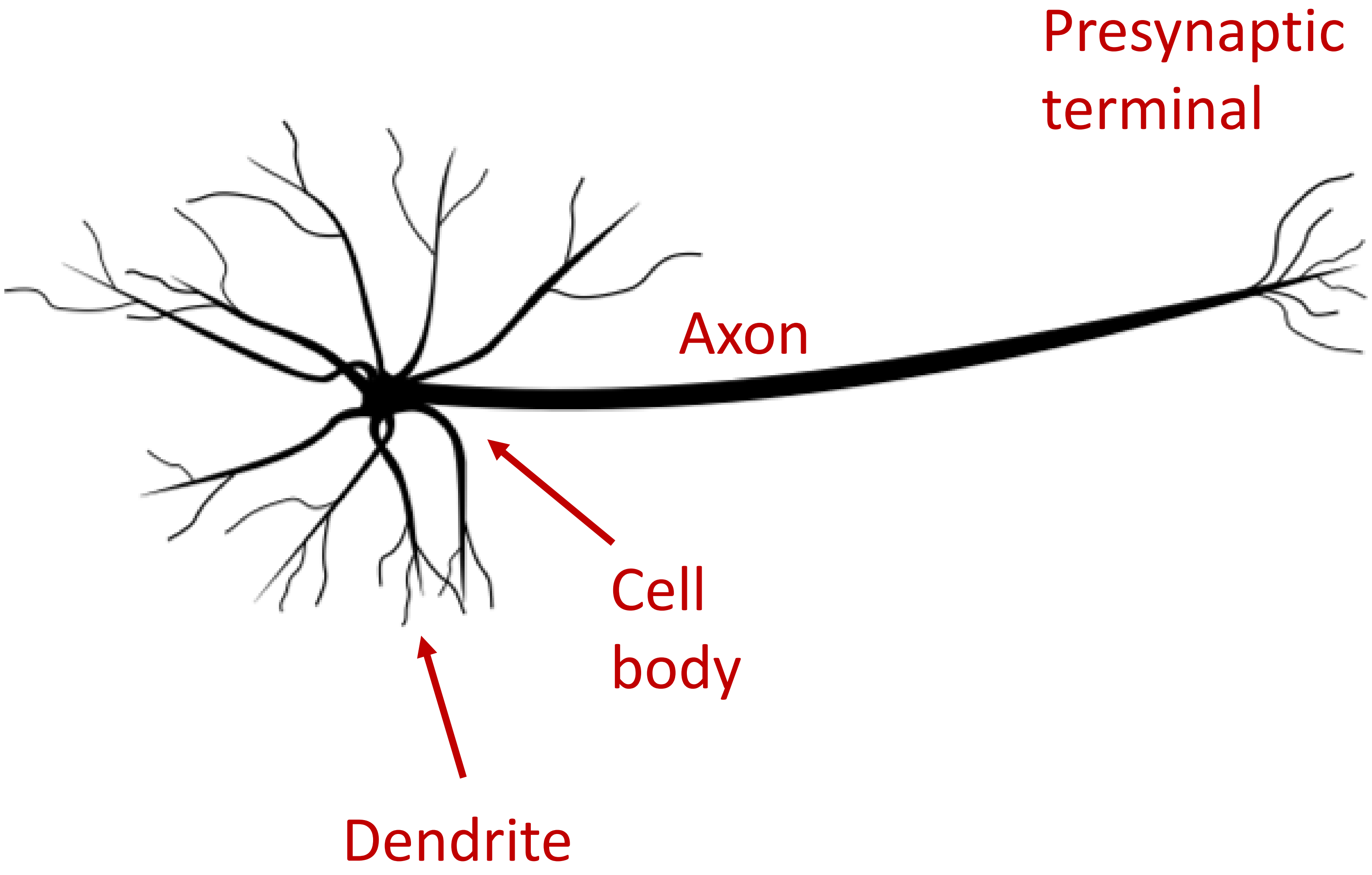
The SVM loss has the form:

$$L_i = \sum_{j \neq y^{(i)}} \max\left(0, s_j^{(i)} - s_{y^{(i)}}^{(i)} + 1\right)$$

Convexity

- Most linear classifiers optimize a convex function
  - Linear layer $s = f(x; W) = Wx$
  - Cross-entropy loss $L_i = -\log(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}})$
  - SVM $L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$
  - L1/L2 regularization $L = \frac{1}{N} \sum_{i=1}^{N} L_i + R(W)$
- Most neural networks need non-convex optimization
  - Few or no guarantees about convergence (mostly falls in a local optimum)
  - Empirically it seems to work anyway
  - Active area of research

Our brains are made of Neurons



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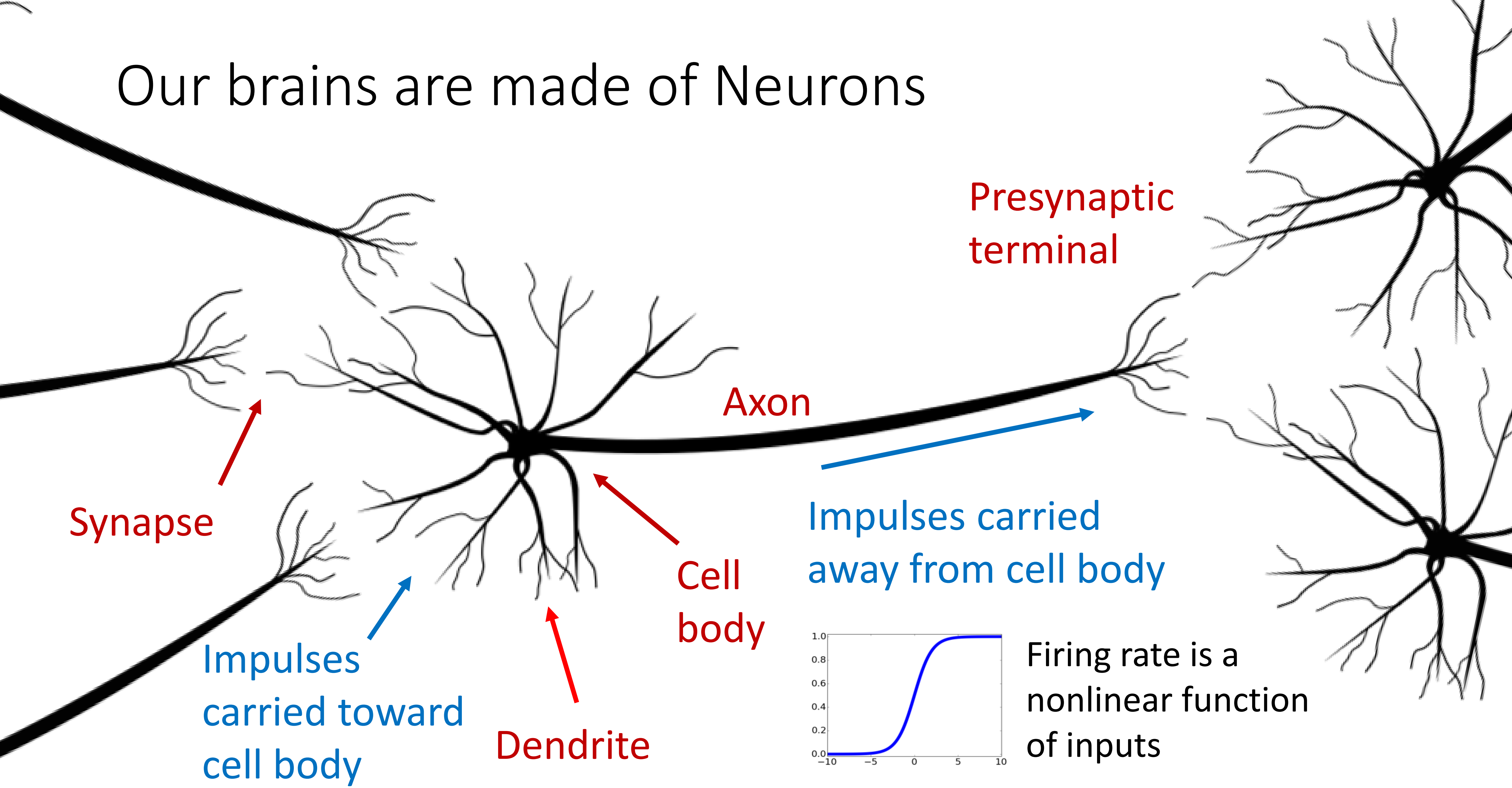
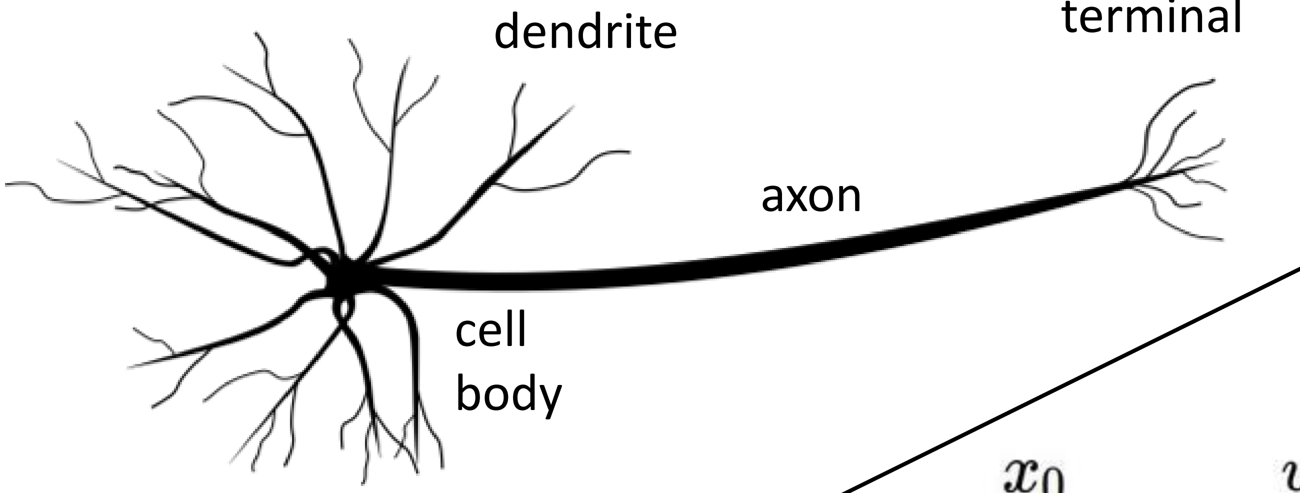
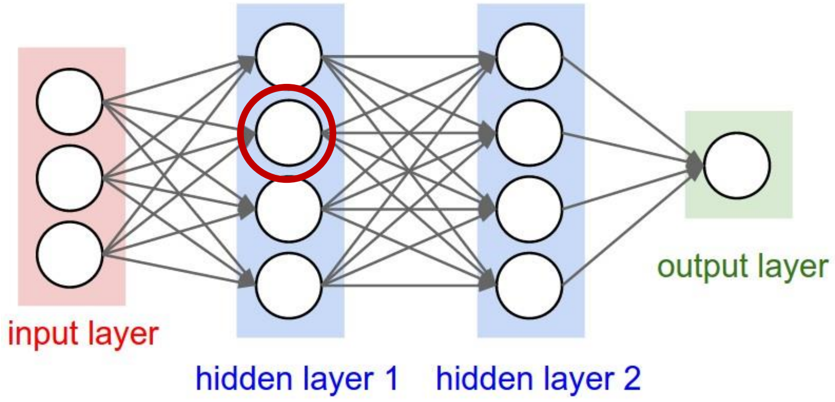


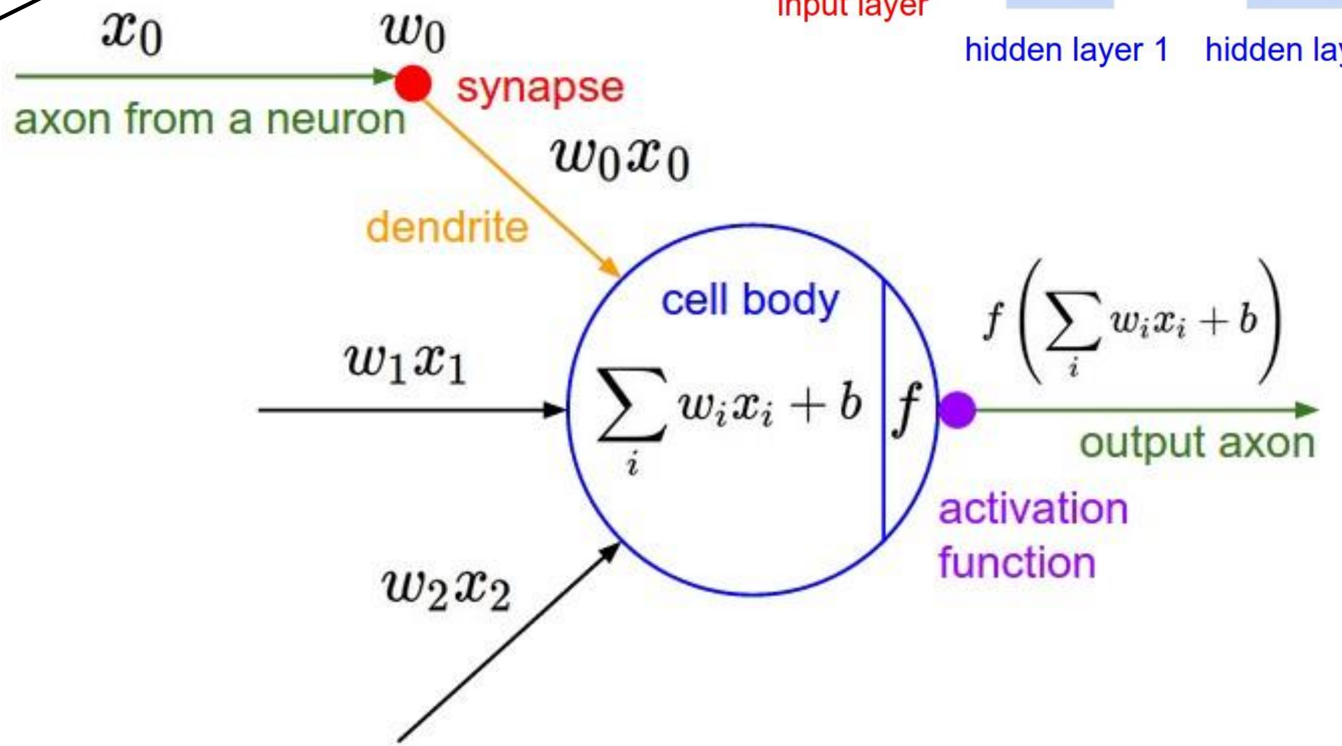
Firing rate is a nonlinear function of inputs

Biological Neuron

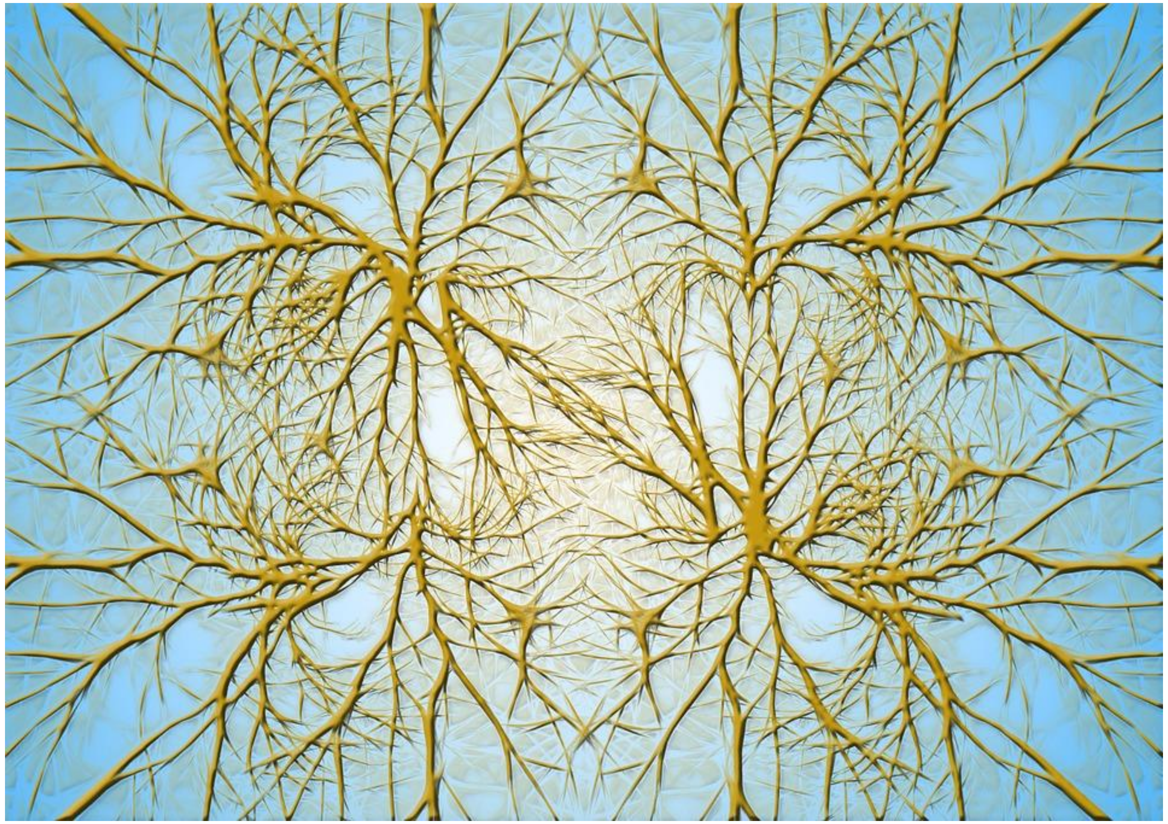


Artificial Neuron





Biological Neurons:
Complex connectivity patterns



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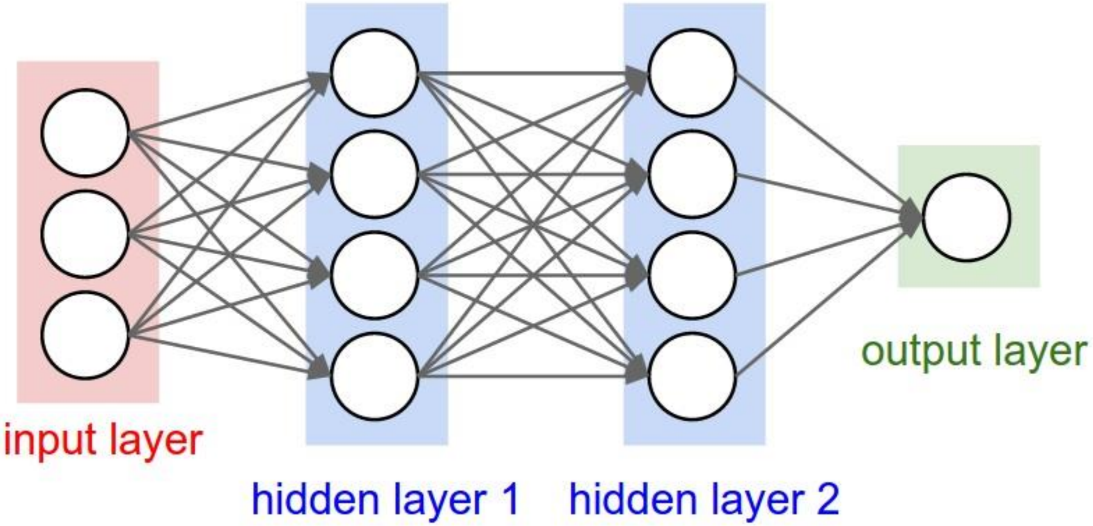
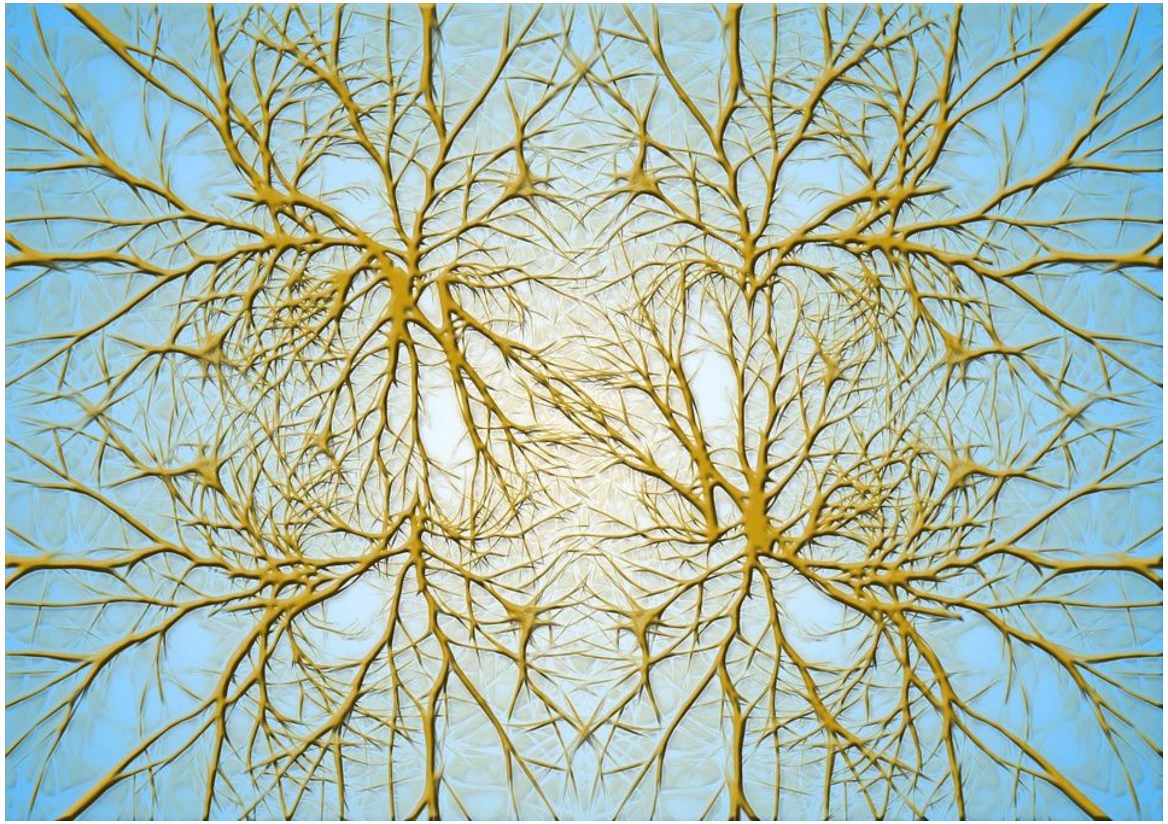
Neurons in a neural network:
Organized into regular layers for computational efficiency



Biological Neurons:
Complex connectivity patterns



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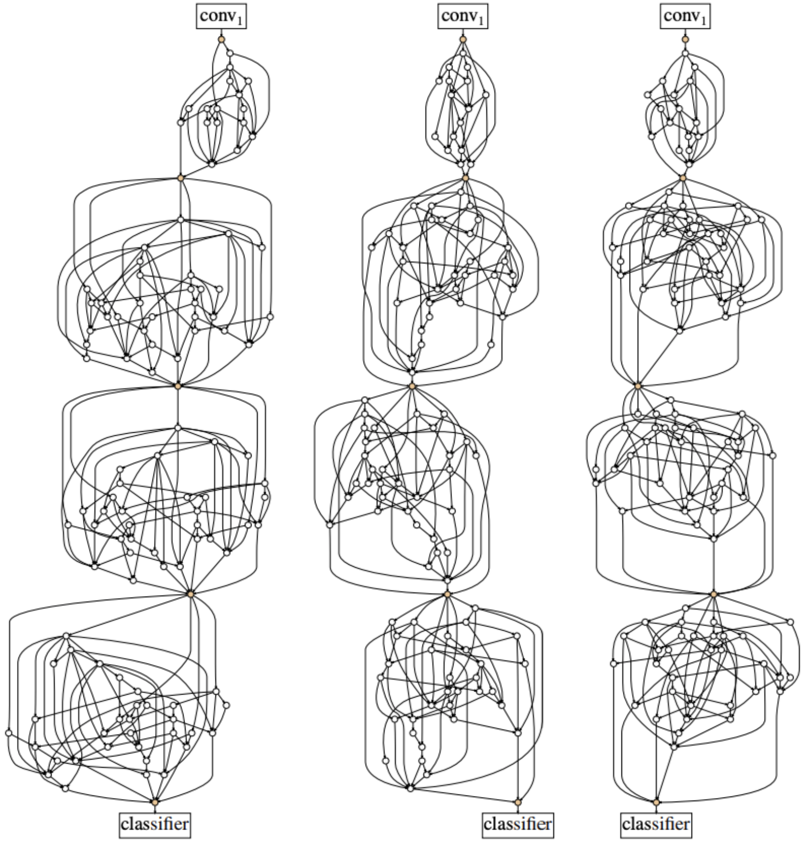
But neural networks with random connections can work too!



Xie et al, "Exploring Randomly Wired Neural Networks for Image Recognition", ICCV 2019

Be very careful with brain analogies!

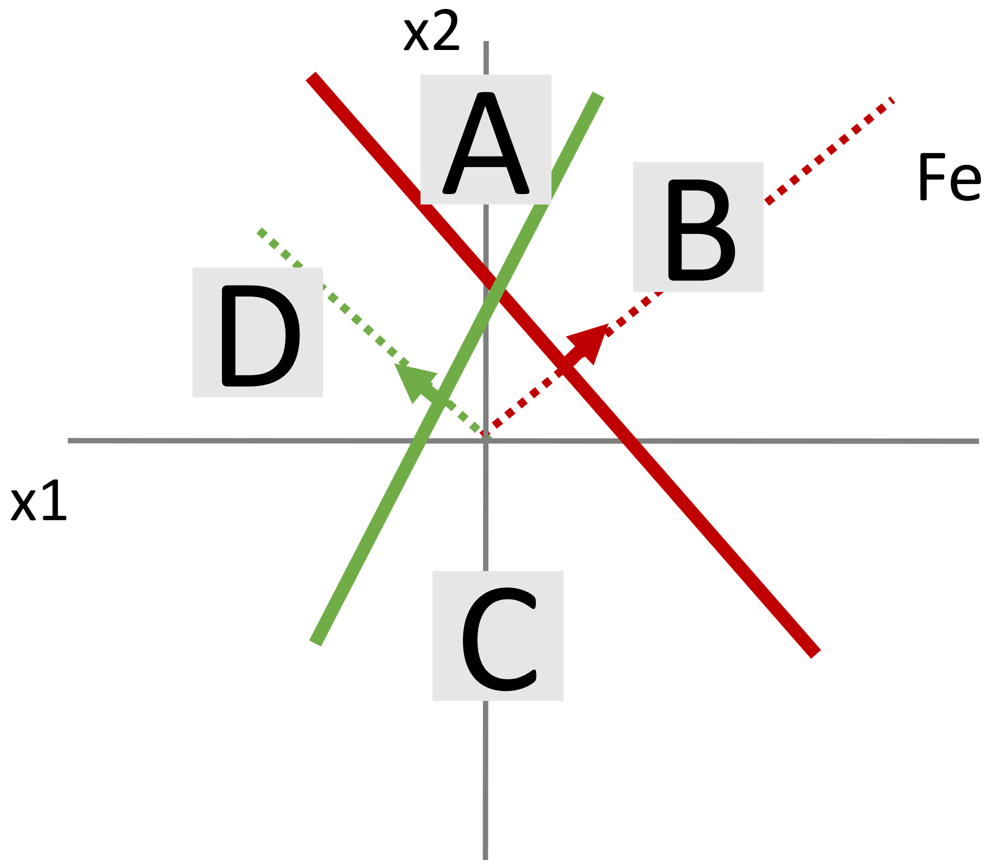
Biological Neurons:

- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Abstracting a neuron by “firing rate” isn’t enough; temporal sequences of activations matter too (spiking neural networks)

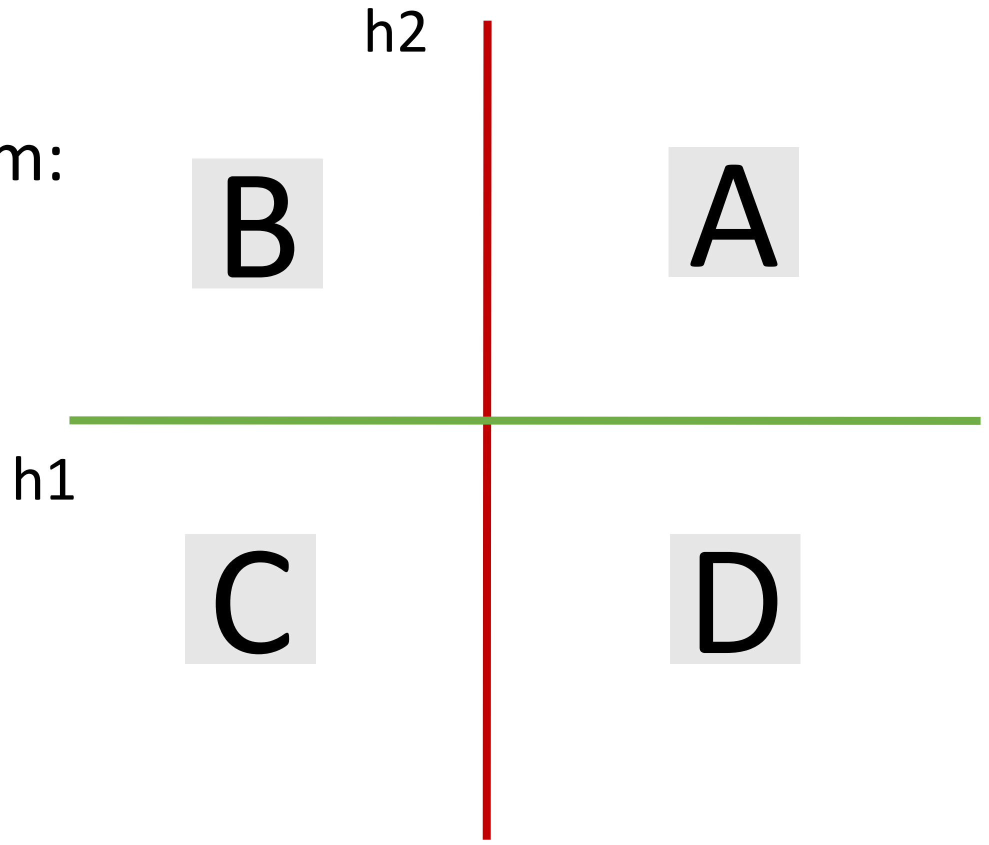
[Dendritic Computation. London and Hausser]

Space Warping

Consider a linear transform: $h = Wx$
Where x, h are both 2-dimensional



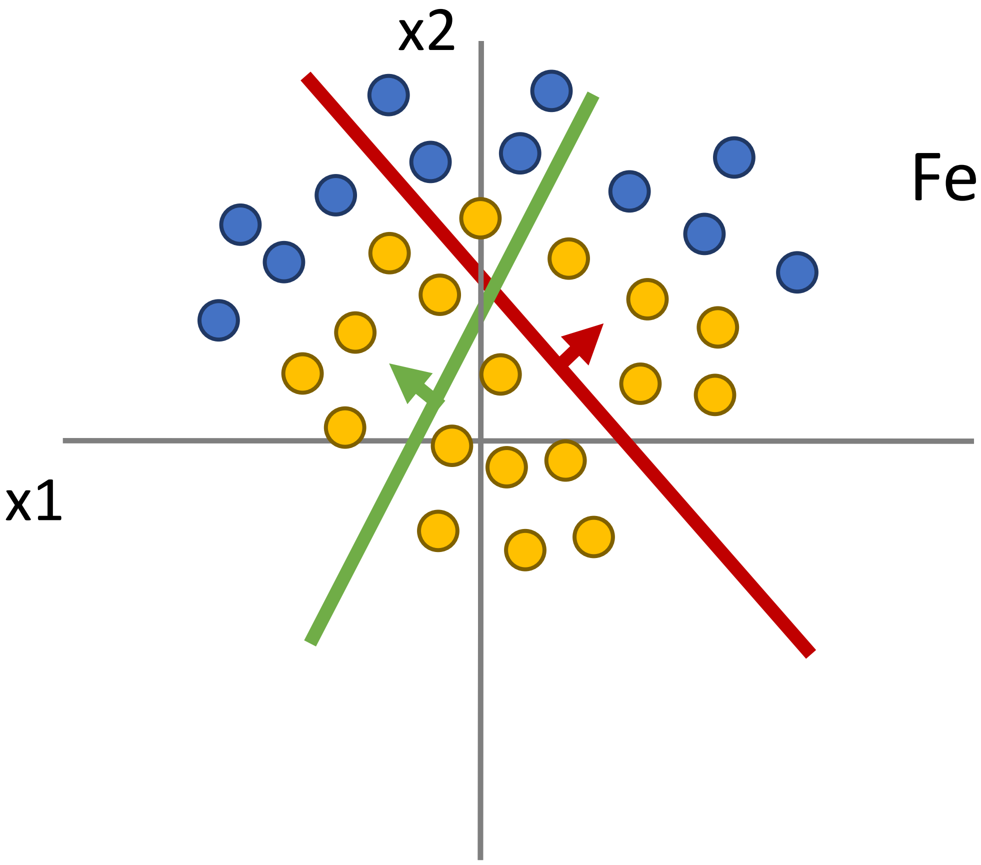
Feature transform:
$h = Wx$



Space Warping

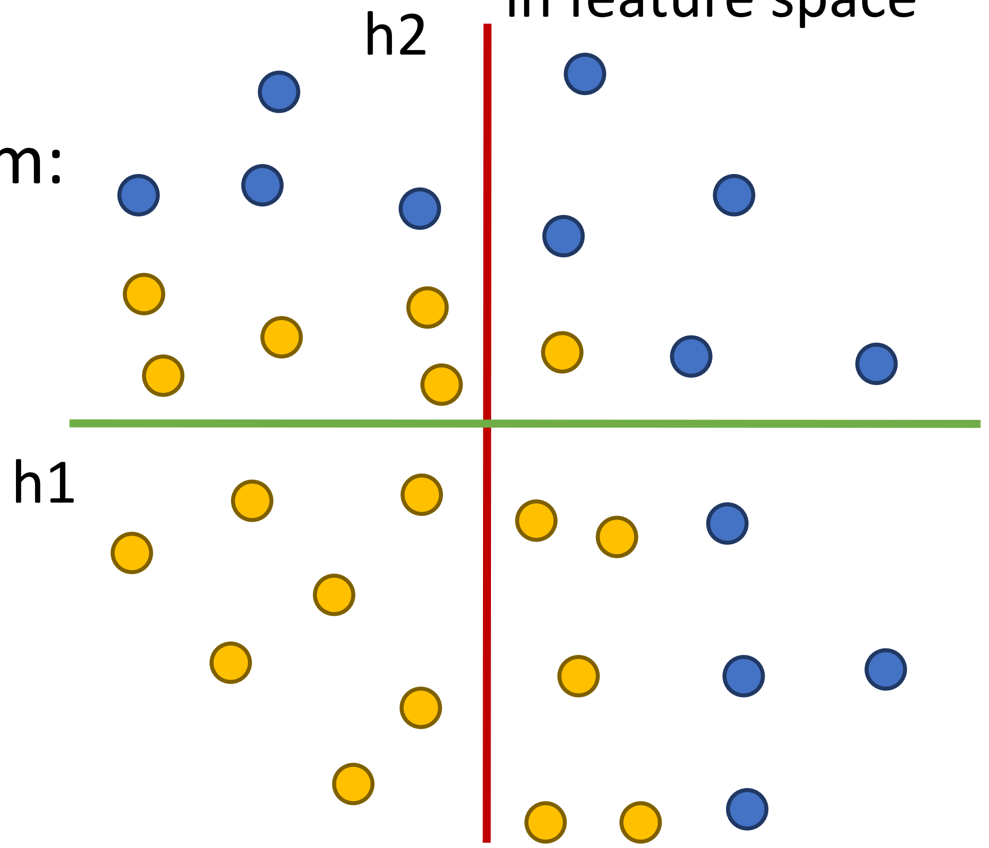
Consider a linear transform: h = Wx
Where x, h are both 2-dimensional

Points not linearly separable in original space



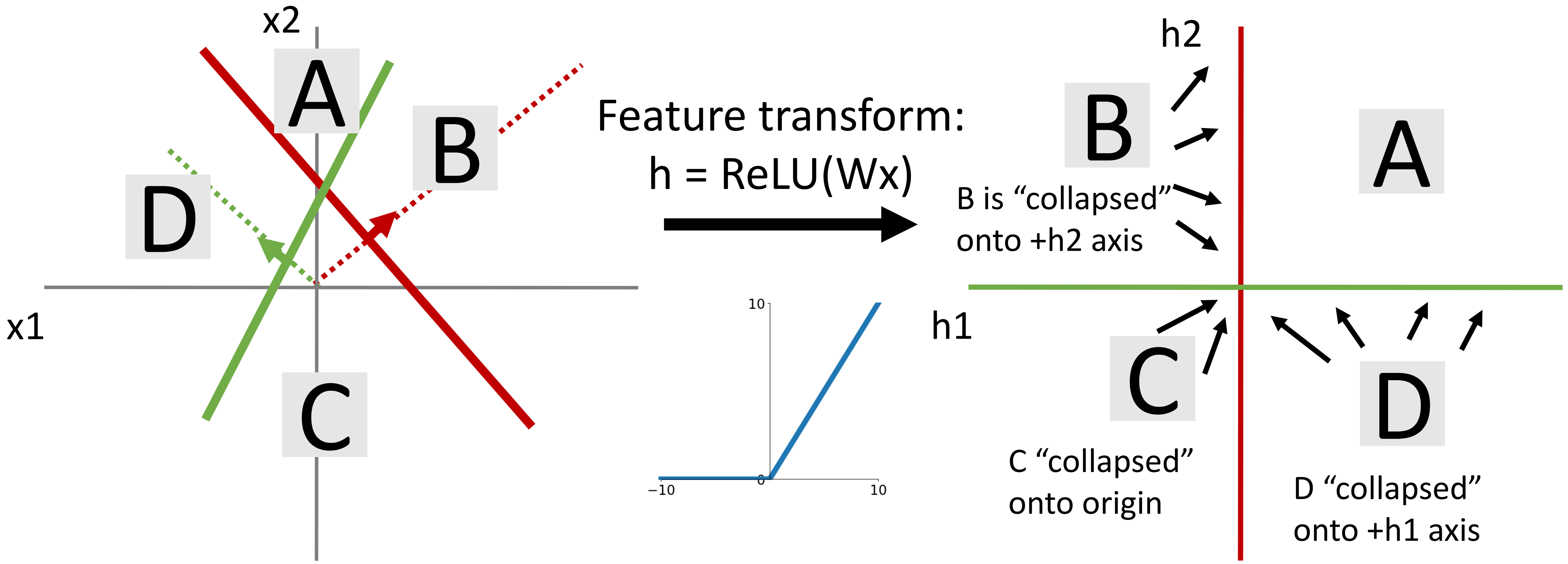
Feature transform:
h = Wx

Not linearly separable in feature space



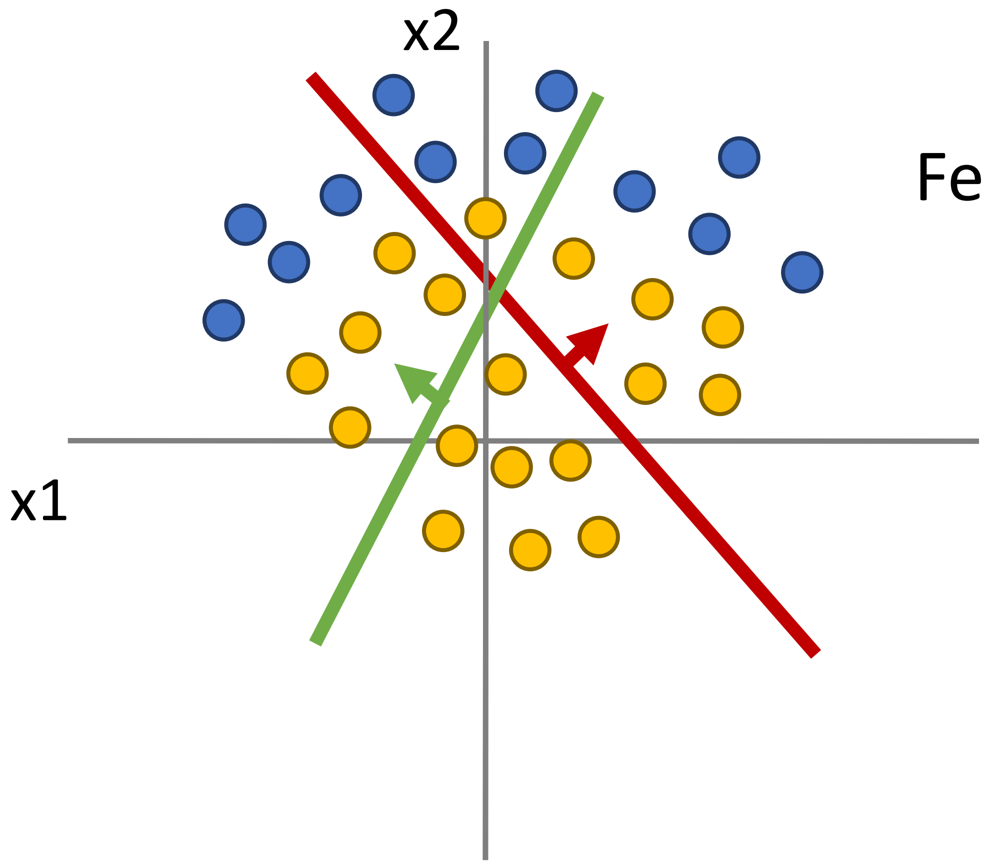
Space Warping

Consider a neural net hidden layer:
h = ReLU(Wx) = max(0, Wx)
Where x, h are both 2-dimensional



Space Warping

Points not linearly separable in original space



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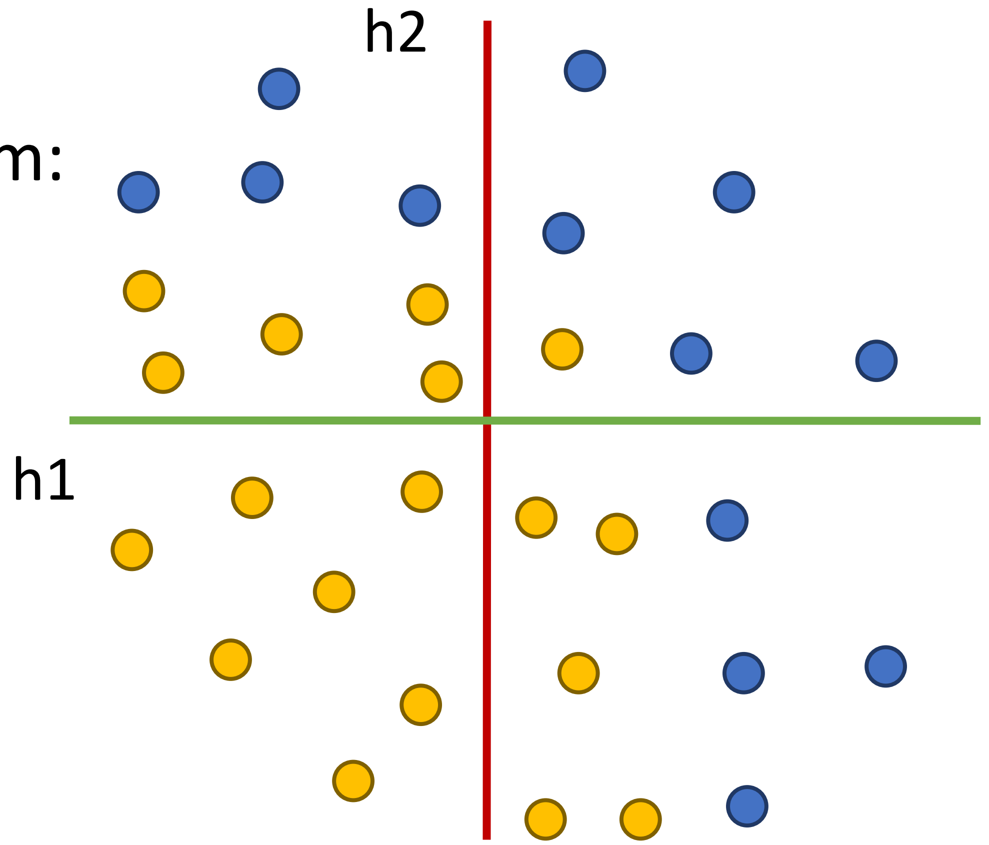
Where x, h are both 2-dimensional

Feature transform:

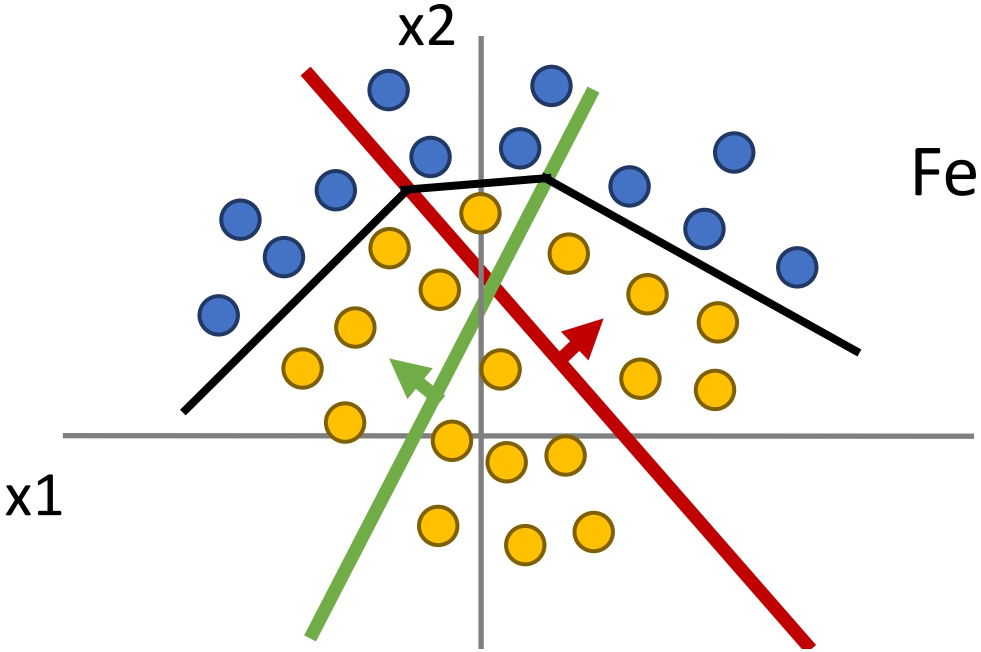
h = Wx



Space Warping

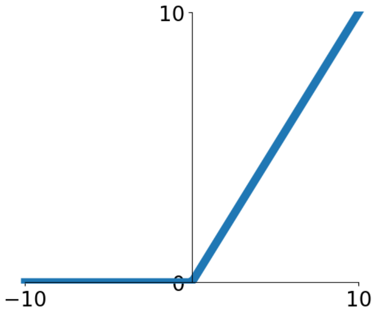
Consider a neural net hidden layer:
$h = \text{ReLU}(Wx) = \max(0, Wx)$
Where x, h are both 2-dimensional

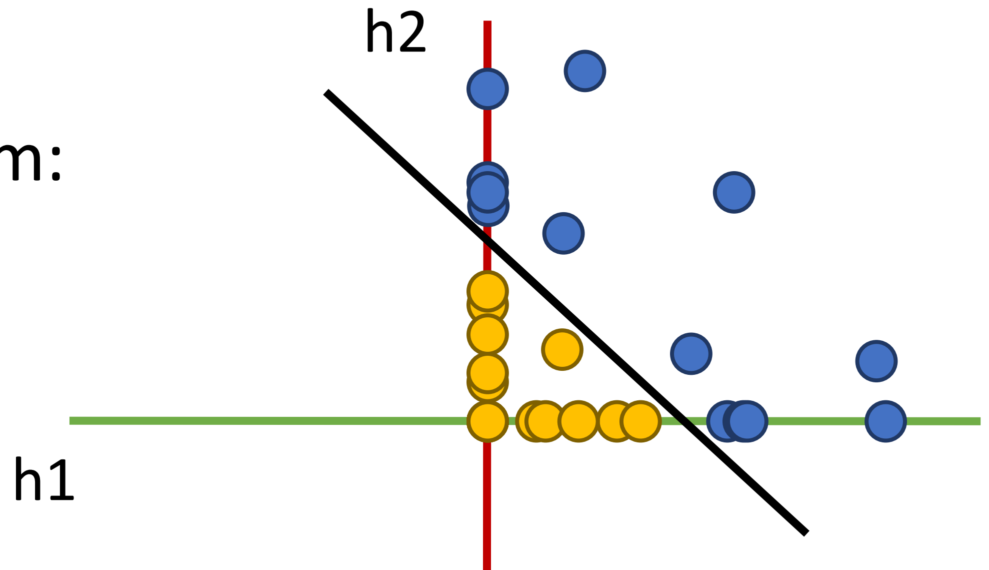
Points not linearly separable in original space



Linear classifier in feature space gives nonlinear classifier in original space

Feature transform:
$h = \text{ReLU}(Wx)$

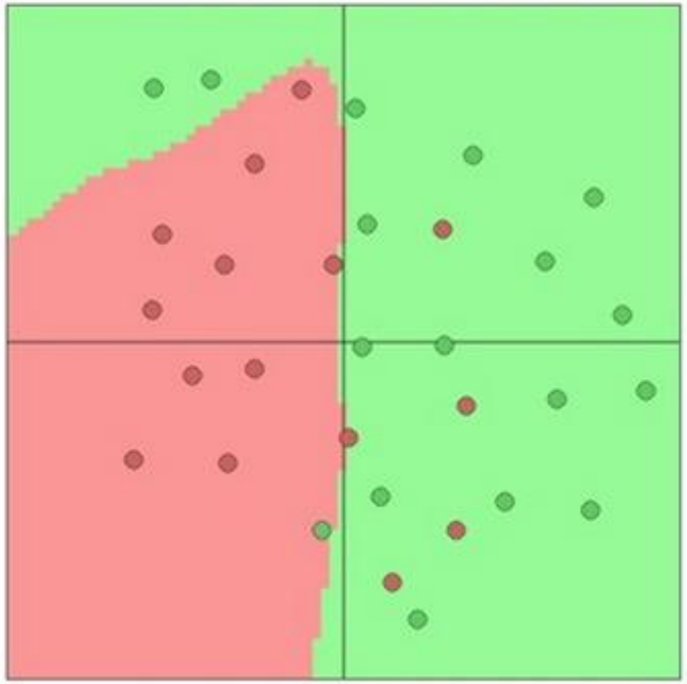




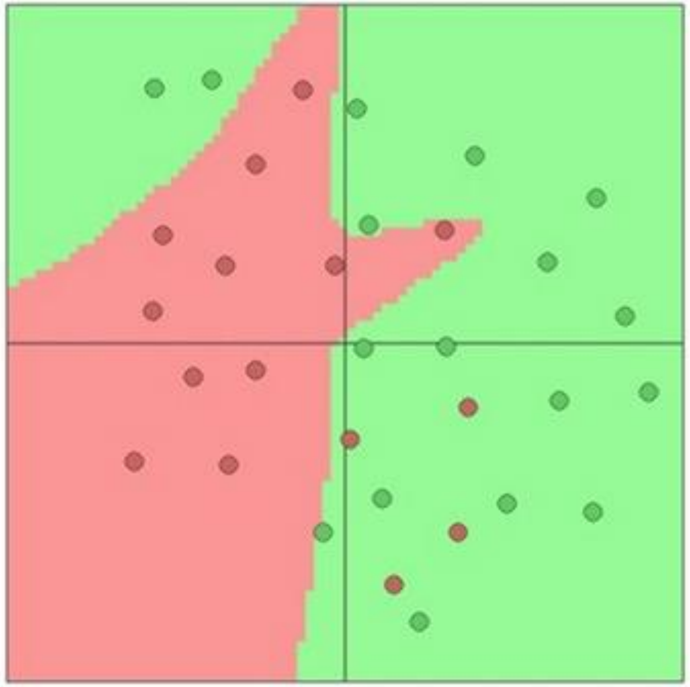
Points are linearly separable in features space!

Setting the number of layers and their sizes

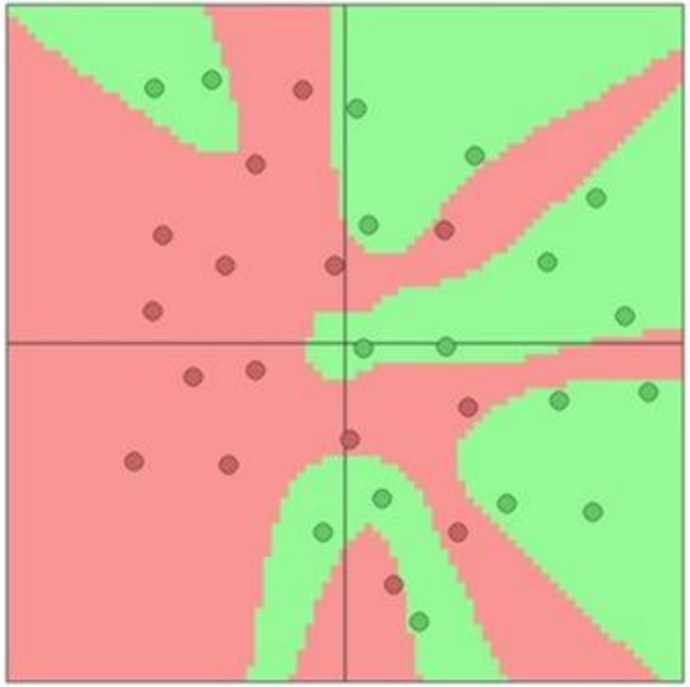
3 hidden units



6 hidden units

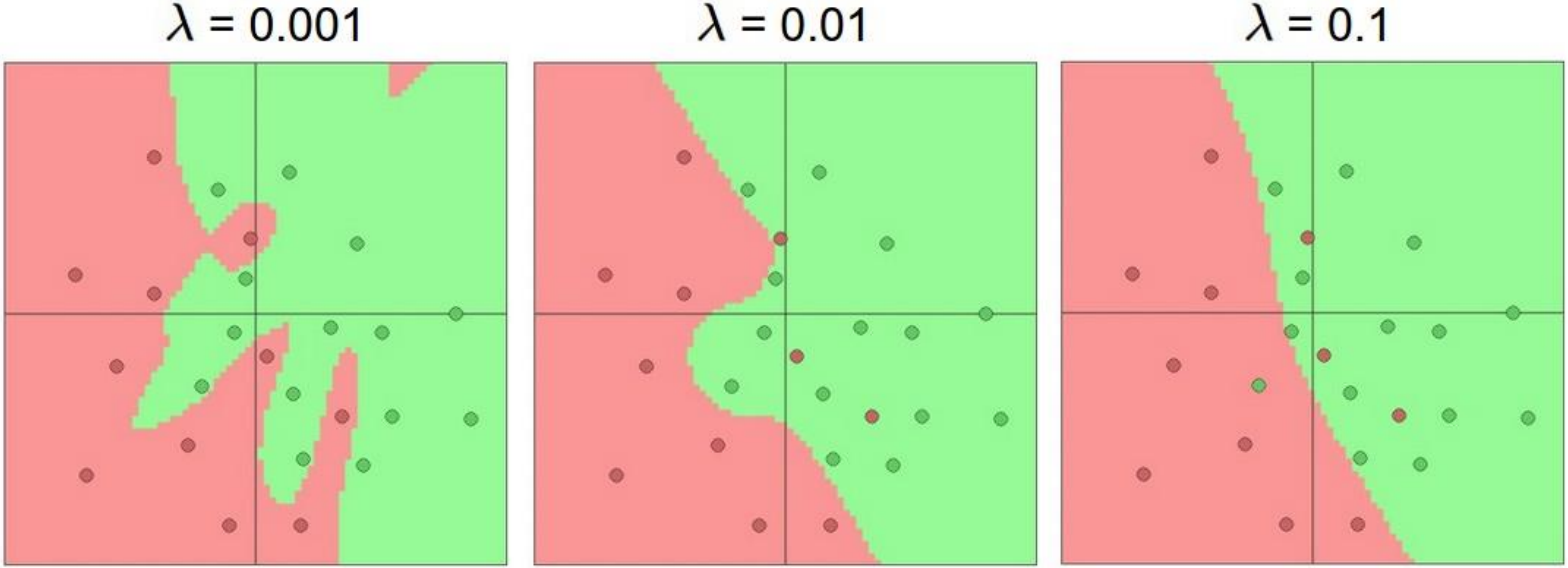


20 hidden units



More hidden units = more capacity

Don’t regularize with size; instead use stronger L2



(Web demo with ConvNetJS:
http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html)

Dropout as Regularization

Regularization: Add term to the loss

$$L = \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1) + \boxed{\lambda R(W)}$$

In common use:

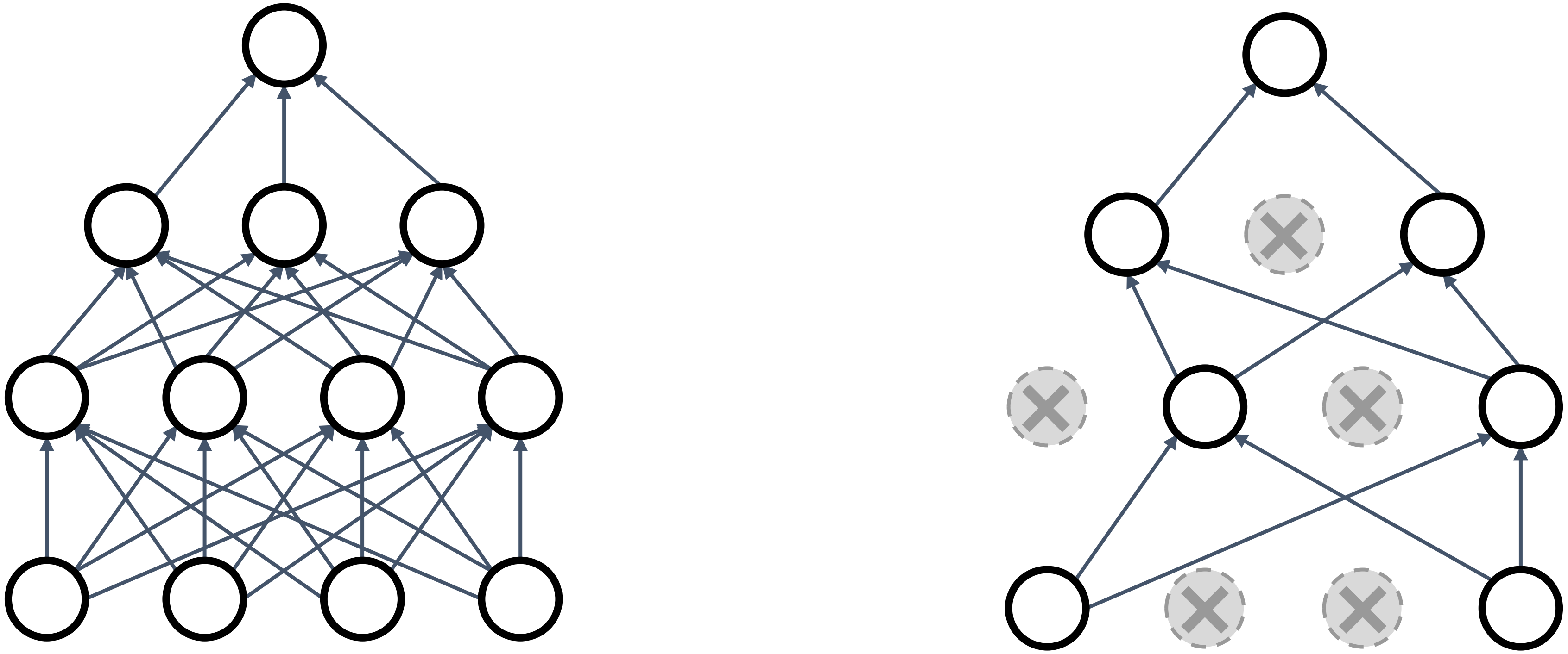
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Dropout

In each forward pass, randomly set some neurons to zero
Probability of dropping is a hyperparameter; 0.5 is common

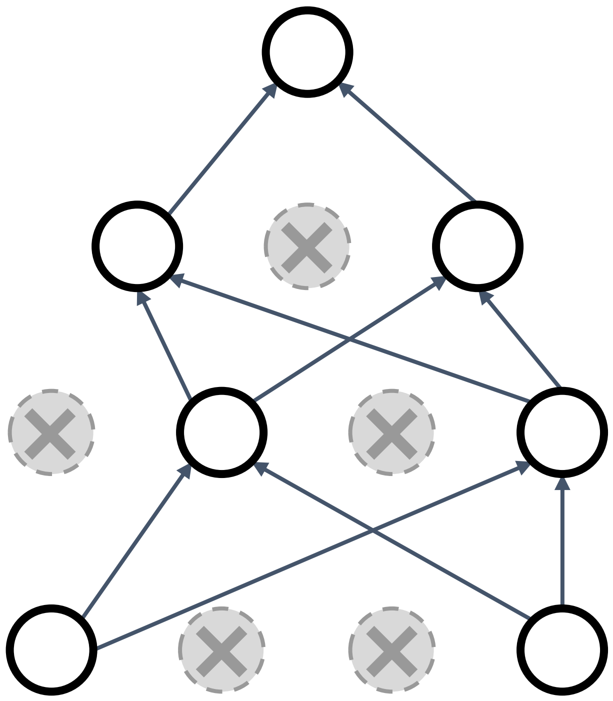


Srivastava et al, "Dropout: A simple way to prevent neural networks from overfitting", JMLR 2014

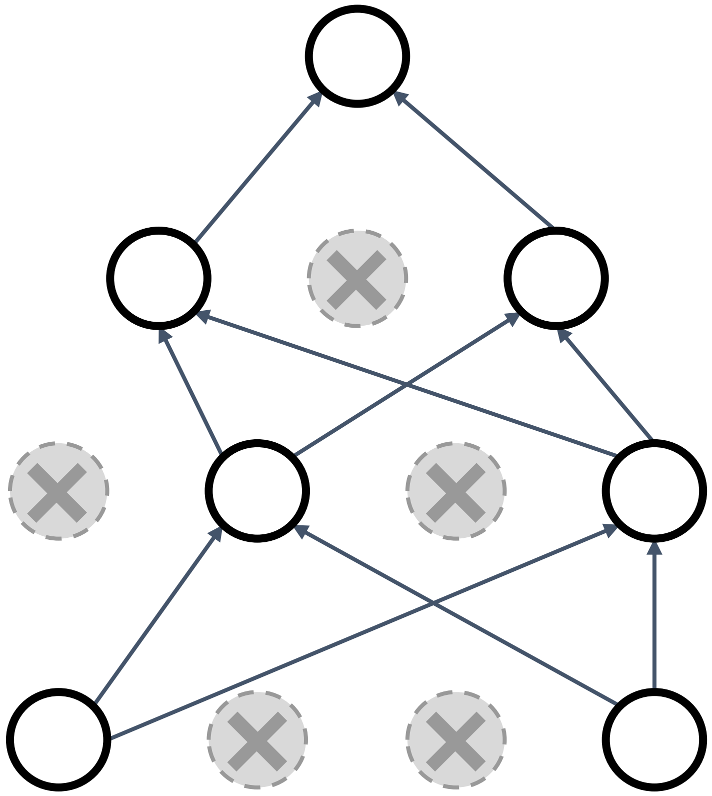
Dropout

```
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)
```

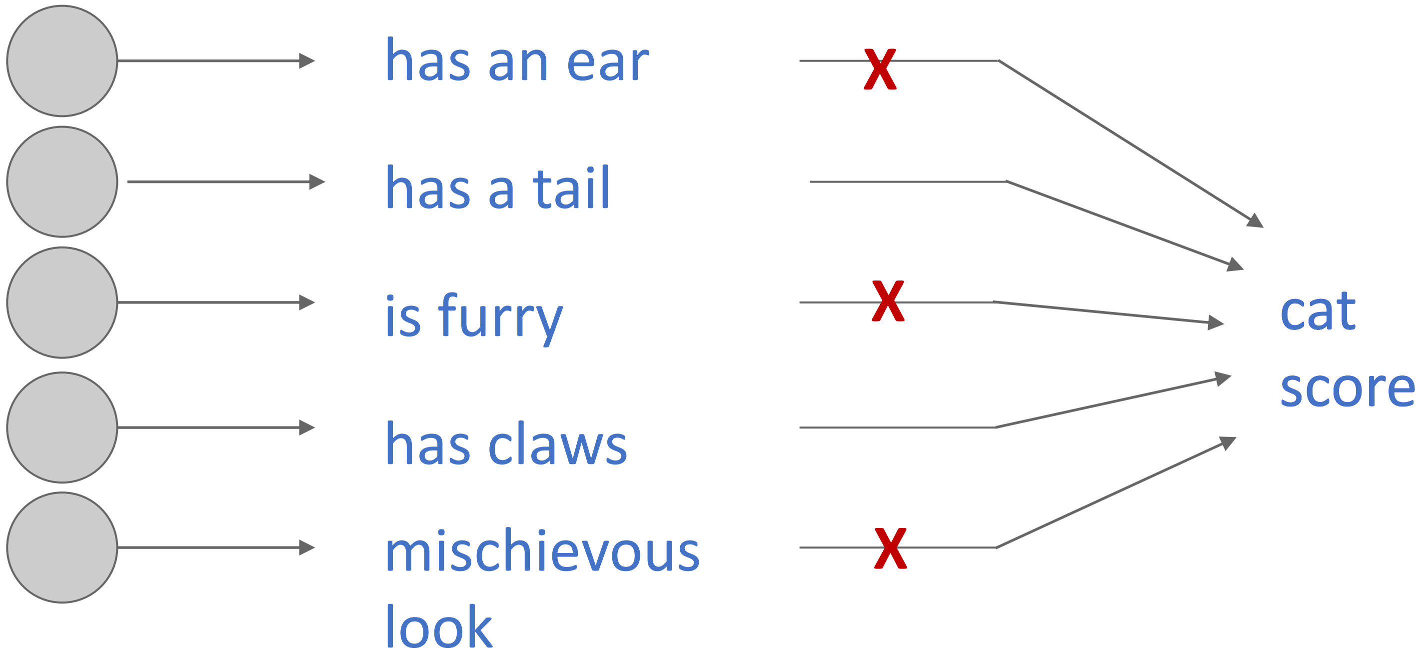
Example forward pass with a 3-layer network using dropout



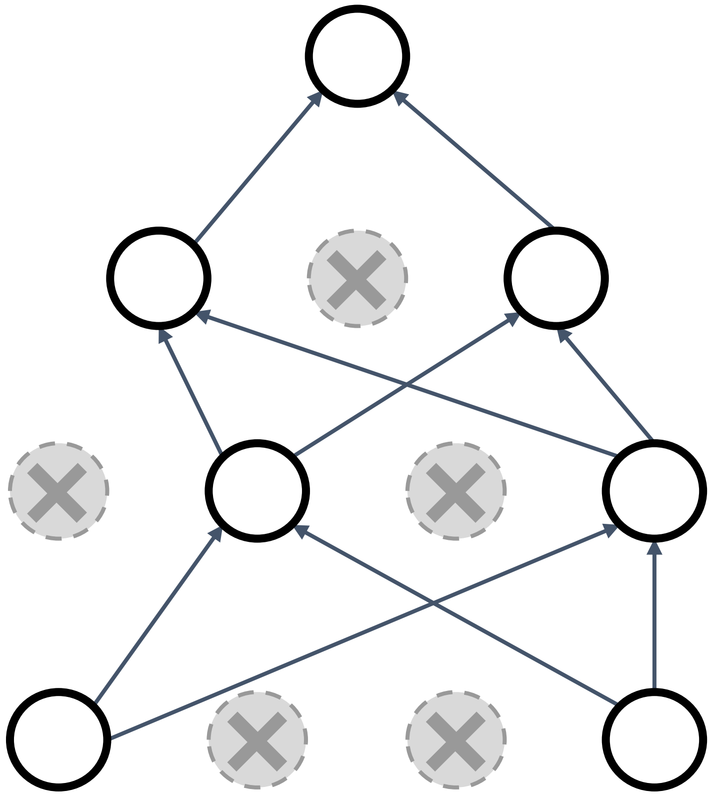
Dropout



Forces the network to have a redundant representation; Prevents **co-adaptation** of features



Dropout



Another interpretation:

Dropout is training a large **ensemble** of models (that share parameters).

Each binary-masked one is one model

An FC layer with 4096 units has $2^{4096} \sim 10^{1233}$ possible masks!
Only $\sim 10^{82}$ atoms in the universe...

Dropout: Test Time

Output (label)

Input (image)

Dropout makes our output random!

$$\boldsymbol{y} = f_W(\boldsymbol{x}, \boldsymbol{z})$$

Random mask

Want to "average out" the randomness at test-time

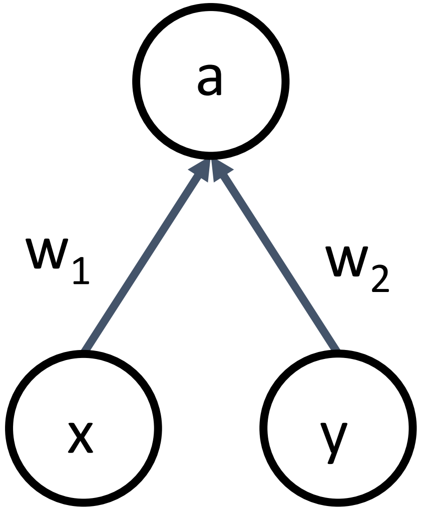
$$y = f(x) = E_z[f(x,z)] = \int p(z) f(x,z) dz$$

But this integral seems hard …

Dropout: Test Time

Want to approximate the integral $y = f(x) = E_z[f(x,z)] = \int p(z) f(x,z) dz$

Consider a single neuron:



At test time we have: $E[a] = w_1 x + w_2 y$

During training we have: $E[a] = \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y)$
$+ \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y)$
$= \frac{1}{2}(w_1 x + w_2 y)$

At test time, drop nothing and **multiply** by dropout probability

Dropout: Test Time

```python
def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
  H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
  out = np.dot(W3, H2) + b3
```

At test time all neurons are active always

=> We must scale the activations so that for each neuron:

<u>output at test time</u> = <u>expected output at training time</u>

Dropout: Summary

```python
""" Vanilla Dropout: Not recommended implementation (see notes below) """

p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
  H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
  out = np.dot(W3, H2) + b3
```

drop in forward pass

scale at test time

“Inverted Dropout” Is More Common in Practice

```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  out = np.dot(W3, H2) + b3
```

Drop and scale during training

test time is unchanged!

NN as a Universal Approximator

Neural Networks as Universal Approximation

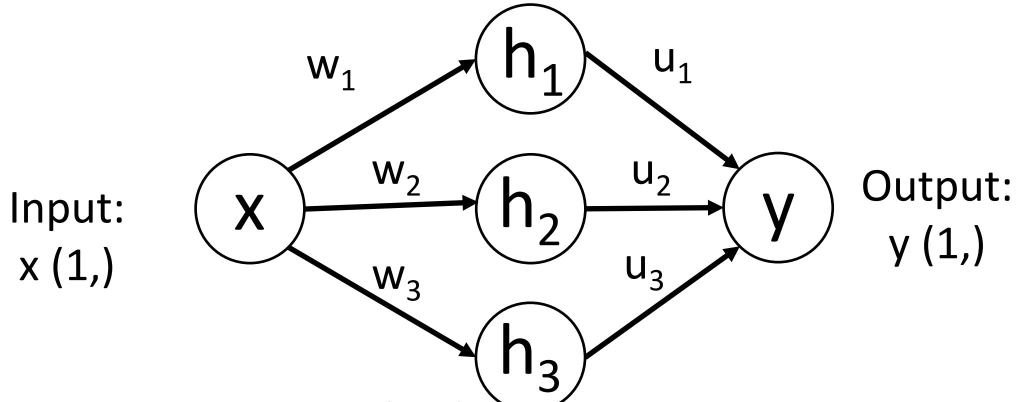
- A neural network with one hidden layer can approximate any(*) function $f: R^N \rightarrow R^M$ with arbitrary precision.

- For example, two-layer Sigmoid/ReLU networks with arbitrary number of hidden units

(*) Many technical conditions: Only holds on compact subsets of R^N; function must be continuous; need to define "arbitrary precision"; etc.

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network



First layer weights: w (3,1)
First layer bias: b (3,)

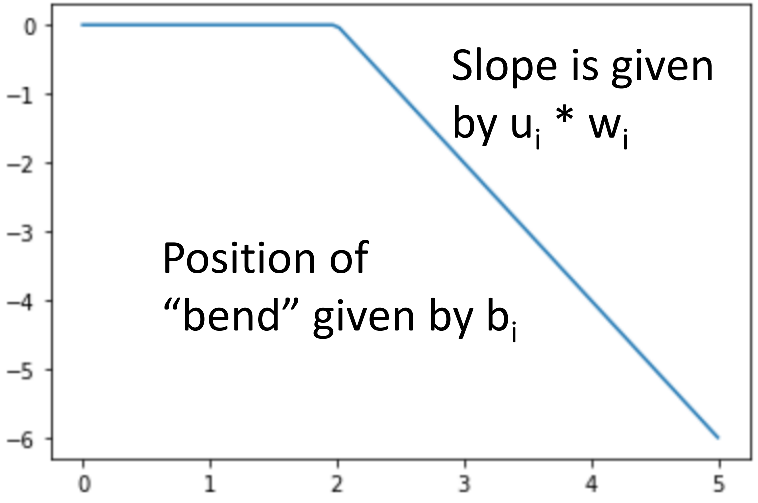
Second layer weights: u (1,3)
First layer bias: p (1,)

h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
+ u2 * max(0, w2 * x + b2)
+ u3 * max(0, w3 * x + b3)
+ p

Output is a sum of shifted, scaled ReLUs:

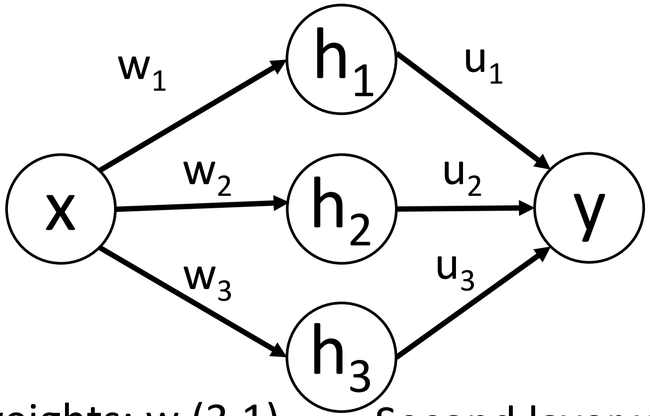
Flip left / right based on sign of w_i



Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network

Input:
x (1,)

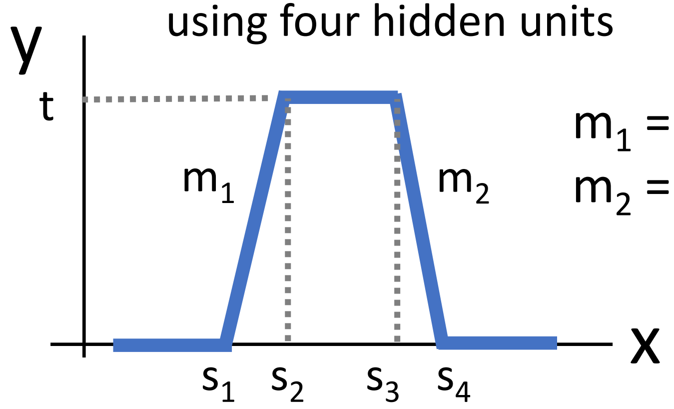


Output:
y (1,)

First layer weights: w (3,1)
First layer bias: b (3,)

Second layer weights: u (1,3)
First layer bias: p (1,)

We can build a "bump function" using four hidden units



$m_1 = t / (s_2 - s_1)$
$m_2 = t / (s_4 - s_3)$

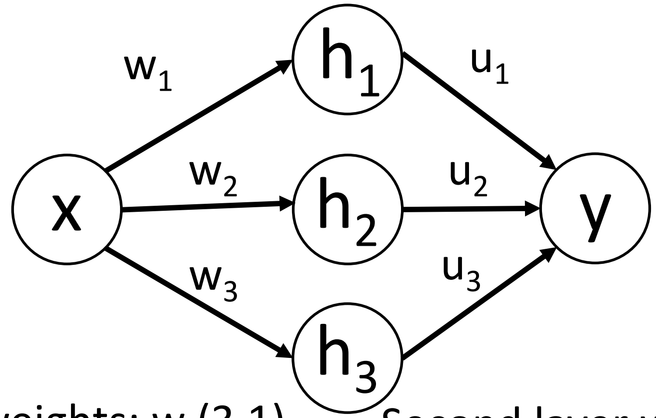
h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
+ u2 * max(0, w2 * x + b2)
+ u3 * max(0, w3 * x + b3)
+ p

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network

Input:
x (1,)



Output:
y (1,)

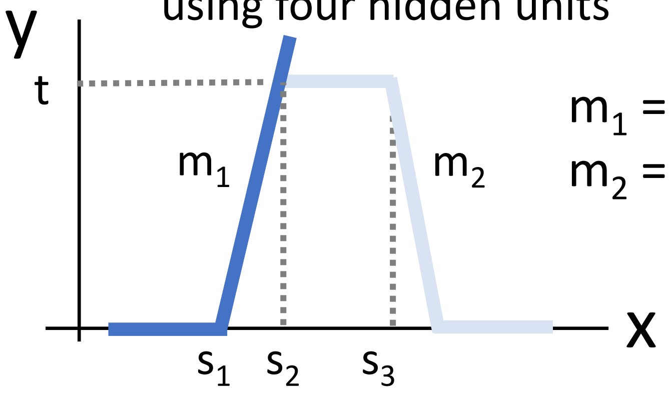
First layer weights: w (3,1)
First layer bias: b (3,)

Second layer weights: u (1,3)
First layer bias: p (1,)

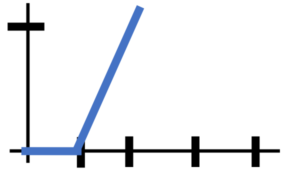
h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
+ u2 * max(0, w2 * x + b2)
+ u3 * max(0, w3 * x + b3)
+ p

We can build a "bump function" using four hidden units



$m_1 = t / (s_2 – s_1)$
$m_2 = t / (s_4 – s_3)$

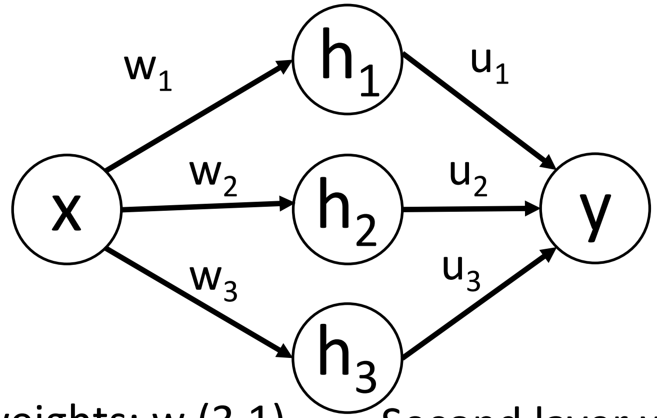


m_1 * max(0, x – s_1)

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network

Input:
x (1,)



Output:
y (1,)

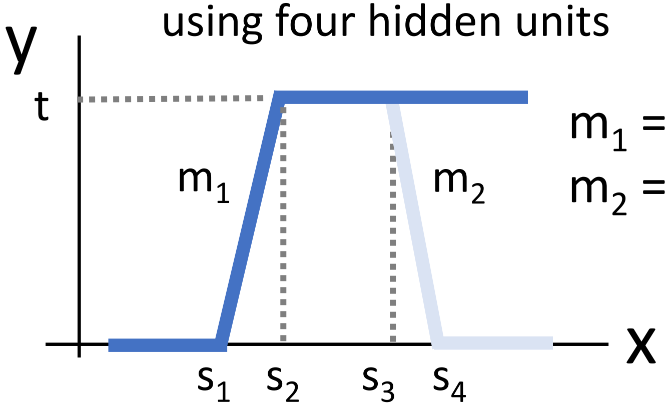
First layer weights: w (3,1)
First layer bias: b (3,)

Second layer weights: u (1,3)
First layer bias: p (1,)

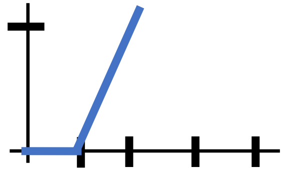
h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
+ u2 * max(0, w2 * x + b2)
+ u3 * max(0, w3 * x + b3)
+ p

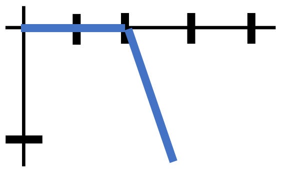
We can build a "bump function" using four hidden units



$m_1 = t / (s_2 - s_1)$
$m_2 = t / (s_4 - s_3)$



m_1 * max(0, x – s_1)

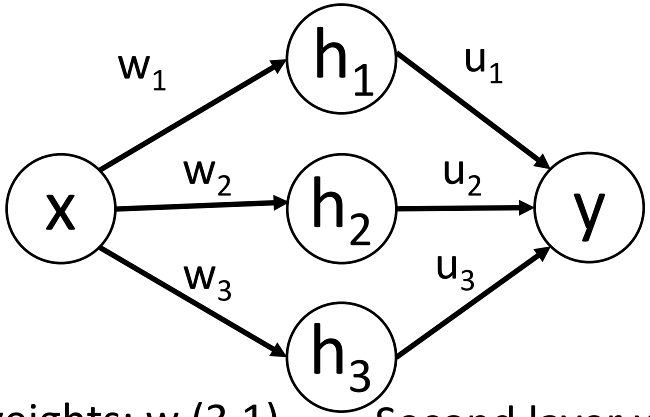


-m_1 * max(0, x – s_2)

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network

Input:
x (1,)



Output:
y (1,)

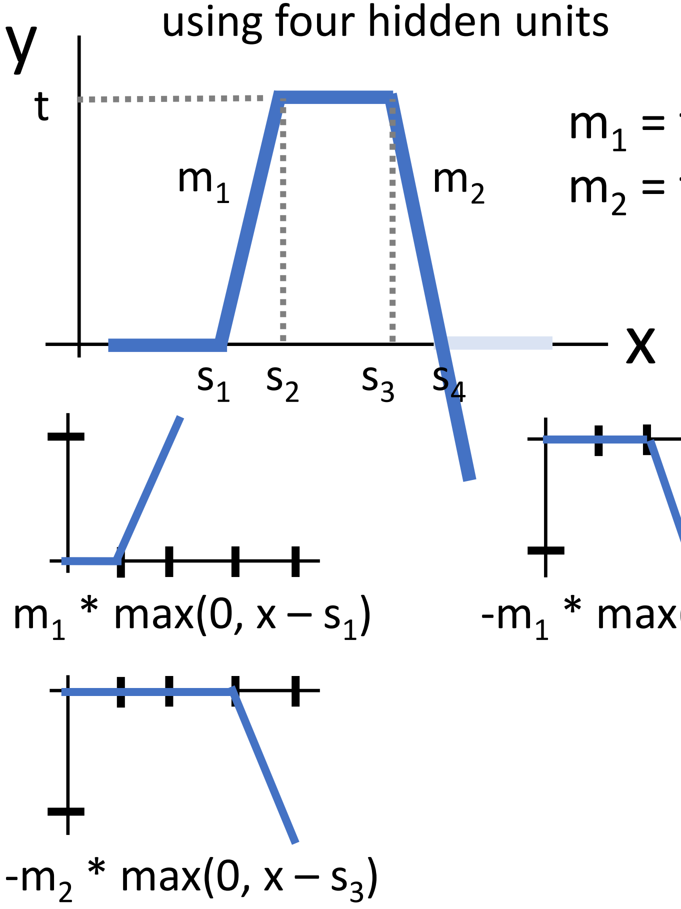
First layer weights: w (3,1)
First layer bias: b (3,)

Second layer weights: u (1,3)
First layer bias: p (1,)

h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
+ u2 * max(0, w2 * x + b2)
+ u3 * max(0, w3 * x + b3)
+ p

We can build a “bump function” using four hidden units

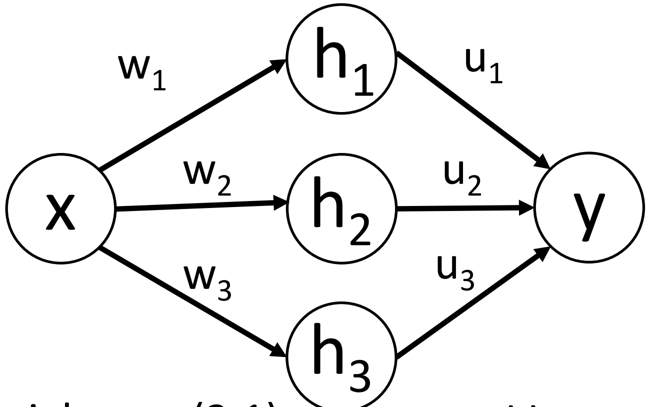


$m_1 = t / (s_2 – s_1)$
$m_2 = t / (s_4 – s_3)$

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network

Input:
x (1,)



Output:
y (1,)

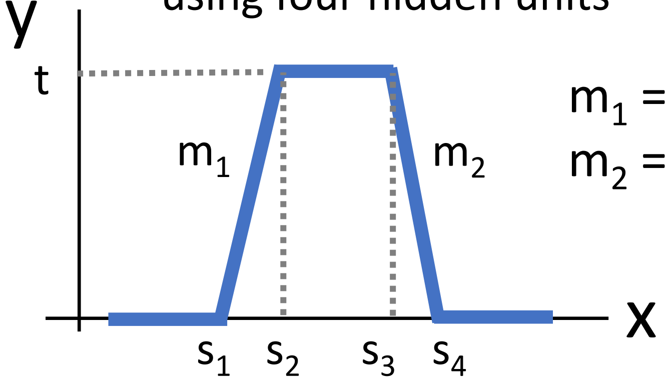
First layer weights: w (3,1)
First layer bias: b (3,)

Second layer weights: u (1,3)
First layer bias: p (1,)

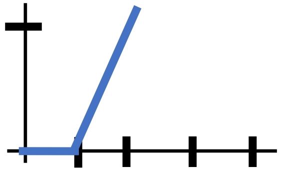
h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
 + u2 * max(0, w2 * x + b2)
 + u3 * max(0, w3 * x + b3)
 + p

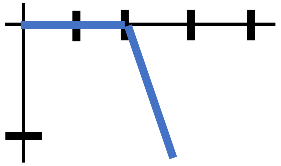
We can build a "bump function" using four hidden units



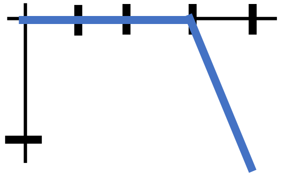
$m_1 = t / (s_2 - s_1)$
$m_2 = t / (s_4 - s_3)$



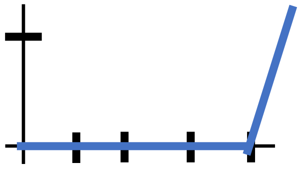
$m_1 * \max(0, x - s_1)$



$-m_1 * \max(0, x - s_2)$



$-m_2 * \max(0, x - s_3)$

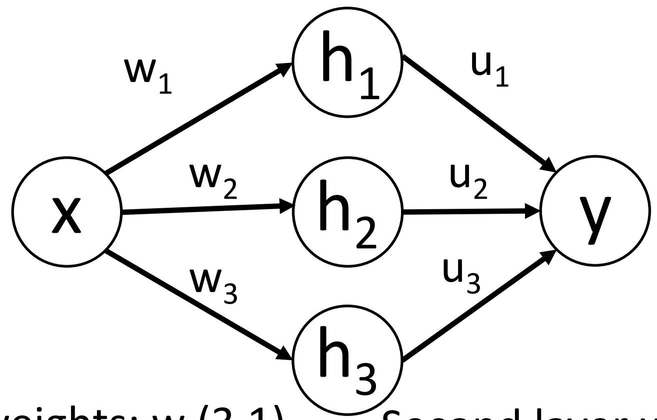


$m_2 * \max(0, x - s_4)$

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network

Input:
x (1,)



Output:
y (1,)

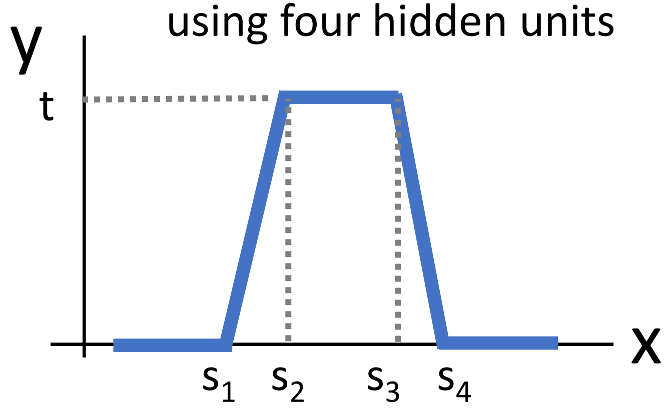
First layer weights: w (3,1)
First layer bias: b (3,)

Second layer weights: u (1,3)
First layer bias: p (1,)

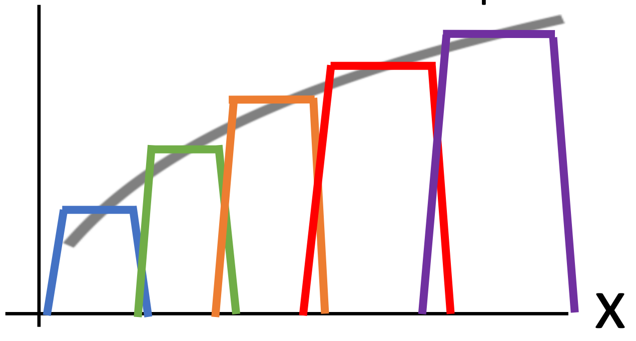
h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
 + u2 * max(0, w2 * x + b2)
 + u3 * max(0, w3 * x + b3)
 + p

We can build a "bump function" using four hidden units



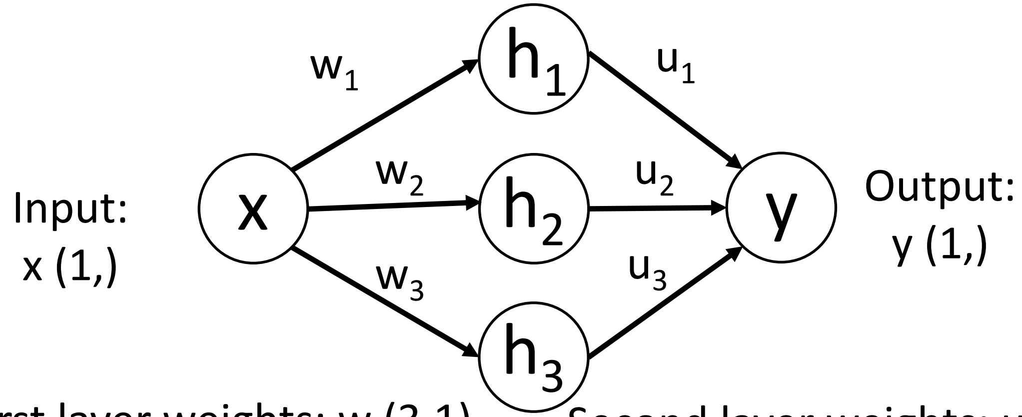
With 4K hidden units, we can build a sum of K bumps



Approximate functions with bumps!

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network



First layer weights: w (3,1)
First layer bias: b (3,)

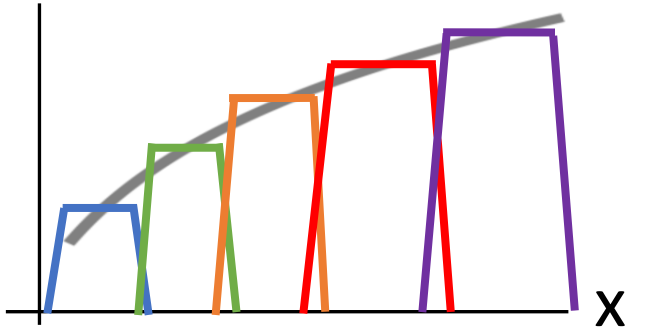
Second layer weights: u (1,3)
First layer bias: p (1,)

$$
\begin{aligned}
h1 &= \max(0, w1 * x + b1) \\
h2 &= \max(0, w2 * x + b2) \\
h3 &= \max(0, w3 * x + b3) \\
y &= u1 * h1 + u2 * h2 + u3 * h3 + p
\end{aligned}
$$

$$
\begin{aligned}
y = u1 &* \max(0, w1 * x + b1) \\
+ u2 &* \max(0, w2 * x + b2) \\
+ u3 &* \max(0, w3 * x + b3) \\
+ p &
\end{aligned}
$$

What about…
- Gaps between bumps?
- Other nonlinearities?
- Higher-dimensional functions?

See [Nielsen, Chapter 4]

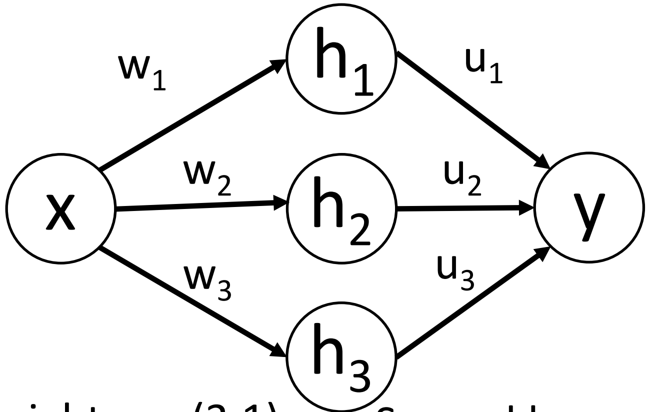


Approximate functions with bumps!

Universal Approximation

Example: Approximating a function f: R -> R with a two-layer ReLU network

Input:
x (1,)

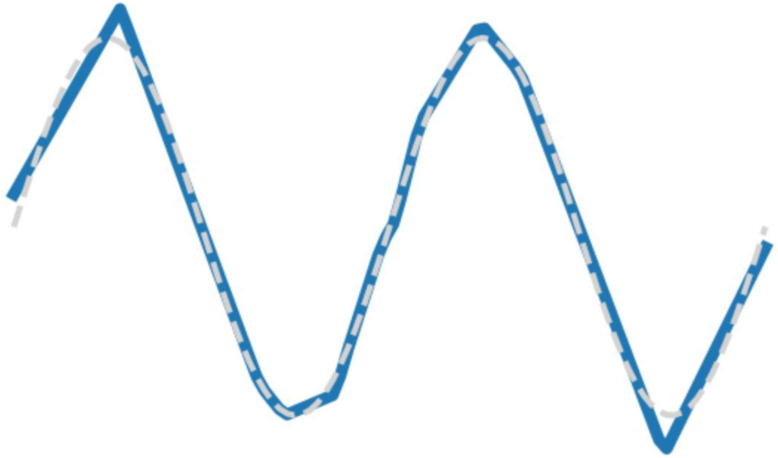


Output:
y (1,)

First layer weights: w (3,1)
First layer bias: b (3,)

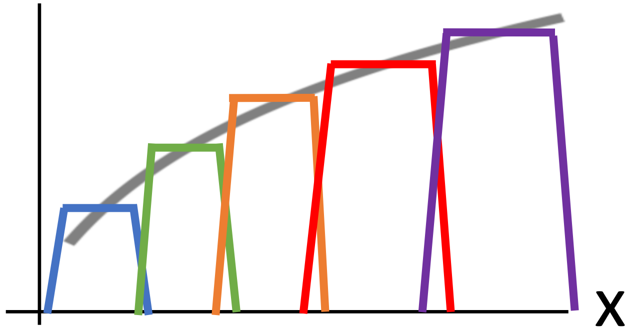
Second layer weights: u (1,3)
First layer bias: p (1,)

Reality check: Networks don’t really learn bumps!



h1 = max(0, w1 * x + b1)
h2 = max(0, w2 * x + b2)
h3 = max(0, w3 * x + b3)
y = u1 * h1 + u2 * h2 + u3 * h3 + p

y = u1 * max(0, w1 * x + b1)
+ u2 * max(0, w2 * x + b2)
+ u3 * max(0, w3 * x + b3)
+ p



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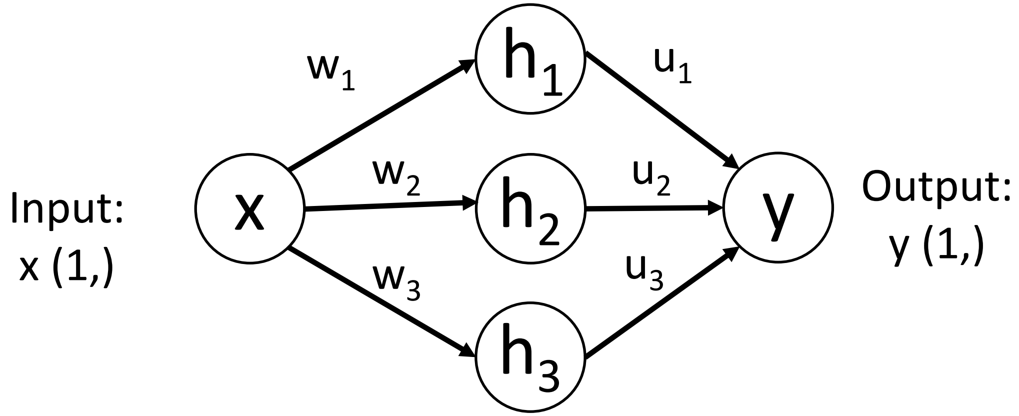

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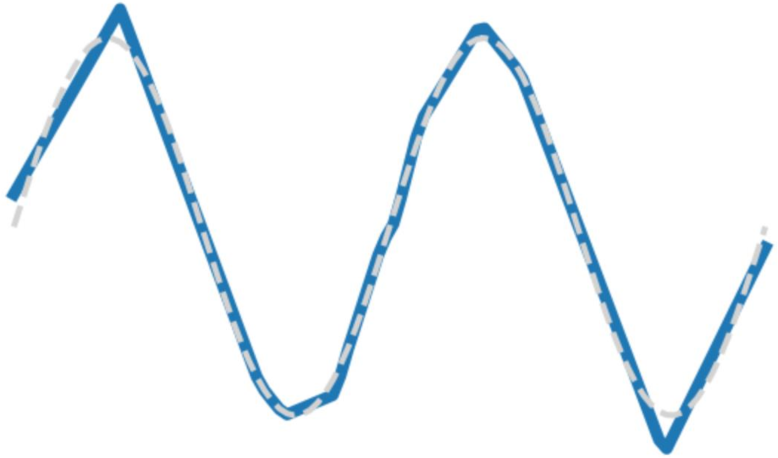
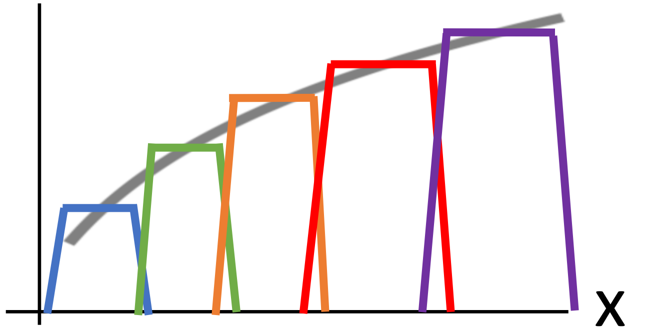


Universal approximation tells us:
- Neural nets can represent any function

Universal approximation DOES NOT tell us:
- Whether we can actually learn any function with SGD
- How much data we need to learn a function

Remember: k-NN is also a universal approximator!



Approximate functions with bumps!

NN Optimization

Problem: How to compute (complex) gradients?

$$s = W_2\, g(W_1 x + b_1) + b_2$$ Nonlinear score function

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$ Per-element data loss

$$R(W) = \sum_k W_k^2$$ L2 Regularization

$$L(W_1, W_2, b_1, b_2) = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda R(W_1) + \lambda R(W_2)$$ Total loss

If we can compute $\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}, \frac{\partial L}{\partial b_1}, \frac{\partial L}{\partial b_2}$ then we can optimize with SGD

(Bad) Idea: Derive $\nabla_W L$ on paper

$$s = f(x; W) = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

$$= \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1)$$

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda \sum_k W_k^2$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2$$

$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

Problem: Very tedious: Lots of matrix calculus, need lots of paper

Problem: What if we want to change loss? e.g., use softmax instead of SVM? Need to re-derive from scratch. Not modular!

Problem: Not feasible for very complex models!

Better Idea: Backpropagation by **Chain Rule**

$$x \xrightarrow{W_1} h_1 \xrightarrow{W_2} h_2 \xrightarrow{W_3} h_3 \xrightarrow{W_4} L$$

D_0 $\quad$ D_1 $\quad$ D_2 $\quad$ D_3 $\quad$ scalar

Chain rule

$$\frac{\partial L}{\partial x} = \left(\frac{\partial h_1}{\partial x}\right)\left(\frac{\partial h_2}{\partial h_1}\right)\left(\frac{\partial h_3}{\partial h_2}\right)\left(\frac{\partial L}{\partial h_3}\right)$$

[D_0 x D_1] [D_1 x D_2] [D_2 x D_3] [D_3]

e.g., (i, j)-th element in W_2

$$\frac{\partial L}{\partial W_2(i,j)} = \left(\frac{\partial h_2}{\partial W_2(i,j)}\right)\left(\frac{\partial h_3}{\partial h_2}\right)\left(\frac{\partial L}{\partial h_3}\right)$$

[D_2] [D_2 x D_3] [D_3]

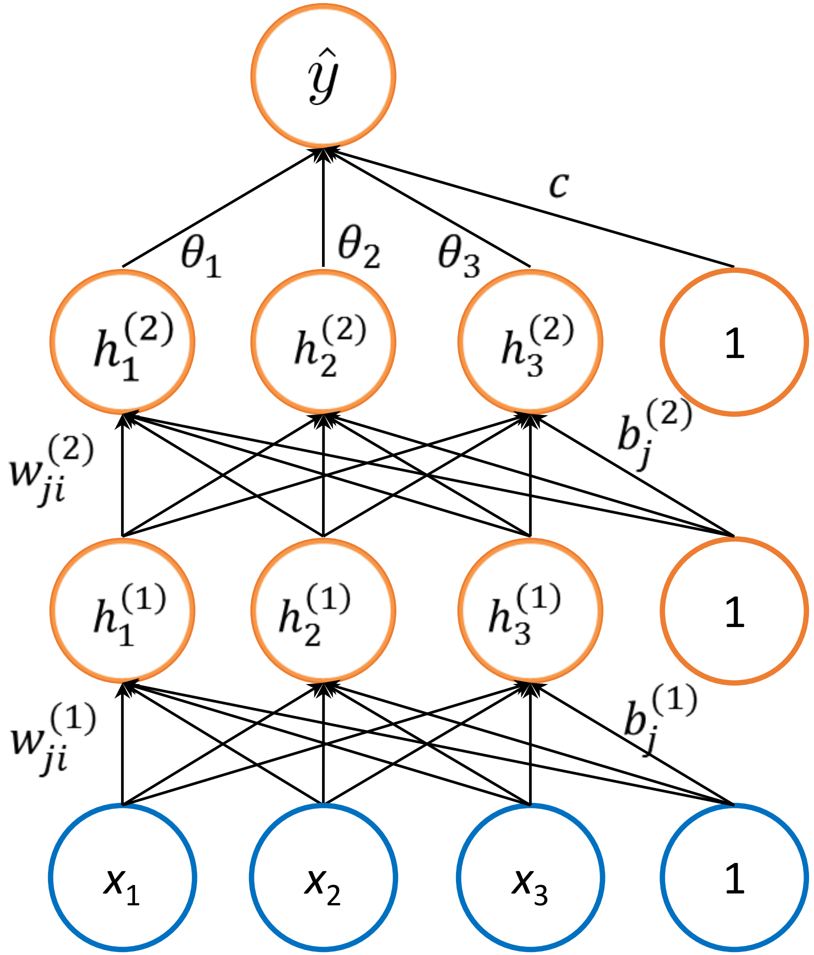
Example: 2-Layer NN Forward Pass

- Input $\mathbf{x}$
- Output $\hat{y}$
- Target y
- L2 Loss function $L = (\hat{y} - y)^2$

First hidden layer $$h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)})$$

Second hidden layer $$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(1)} + b_j^{(2)})$$

Output $$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$



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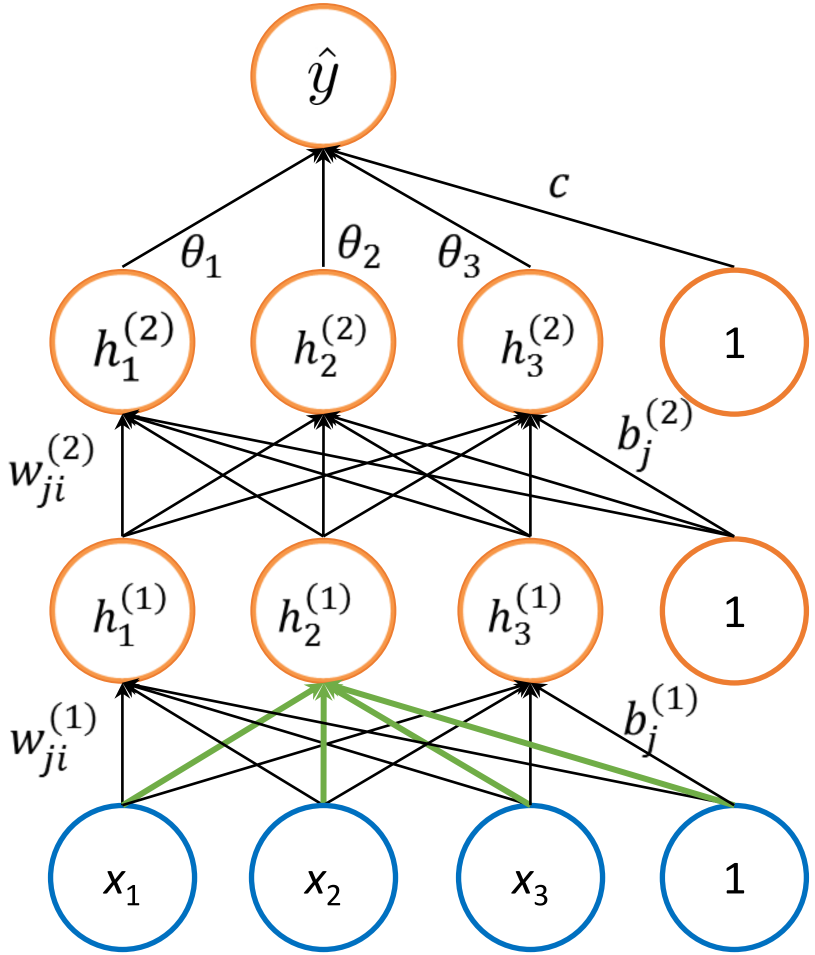

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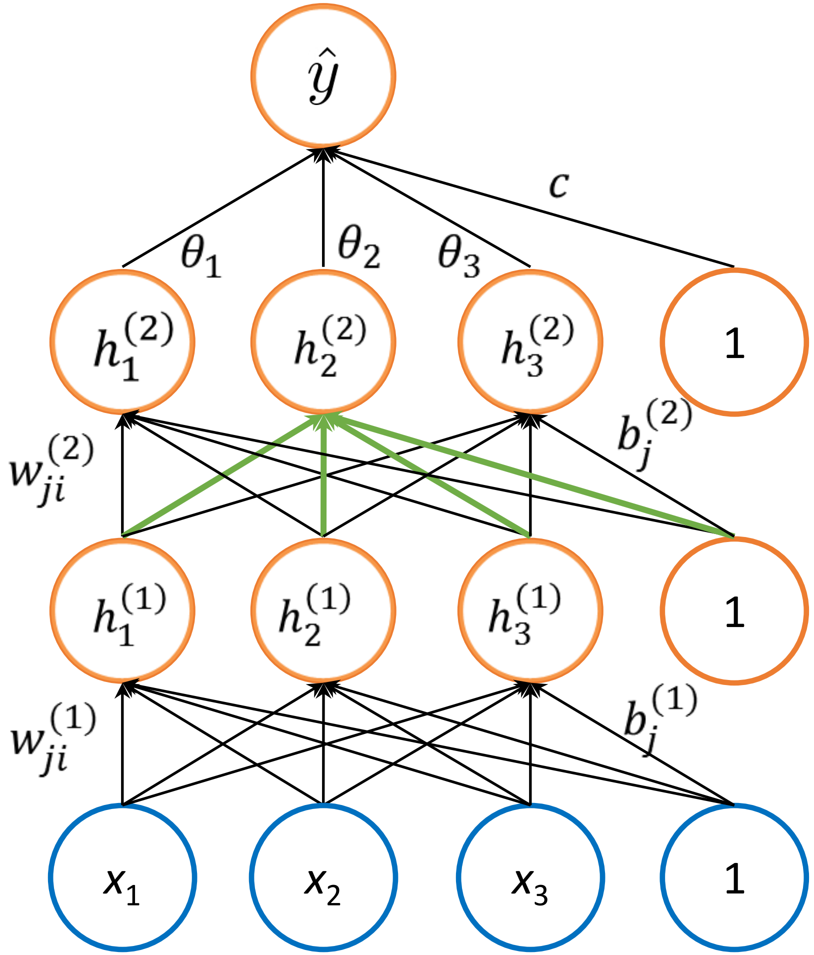
Second hidden layer $$\boxed{h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(1)} + b_j^{(2)})}$$

Output $$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$



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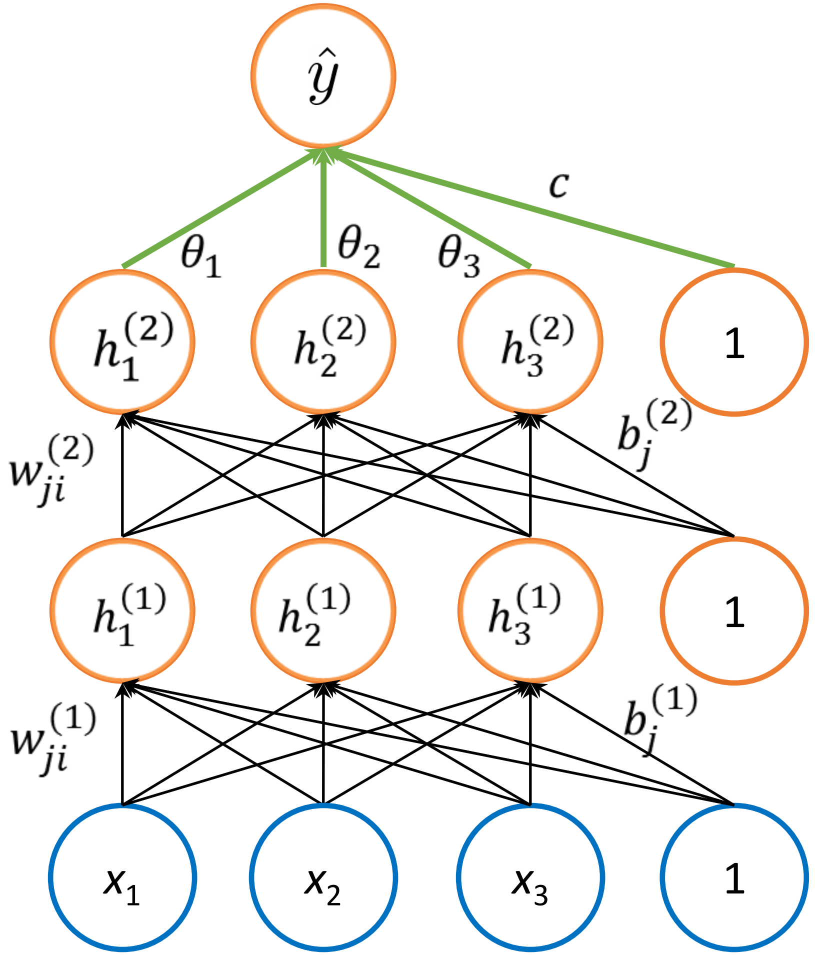
Output $$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$



Example: 2-Layer NN Backward Pass

- Compute gradients w.r.t.

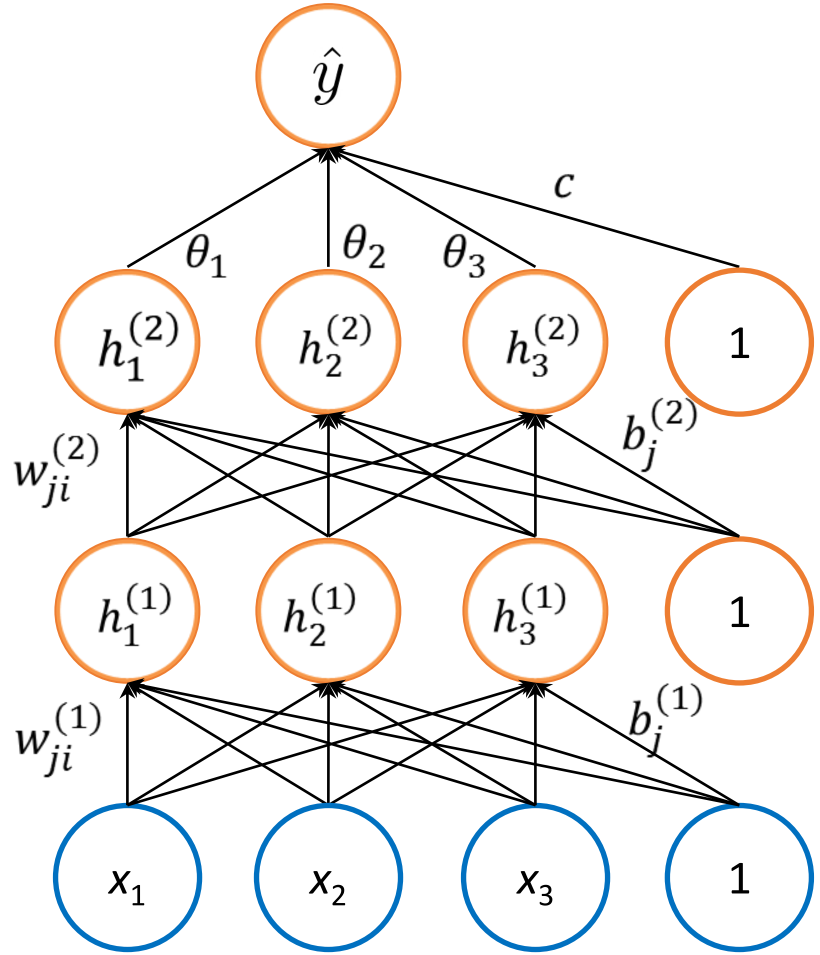
$$\{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \theta, c\}$$

$$h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)}), \forall j$$

$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(i)} + b_j^{(2)}), \forall j$$

$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

$$L = (\hat{y} - y)^2$$



Example: 2-Layer NN Backward Pass

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

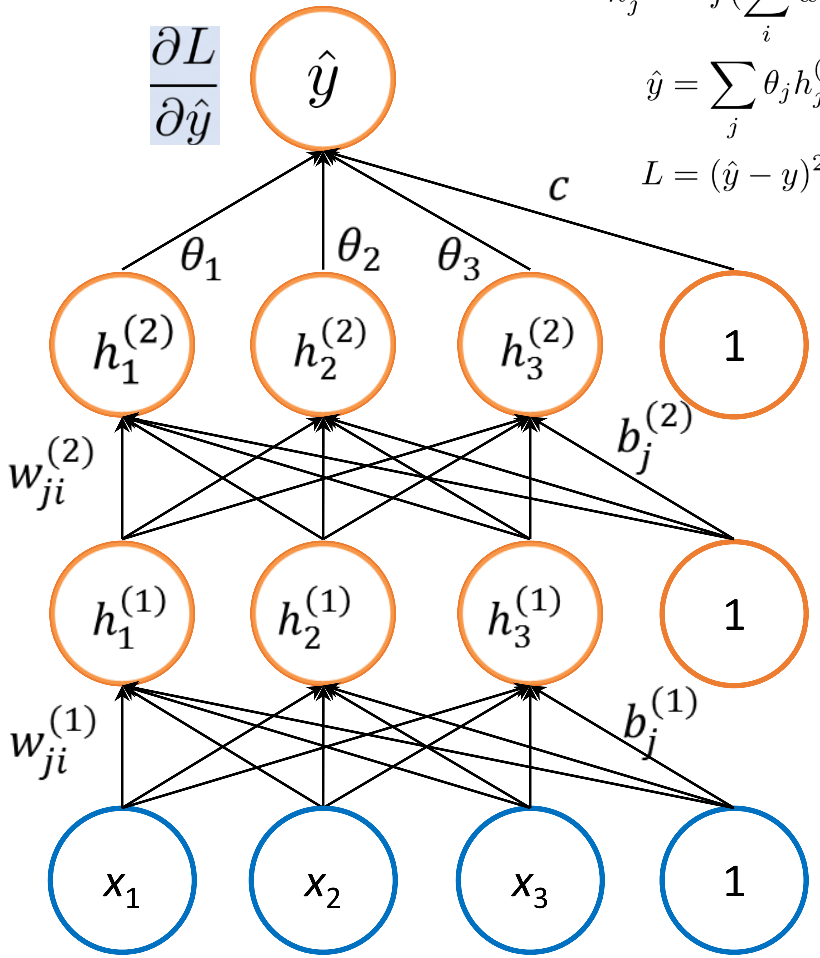
$$\{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \theta, c\}$$

$$h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)}), \forall j$$

$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(i)} + b_j^{(2)}), \forall j$$

$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

$$L = (\hat{y} - y)^2$$



Example: 2-Layer NN Backward Pass

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$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

$$L = (\hat{y} - y)^2$$

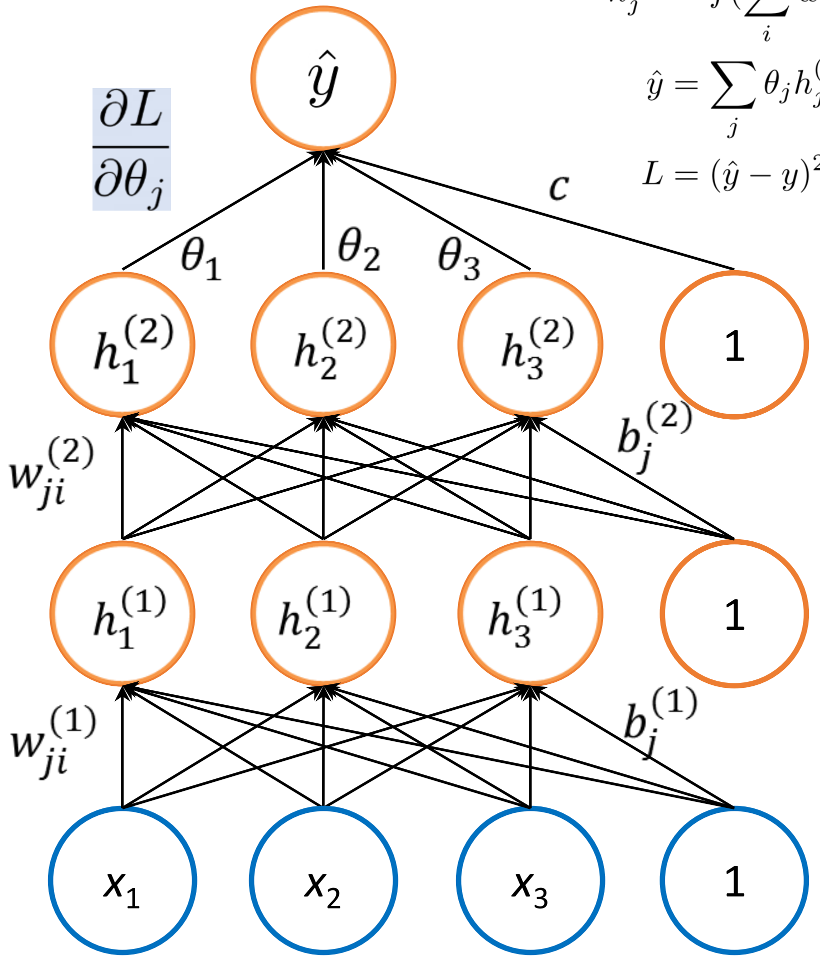
$$\frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\frac{\partial L}{\partial \theta_j} = \frac{\partial \hat{y}}{\partial \theta_j} \frac{\partial L}{\partial \hat{y}} = h_j^{(2)} \frac{\partial L}{\partial \hat{y}}$$

Downstream gradient

Local gradient

Upstream gradient



Example: 2-Layer NN Backward Pass

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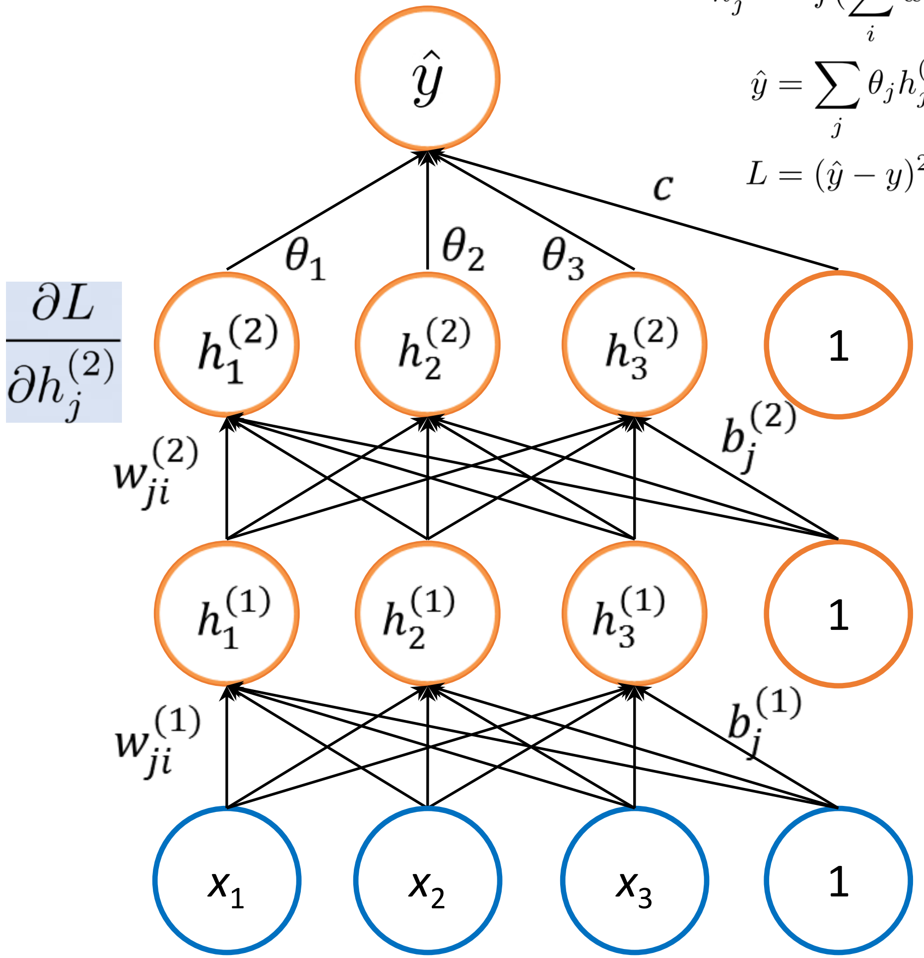
$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

$$L = (\hat{y} - y)^2$$

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

$$\frac{\partial L}{\partial \theta_j} = \frac{\partial \hat{y}}{\partial \theta_j} \frac{\partial L}{\partial \hat{y}} = h_j^{(2)} \frac{\partial L}{\partial \hat{y}}$$

$$\frac{\partial L}{\partial h_j^{(2)}} = \frac{\partial \hat{y}}{\partial h_j^{(2)}} \frac{\partial L}{\partial \hat{y}} = \theta_j \frac{\partial L}{\partial \hat{y}}$$



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$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(i)} + b_j^{(2)}), \forall j$$

$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

$$L = (\hat{y} - y)^2$$

$$z_j^{(2)} = \sum_i h_i^{(1)} w_{ji}^{(2)} + b_j^{(2)}$$

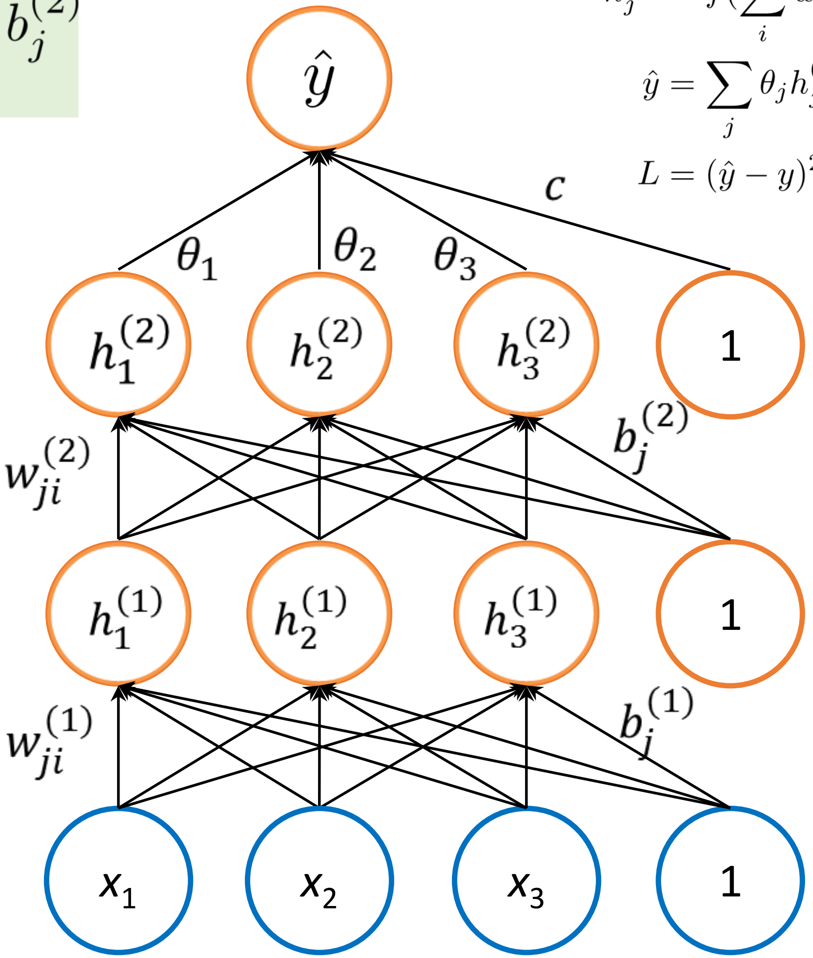
$$\frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\frac{\partial L}{\partial \theta_j} = \frac{\partial \hat{y}}{\partial \theta_j}\frac{\partial L}{\partial \hat{y}} = h_j^{(2)} \frac{\partial L}{\partial \hat{y}}$$

$$\frac{\partial L}{\partial h_j^{(2)}} = \frac{\partial \hat{y}}{\partial h_j^{(2)}}\frac{\partial L}{\partial \hat{y}} = \theta_j \frac{\partial L}{\partial \hat{y}}$$

$$\frac{\partial L}{\partial w_{ji}^{(2)}} = \frac{\partial h_j^{(2)}}{\partial w_{ji}^{(2)}} \frac{\partial L}{\partial h_j^{(2)}} = f'(z_j^{(2)}) h_i^{(1)} \frac{\partial L}{\partial h_j^{(2)}}$$

$$\frac{\partial L}{\partial w_{ji}^{(2)}}$$



Example: 2-Layer NN Backward Pass

$$\{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \theta, c\}$$

$$h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)}), \forall j$$

$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(i)} + b_j^{(2)}), \forall j$$

$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

$$L = (\hat{y} - y)^2$$

$$z_j^{(2)} = \sum_i h_i^{(1)} w_{ji}^{(2)} + b_j^{(2)}$$

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

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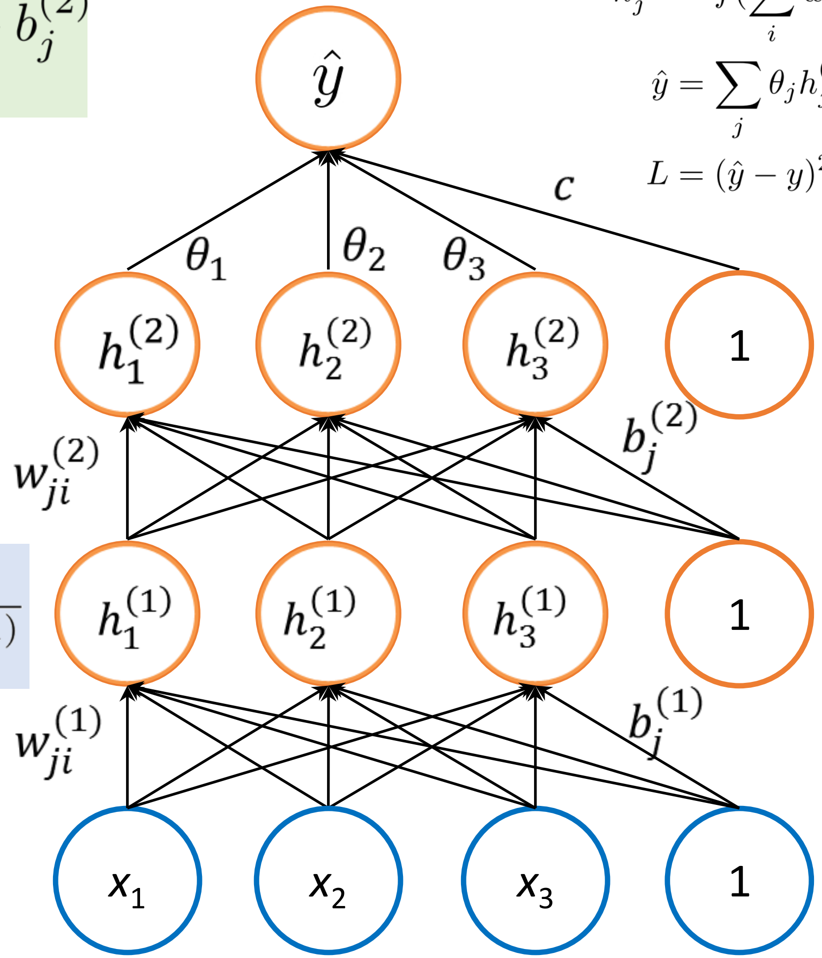
$$\frac{\partial L}{\partial h_i^{(1)}} = \sum_j \frac{\partial h_j^{(2)}}{\partial h_i^{(1)}} \frac{\partial L}{\partial h_j^{(2)}} = \sum_j f'(z_j^{(2)}) w_{ji}^{(2)} \frac{\partial L}{\partial h_j^{(2)}}$$

$$\frac{\partial L}{\partial h_i^{(1)}}$$



Example: 2-Layer NN Backward Pass

$$\{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \theta, c\}$$

$$h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)}), \forall j$$

$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(i)} + b_j^{(2)}), \forall j$$

$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

$$L = (\hat{y} - y)^2$$

$$z_j^{(2)} = \sum_i h_i^{(1)} w_{ji}^{(2)} + b_j^{(2)}$$

$$z_i^{(1)} = \sum_k x_k w_{ik}^{(1)} + b_i^{(1)}$$

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

$$\frac{\partial L}{\partial \theta_j} = \frac{\partial \hat{y}}{\partial \theta_j} \frac{\partial L}{\partial \hat{y}} = h_j^{(2)} \frac{\partial L}{\partial \hat{y}}$$

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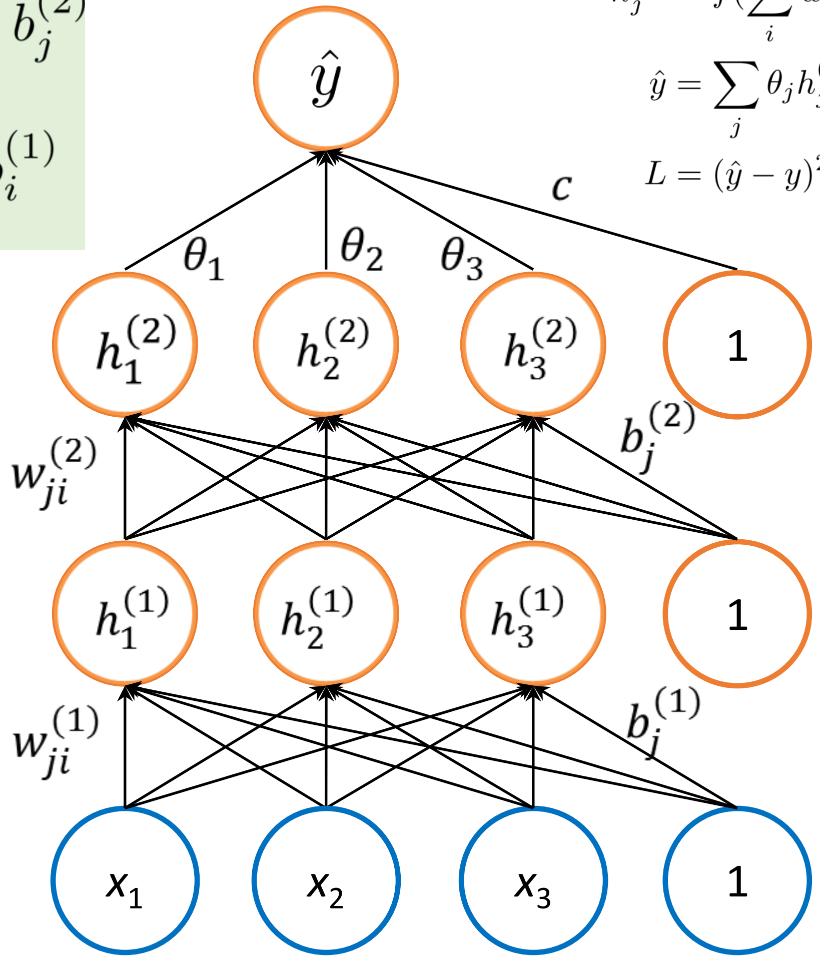
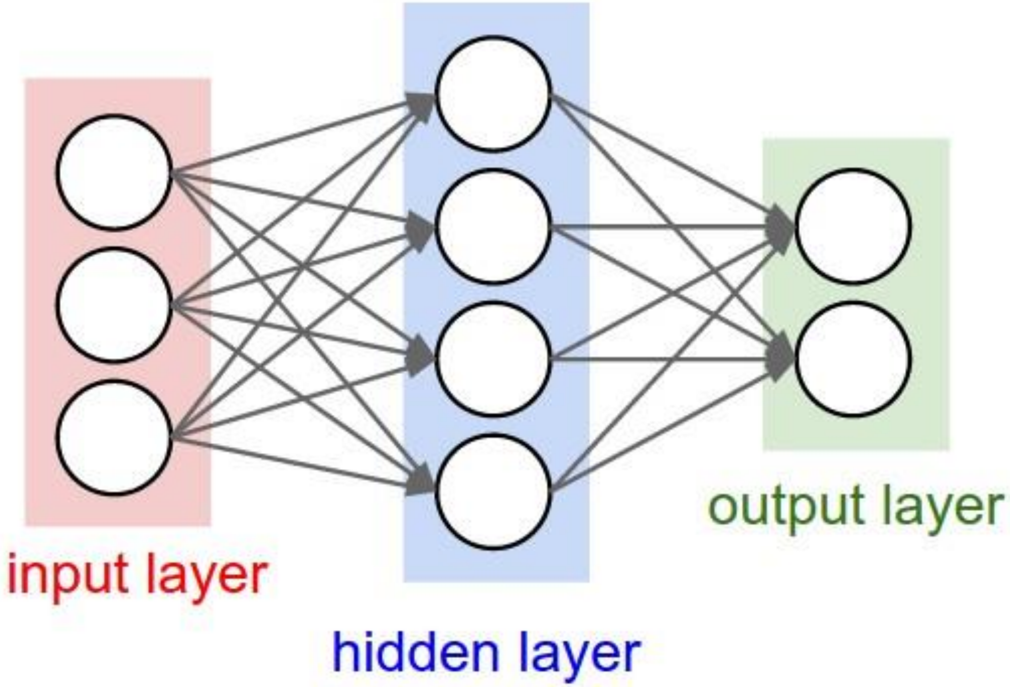
$$\frac{\partial L}{\partial h_i^{(1)}} = \sum_j \frac{\partial h_j^{(2)}}{\partial h_i^{(1)}} \frac{\partial L}{\partial h_j^{(2)}} = \sum_j f'(z_j^{(2)}) w_{ji}^{(2)} \frac{\partial L}{\partial h_j^{(2)}}$$

$$\frac{\partial L}{\partial w_{ik}^{(1)}}$$

$$\frac{\partial L}{\partial w_{ik}^{(1)}} = \frac{\partial h_i^{(1)}}{\partial w_{ik}^{(1)}} \frac{\partial L}{\partial h_i^{(1)}} = f'(z_i^{(1)}) x_k \frac{\partial L}{\partial h_i^{(1)}}$$



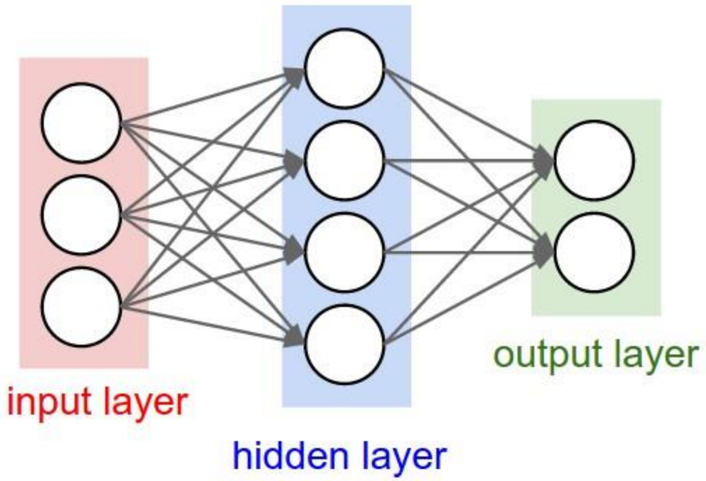
Neural Net in <20 lines!




```python
import numpy as np
from numpy.random import randn

N, Din, H, Dout = 64, 1000, 100, 10
x, y = randn(N, Din), randn(N, Dout)
w1, w2 = randn(Din, H), randn(H, Dout)
for t in range(10000):
  h = 1.0 / (1.0 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  dy_pred = 2.0 * (y_pred - y)
  dw2 = h.T.dot(dy_pred)
  dh = dy_pred.dot(w2.T)
  dw1 = x.T.dot(dh * h * (1 - h))
  w1 -= 1e-4 * dw1
  w2 -= 1e-4 * dw2
```

Neural Net in <20 lines!



Initialize weights and data

Compute loss (sigmoid activation, L2 loss)

Compute gradients

SGD step

```python
import numpy as np
from numpy.random import randn

N, Din, H, Dout = 64, 1000, 100, 10
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  dw1 = x.T.dot(dh * h * (1 - h))
  w1 -= 1e-4 * dw1
  w2 -= 1e-4 * dw2
```

Better Idea: Backpropagation by **Chain Rule**

$$x \xrightarrow{W_1} h_1 \xrightarrow{W_2} h_2 \xrightarrow{W_3} h_3 \xrightarrow{W_4} L$$

D_0 D_1 D_2 D_3 scalar

Chain rule

$$\frac{\partial L}{\partial x} = \left(\frac{\partial h_1}{\partial x}\right)\left(\frac{\partial h_2}{\partial h_1}\right)\left(\frac{\partial h_3}{\partial h_2}\right)\left(\frac{\partial L}{\partial h_3}\right)$$

[D_0 x D_1] [D_1 x D_2] [D_2 x D_3] [D_3]

e.g., (i, j)-th element in W_2

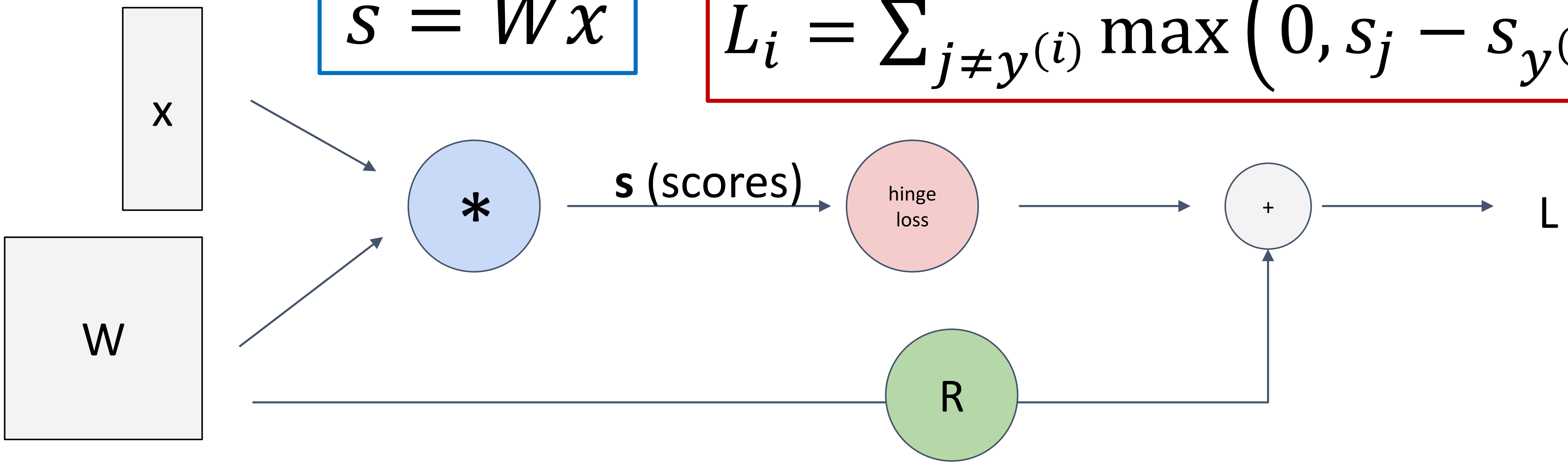
$$\frac{\partial L}{\partial W_2(i,j)} = \left(\frac{\partial h_2}{\partial W_2(i,j)}\right)\left(\frac{\partial h_3}{\partial h_2}\right)\left(\frac{\partial L}{\partial h_3}\right)$$

[D_2] [D_2 x D_3] [D_3]

Better Idea: **Computational Graphs**

$$\boxed{s = Wx}$$

$$\boxed{L_i = \sum_{j \neq y^{(i)}} \max\left(0, s_j - s_{y^{(i)}} + 1\right)}$$



$$\boxed{R(W)}$$

Next: Backpropagation