Neural Networks: Architecture

CS229: Machine Learning

winter

Stanford University, ~~Spring~~ 2024
(Adapted from slides by Matgus Telgarsky and Alexander Schwing)

Goals of this lecture

- Understand the motivation for deep neural networks
- Learn about deep neural network architecture(s) and some standard components

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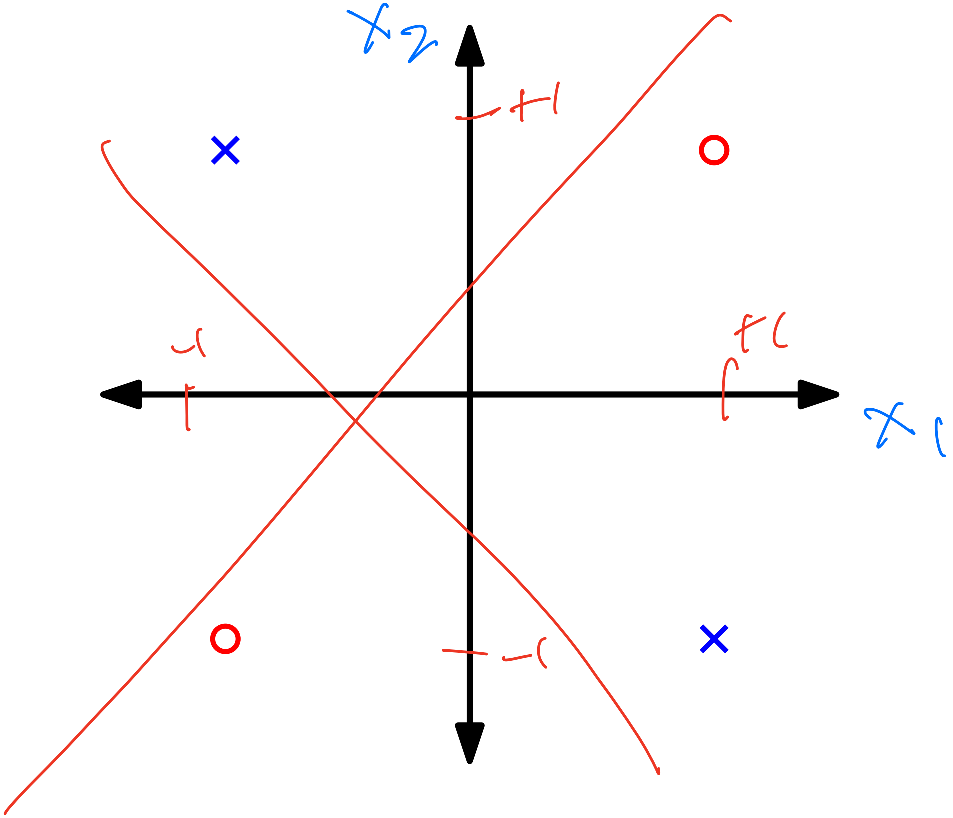
Reading material

- Course Notes, Section 7.1, 7.2
- I. Goodfellow et al.; Deep Learning; Chapters 6-9

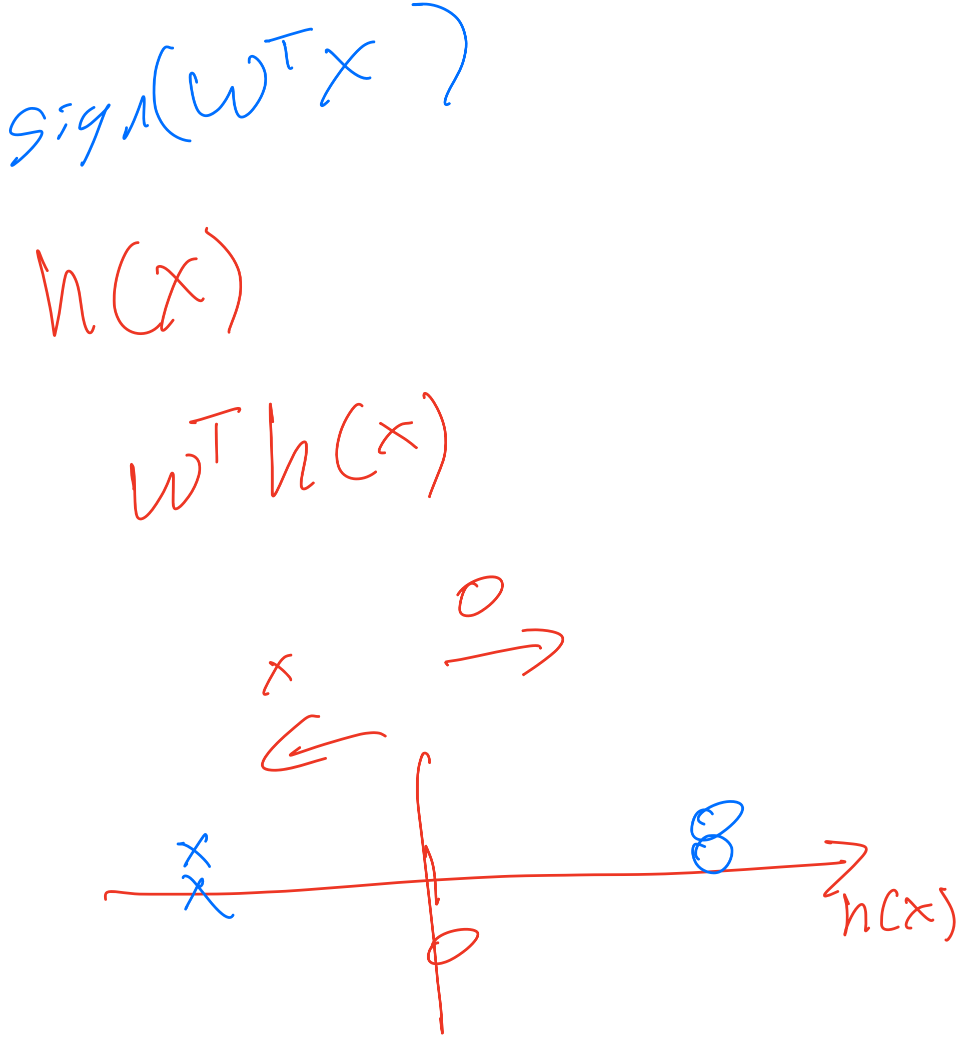
Lecture notation

Notation	Usage
$h(\cdot)$	Feature function; $\overset{\phi}{\cancel{h}}(\cdot)$ in the notes
$f(\cdot)$	Prediction function; $h(\cdot)$ in the notes
$l(\cdot, \cdot)$	Loss function; $J(\cdot)$ in the notes
$\boldsymbol{w}, \boldsymbol{W}$	Model Parameters, θ in the notes
$\boldsymbol{x}^{(i)}, \boldsymbol{x}$	Input(s)
$y^{(i)}, y$	Label(s)
λ	Regularization parameter(s); C in the notes
$\sigma(\cdot)$	Activation function, nonlinearity

Limitations of linear predictors?



No linear separator classifies perfectly!



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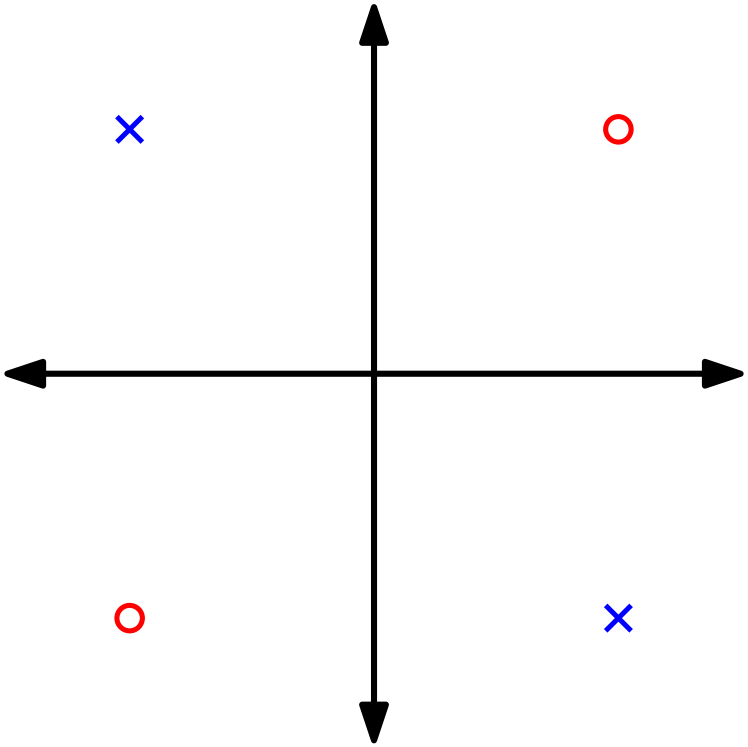

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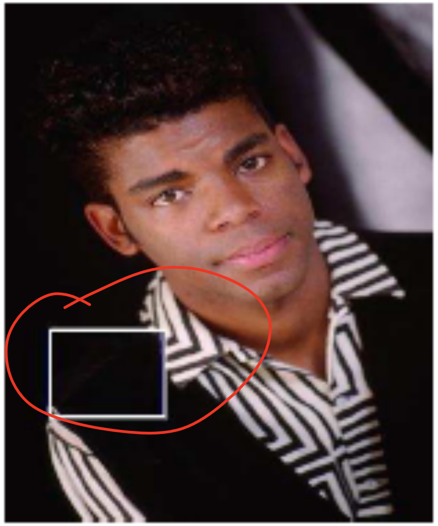
Feature Transformation:
use features $h(\boldsymbol{x}) := \boldsymbol{x}_1^\top \boldsymbol{x}_2$,
with prediction $y = \text{sgn}\left(\boldsymbol{w}^\top h(\boldsymbol{x})\right)$.

Real-world Application: **Edge/Boundary detection:**

What are y, x?

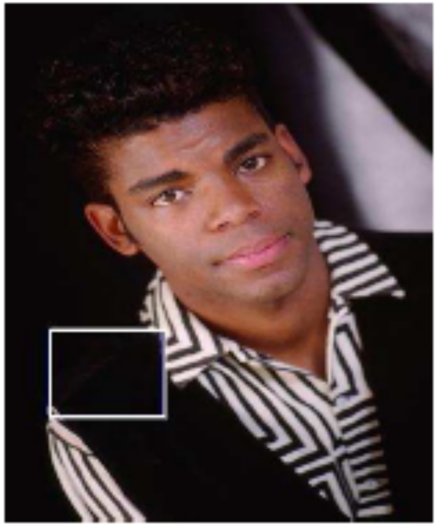


$y :=$ background -1
foreground $+1$

$x :=$ pixels
(intensity, color)

Real-world Application: Edge/Boundary detection:

Issues?



Poor contrast

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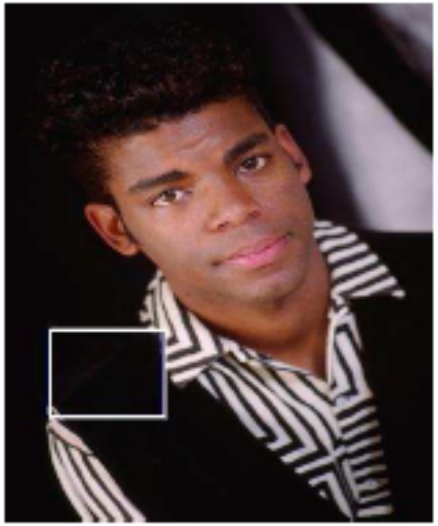

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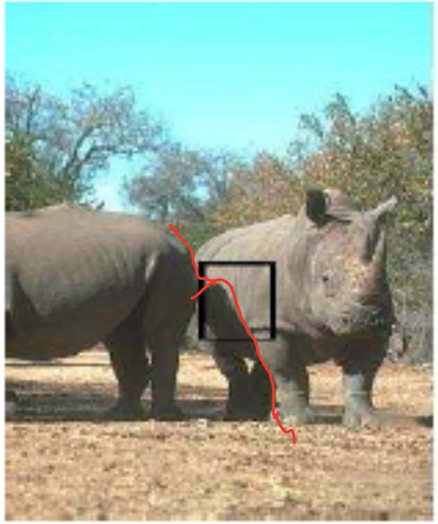

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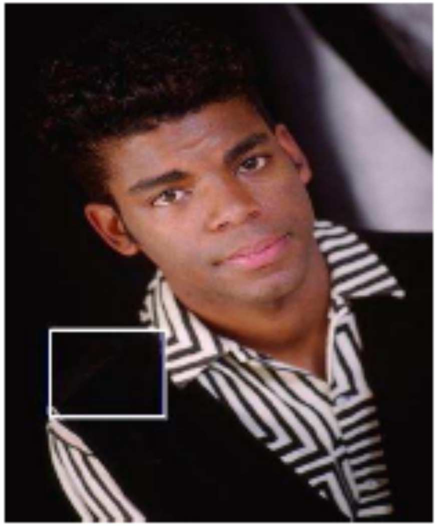

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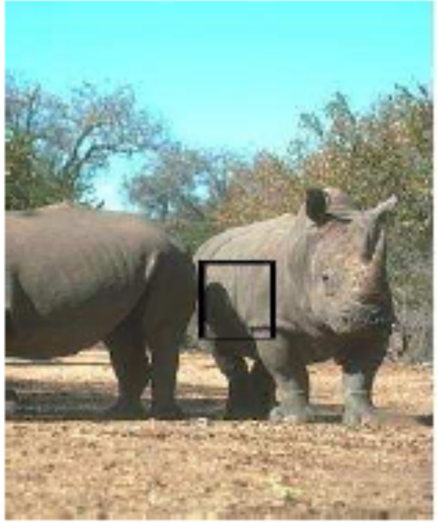

Shadow

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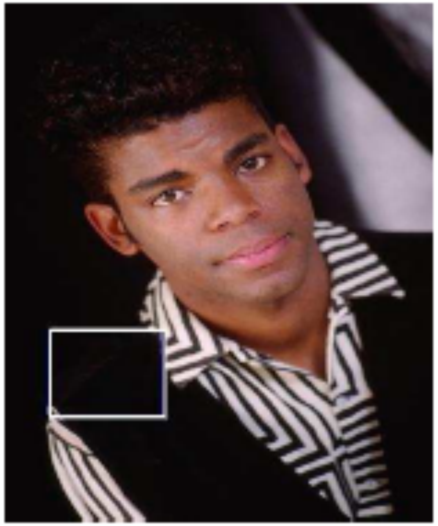

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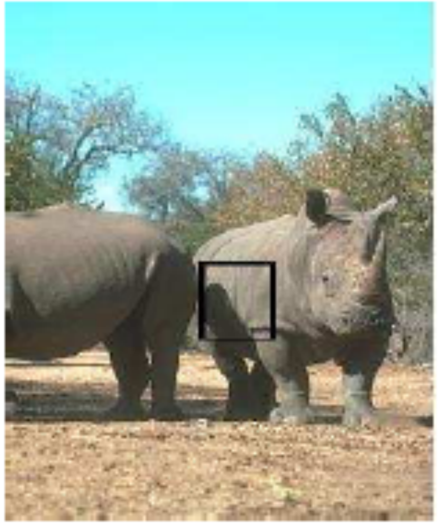

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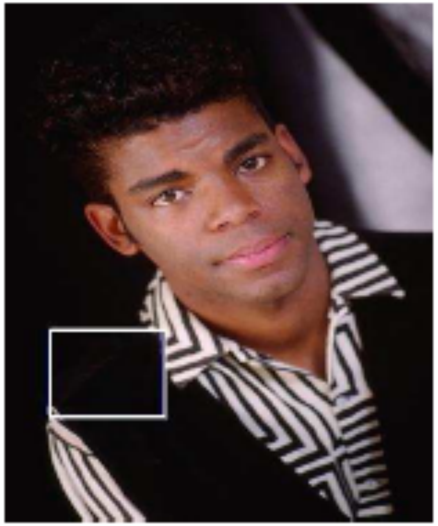

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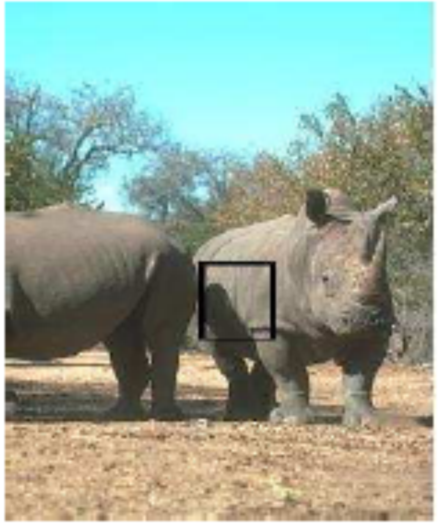

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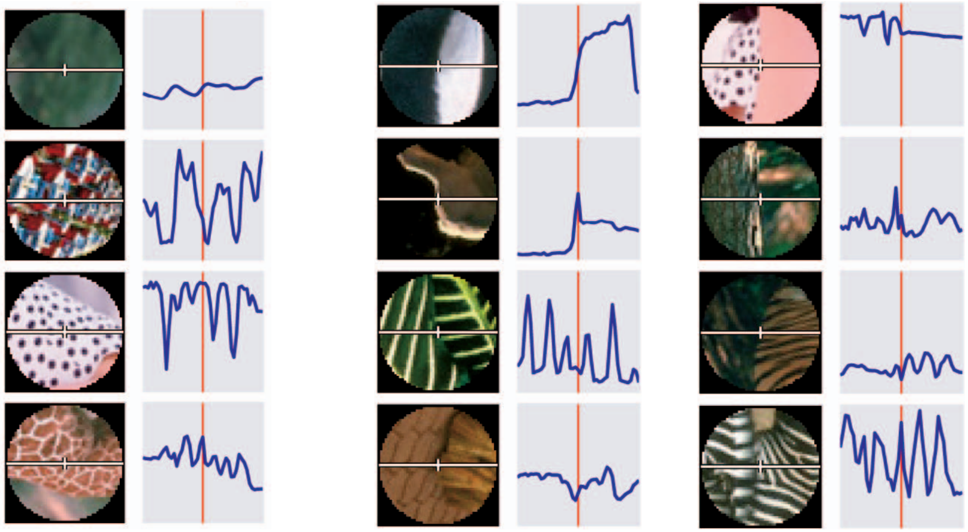
Texture

Edge/Boundary detection: Why is it so difficult?

Let’s look at a local image region and the corresponding intensities:



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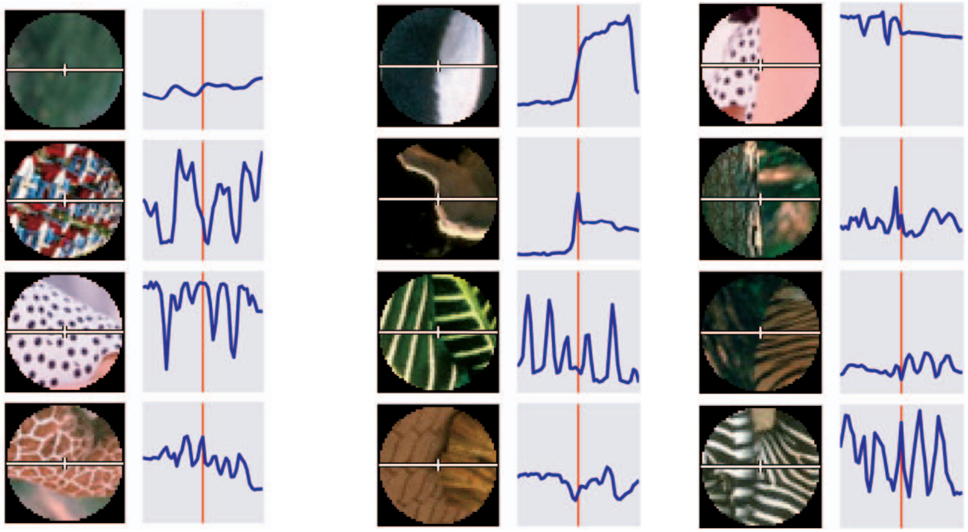

Non-Boundaries

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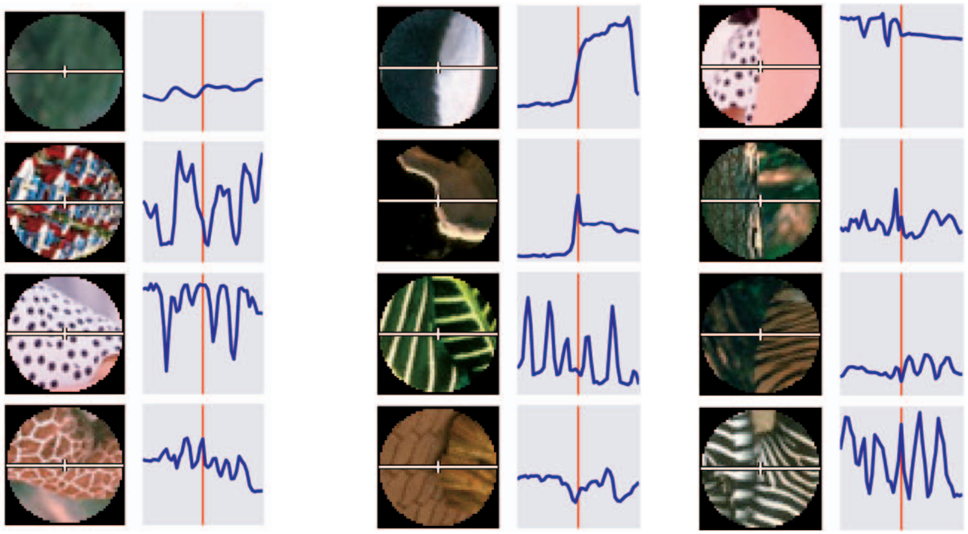

Non-Boundaries Boundaries

$h(x)$ = pixel intensity

⟶ avg local intensity

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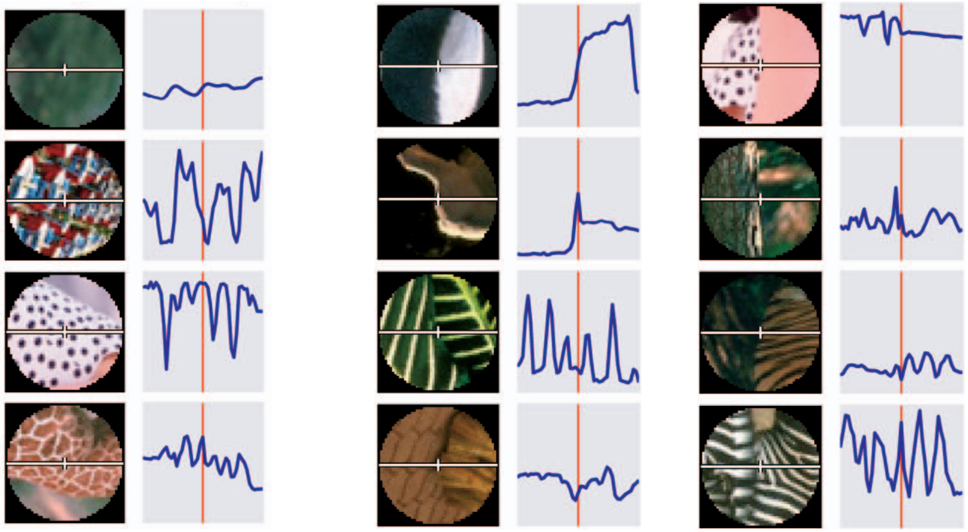

Non-Boundaries Boundaries

Intensity cue is not necessarily a good indicator for boundaries.

Martin et al., *Learning to detect natural Image Boundaries ...*, PAMI 2004

Edge/Boundary detection: What other image cues could be helpful?

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How to combine all those cues?

$h(x_i) = \begin{bmatrix} BG \\ CG \\ \vdots \end{bmatrix}$ $\quad w^T h(x) = f(x)$

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How to combine all those cues? Learn a linear combination of cues

- What is $y^{(i)}$?

- What is $y^{(i)}$? Annotated pixel label

- What is $y^{(i)}$? Annotated pixel label
- What is $x^{(i)}$?

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- What is $x^{(i)}$? Image pixel

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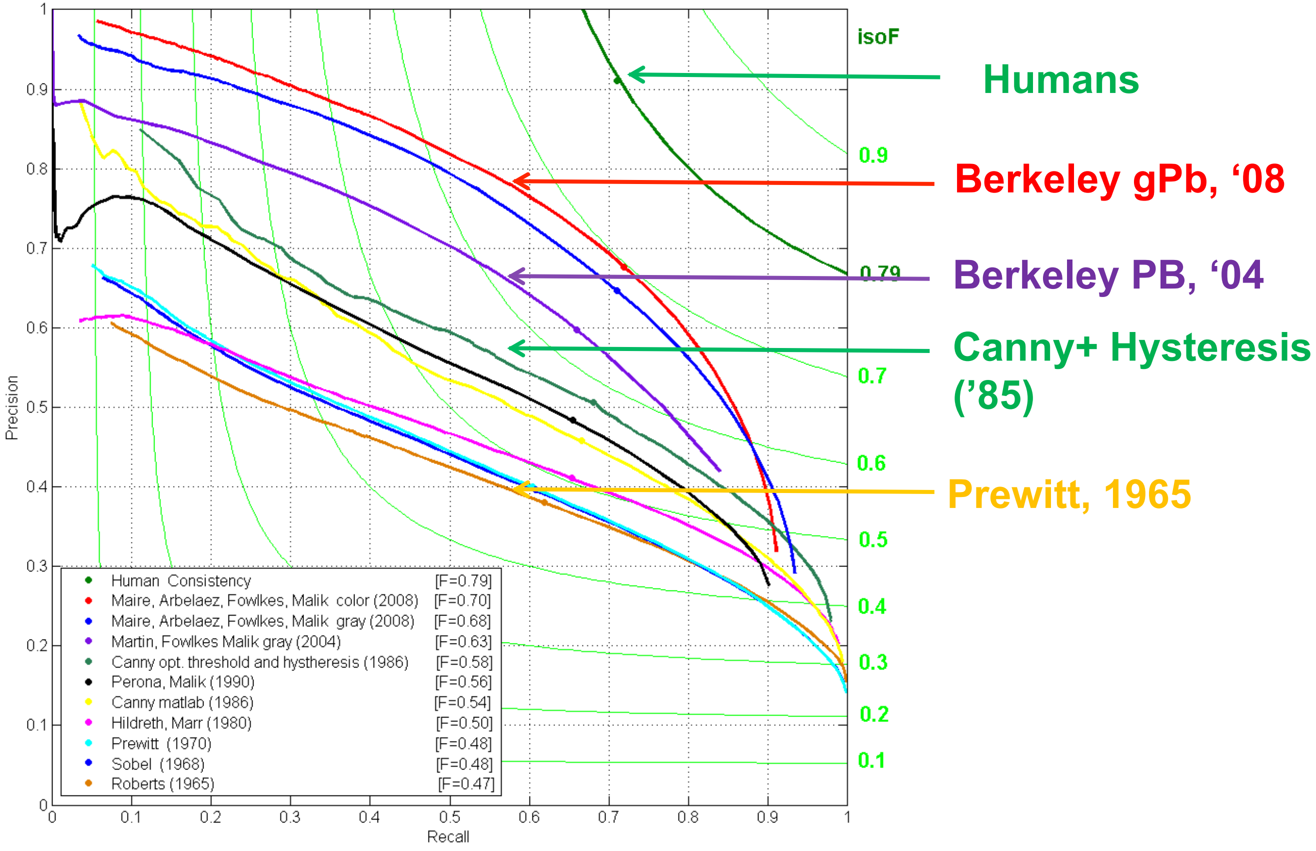
- What is $h(x^{(i)})$?

- What is $y^{(i)}$? Annotated pixel label
- What is $x^{(i)}$? Image pixel
- What is $h(x^{(i)})$? Vector of features computed in the **neighborhood** of pixel i, e.g., intensity, texture gradient, oriented gradient etc.

Boundary detection performance:



Key Takeaways:

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- Selecting good features is often key to the performance of an ML algorithm.
- Most common approach is to apply known heuristics that work well from (community/expert) experience.
- Caution: when/how can adding features hurt performance?
- Next, we will discuss how deep learning can help automate feature extraction.

Neural networks via *features*.

To make a linear predictor nonlinear in x, we rely upon feature mapping h:

$$\boldsymbol{w}^\top \boldsymbol{x} \qquad \text{becomes} \qquad \boldsymbol{w}^\top h(\boldsymbol{x}).$$

We are at the mercy of the quality of h.

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$\ell(w) = -\log P(y \mid x; w)$

Why not *learn* h? e.g.,

$$\min_{\boldsymbol{w}} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y^{(i)}, \boldsymbol{w}^\top \boldsymbol{x}^{(i)}\right) \qquad \text{becomes} \qquad \min_{\boldsymbol{w}, h} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y^{(i)}, \boldsymbol{w}^\top h(\boldsymbol{x}^{(i)})\right)$$

Neural networks as iterated linear prediction (part 1).

Natural choice: build feature maps out of linear predictors!

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$$\boldsymbol{w}^\top \boldsymbol{x} \qquad \text{becomes} \qquad \boldsymbol{v}^\top h(\boldsymbol{x}) \quad \text{where } h(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$$

with $\boldsymbol{w} \in \mathbb{R}^d, \boldsymbol{v} \in \mathbb{R}^m, \boldsymbol{A} \in \mathbb{R}^{m \times d}, \boldsymbol{b} \in \mathbb{R}^m$.

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Gained no additional representation flexibility!

$$\boldsymbol{v}^\top(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}) = (\boldsymbol{A}^\top \boldsymbol{v})^\top \boldsymbol{x} + \boldsymbol{v}^\top \boldsymbol{b}.$$

w

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$$\sigma(v) = \begin{bmatrix} \sigma(v_1) \\ \sigma(v_2) \\ \vdots \\ \sigma(v_m) \end{bmatrix}$$

Fix: introduce **nonlinearity/transfer/activation** $\sigma : \mathbb{R}^m \to \mathbb{R}^m$:

$$h(\boldsymbol{x}) := \sigma\left(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}\right).$$

Neural networks as iterated linear prediction (part 2).

We will predict as

$h(x; A, b, \sigma)$ ← fit

$$\boldsymbol{w}^\top h(\boldsymbol{x}) \qquad \text{where } h(\boldsymbol{x}) = \sigma\left(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}\right).$$

We will train as

$$\min_{\boldsymbol{w}\in\mathbb{R}^m, \boldsymbol{A}\in\mathbb{R}^{m\times d}, \boldsymbol{b}\in\mathbb{R}^m} \frac{1}{n}\sum_{i=1}^{n} \ell\left(y^{(i)}, \boldsymbol{w}^\top \sigma\left(\boldsymbol{A}\boldsymbol{x}^{(i)} + \boldsymbol{b}\right)\right).$$

Question: which training procedure? Gradient Desent

OR SGD

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Why stop there? We can also do

$$\boldsymbol{w}^\top \sigma_1\left(\boldsymbol{A}^{[1]} h(\boldsymbol{x}) + \boldsymbol{b}^{[1]}\right) \qquad \text{where } h(\boldsymbol{x}) = \sigma_2\left(\boldsymbol{A}^{[2]}\boldsymbol{x} + \boldsymbol{b}^{[2]}\right),$$

and iterate further.

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and iterate further. *This is a deep neural network.*

Neural networks as functions.

A linear predictor (**one layer network**) has the form

$$\boldsymbol{w}^\top \boldsymbol{x}.$$

A **two layer network** has the form

$$\boldsymbol{x} \mapsto \boldsymbol{w}^\top \sigma_1\left(\boldsymbol{A}^{[1]}\boldsymbol{x} + \boldsymbol{b}^{[1]}\right).$$

$h(x)$

$\to A^{[i]}, b^{[i]}$

Iterating, a **multi-layer network** has the form

$$\boldsymbol{w}^\top \sigma_1\left(\boldsymbol{A}^{[1]}\sigma_2\left(\cdots \boldsymbol{A}^{[L-2]}\sigma_{L-1}\left(\boldsymbol{A}^{[L-1]}\boldsymbol{x} + \boldsymbol{b}^{[L-1]}\right) + \boldsymbol{b}^{[L-2]}\cdots\right) + \boldsymbol{b}^{[1]}\right).$$

$h(x)$

$\to$ Parameters $\{A^{[i]}, b^{[i]}\}$

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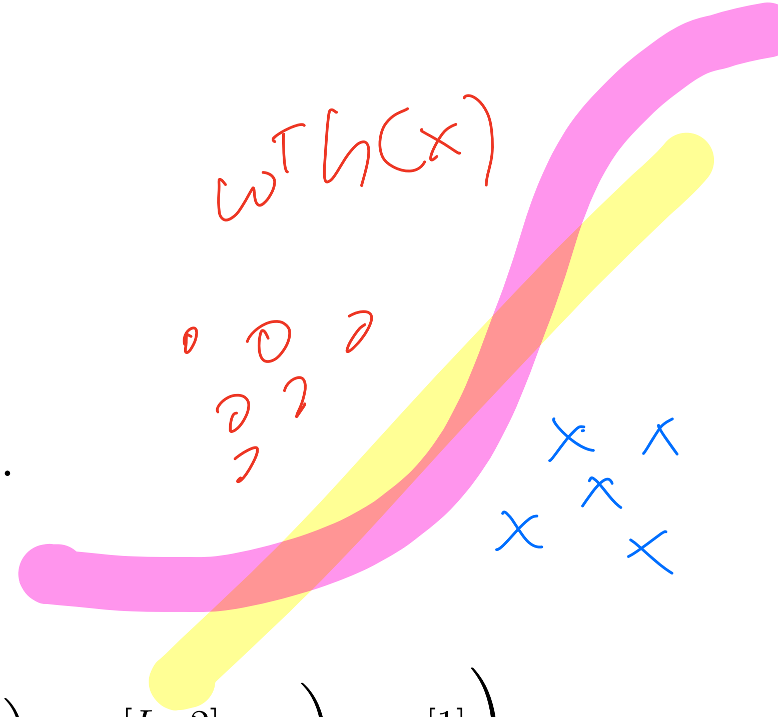
$w^T h(x)$



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Optimization now takes the form

$$\min_{\boldsymbol{w}, \boldsymbol{A}^{[1]}, \ldots, \boldsymbol{A}^{[L-1]}, \boldsymbol{b}_1, \ldots, \boldsymbol{b}_{L-1}} \frac{1}{n} \sum_{i=1}^{n} \ell \left(y^{(i)}, \boldsymbol{w}^\top \sigma_1 \left(\cdots \sigma_{L-1} \left(\boldsymbol{A}^{[L-1]} \boldsymbol{x}^{(i)} + \boldsymbol{b}^{[L-1]} \right) \cdots \right) \right).$$

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Node j in this graph:

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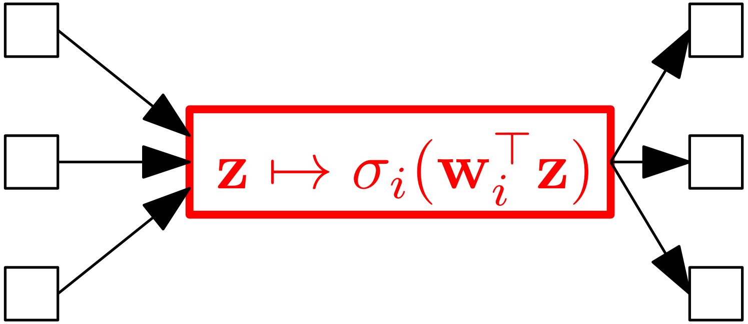

one layer

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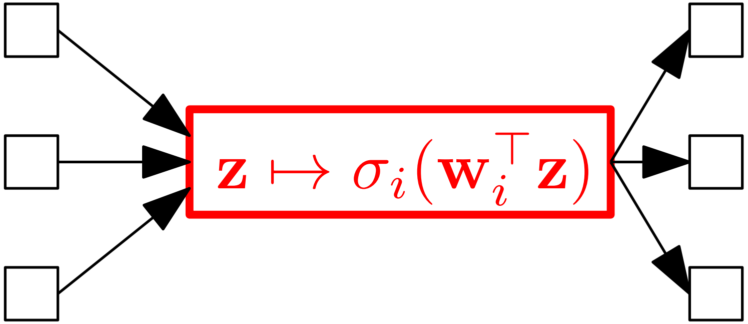

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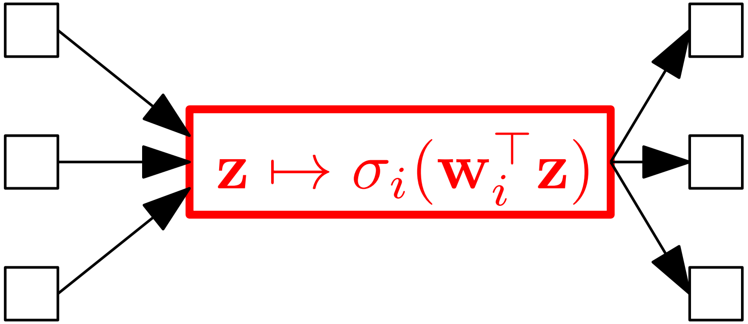

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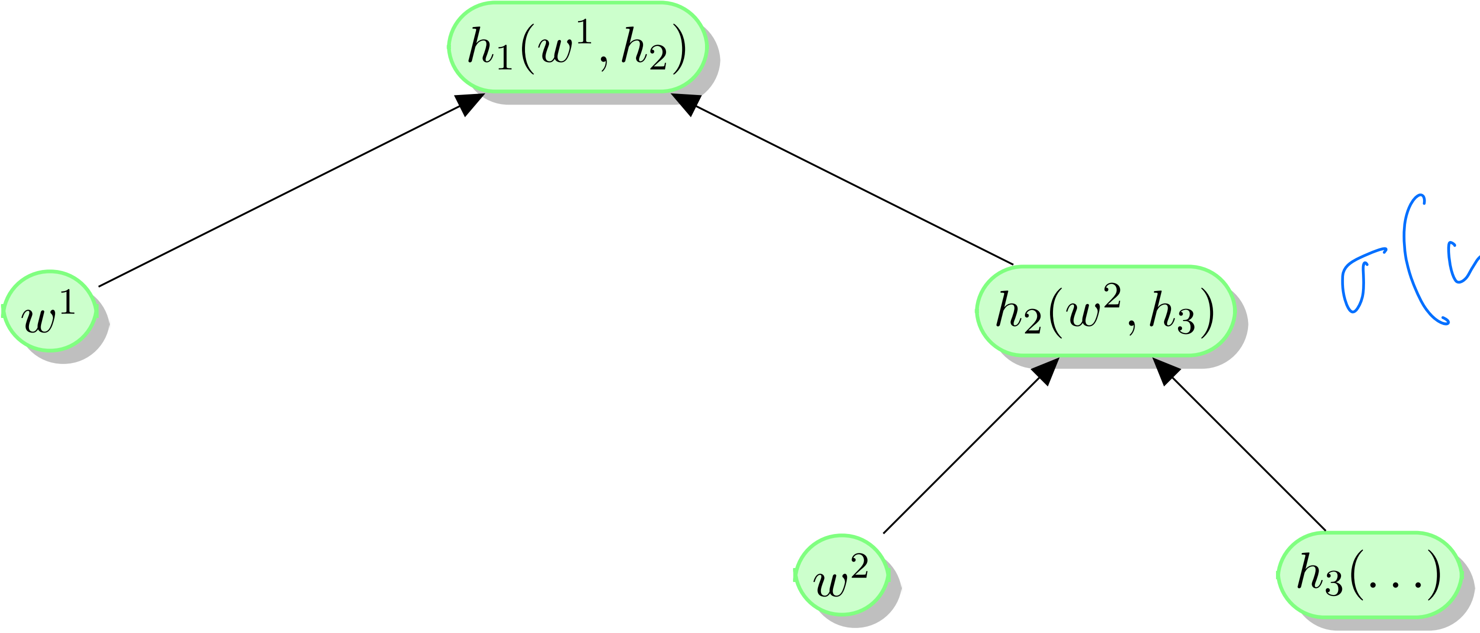
Tensorflow computation graphs: everything needed to train is in the graph; e.g., parameters are also assigned to nodes.

Internal representation used by deep net packages

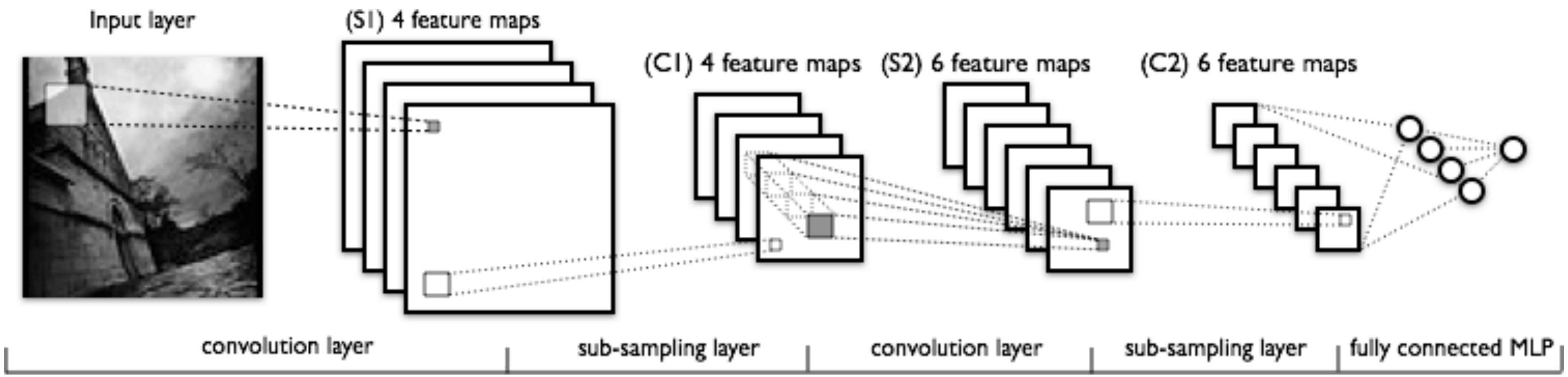
$$f(\boldsymbol{w}, x, y) = h_1(w^1, h_2(w^2, h_3(\ldots)))$$

Nodes are weights, data, and functions



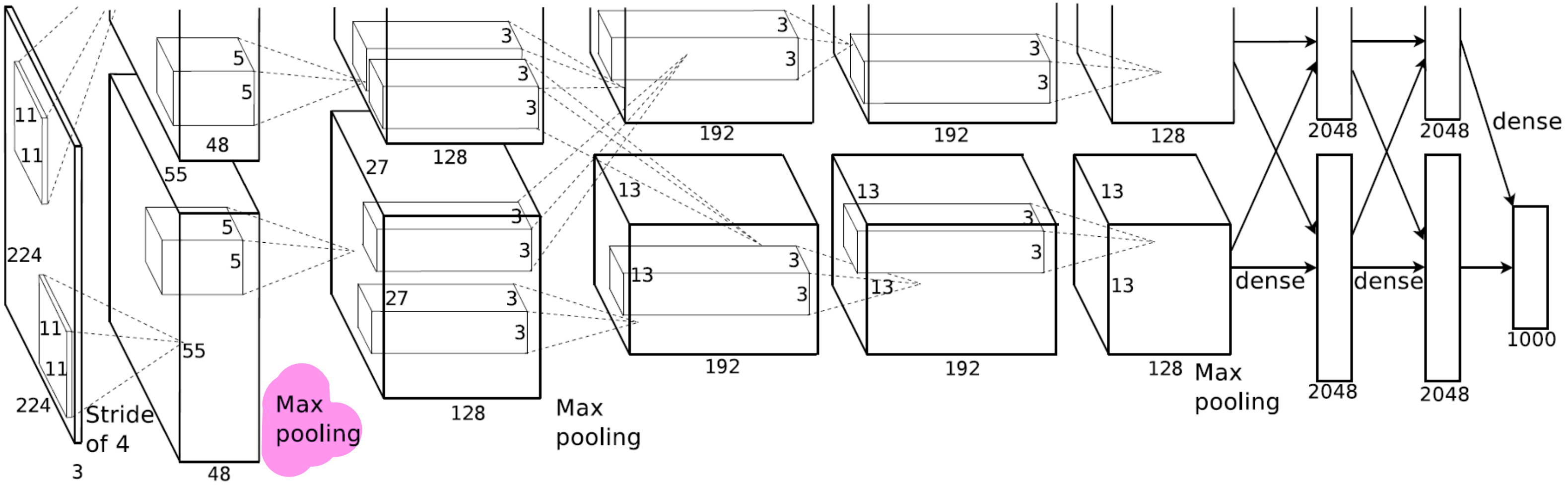
$\sigma(w^{2T} h_3())$

Example function architecture: LeNet



Decreasing spatial resolution and the increasing number of channels (dimension of feature maps)

Example function architecture: AlexNet



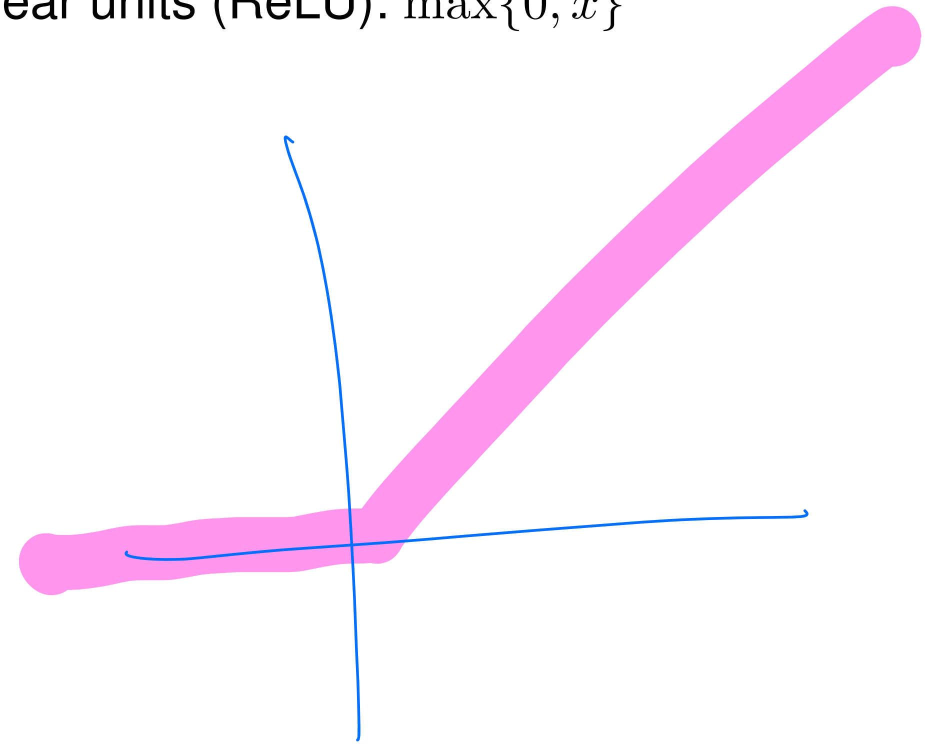
Decreasing spatial resolution and the increasing number of channels (dimension of feature maps)

Why is the output 1000-dimensional?

Common functions/layers in a deep network

Common functions/layers in a deep network

- Univariate activations e.g. rectified linear units (ReLU): $\max\{0, x\}$
- Fully connected layers
- Convolution layers
- Maximum-/Average- pooling
- Soft-max layer
- Dropout



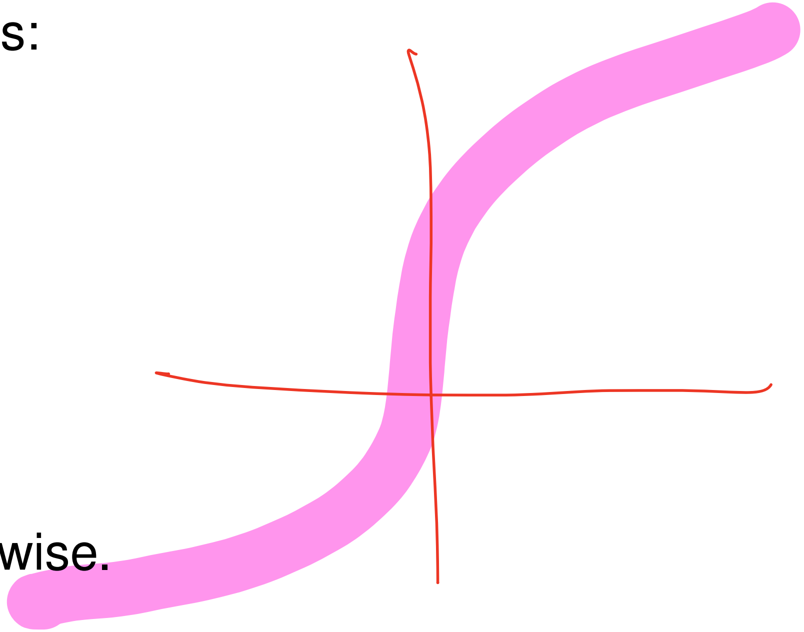
Neural network (univariate) activations.

We mentioned that **nodes** compute

$$\sigma\left(\boldsymbol{v}^\top \boldsymbol{z}\right),$$

where *activation/transfer/nonlinearity* $\sigma : \mathbb{R} \to \mathbb{R}$ is:

- ReLU (Rectified Linear Unit) $\max\{0, z\}$;
- Sigmoid $\frac{1}{1+\exp(-z)}$;
- $\dots$.



For

$$\sigma(\boldsymbol{A}\boldsymbol{z} + \boldsymbol{b}),$$

this implies applying the univariate σ coordinate-wise.

Fully connected layer

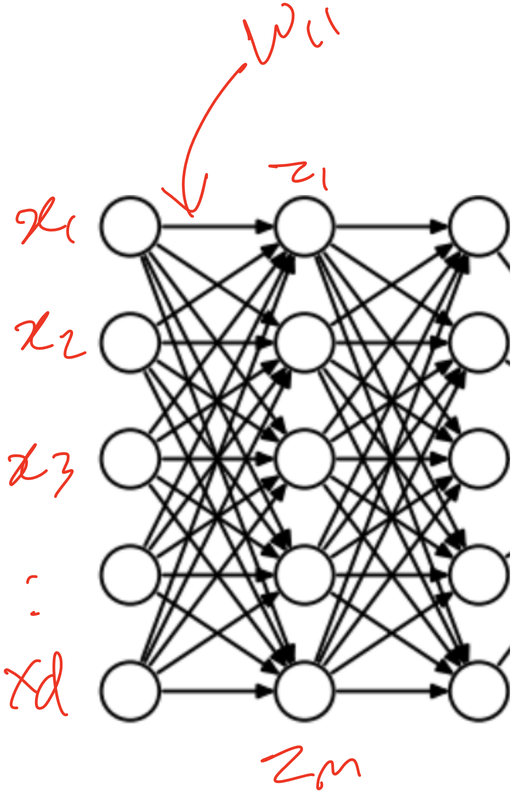
$\mathbb{R}^{m \times d}$

$\in \mathbb{R}^d$

$$\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

Trainable parameters $\boldsymbol{w}$:

- Weight matrix
- Bias



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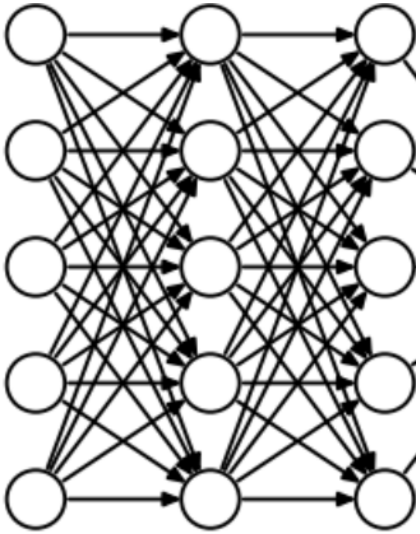

What's an issue with fully connected layers?

Issue with fully connected layers

- Suppose the input is an image of size 256×256
- Let the output of this layer have identical size
- How many weights are necessary?

$(256 \times 256)^2$

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- Let the output of this layer have identical size
- How many weights are necessary?

$$(256 \times 256)^2 = 2^{32} = 4,294,967,296$$

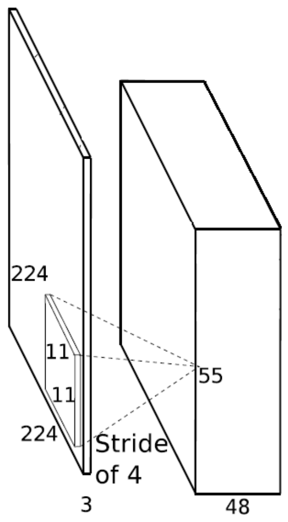
Issue with fully connected layers

- Suppose the input is an image of size 256×256
- Let the output of this layer have identical size
- How many weights are necessary?

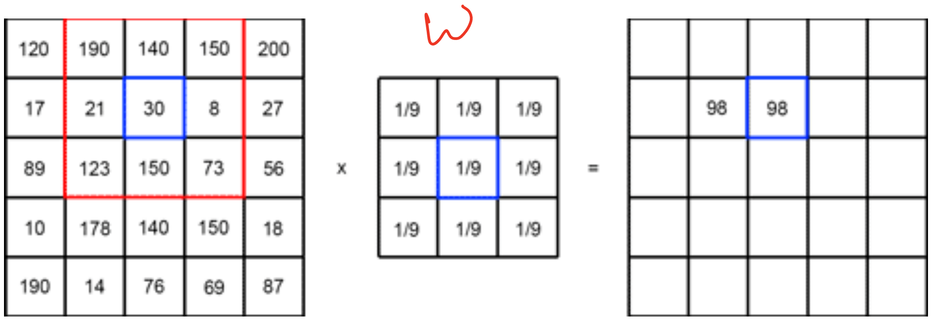
$$(256 \times 256)^2 = 2^{32} = 4,294,967,296$$

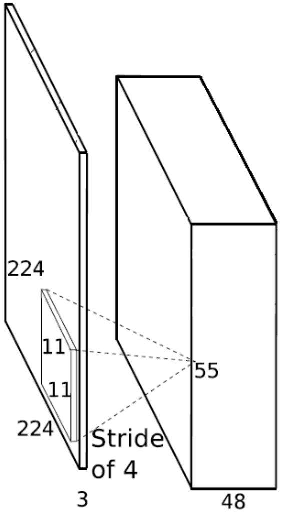
- A solution: share weights

Convolutions

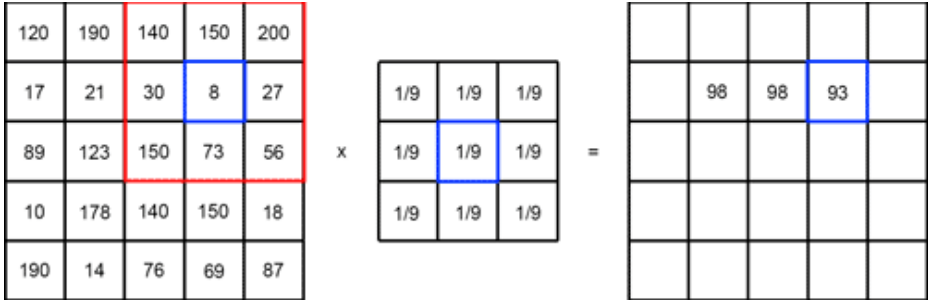


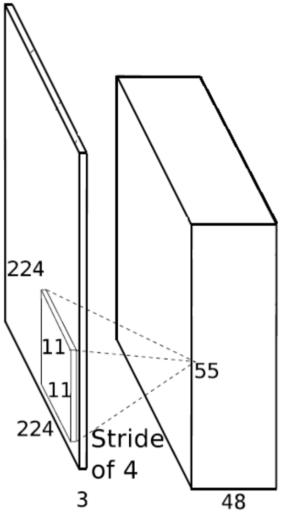
Convolutions





Convolutions





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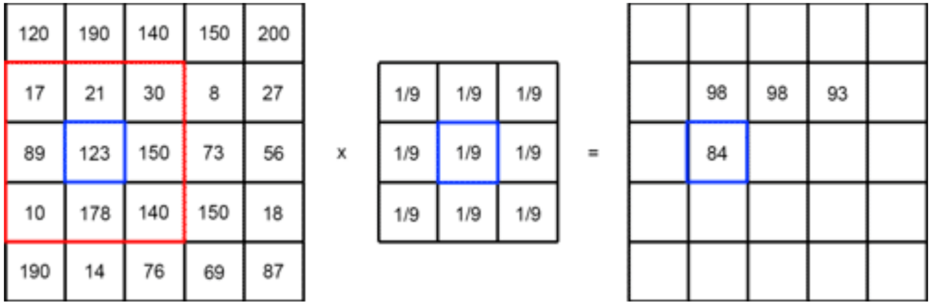

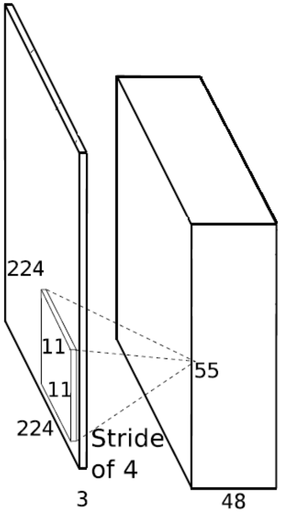

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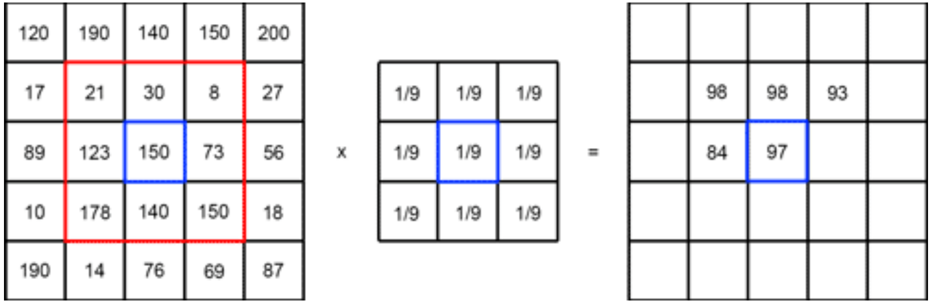

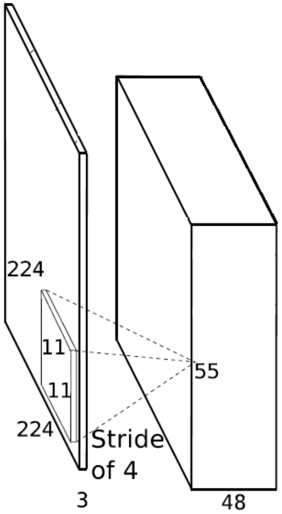

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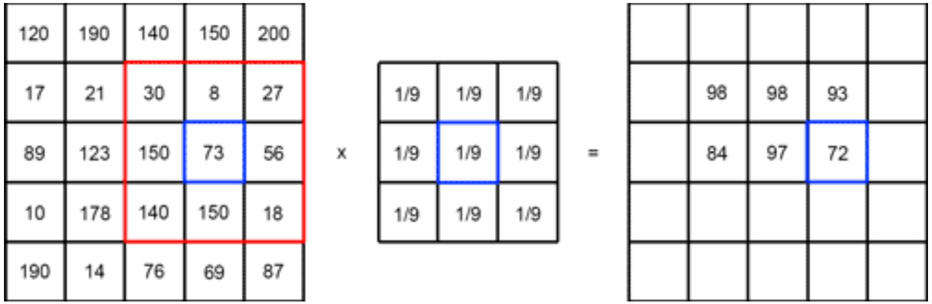

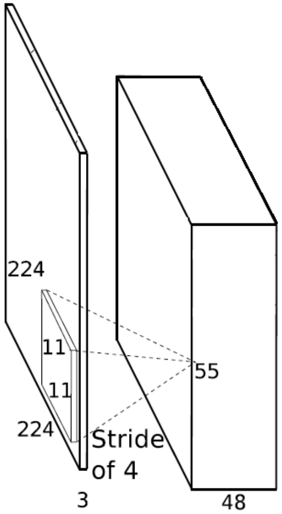

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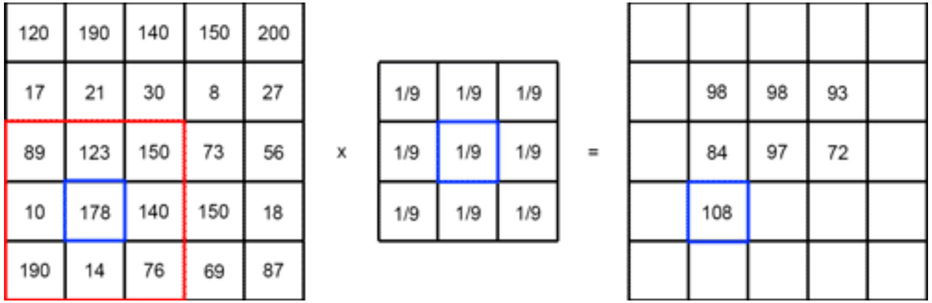
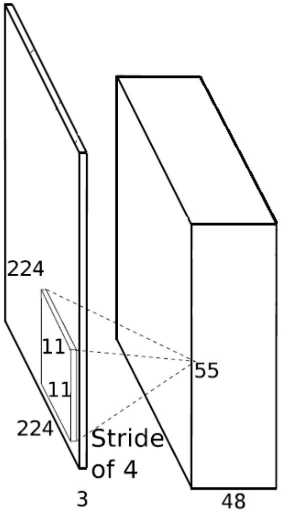




Convolutions

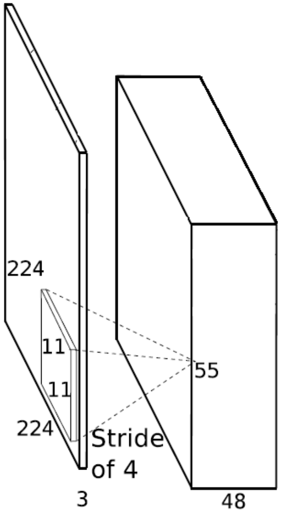
120	190	140	150	200
17	21	30	8	27
89	123	150	73	56
10	178	140	150	18
190	14	76	69	87

x

1/9	1/9	1/9
1/9	1/9	1/9
1/9	1/9	1/9

=

	98	98	93	
	84	97	72	
	108	108		



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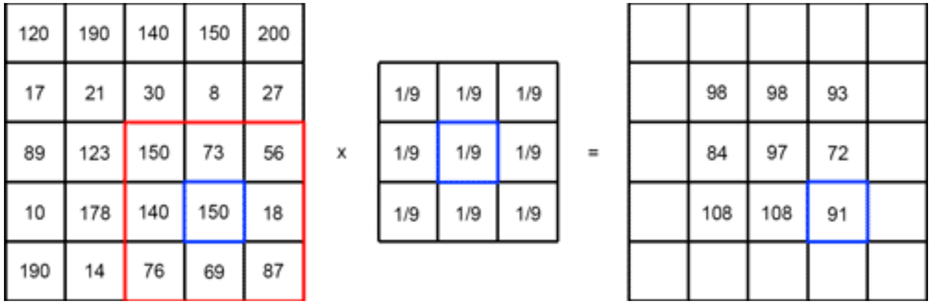

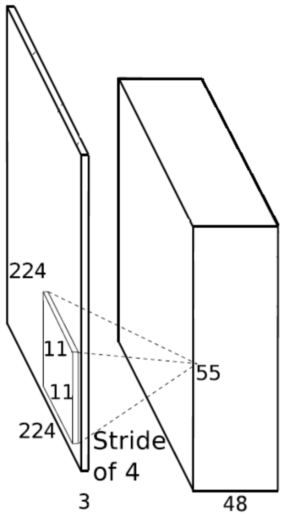

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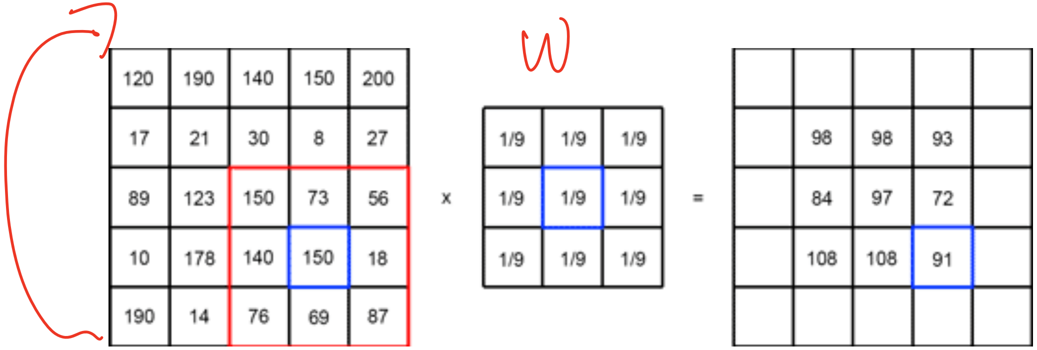
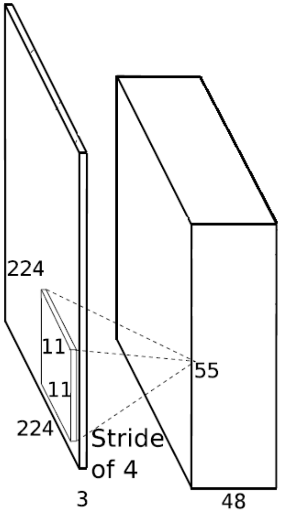




Trainable parameters w:

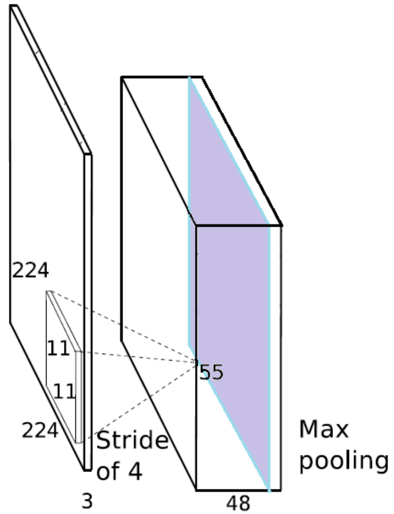
- Filters (width, height, depth, number)
- Bias

Maximum-/Average- pooling

Maximum or average over a spatial region

Trainable parameters w:

- None



Soft-max layer

$$\frac{\exp z_i}{\sum_j \exp z_j}$$

Trainable parameters $\boldsymbol{w}$:

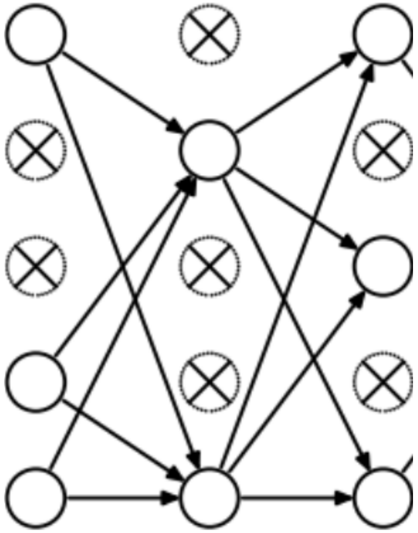
- None

Dropout layer

Randomly set activations to zero

Trainable parameters w:

- None



Multiclass output.

Modern networks often end with **softmax** nonlinearity:

$$\sum_{i=1}^{k} \frac{\exp(\boldsymbol{z}_i)\mathbf{e}_i}{\sum_{j=1}^{k}\exp(\boldsymbol{z}_j)}$$

(where $\mathbf{e}_i$ is i^{th} standard basis vector.)
Output is now a probability vector!

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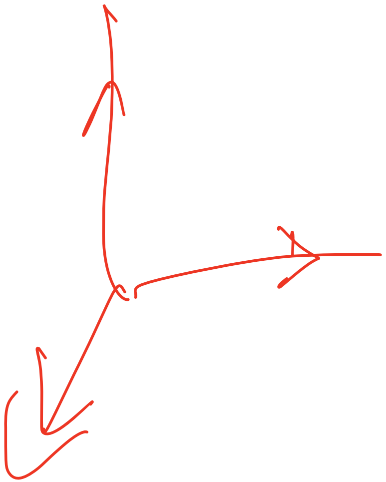
(where $\mathbf{e}_i$ is i^{th} standard basis vector.)
Output is now a probability vector!

Alternate notation: output vector $\boldsymbol{v}_i \propto \exp(\boldsymbol{z}_i)$.

Cross-entropy loss.

Given *one hot* $\boldsymbol{y} \in \{\mathbf{e}_1, \ldots, \mathbf{e}_k\}$ and probability vector $\hat{\boldsymbol{y}} \in \mathbb{R}^k$,

$$\ell(y, \hat{y}) = -\sum_{i=1}^{k} \boldsymbol{y}_i \ln(\hat{\boldsymbol{y}}_i).$$



$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} \quad \cdots \quad \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

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Combined with softmax $\hat{\boldsymbol{y}} \propto \exp(\boldsymbol{z})$:

$$-\sum_{i=1}^{k} \boldsymbol{y}_i \ln\left(\frac{\exp(\boldsymbol{z}_i)}{\sum_j \exp(\boldsymbol{z}_j)}\right) = -\sum_{i=1}^{k} \boldsymbol{y}_i \boldsymbol{z}_i + \ln\left(\sum_{i=1}^{k} \exp(\boldsymbol{z}_i)\right).$$

Note: For numerical stability, use $\ln \sum_i \exp v_i = c + \ln \sum_i \exp(v_i - c)$.

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Equivalent to multinomial logistic loss.

Regularization.

- "Weight decay": $+\lambda\|\boldsymbol{w}\|^2$ in objective (where $\boldsymbol{w}$ are all parameters).
- Dropout: randomly nullify node outputs in training.
- Batch normalization: "standardize" node output distribution.

Optimization.

Regularized learning now takes the form

$$\min_{\boldsymbol{W}^{[1]},\ldots,\boldsymbol{W}^{[L]},\boldsymbol{b}^{[1]},\ldots,\boldsymbol{b}^{[L]}} \frac{1}{n}\sum_{i=1}^{n} \ell\left(y^{(i)}, \boldsymbol{W}^{[L]}\sigma_{L-1}\left(\cdots\sigma_1\left(\boldsymbol{W}^{[1]}\boldsymbol{x}^{(i)}+\boldsymbol{b}^{[1]}\right)\cdots\right)\right) + \lambda\sum_{l=1}^{L}\|\boldsymbol{W}^{[l]}\|_2^2$$

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Implications:

- Gradient-based optimization approaches is no longer guaranteed to find the global optimum
- Initialization of parameters matters

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In general, resulting optimization is "harder" than linear regression

Implications:

- Gradient-based optimization approaches is no longer guaranteed to find the global optimum
- Initialization of parameters matters
- Stochastic gradient descent works well in practice

Quiz:

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- How can you interpret deep nets as learning feature transformations?
- How can you interpret deep nets as function graphs?
- What are some standard components of deep nets?
- What algorithm can be used to train deep nets?

Important topics of this lecture

- Deep nets as functions and graphs
- Components of deep nets

Up next:

- Backpropagation