

Machine Learning: Lecture 2

Jennifer Ngadiuba (Fermilab)
University of Pavia, May 8-12 2023

Overview of the lectures

- **Day 1:**

- Introduction to Machine Learning fundamentals
- Linear Models

- **Day 2:**

- Neural Networks
- Deep Neural Networks
- Convolutional Neural Networks

- **Day 3:**

- Recurrent Neural Networks
- Graph Neural Networks (part 1)

- **Day 4:**

- Graph Neural Networks (part 2)
- Transformers

- **Day 5:**

- Unsupervised learning
- Autoencoders
- Generative Adversarial Networks
- Normalizing Flows

Hands on sessions each day will closely follow the lectures topics

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- Intro to neural networks
- Training
- Activation functions
- Deep Neural Networks
- Convolutional Neural Networks
- Batch Normalization
- Summary

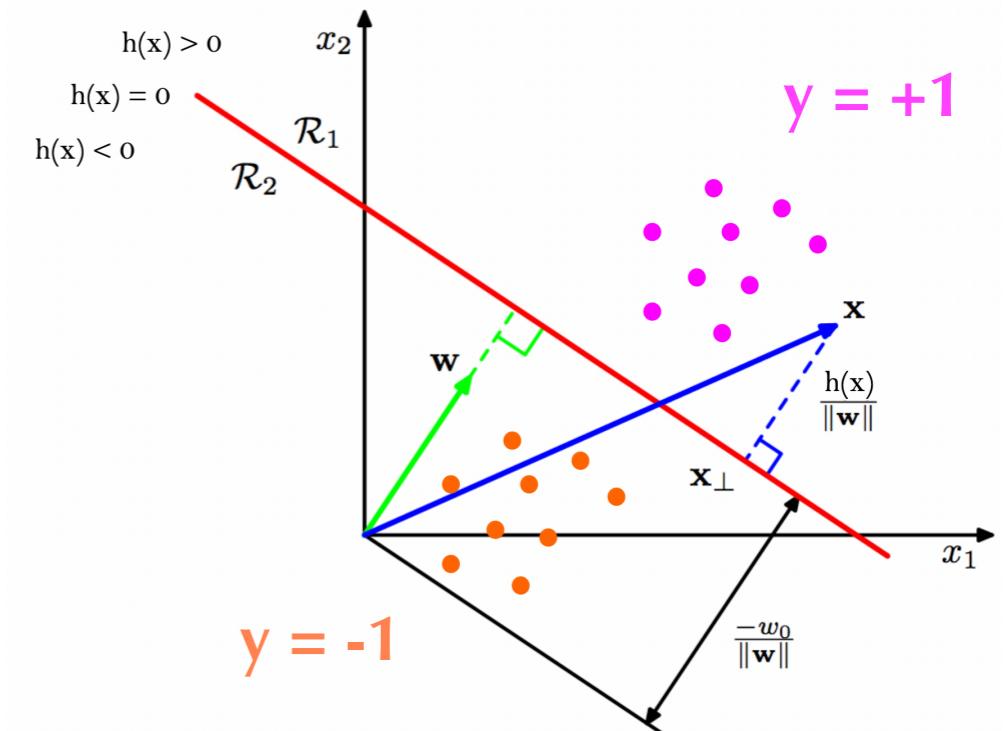
Intro to neural networks

Recap: logistic regression

- Task: learn a function to **separate different classes of data** — for two classes we call this “binary classification”:

- $\mathbf{x}_i \in \mathbb{R}^m$
- $y_i \in \{-1, 1\}$ — we call these “true labels”

- **Linear decision boundary:** $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T \mathbf{x}$



Recap: logistic regression

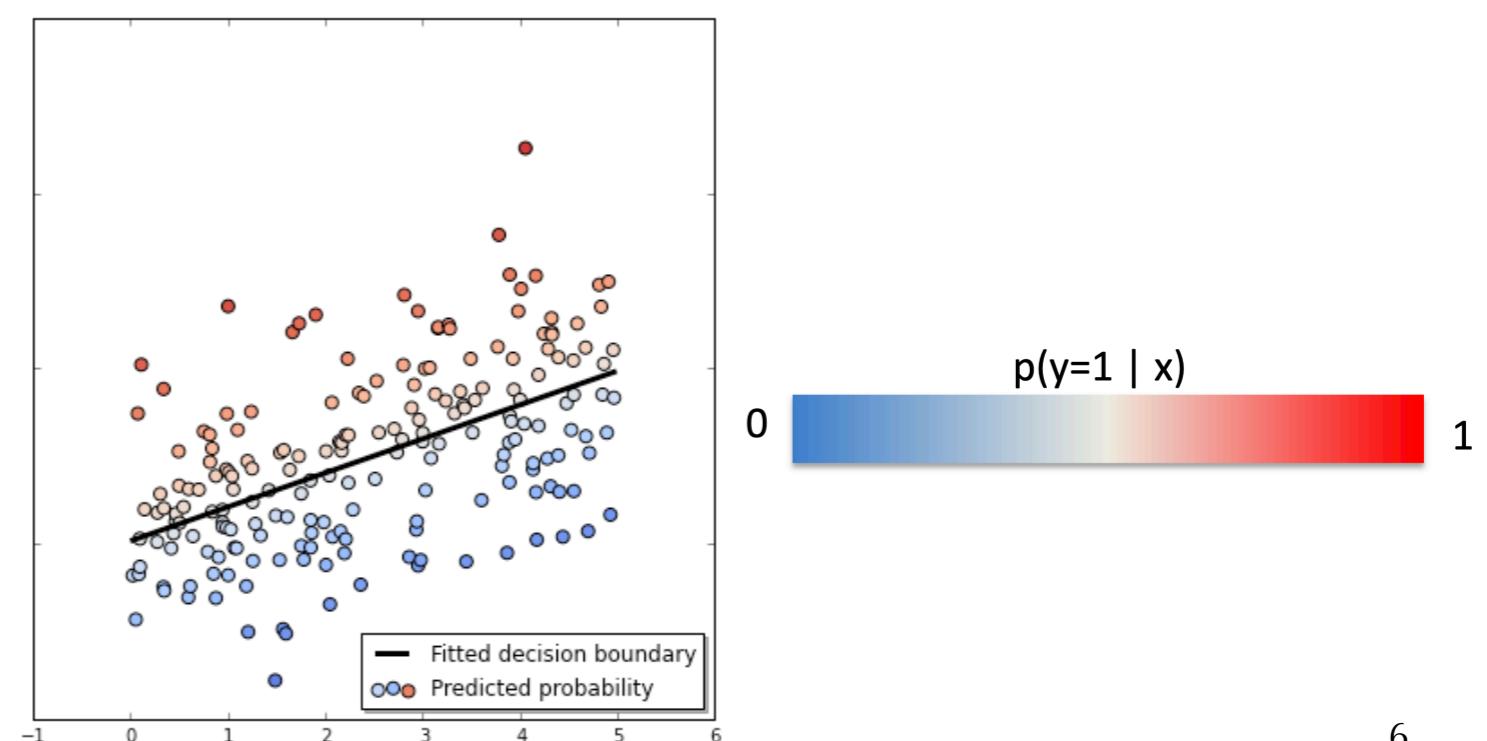
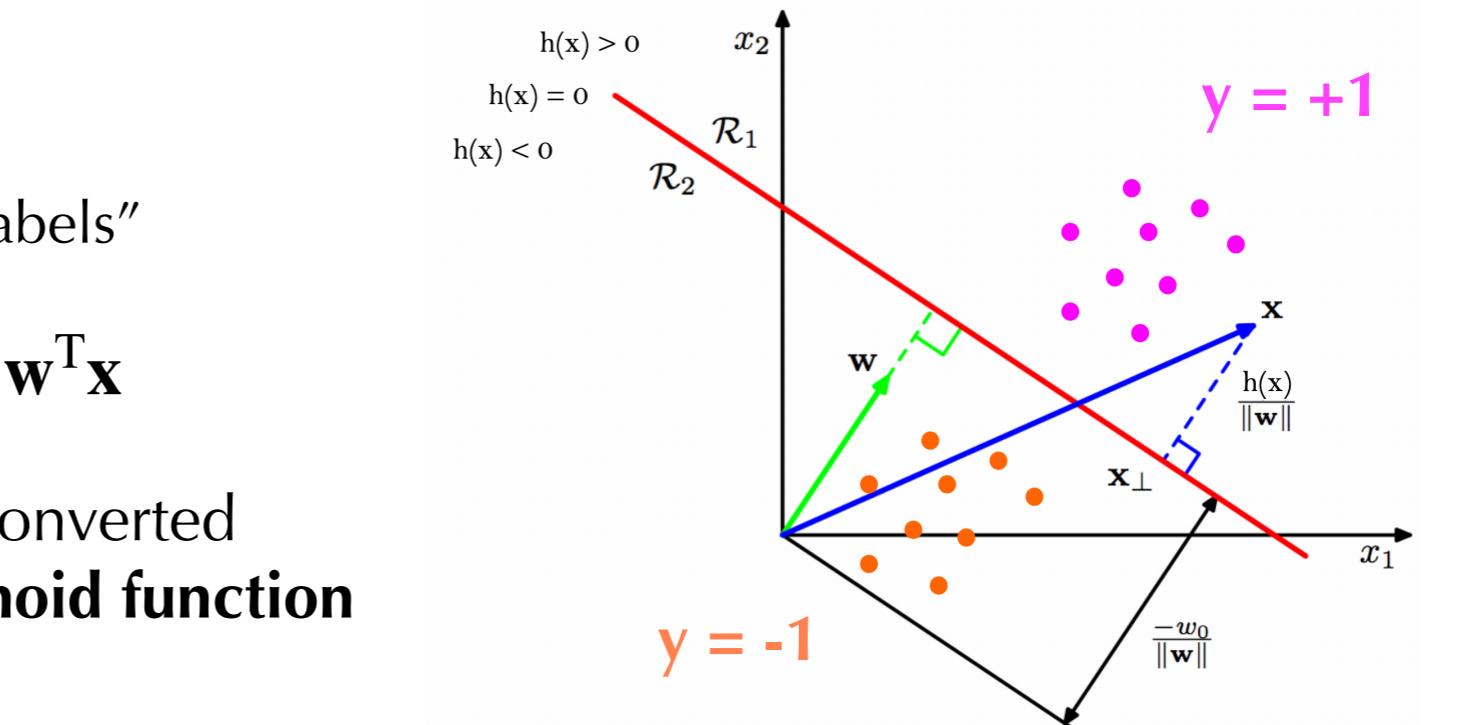
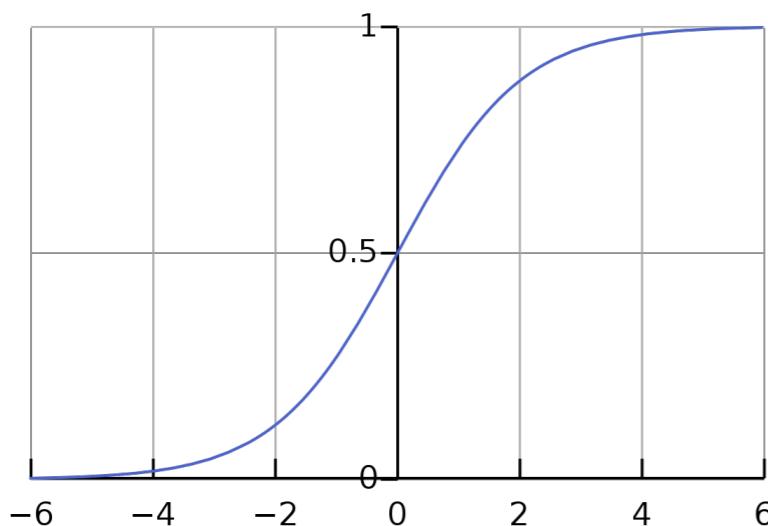
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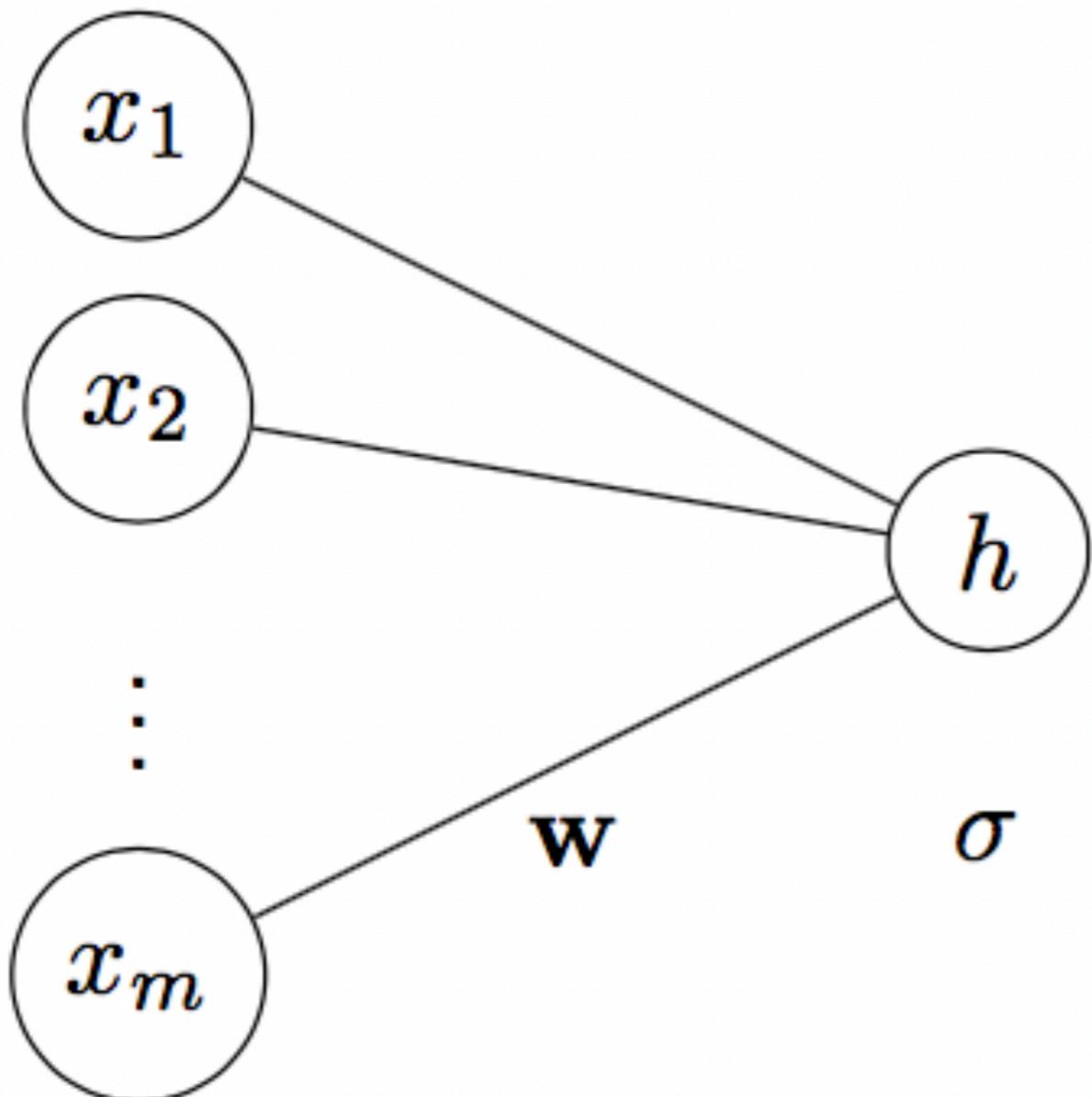
- **Linear decision boundary:** $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T \mathbf{x}$

- Distance from decision boundary is converted to class probability using **logistic sigmoid function**

$$p(y=1 | \mathbf{x}) \equiv p_i = \frac{1}{1 + e^{-h(\mathbf{x}; \mathbf{w})}} = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$



Recap: logistic regression



Represent logistic regression as a graph:
this unit is the main building block of a Neural Network!

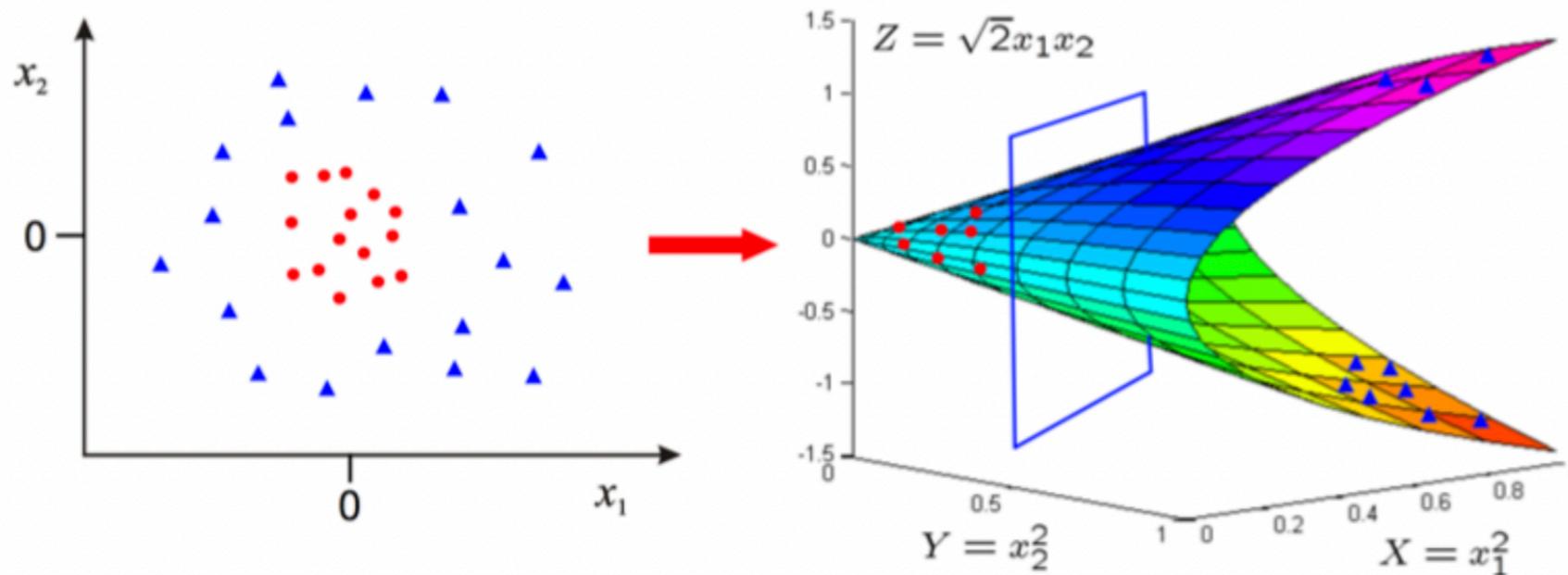
$$p(y = 1 | \mathbf{x}) = \sigma(h(\mathbf{x}, \mathbf{w})) = \frac{1}{1 + e^{-h(\mathbf{x}; \mathbf{w})}} = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

Adding non-linearity

- What if we want a non-linear decision boundary?

- chose basis, e.g.: $\phi(x) \sim \{x^2, \sin(x), \log(x), \dots\}$

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \quad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$



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- Learn the basis functions directly from data

$$\phi(\mathbf{x}; \mathbf{u}) : \mathbb{R}^m \longrightarrow \mathbb{R}^d$$

- where \mathbf{u} is a set of parameters for the transformation

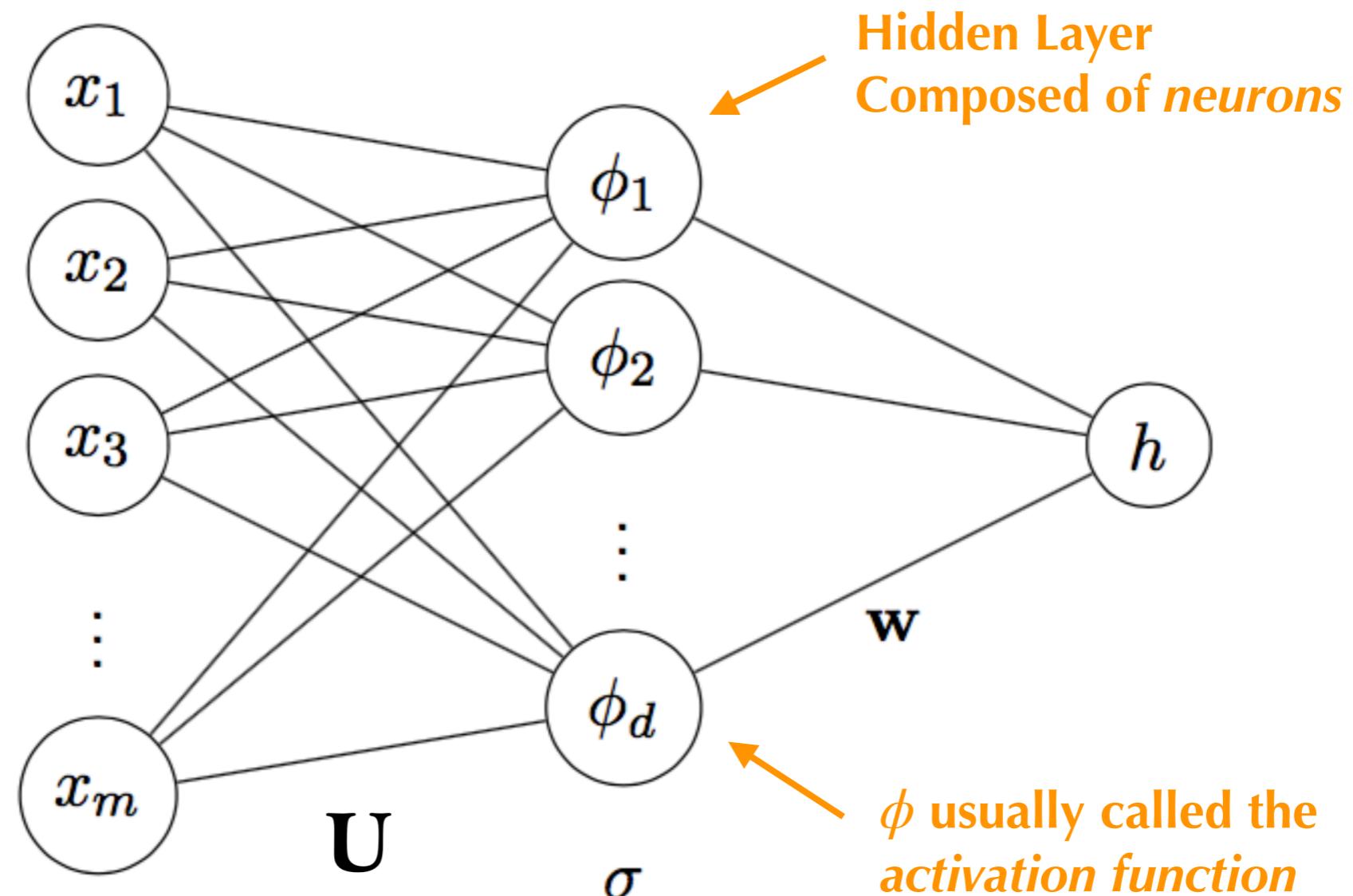
Neural Networks

- Define the basis functions $j = \{1, \dots, d\}$: $\phi_j(\mathbf{x}; \mathbf{u}) = \sigma(\mathbf{u}_j^T \mathbf{x})$
- Put all $\mathbf{u}_j \in \mathbb{R}^m$ vectors into matrix \mathbf{U}

$$\phi(\mathbf{x}; \mathbf{U}) = \sigma(\mathbf{U}\mathbf{x}) = \begin{bmatrix} \sigma(\mathbf{u}_1^T \mathbf{x}) \\ \sigma(\mathbf{u}_2^T \mathbf{x}) \\ \vdots \\ \sigma(\mathbf{u}_d^T \mathbf{x}) \end{bmatrix} \in \mathbb{R}^d$$

- σ is a pointwise sigmoid acting on each vector element
- Full model becomes $h(\mathbf{x}; \mathbf{w}, \mathbf{U}) = \mathbf{w}^T \phi(\mathbf{x}; \mathbf{U})$

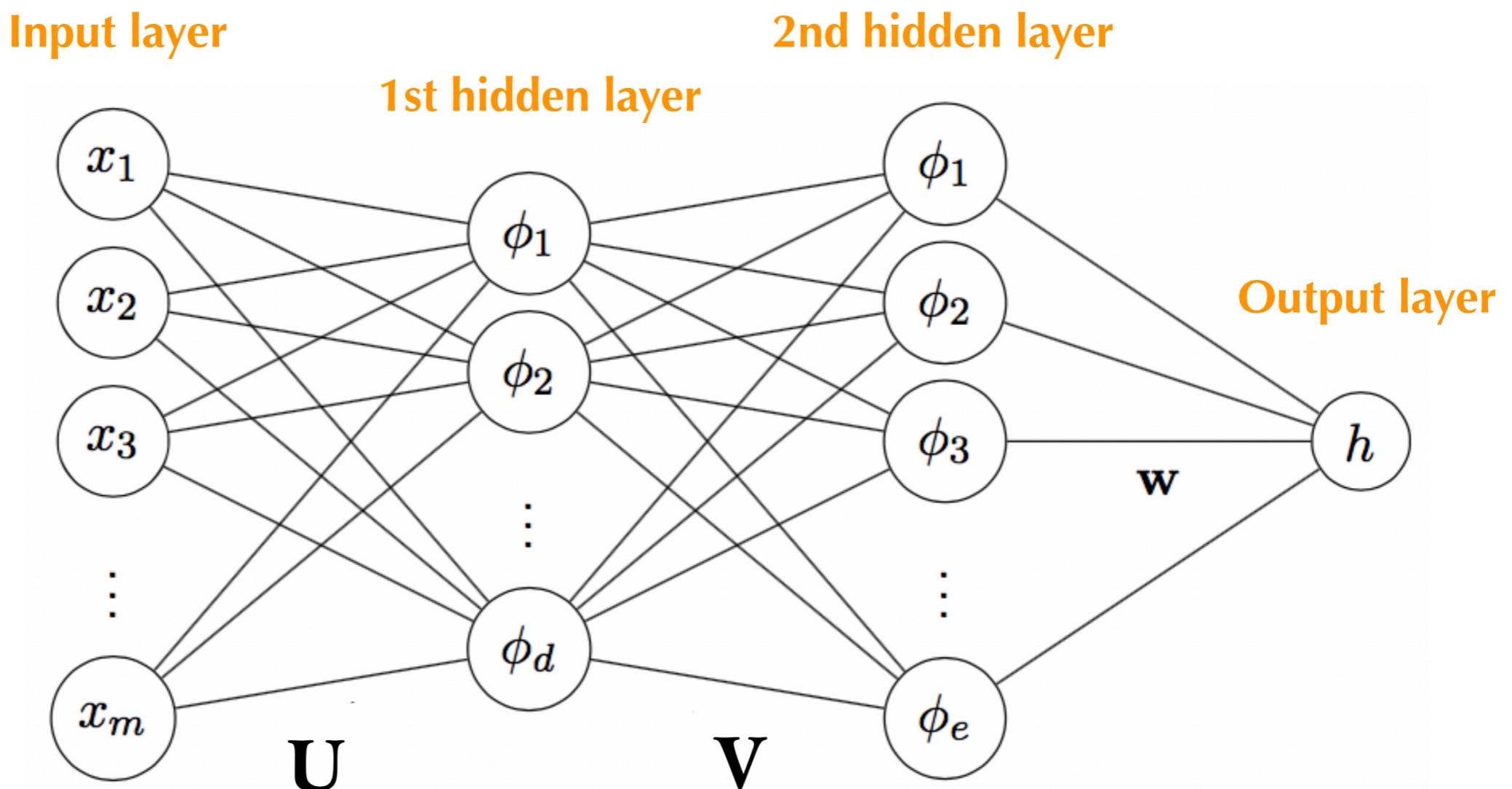
Neural Networks



$$\phi(\mathbf{x}) = \sigma(\mathbf{U}\mathbf{x})$$

$$h(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$$

Multi-layer Neural Networks



Each layer adapts basis based on previous layer

These types of networks are called **Multi Layer Perceptrons (MLP)**

Universal approximation theorem

- Feed-forward neural network with a single hidden layer containing a finite number of neurons can approximate continuous functions arbitrarily well on a space \mathbb{R}^n
 - only mild assumptions on non-linear activation function needed. Sigmoid functions work, as do others.
- But no other information are added on how many neurons needed, or how much data!
- How to find the parameters, given a dataset, to perform this approximation?

Training

Neural Networks optimization

- Neural Network model:
$$h(\mathbf{x}; \mathbf{w}, \mathbf{U}) = \mathbf{w}^T \sigma(\mathbf{U}\mathbf{x})$$

- **Classification:** cross-entropy loss function

$$\mathcal{L}(\mathbf{w}, \mathbf{U}) = - \sum_i y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i)$$

$$p_i = p(y_i = 1 | \mathbf{x}_i) = \sigma(h(\mathbf{x}_i))$$

- **Regression:** mean squared error loss function

$$\mathcal{L}(\mathbf{w}, \mathbf{U}) = \frac{1}{n} \sum_{i=1}^n (y_i - h(\mathbf{x}_i))^2$$

- **Minimize loss with respect to weights \mathbf{w}, \mathbf{U} with gradient descent**

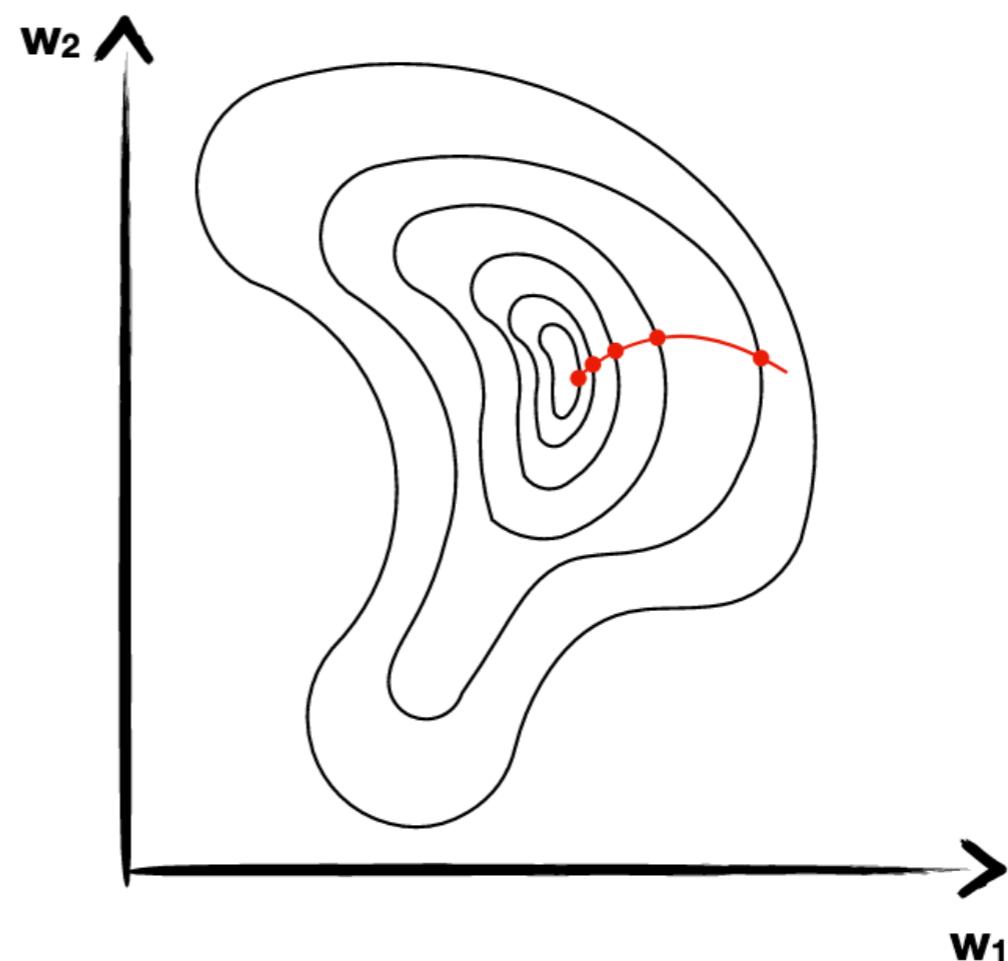
Gradient Descent

- Parameters update:

$$\mathbf{w}' \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \mathbf{U})$$

$$\mathbf{U}' \leftarrow \mathbf{U} - \eta \nabla_{\mathbf{U}} \mathcal{L}(\mathbf{w}, \mathbf{U})$$

- How to compute the gradients?



Chain rule

- The loss function: $\mathcal{L}(\mathbf{w}, \mathbf{U}) = - \sum_i y_i \ln(\sigma(h(\mathbf{x}_i))) + (1 - y_i) \ln(1 - \sigma(h(\mathbf{x}_i)))$
- Derivative of sigmoid: $\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1 - \sigma(x))$
- Apply chain rule to compute gradient w.r.t \mathbf{w}

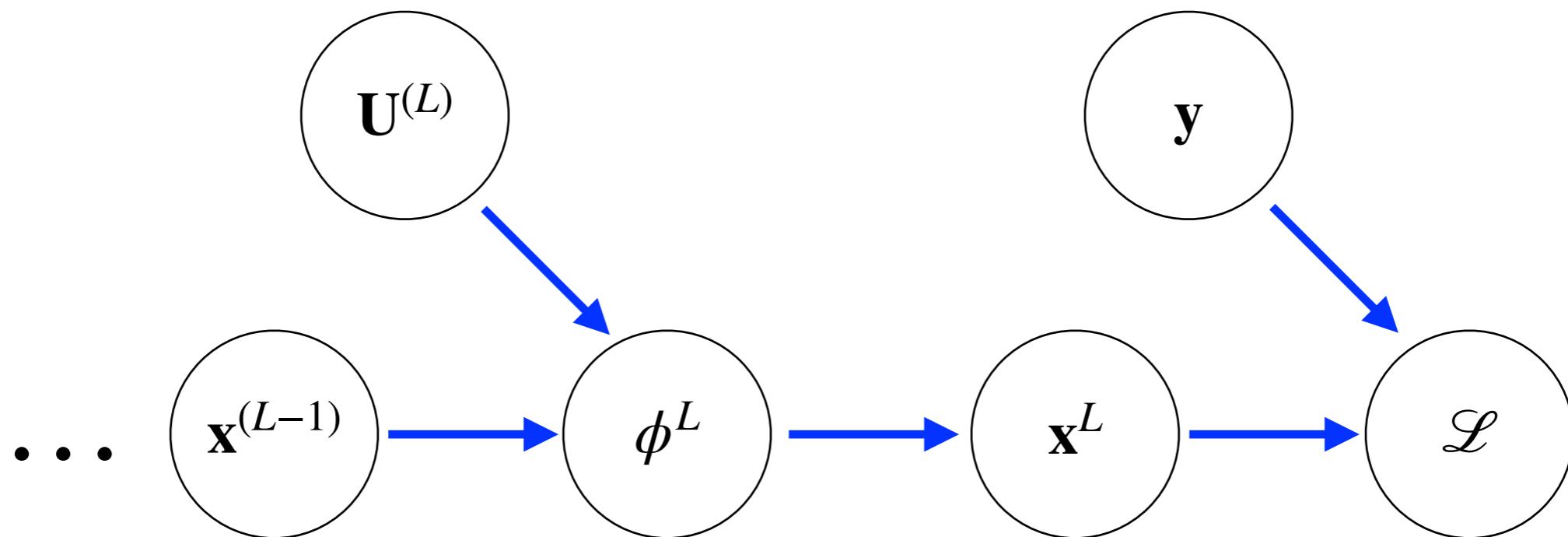
$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \frac{\partial \mathcal{L}}{\partial h} \frac{\partial h}{\partial \mathbf{w}} = \sum_i y_i(1 - \sigma(h(\mathbf{x}_i)))\sigma(\mathbf{U}\mathbf{x}_i) + (1 - y_i)\sigma(h(\mathbf{x}_i))\sigma(\mathbf{U}\mathbf{x}_i)$$

- Apply chain rule to compute gradient w.r.t. \mathbf{u}_j

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{u}_j} &= \frac{\partial \mathcal{L}}{\partial h} \frac{\partial h}{\partial \sigma} \frac{\partial \sigma}{\partial \mathbf{u}_j} = \sum_i y_i(1 - \sigma(h(\mathbf{x}_i)))w_j\sigma(\mathbf{u}_j\mathbf{x}_i)(1 - \sigma(\mathbf{u}_j\mathbf{x}_i))\mathbf{x}_i \\ &\quad + (1 - y_i)\sigma(h(\mathbf{x}_i))w_j\sigma(\mathbf{u}_j\mathbf{x}_i)((1 - \sigma(\mathbf{u}_j\mathbf{x}_i))\mathbf{x}_i) \end{aligned}$$

Backpropagation

- Loss function composed of L layers of non linearity $\mathcal{L}(\phi^{(L)}(\dots\phi^{(1)}(\mathbf{x})))$
- **Forward step (forward propagation)**
 - compute and save intermediate computations $\phi^{(1)}(\mathbf{x}), \dots, \phi^{(L)}(\mathbf{x})$

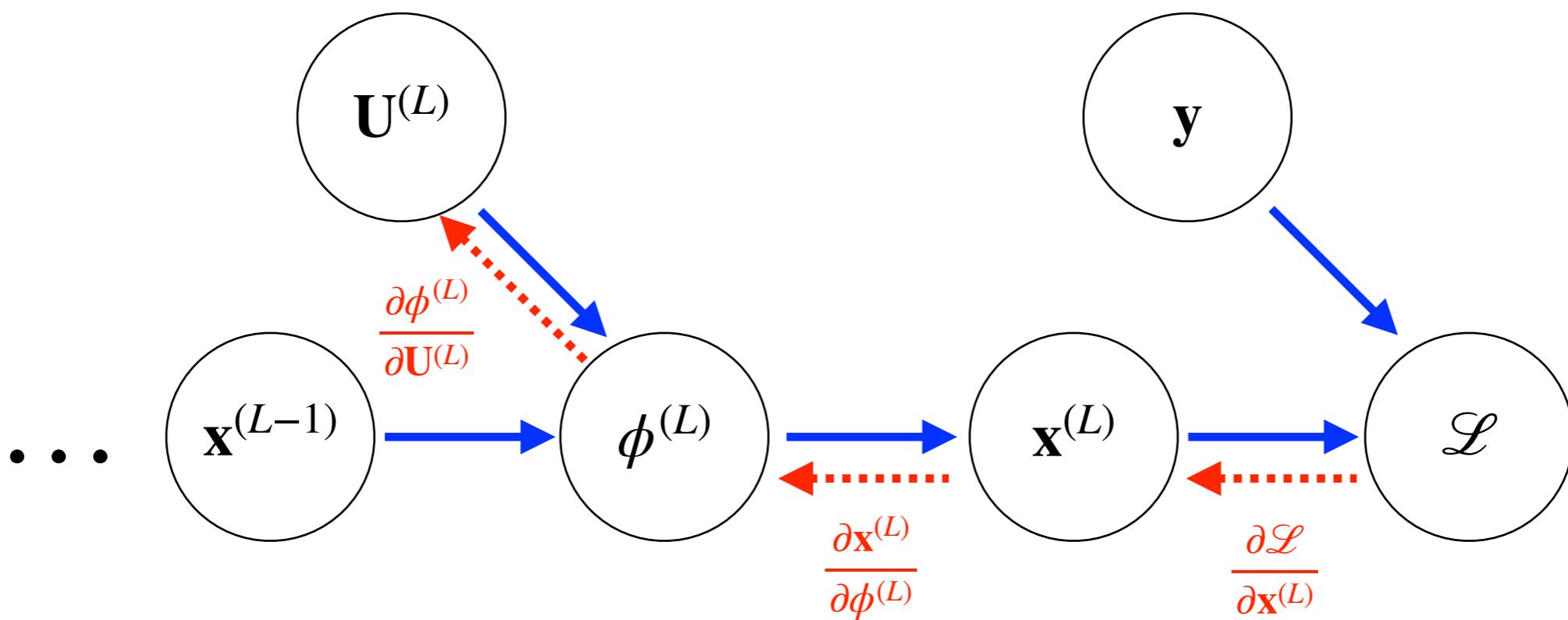


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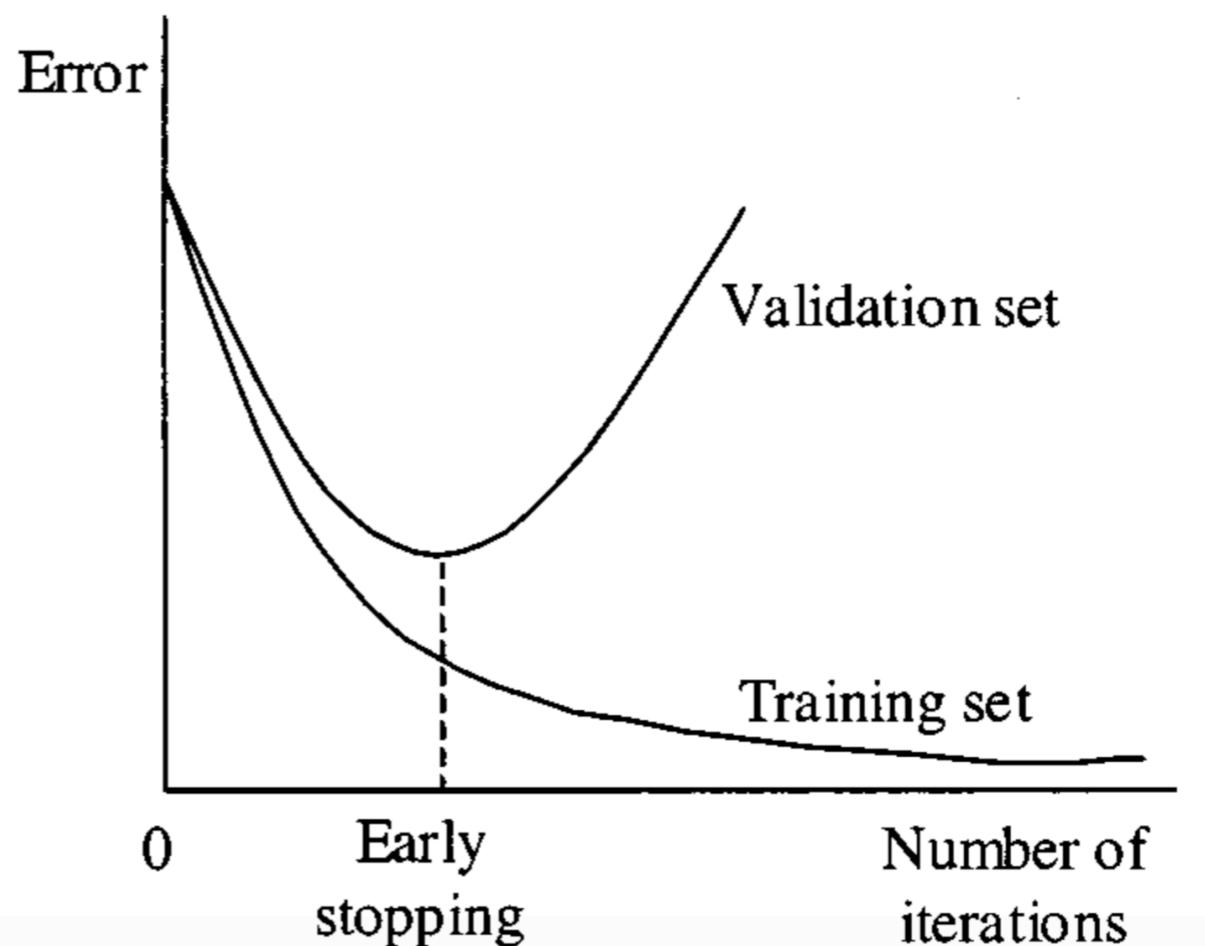
- compute and save intermediate computations $\phi^{(1)}(\mathbf{x}), \dots, \phi^{(L)}(\mathbf{x})$

- **Backward step (backpropagation) \rightarrow**
$$\frac{\partial \mathcal{L}}{\partial \mathbf{U}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \phi^{(L)}} \frac{\partial \phi^{(L)}}{\partial \mathbf{U}^{(L)}}$$



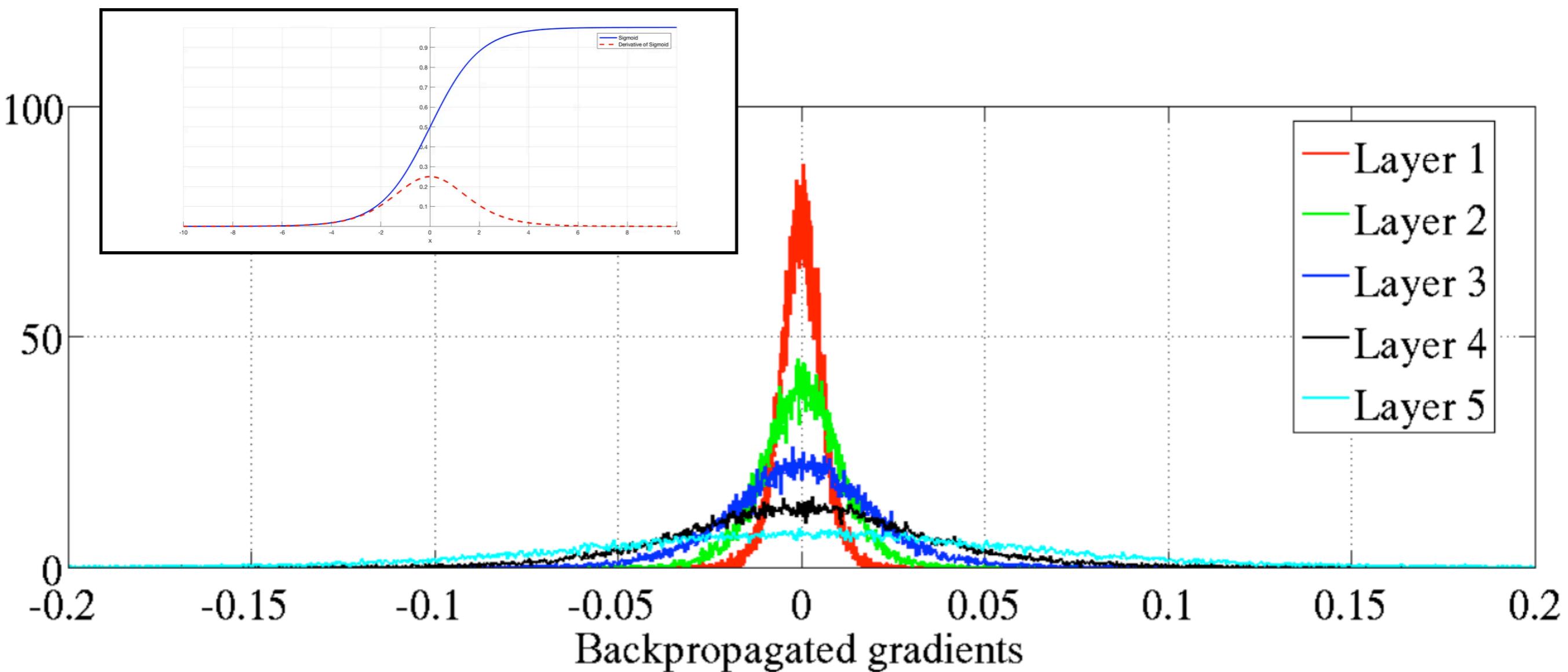
Training

- The gradient is typically computed through [Automatic Differentiation](#) (fast and exact)
- Repeat gradient update of weights to reduce loss
 - each iteration through the full dataset (in mini batches) is called an epoch
- Use validation set to examine for overtraining, and determine when to stop training



Vanishing gradient

- As more layers using certain activation functions are added to neural networks, the gradients of the loss function might approach zero, making the network hard to train
 - small gradients slow down, and eventually block, stochastic gradient descent
 - this results in a limited capacity of learning

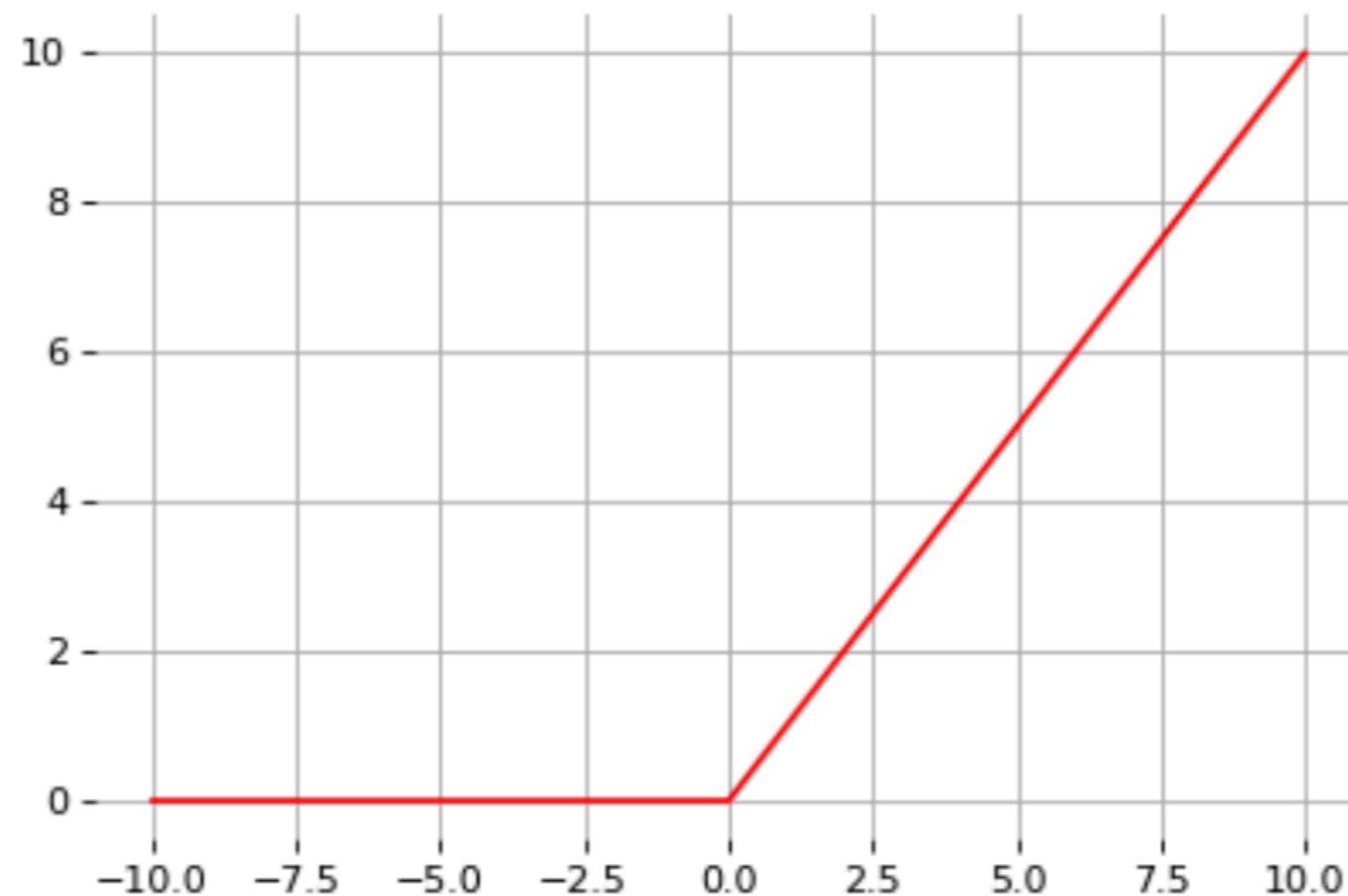


Activation functions

Activation functions

- Instead of the sigmoid (activation) function , modern NN are for most based on **rectified linear units (ReLU)**

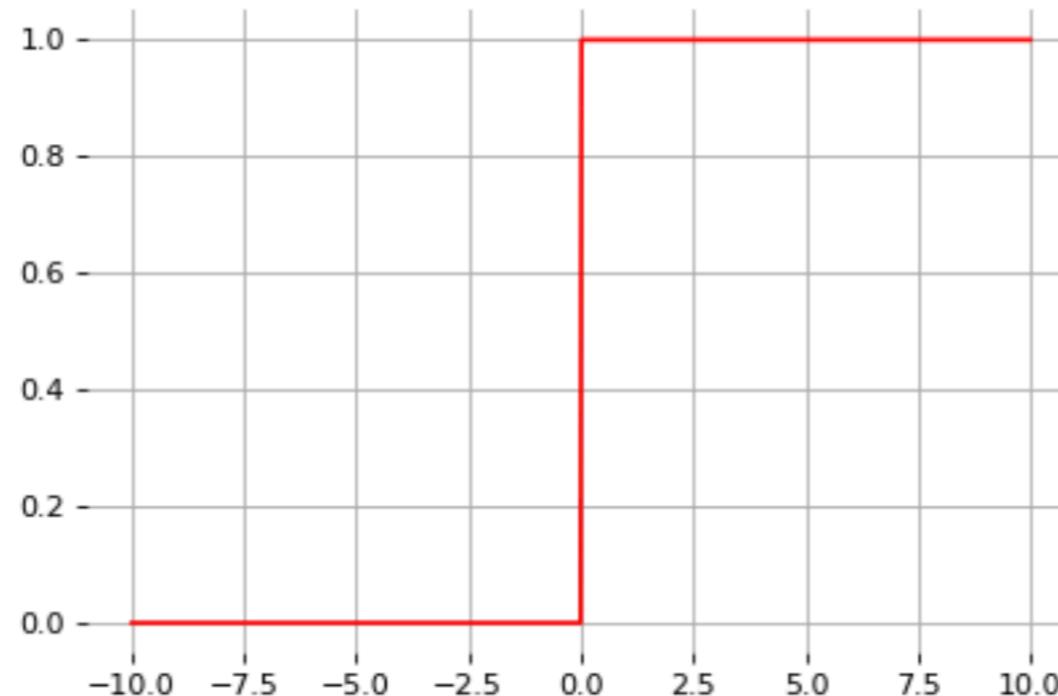
$$\text{ReLU}(x) = \max(0, x)$$



Activation functions

- Note that the derivative of the ReLU function is

$$\frac{\partial}{\partial x} \text{ReLU}(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ 1 & \text{otherwise} \end{cases}$$



- For $\mathbf{x} = \mathbf{0}$ the derivative is undefined. In practice, it is set to zero.

Activation functions

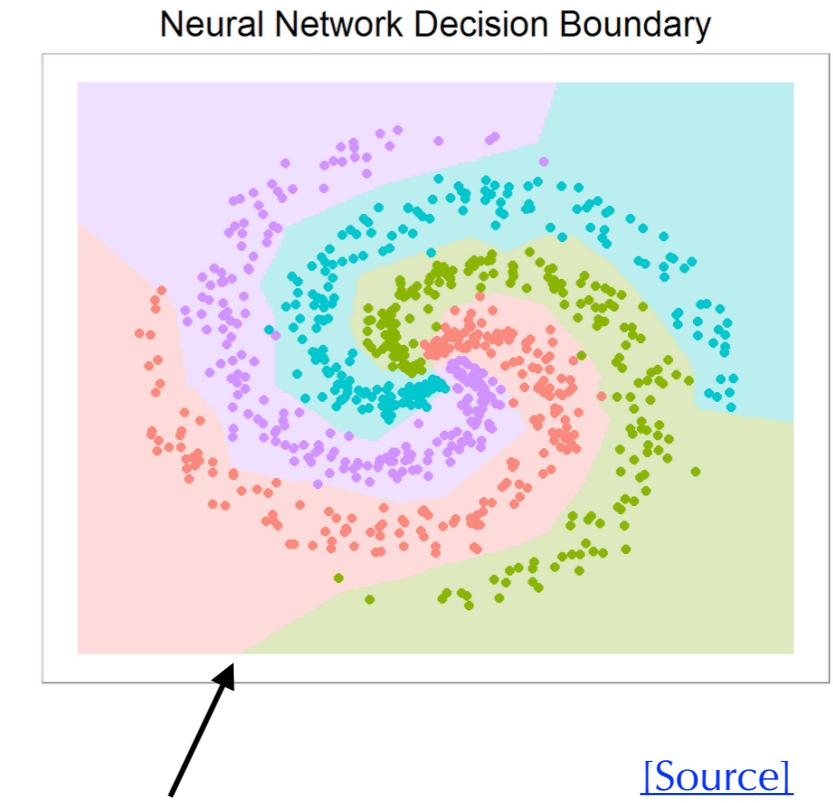
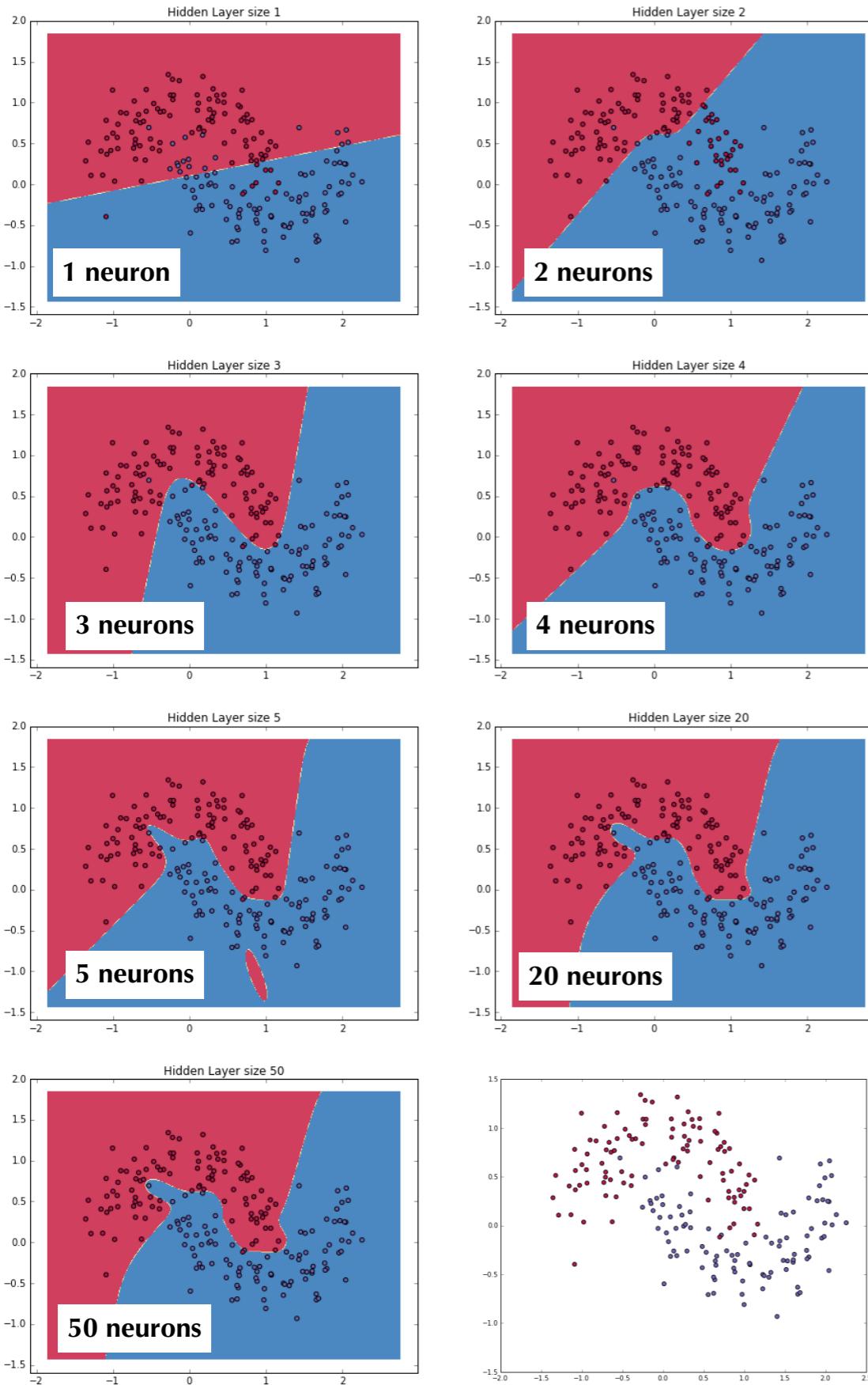
- With ReLU you end up with products of ones or zeros rather than products of very small numbers when doing backpropagation
 - the ReLU unit dies when its input is negative
 - this is actually a useful property to induce *sparsity*
- Drawback: a “dead” neuron is unlikely to recover and if there are too many of these you may end up with a large part of the NN doing nothing
 - in practice this happens if the learning rate is off or if there is a large negative bias
- Several ways to mitigate this, e.g. LeakyReLU



Activation functions

Name	Plot	Function, $g(x)$	Derivative of g , $g'(x)$	Range	Order of continuity
Identity		x	1	$(-\infty, \infty)$	C^∞
Binary step		$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	0	{0, 1}	C^{-1}
Logistic, sigmoid, or soft step		$\sigma(x) \doteq \frac{1}{1 + e^{-x}}$	$g(x)(1 - g(x))$	$(0, 1)$	C^∞
Hyperbolic tangent (tanh)		$\tanh(x) \doteq \frac{e^x - e^{-x}}{e^x + e^{-x}}$	$1 - g(x)^2$	$(-1, 1)$	C^∞
Rectified linear unit (ReLU) ^[8]		$(x)^+ \doteq \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases} = \max(0, x) = x\mathbf{1}_{x>0}$	$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$[0, \infty)$	C^0
Gaussian Error Linear Unit (GELU) ^[5]		$\frac{1}{2}x \left(1 + \text{erf}\left(\frac{x}{\sqrt{2}}\right)\right) = x\Phi(x)$	$\Phi(x) + x\phi(x)$	$(-0.17\dots, \infty)$	C^∞
Softplus ^[9]		$\ln(1 + e^x)$	$\frac{1}{1 + e^{-x}}$	$(0, \infty)$	C^∞
Exponential linear unit (ELU) ^[10]		$\begin{cases} \alpha(e^x - 1) & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$ with parameter α	$\begin{cases} \alpha e^x & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ 1 & \text{if } x = 0 \text{ and } \alpha = 1 \end{cases}$	$(-\alpha, \infty)$	$\begin{cases} C^1 & \text{if } \alpha = 1 \\ C^0 & \text{otherwise} \end{cases}$
Scaled exponential linear unit (SELU) ^[11]		$\lambda \begin{cases} \alpha(e^x - 1) & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$ with parameters $\lambda = 1.0507$ and $\alpha = 1.67326$	$\lambda \begin{cases} \alpha e^x & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	$(-\lambda\alpha, \infty)$	C^0
Leaky rectified linear unit (Leaky ReLU) ^[12]		$\begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$	$\begin{cases} 0.01 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$(-\infty, \infty)$	C^0
Parametric rectified linear unit (PReLU) ^[13]		$\begin{cases} \alpha x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$ with parameter α	$\begin{cases} \alpha & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	$(-\infty, \infty)$	C^0
Sigmoid linear unit (SiLU, ^[5] Sigmoid shrinkage, ^[14] SiL, ^[15] or Swish-1 ^[16])		$\frac{x}{1 + e^{-x}}$	$\frac{1 + e^{-x} + xe^{-x}}{(1 + e^{-x})^2}$	$[-0.278\dots, \infty)$	C^∞
Gaussian		e^{-x^2}	$-2xe^{-x^2}$	$(0, 1]$	C^∞

Non-linear decision boundaries



[\[Source\]](#)

4-class classification
2-hidden layer NN
ReLU activations
L2 regularization

Binary classification
1-hidden layer NN
Varying number of nodes
L2 regularization

[\[Source\]](#)

Universal approximation theorem

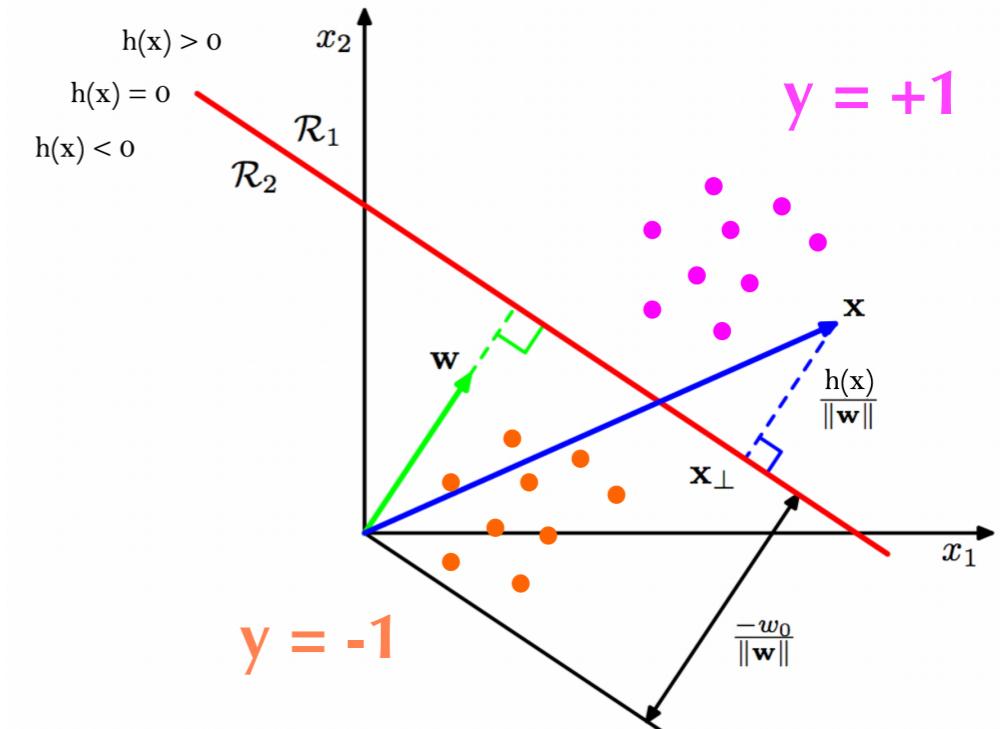
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- How to find the parameters, given a dataset, to perform this approximation?

Recap: logistic regression

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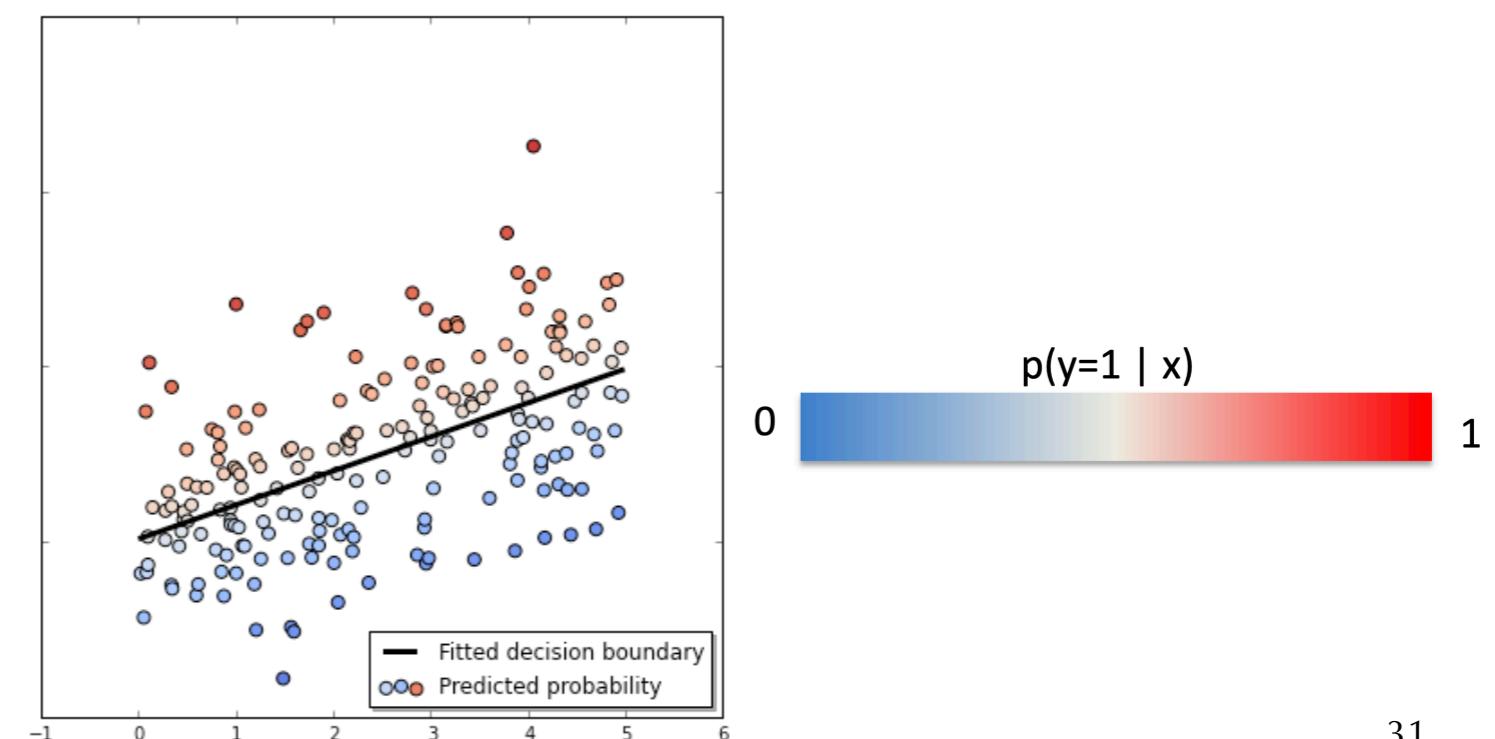
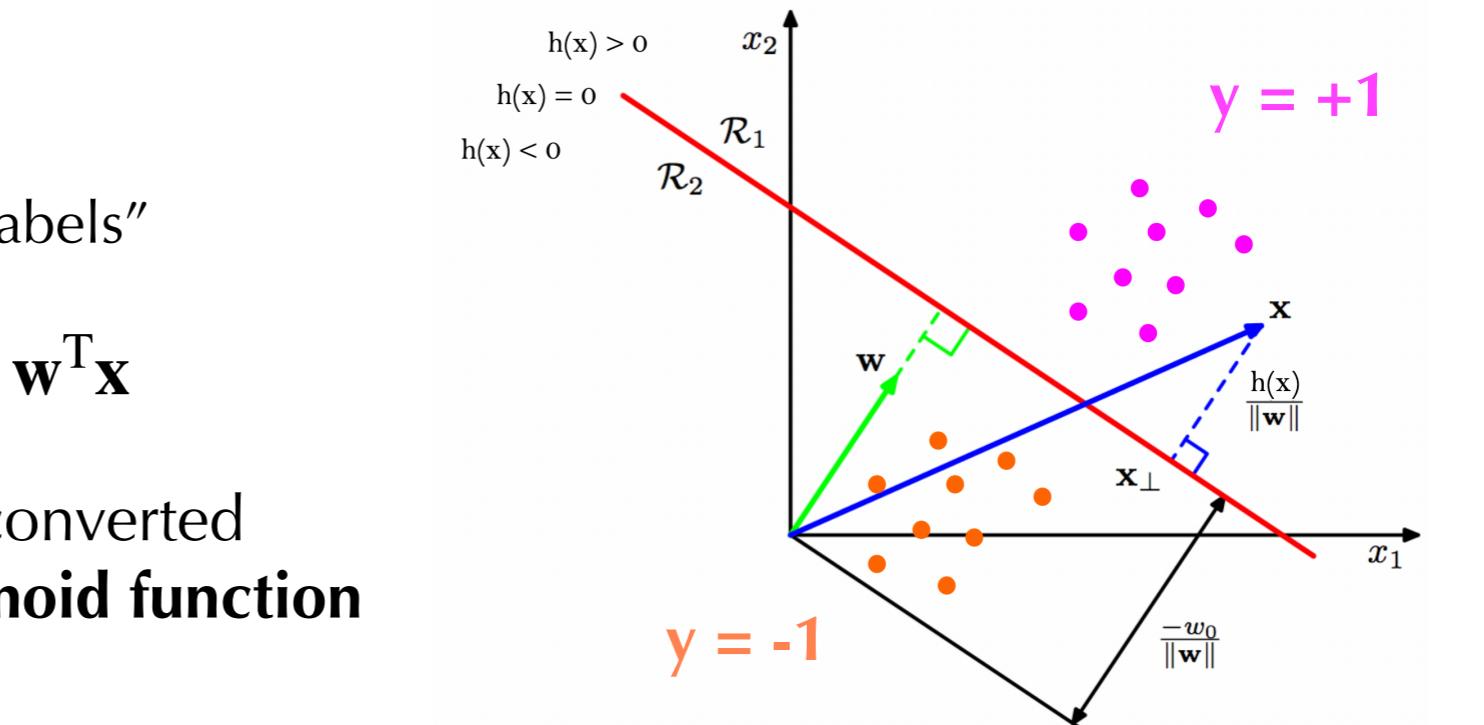
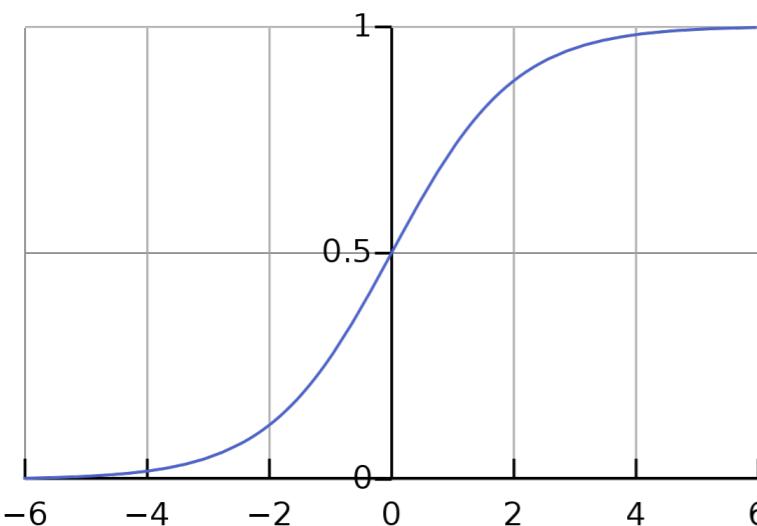
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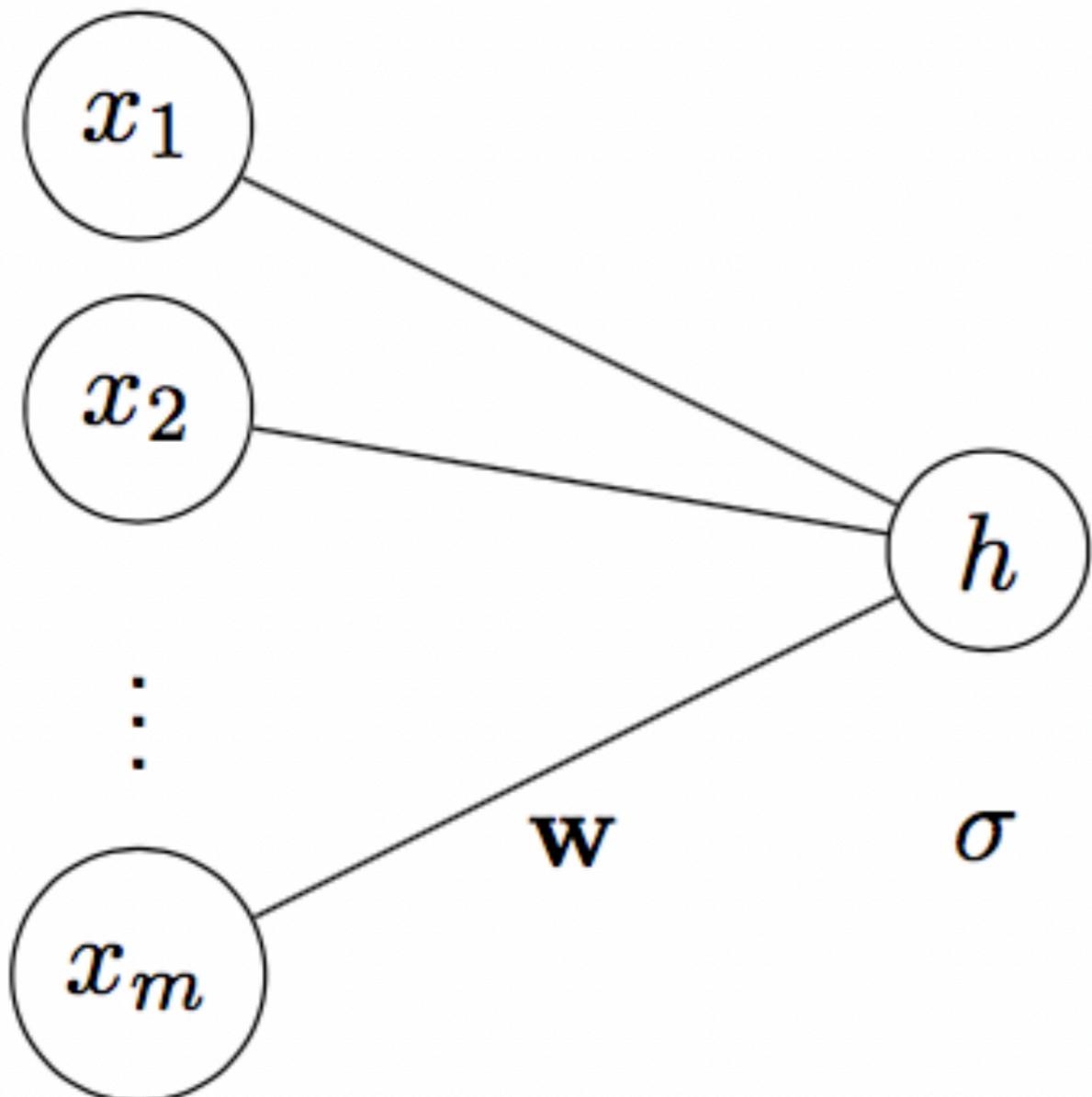
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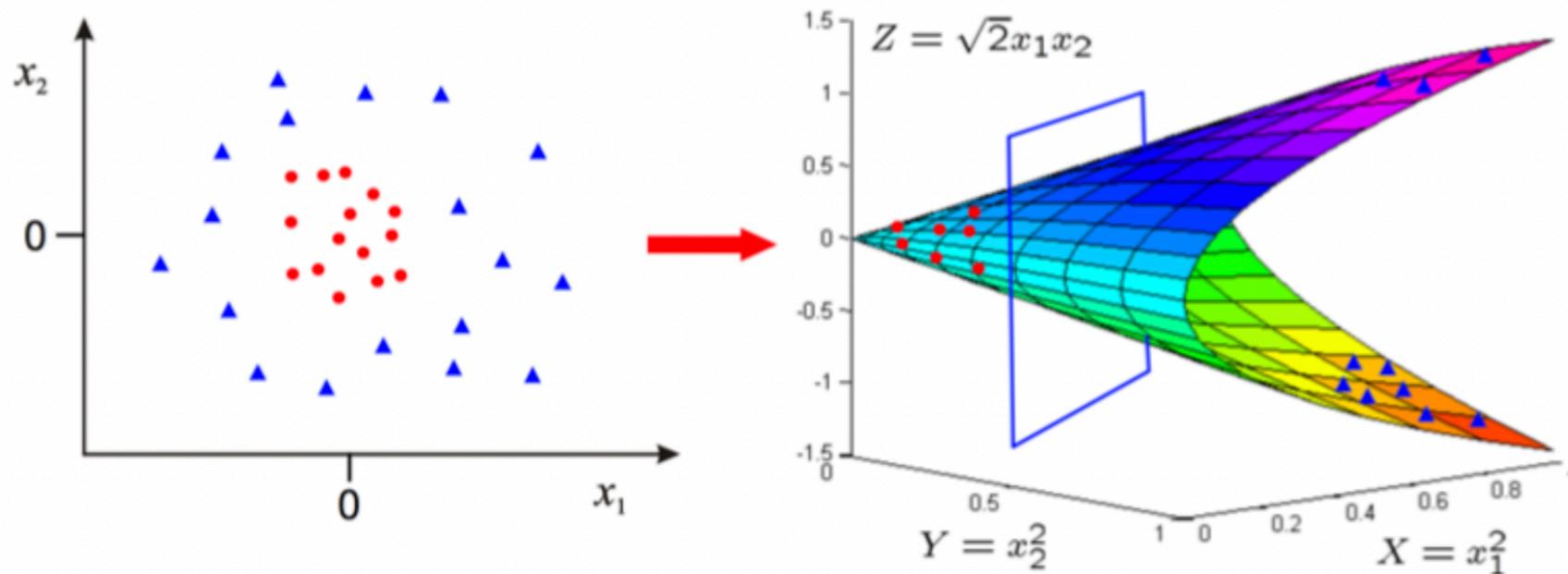
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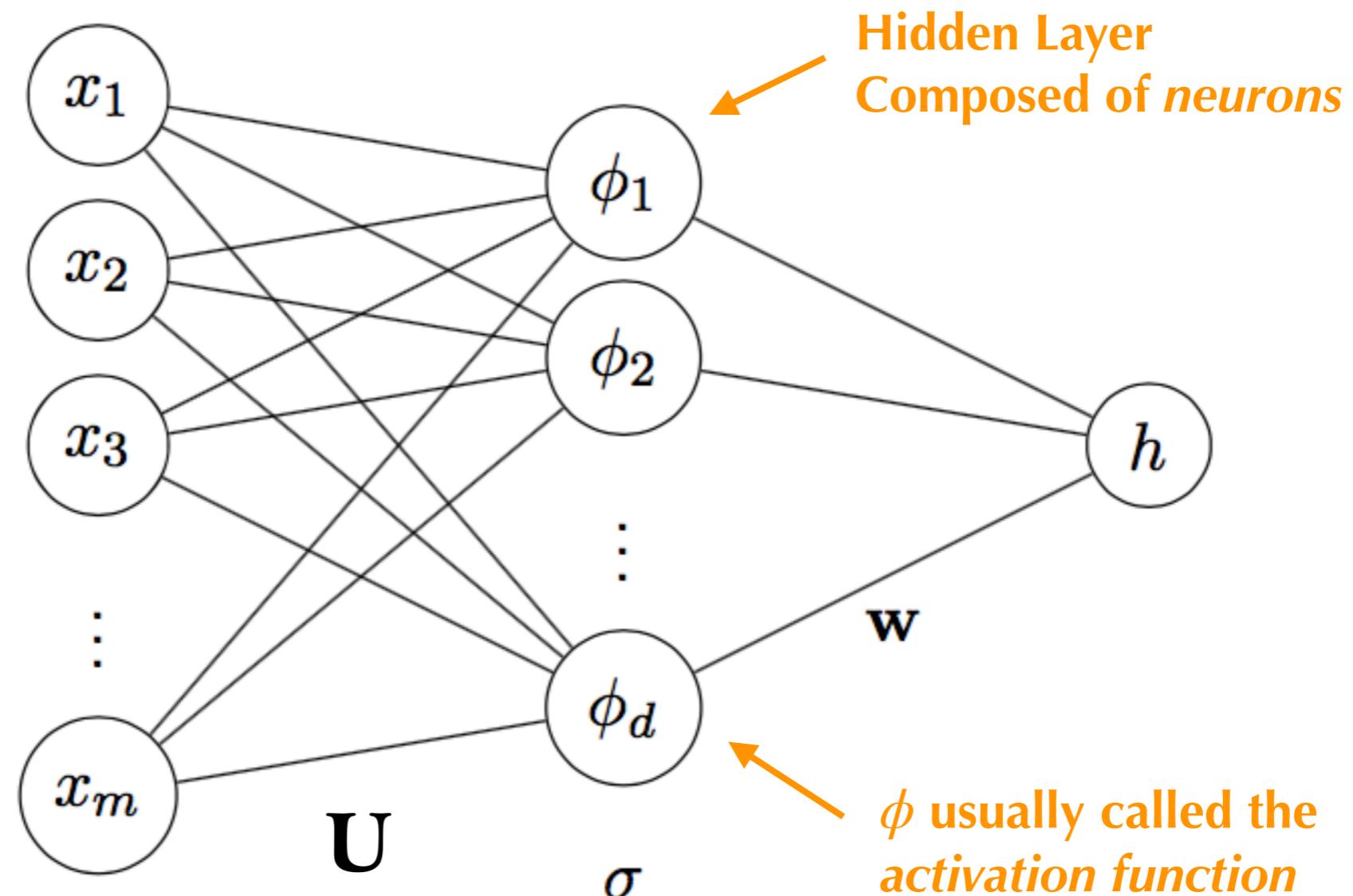
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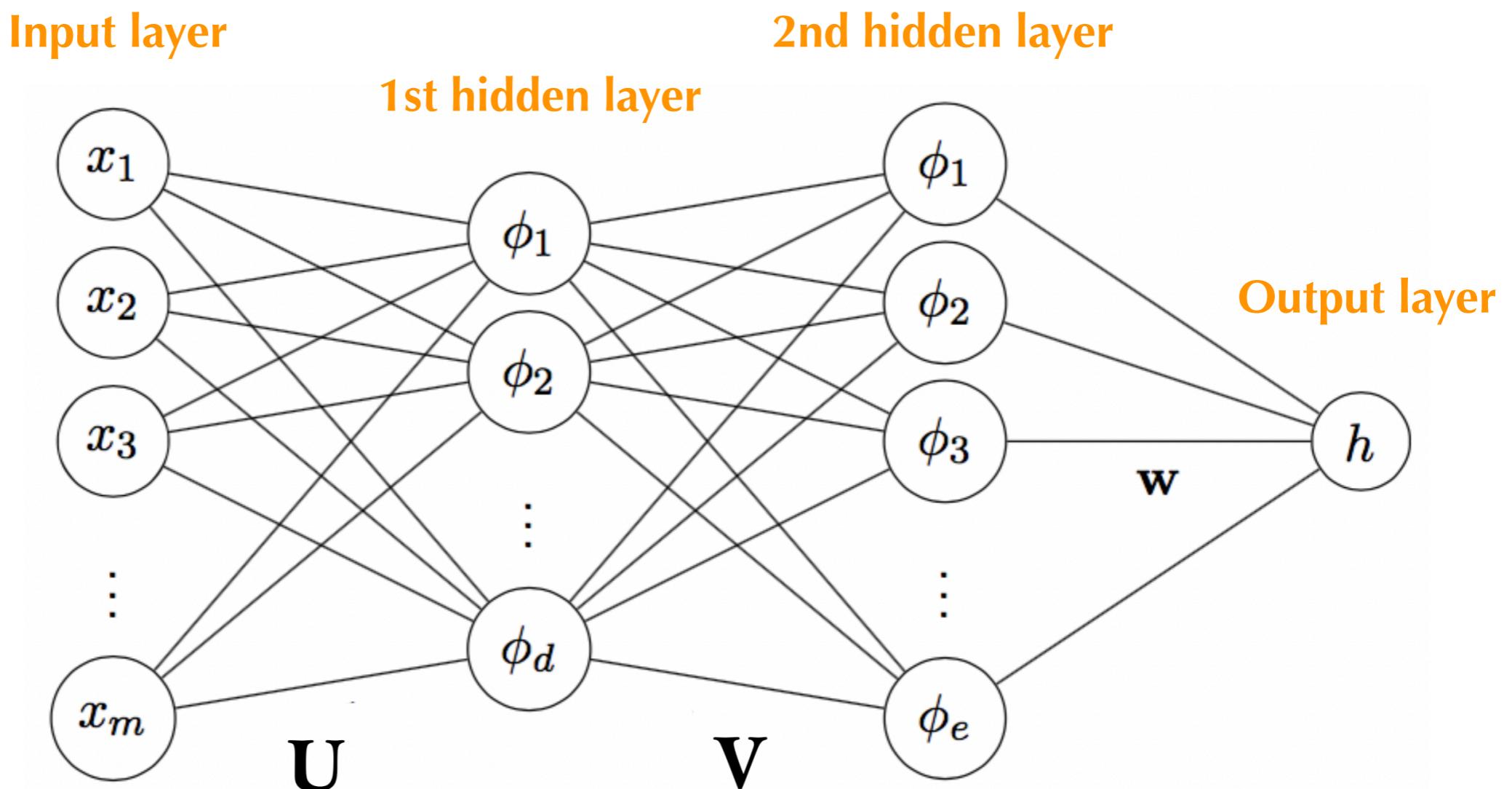
Neural Networks



$$\phi(\mathbf{x}) = \sigma(\mathbf{Ux})$$

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Multi-layer Neural Networks



Each layer adapts basis based on previous layer

These types of networks are called **Multi Layer Perceptrons (MLP)**

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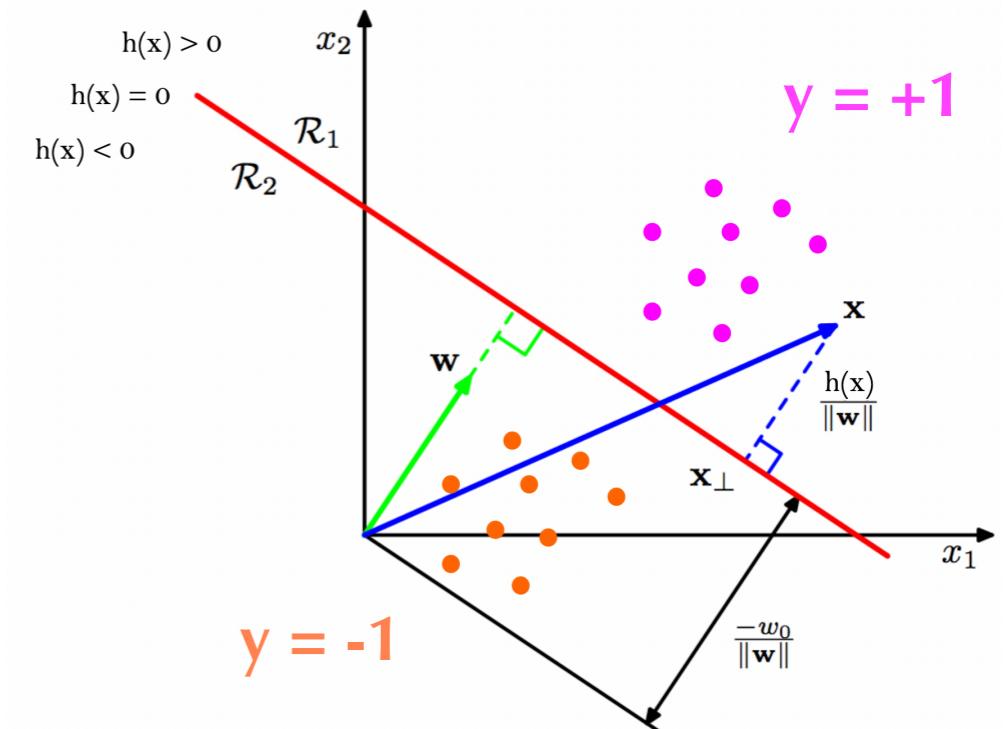
Deep Neural Networks

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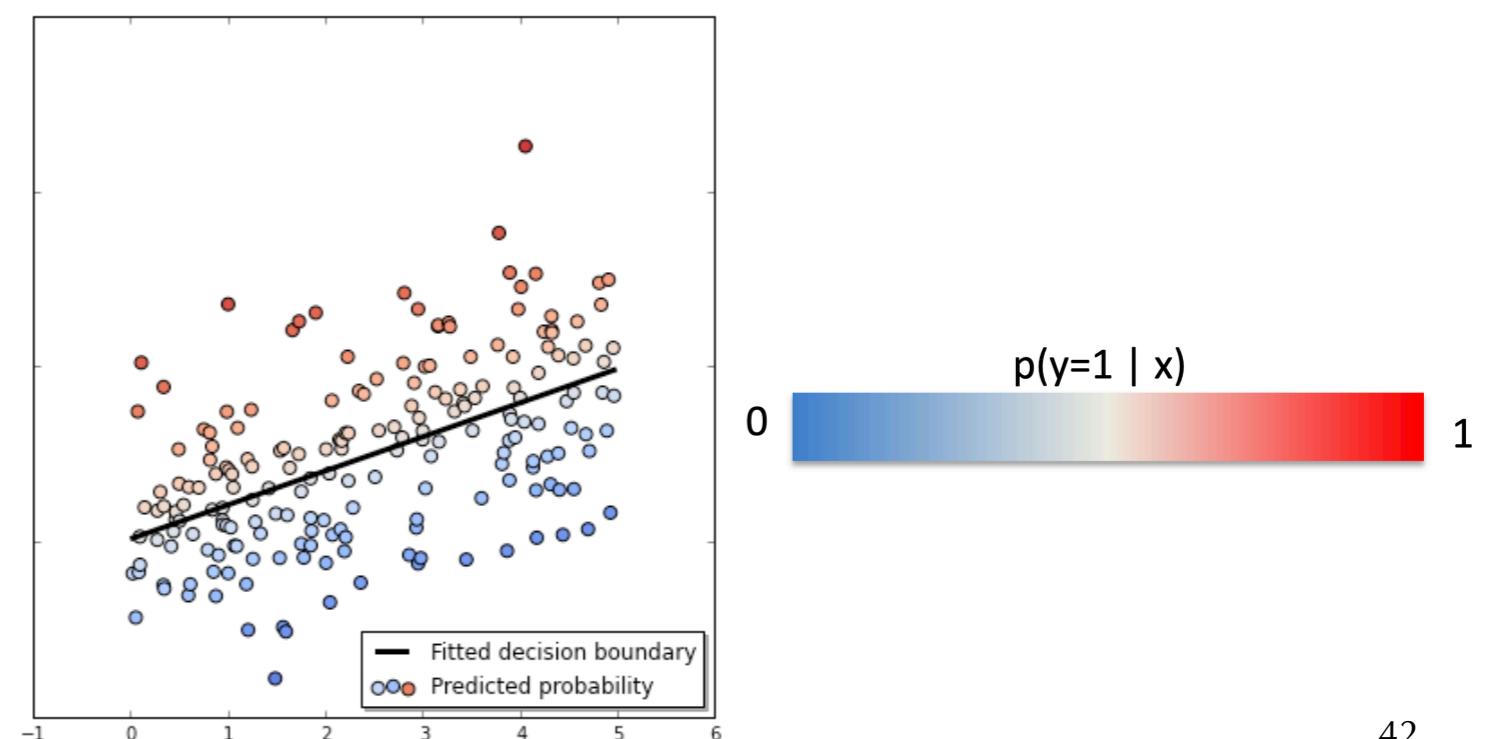
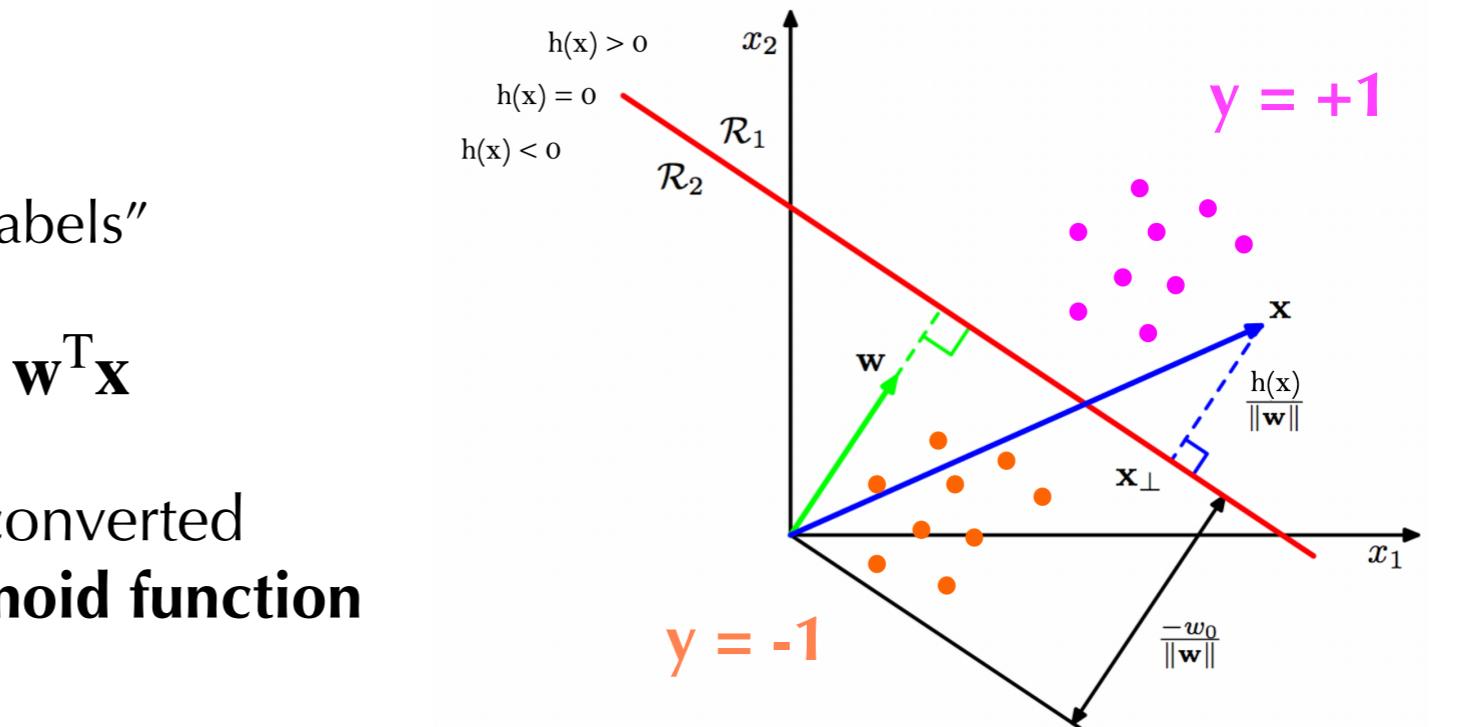
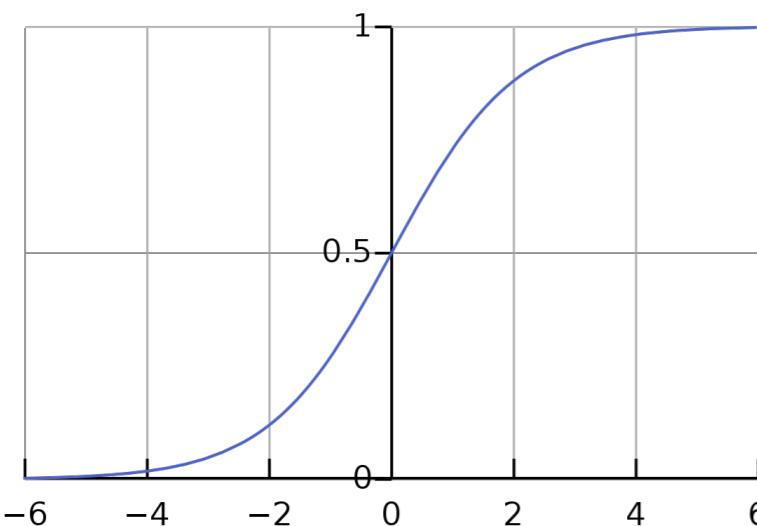
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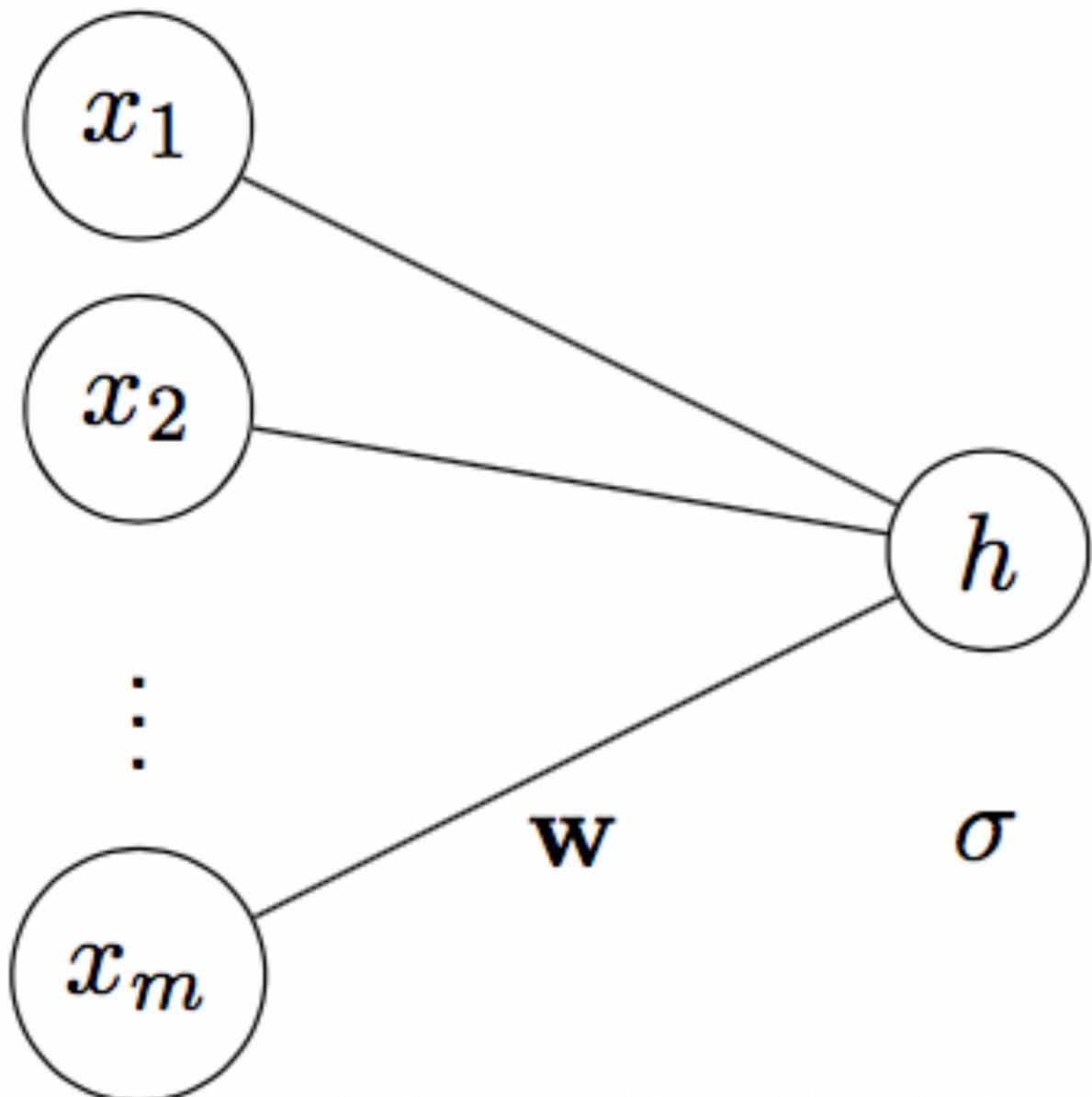
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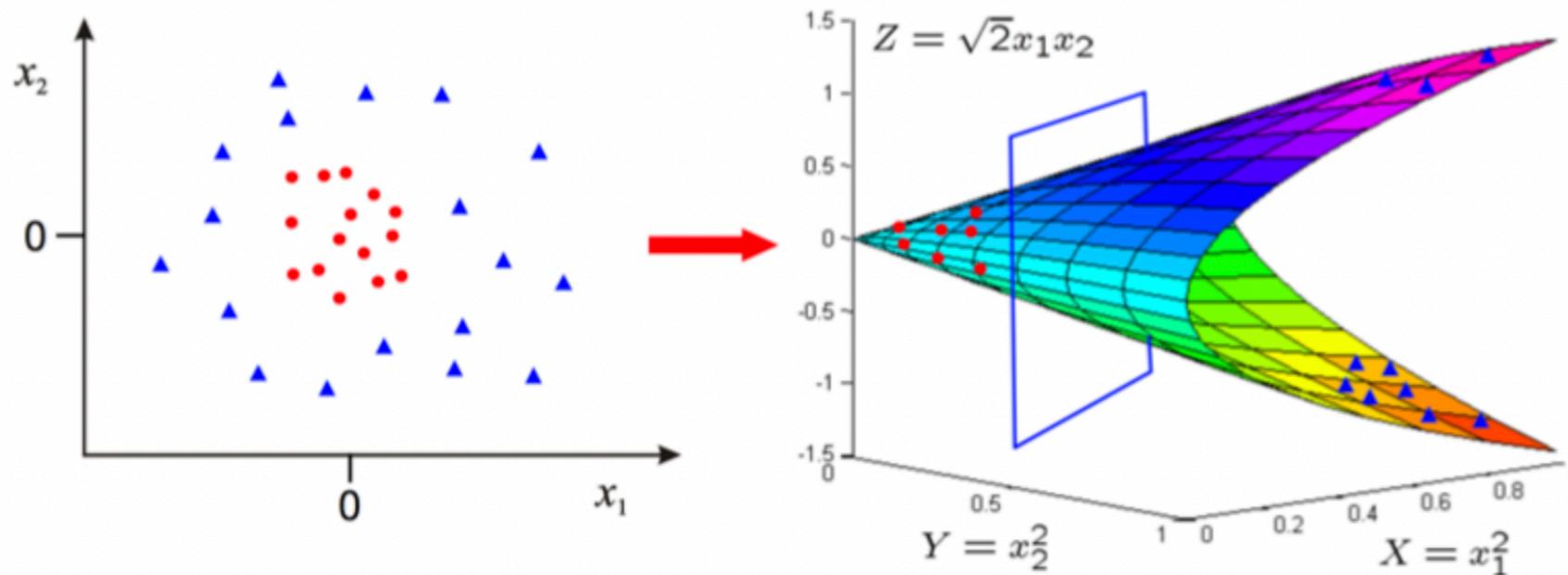
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Adding non-linearity

- What if we want a non-linear decision boundary?

- chose basis, e.g.: $\phi(x) \sim \{x^2, \sin(x), \log(x), \dots\}$

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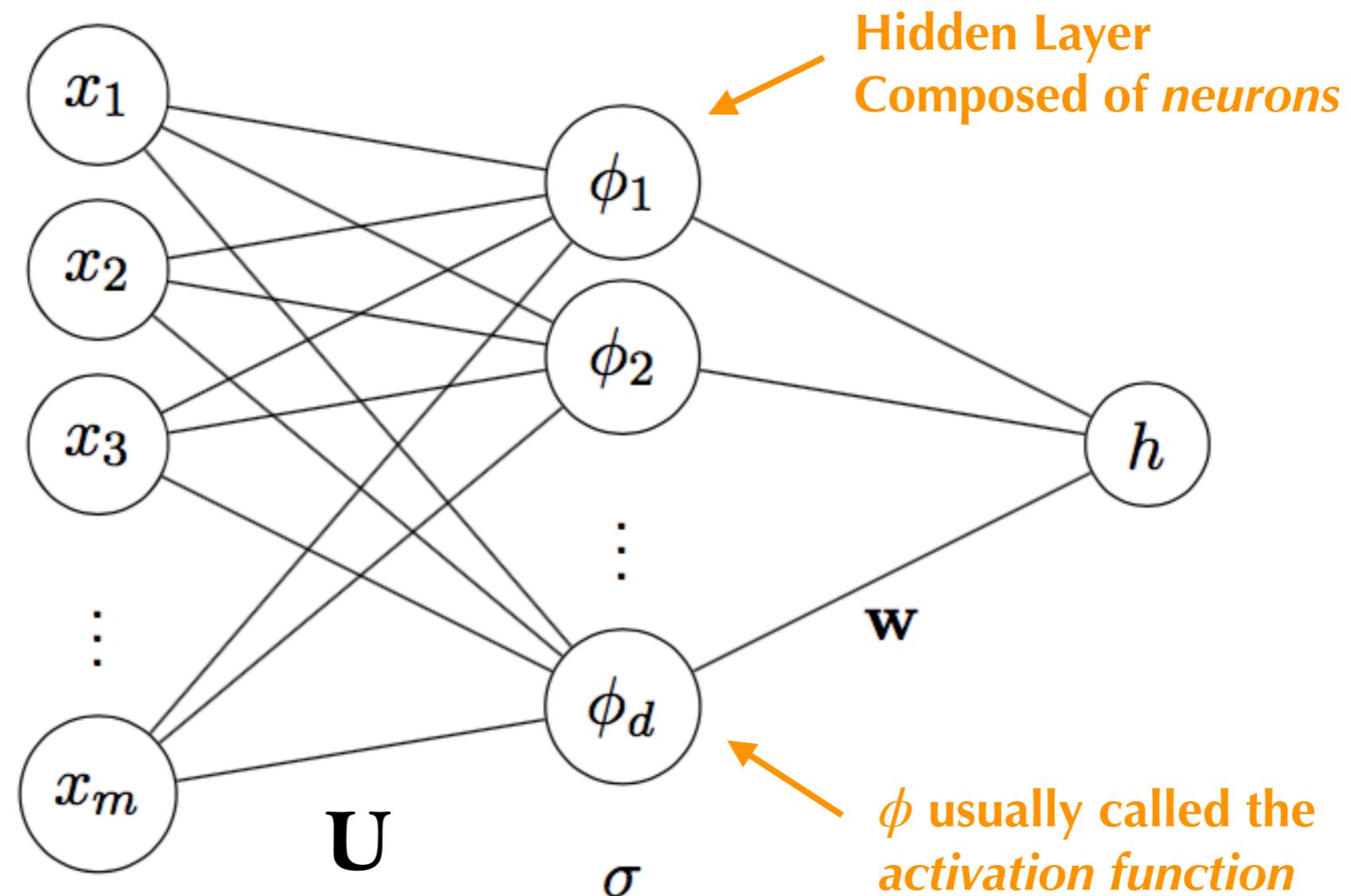
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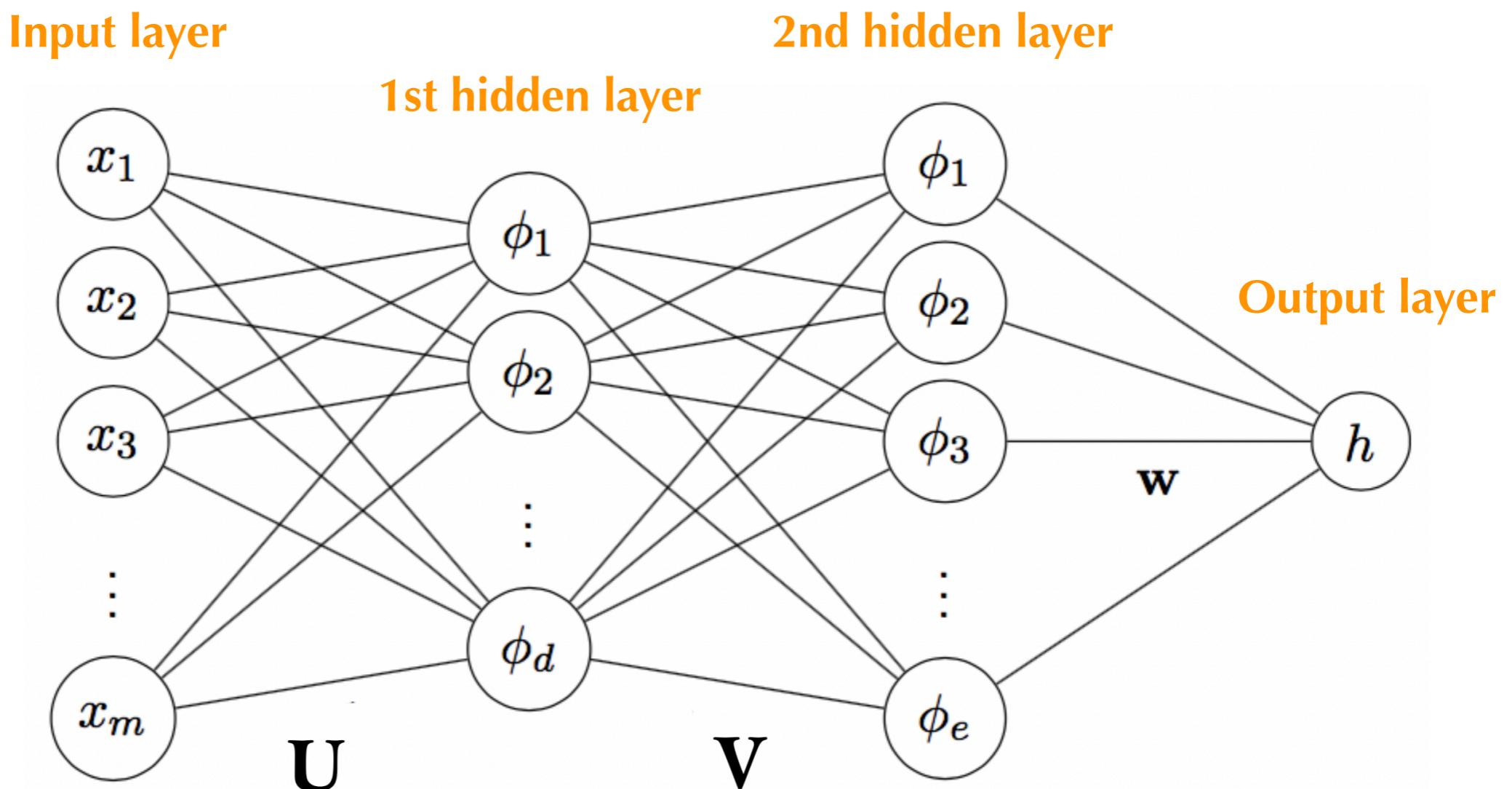
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Multi-layer Neural Networks

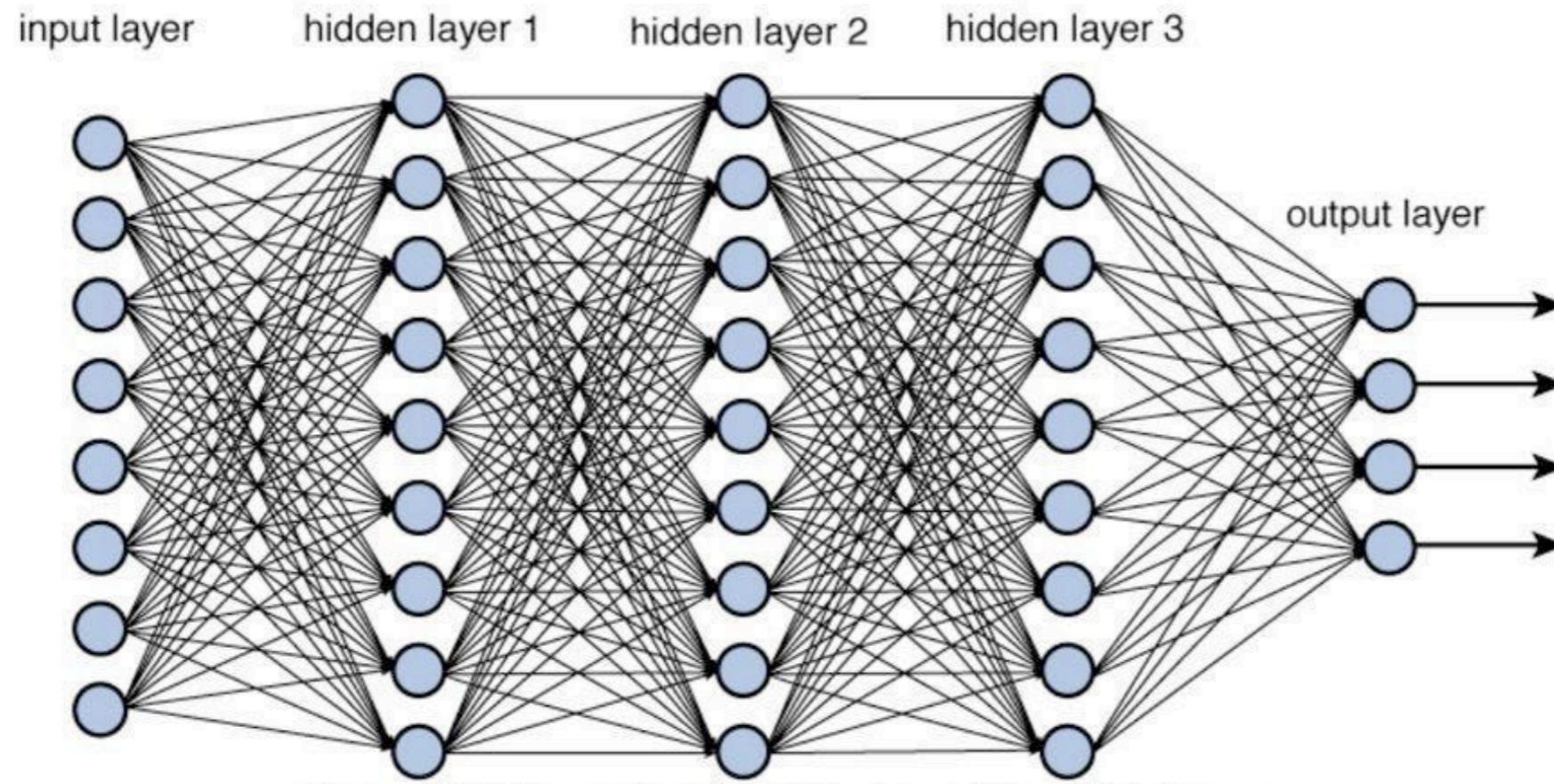


These types of networks are called **Multi Layer Perceptrons (MLP)**

Universal approximation theorem

- Feed-forward neural network with a single hidden layer containing a finite number of neurons can approximate continuous functions arbitrarily well on a space \mathbb{R}^n
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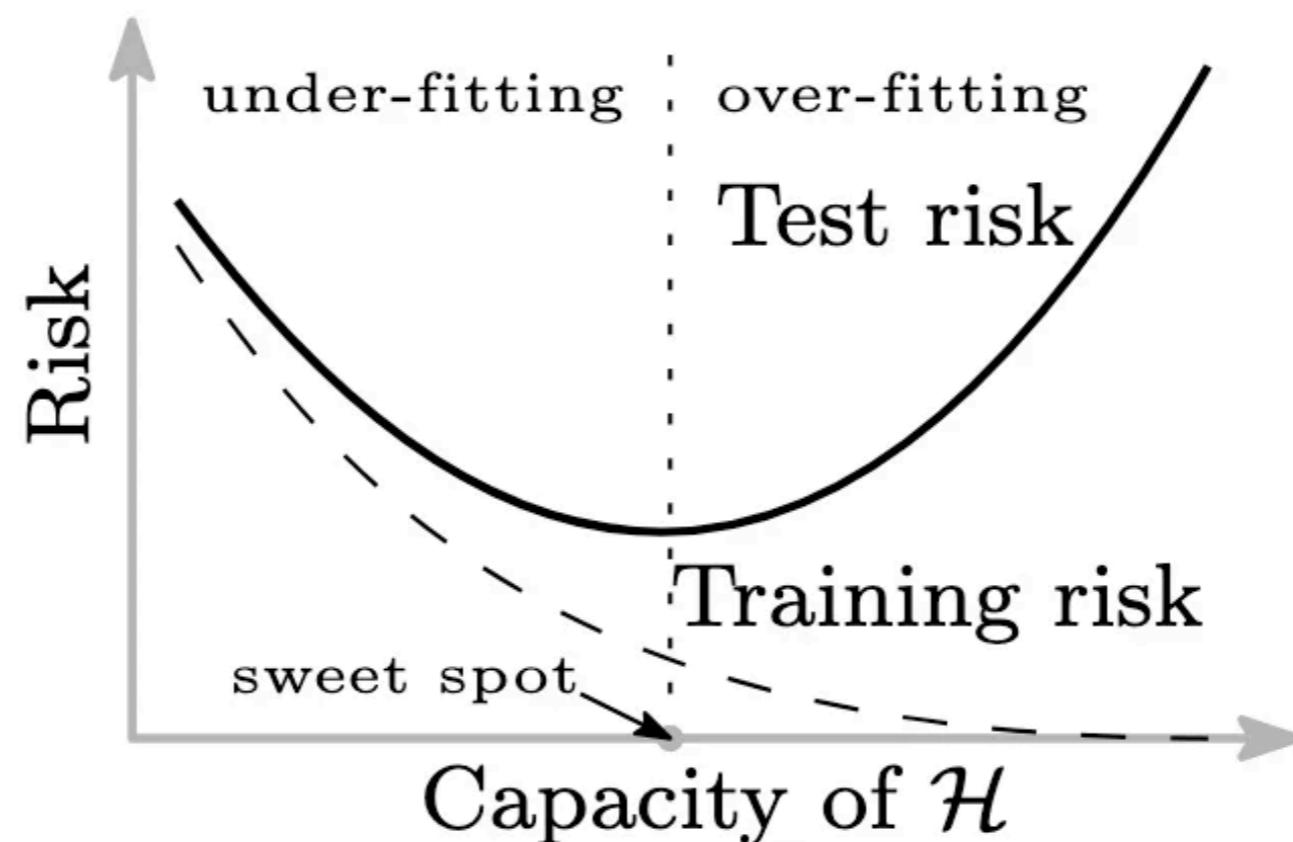
Deep Neural Networks



- As data complexity grows, need exponentially large number of neurons in a single-hidden-layer network to capture all structure in data
- Deep neural networks factorize the learning of structure in data across many layers
- Difficult to train, only recently possible with large datasets, fast computing (GPU/TPU), and new training procedures / NN architectures

Double Descent

- What we learned yesterday: “**complex models are worse**” — the bias-variance trade off



Double Descent

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Not entirely true...

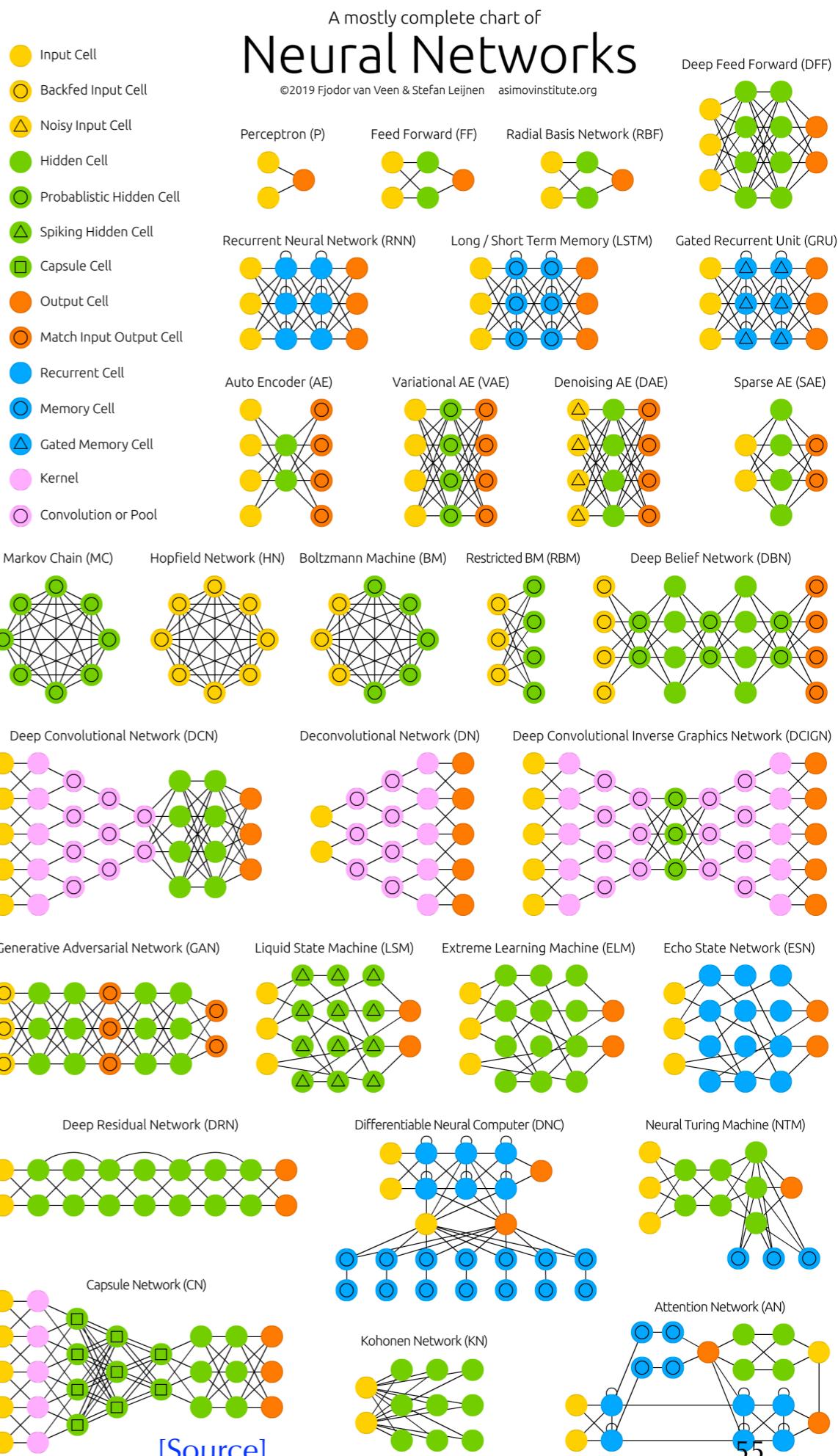
- GPT-3: 175 billion parameters
 - Cost (2020): \$4.6 million
- GPT-4 (Human Brain): 100 trillion parameters
 - Cost (2020): \$2.6 billion
 - Cost (2024): \$325 million
 - Cost (2028): \$40 million
 - Cost (2032): \$5 million

Double Descent

- What we learned yesterday: “**complex models are worse**” — the bias-variance trade off
- For modern DNN architectures this is not entirely true → so-called **double descent** behaviour observed by Belkin et al. in 2018
- **Double Descent:** over-parametrizing a deep model often improves test performance, contrary to bias-variance tradeoff prediction
- **But we must control that gradient does not vanish or that sparsity is under control**
- Major part of deep learning is to **choose the right function and engineer the data properly** for the architecture
 - instead of trying to improve training with regularization and/or new optimizers
 - need to make gradient descent work, even at the cost of substantially engineering the model

Neural Network Zoo

- The NN architecture and the node connectivity can be adapted for problem at hand
- Moving inductive bias from feature engineering to model design
 - Inductive bias:*
Knowledge about the problem
 - Feature engineering:*
Hand crafter variables
 - Model design:*
The data representation and the NN architecture



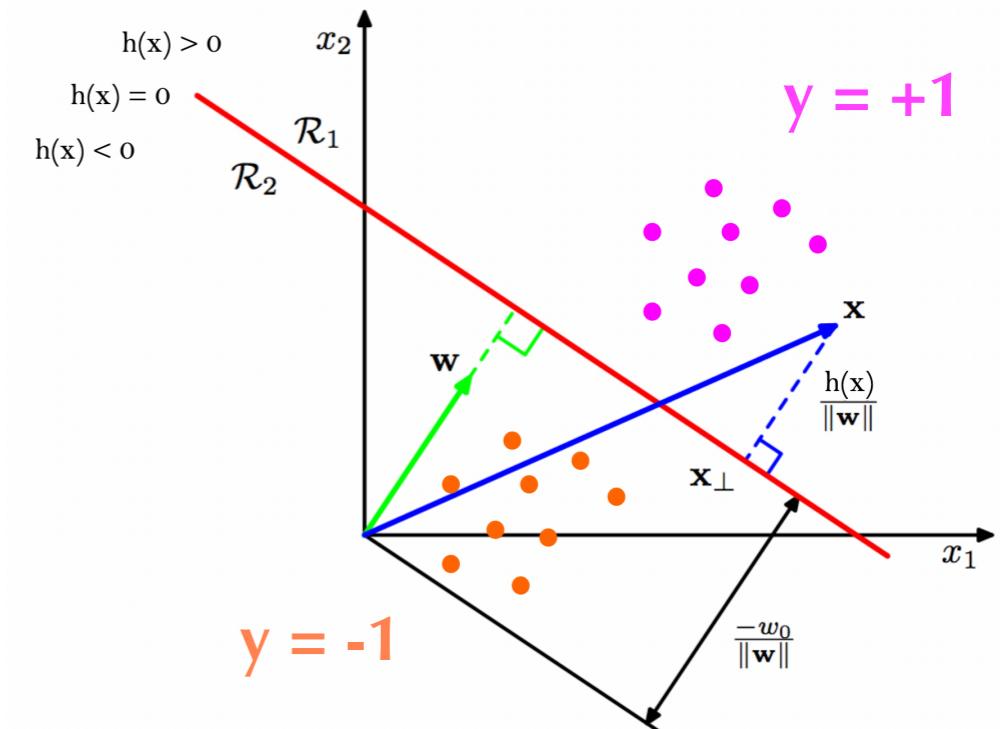
Convolutional Neural Networks

Recap: logistic regression

- Task: learn a function to **separate different classes of data** — for two classes we call this “binary classification”:

- $\mathbf{x}_i \in \mathbb{R}^m$
- $y_i \in \{-1, 1\}$ — we call these “true labels”

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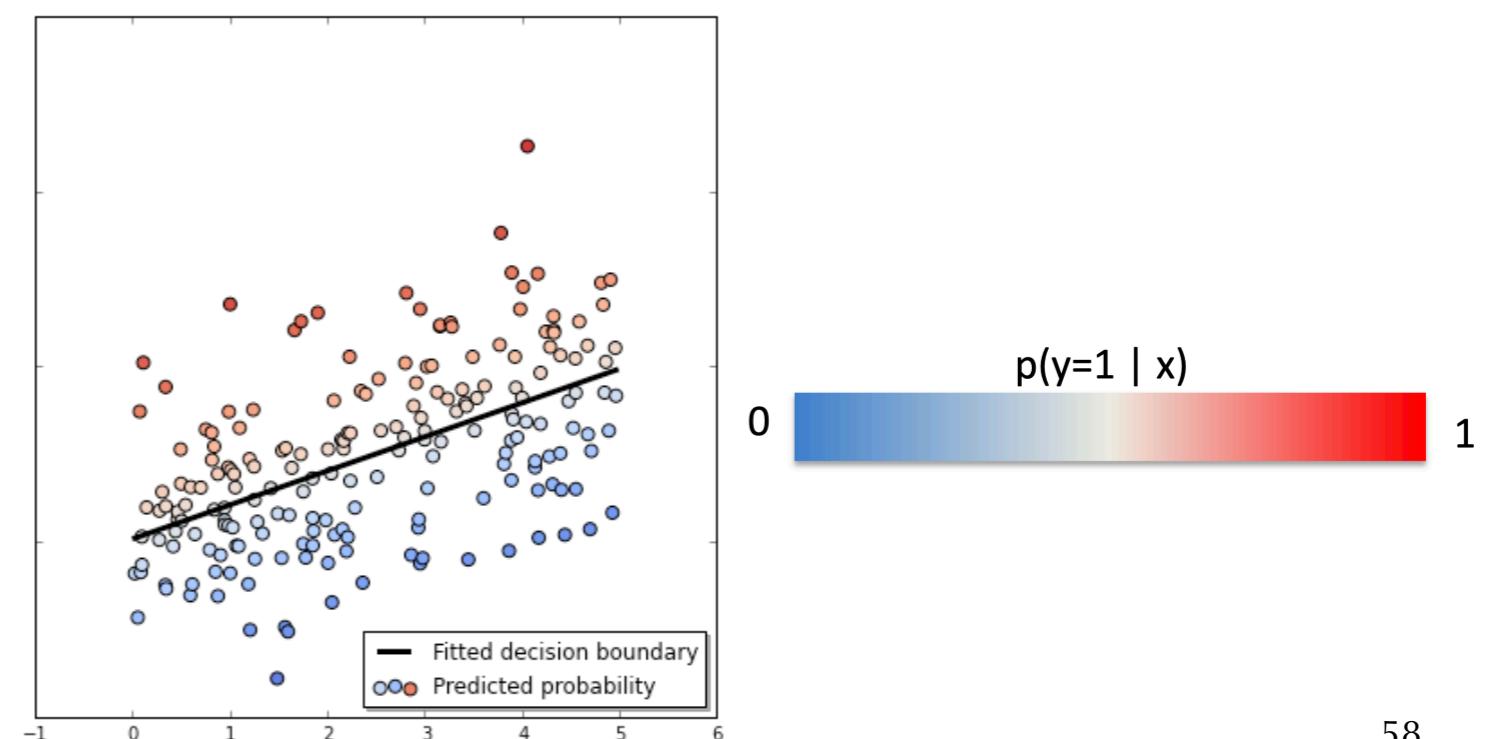
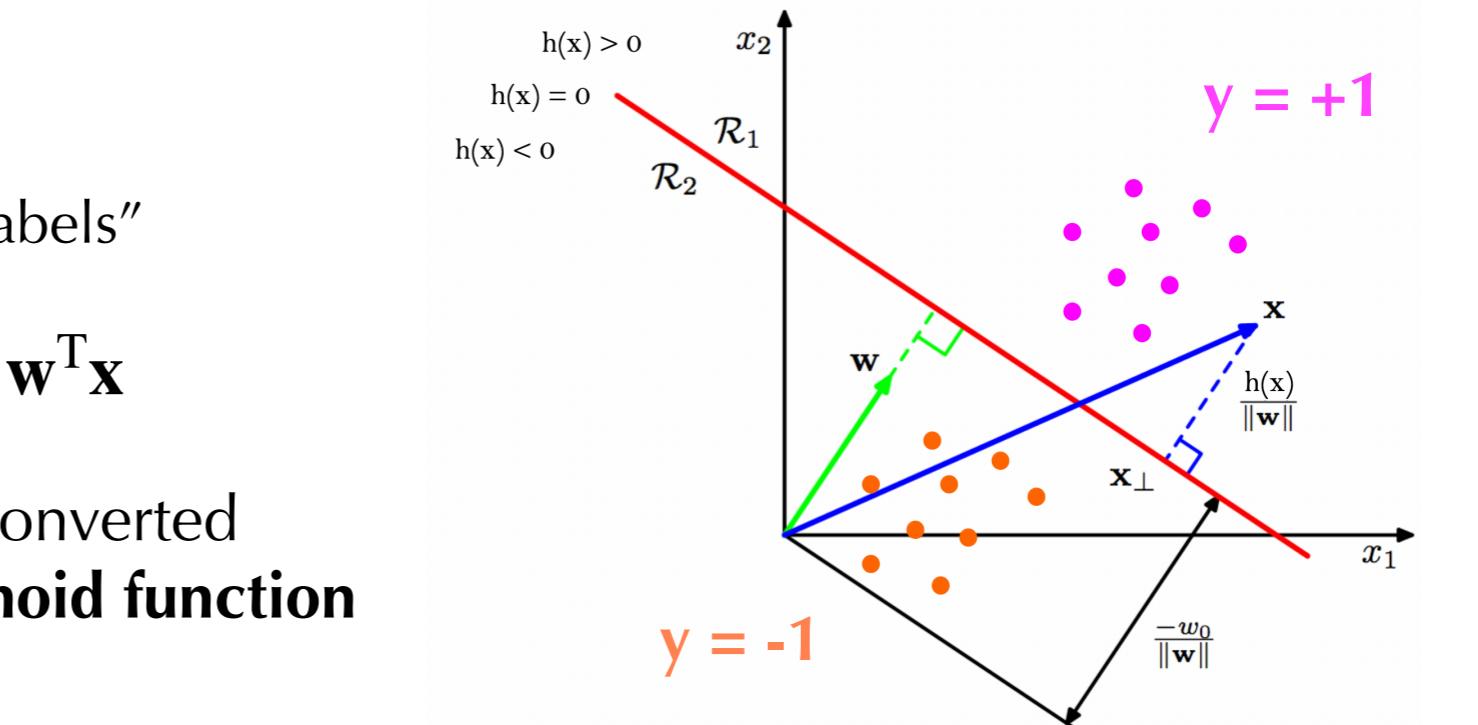
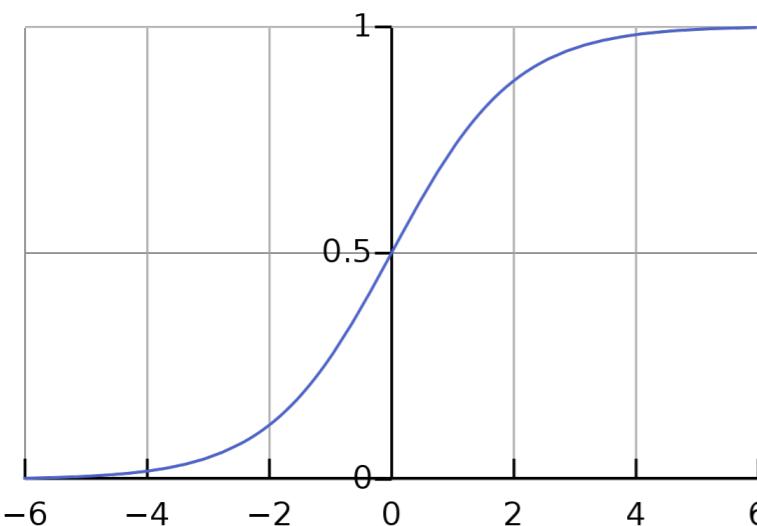
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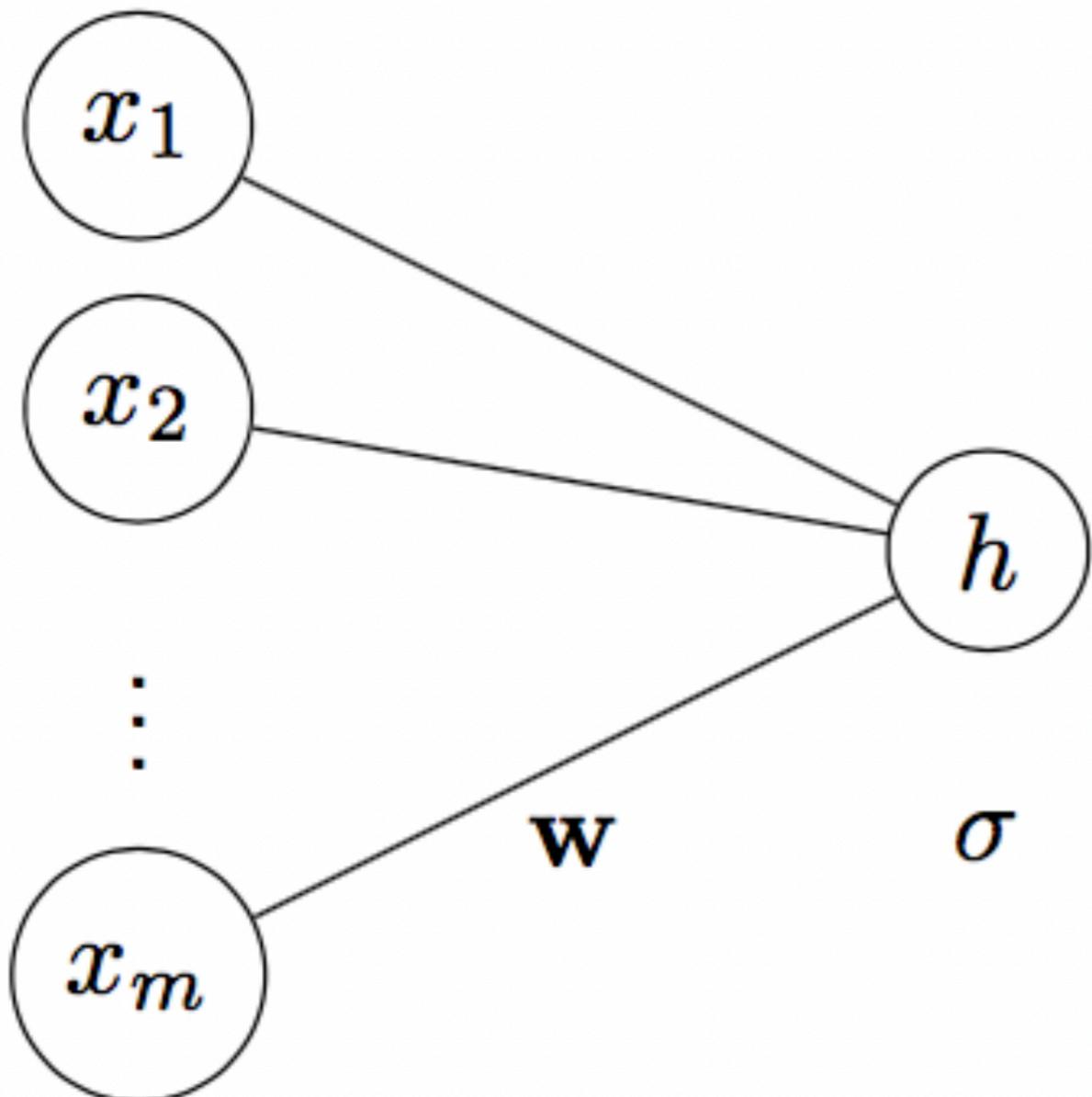
- **Linear decision boundary:** $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T \mathbf{x}$

- Distance from decision boundary is converted to class probability using **logistic sigmoid function**

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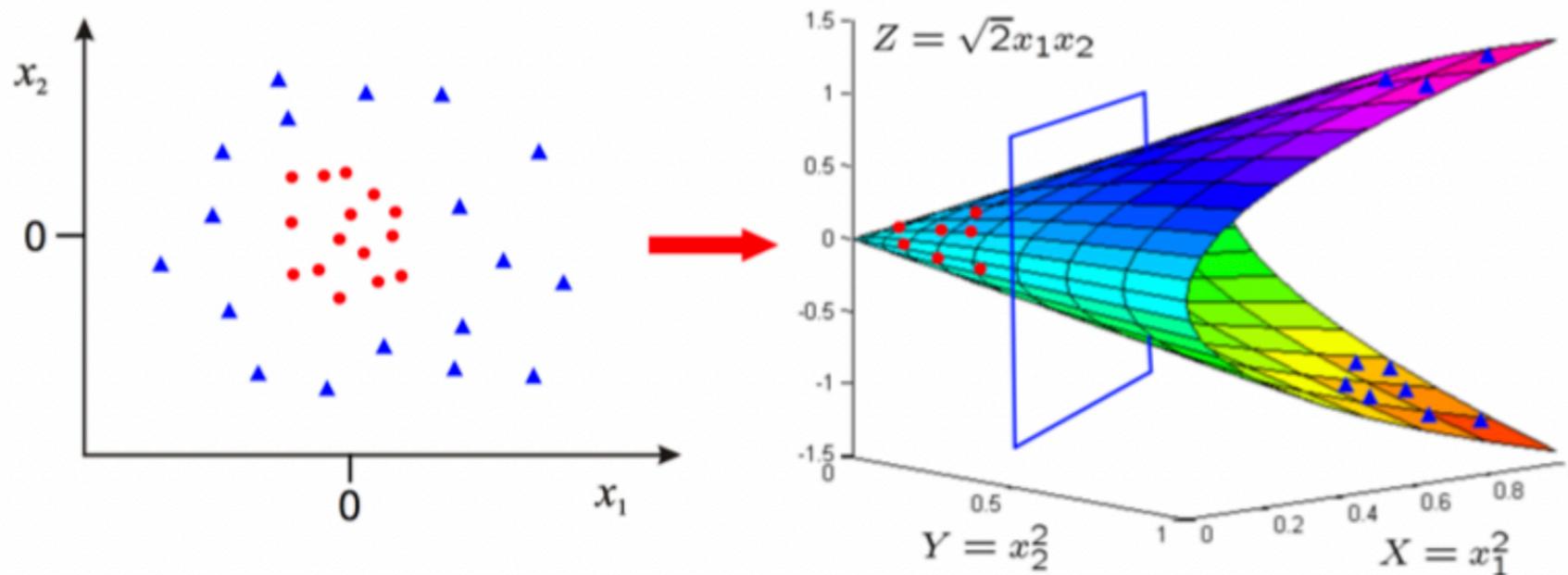
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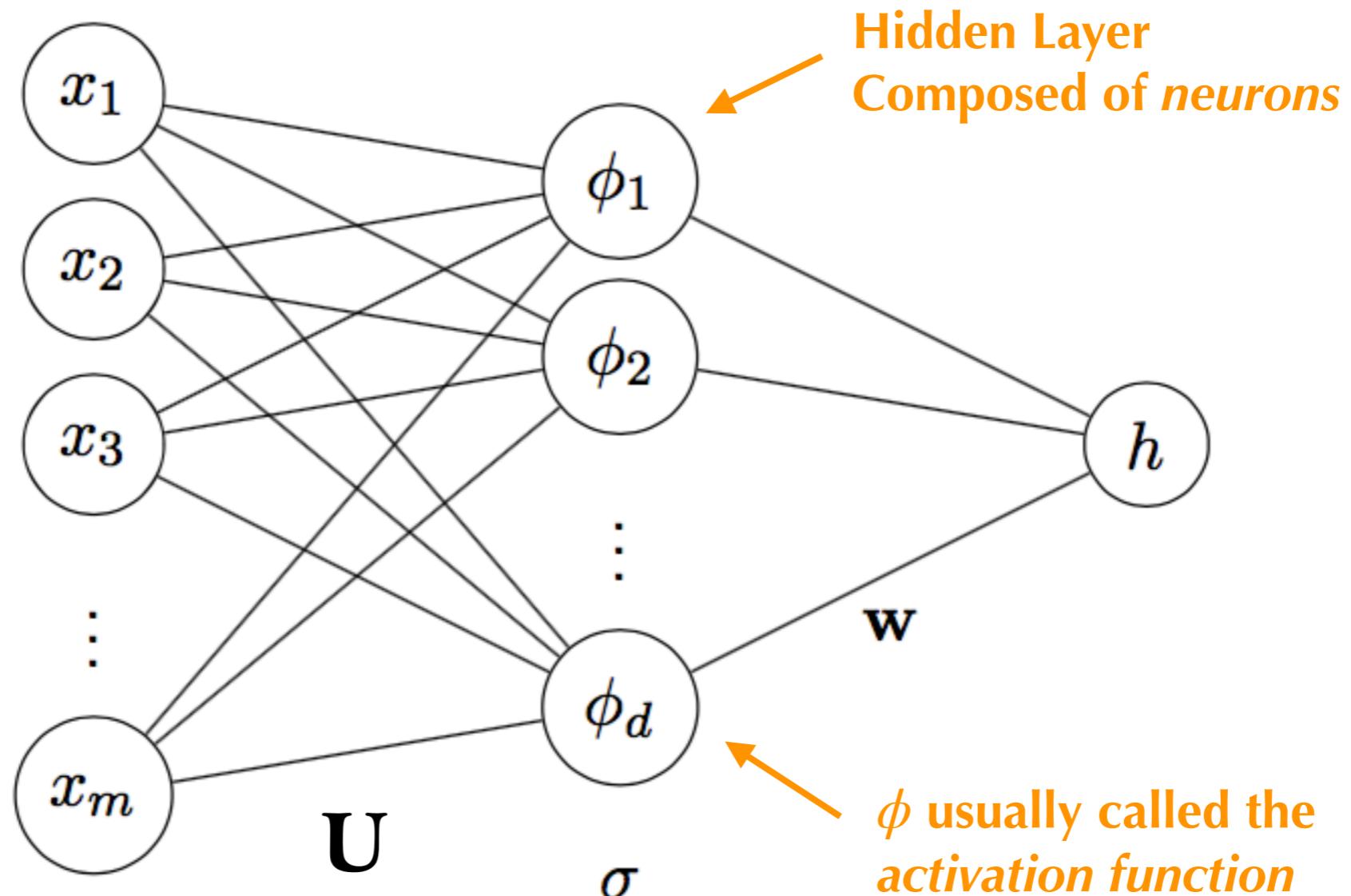
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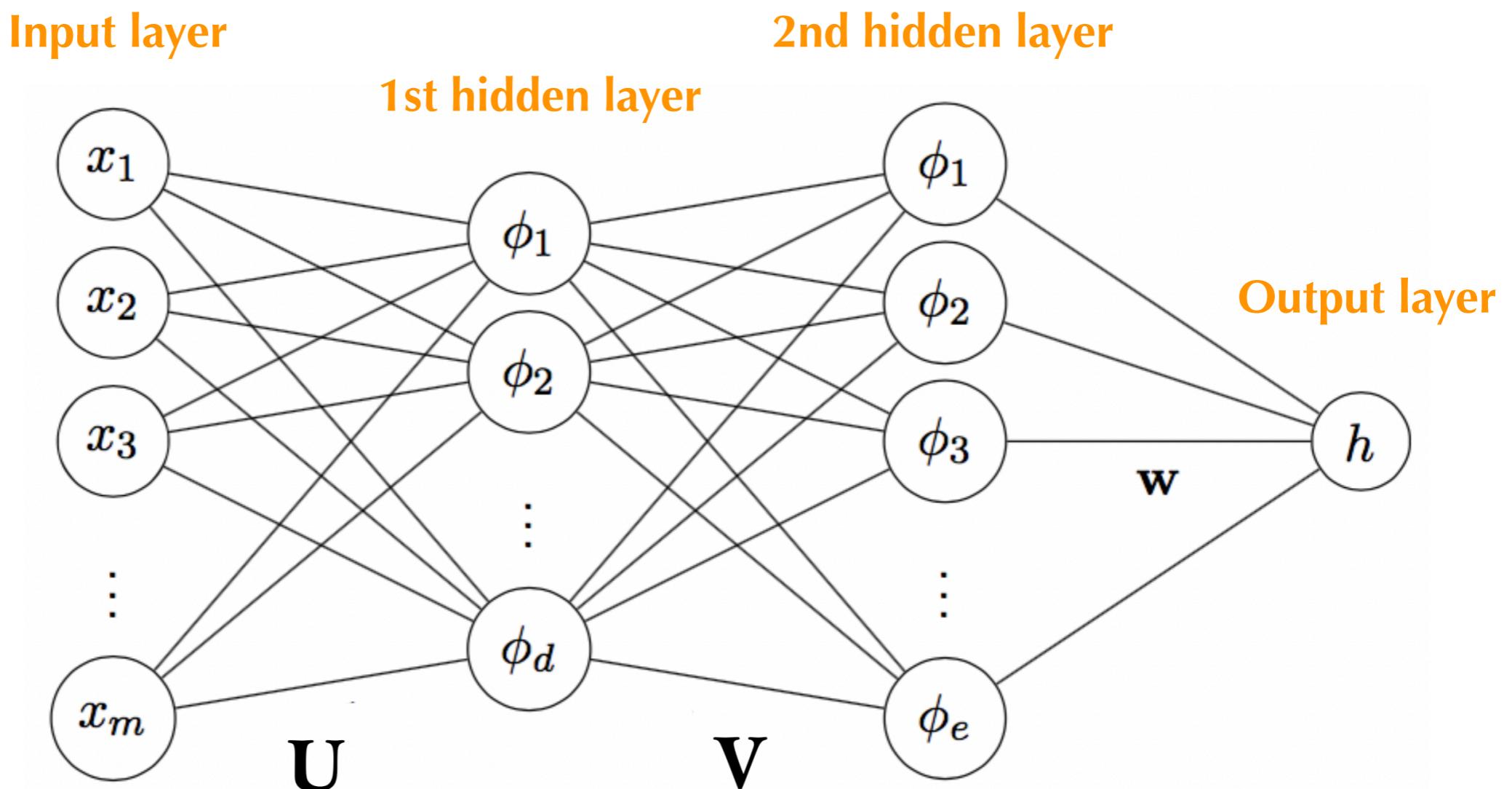
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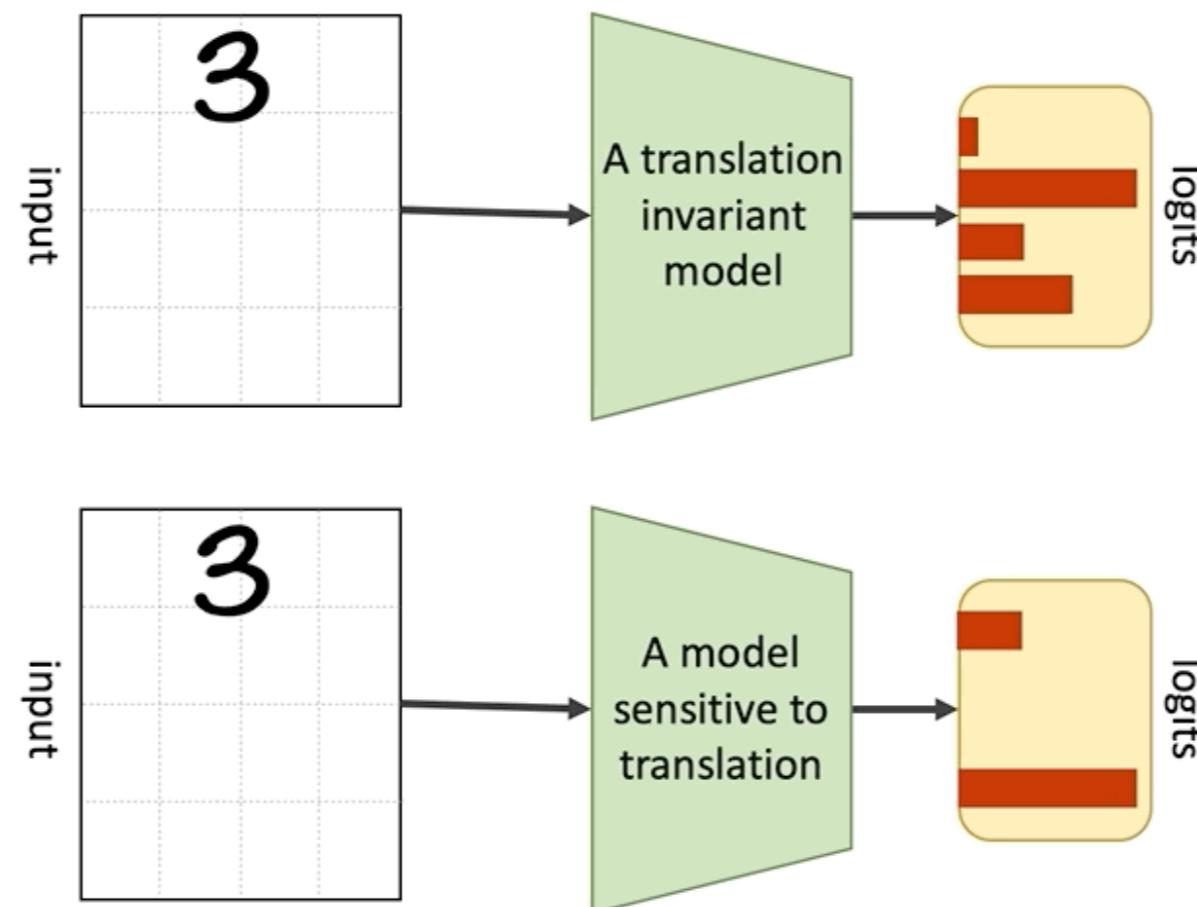
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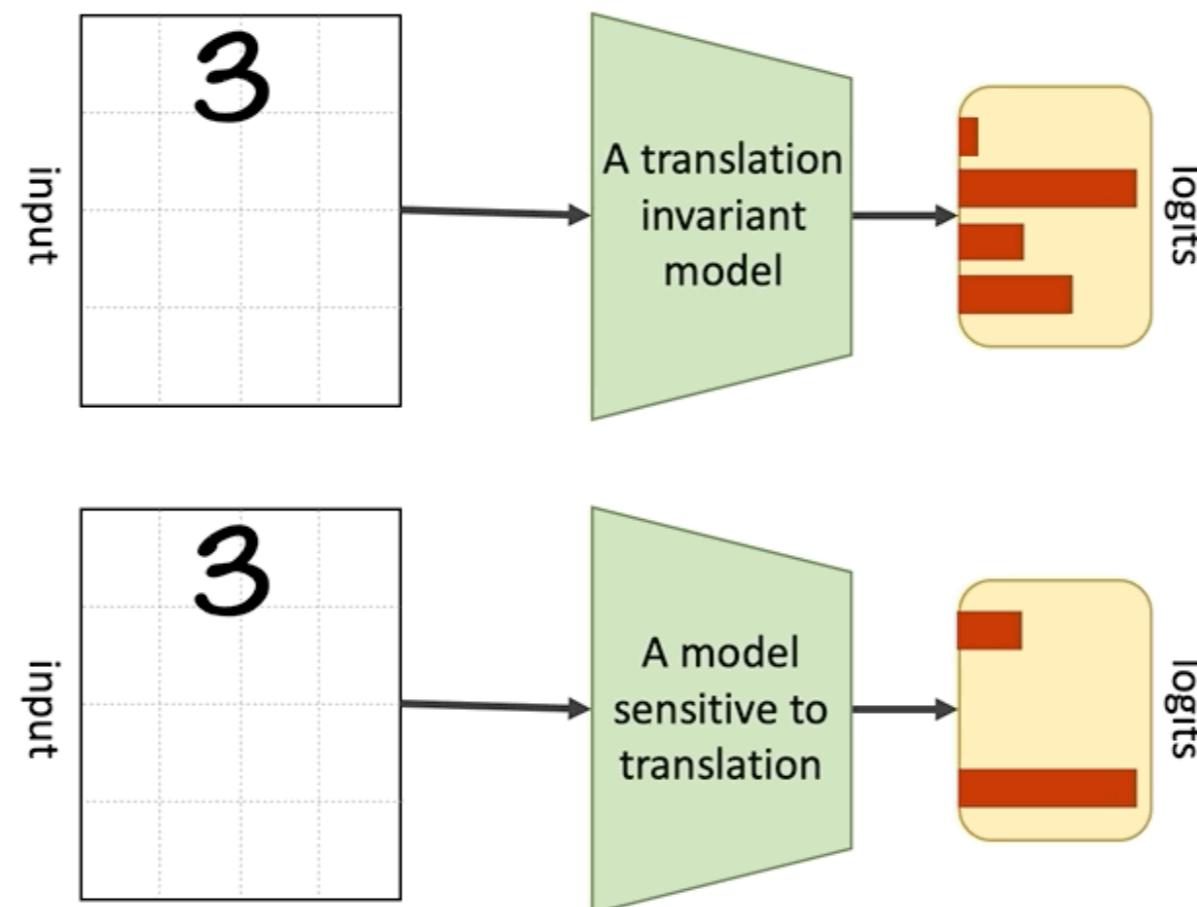
- When the structure of data includes “**equivariance to translation**”, a representation meaningful at a certain location can / should be used everywhere



- Convolutional layers build on this idea, that the same “local” transformation is applied everywhere and preserves the final output

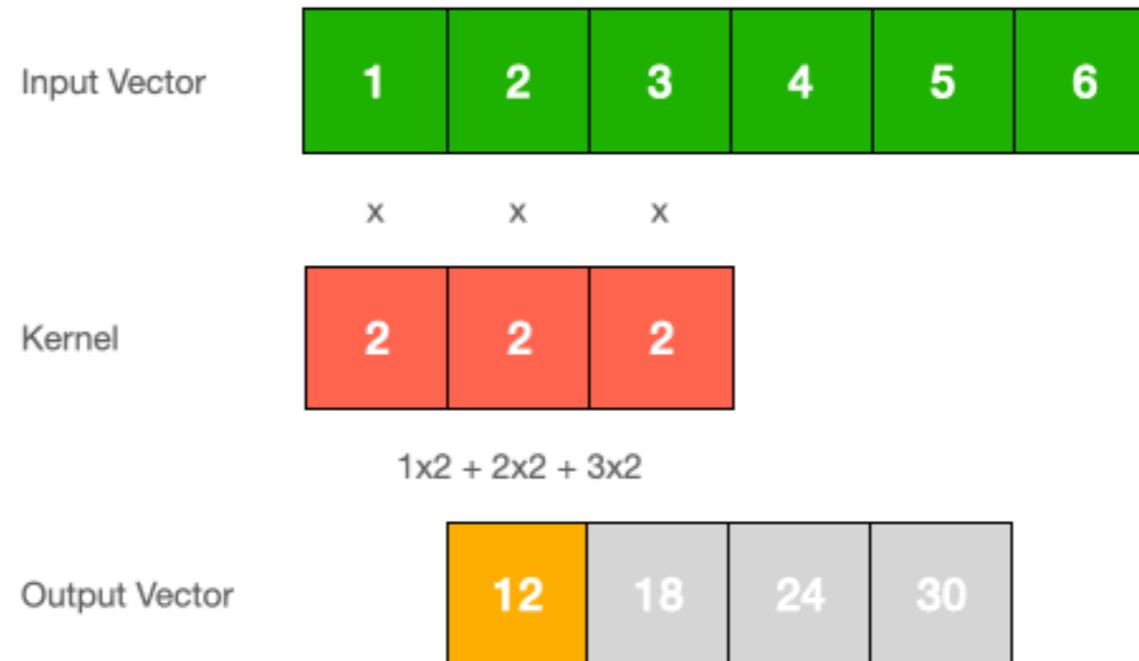
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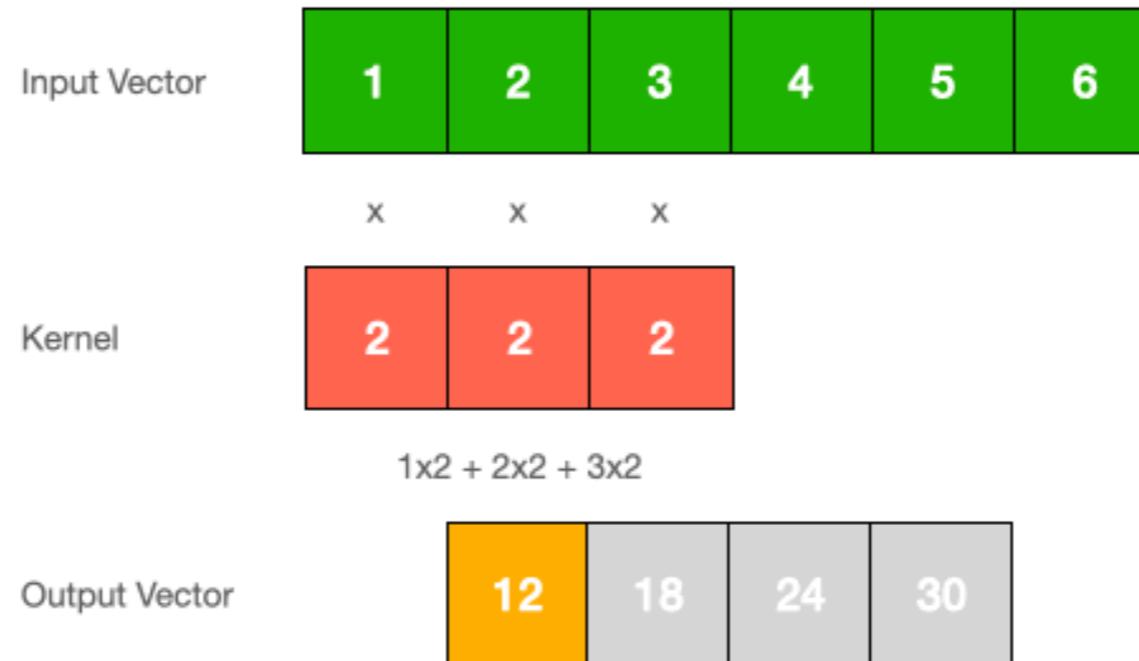
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1D convolutional layers



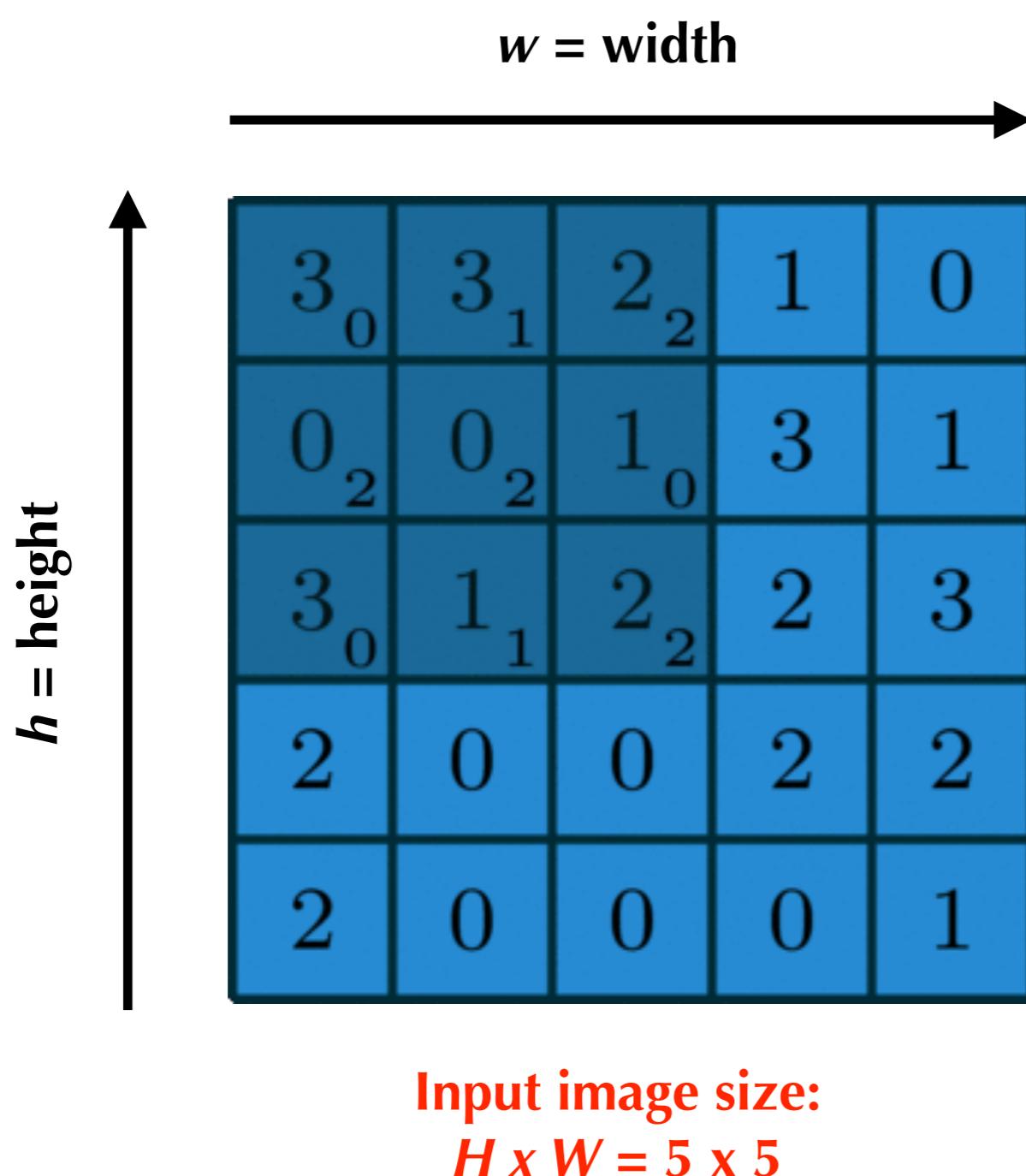
- **Data** (one vector of m features for simplicity): $\mathbf{x} \in \mathbb{R}^m$
- **Convolutional filter of width k :** $\mathbf{u} \in \mathbb{R}^k$
- Convolution $\mathbf{x} \circledast \mathbf{u}$ is a vector of size $m - k + 1$ with element j : $(\mathbf{x} \circledast \mathbf{u})_j = \sum_{b=0}^{k-1} x_{i+b} u_b$
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2D convolutional layers



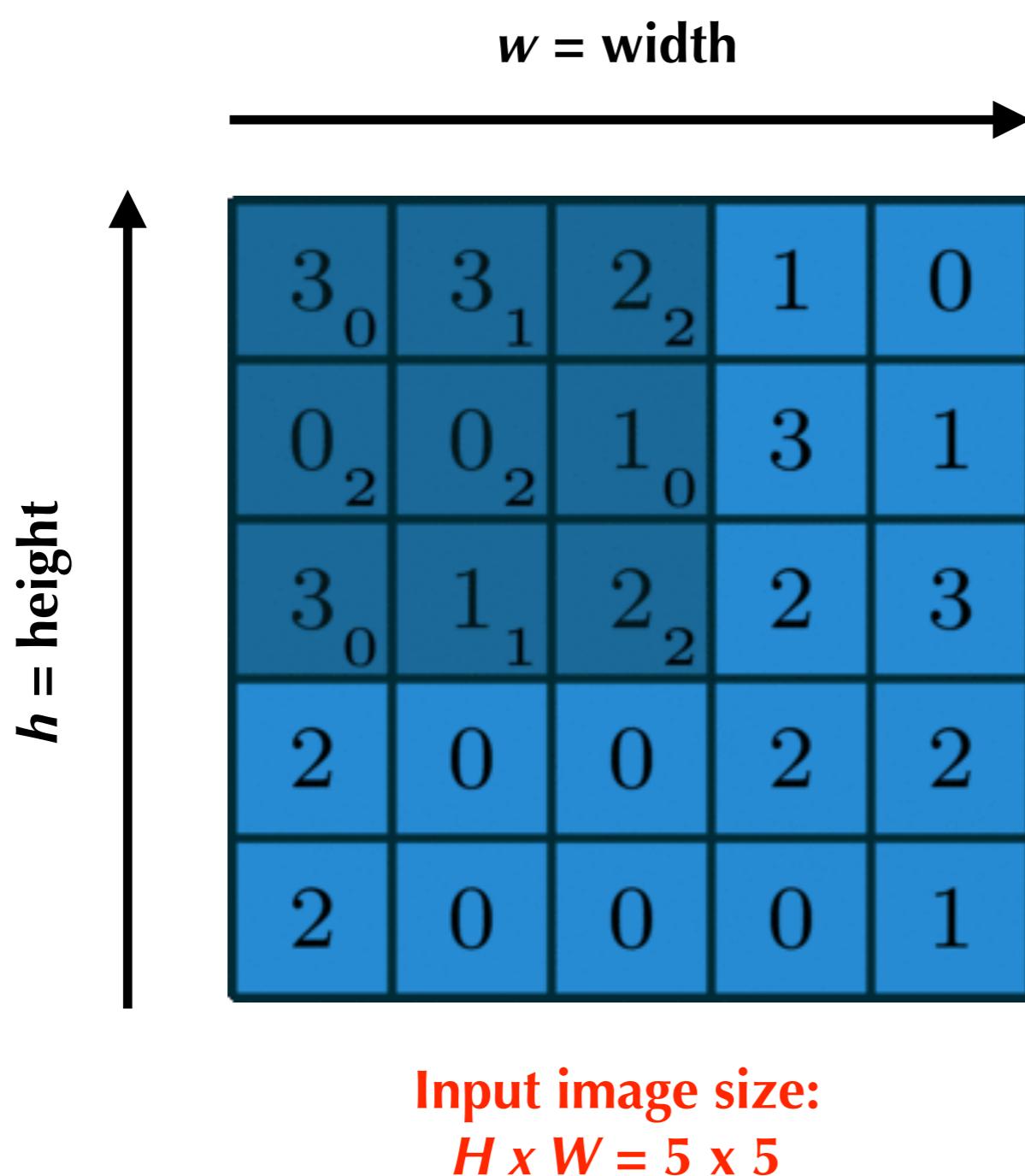
Filter size:
height = $h_k = 3$
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12.0	12.0	17.0
10.0	17.0	19.0
9.0	6.0	14.0

Output image size:
height = $h - h_k + 1 = 3$
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Same principle but over a 2D matrix

2D convolutional layers



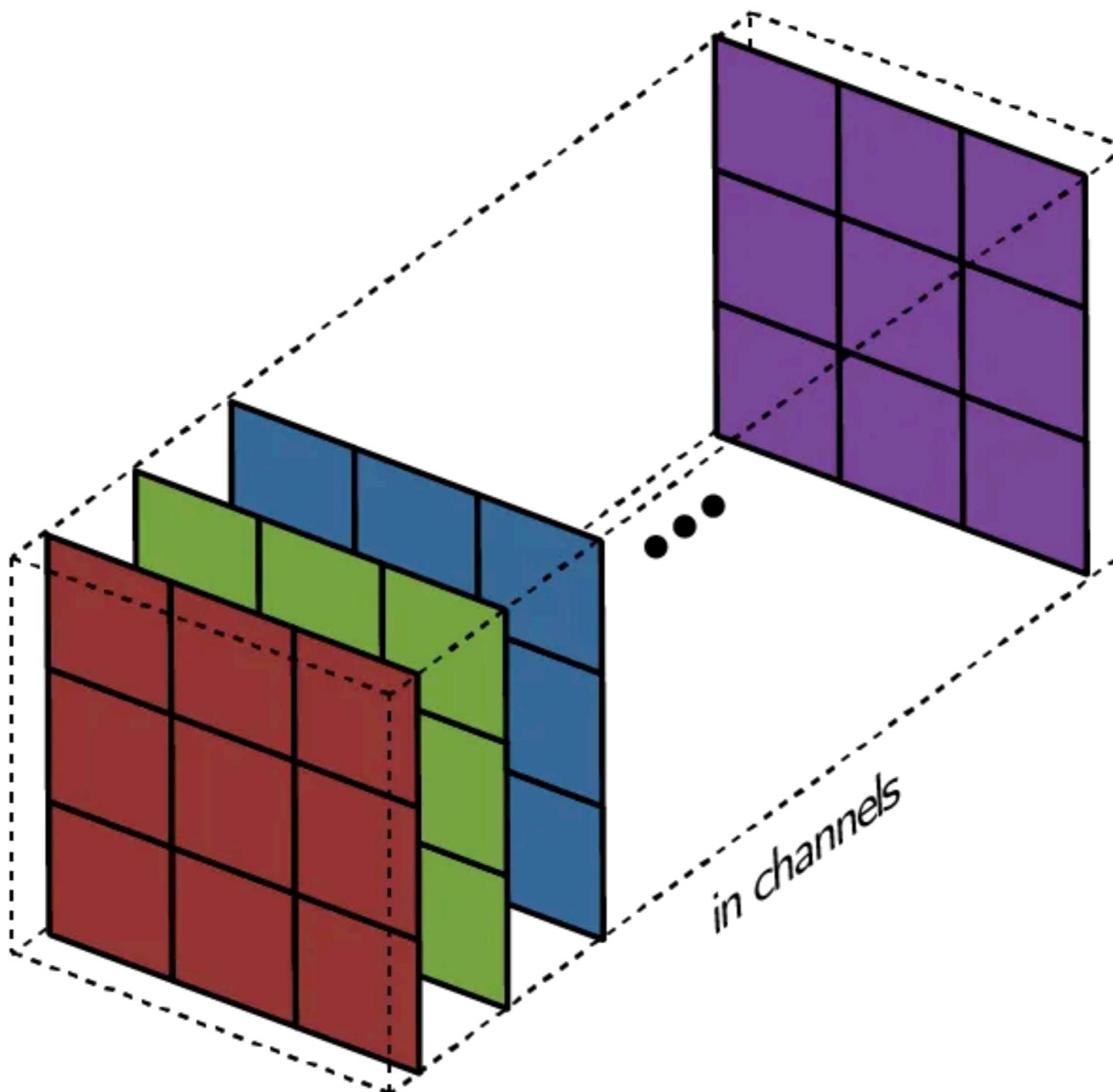
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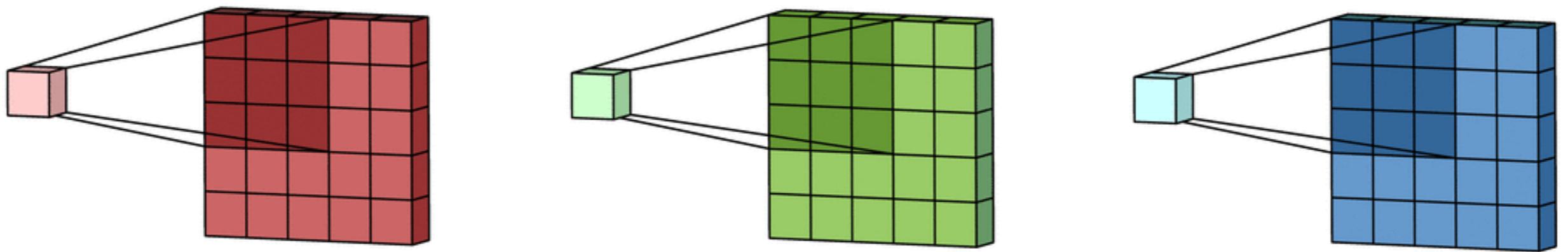
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2D CNNs with multiple channels



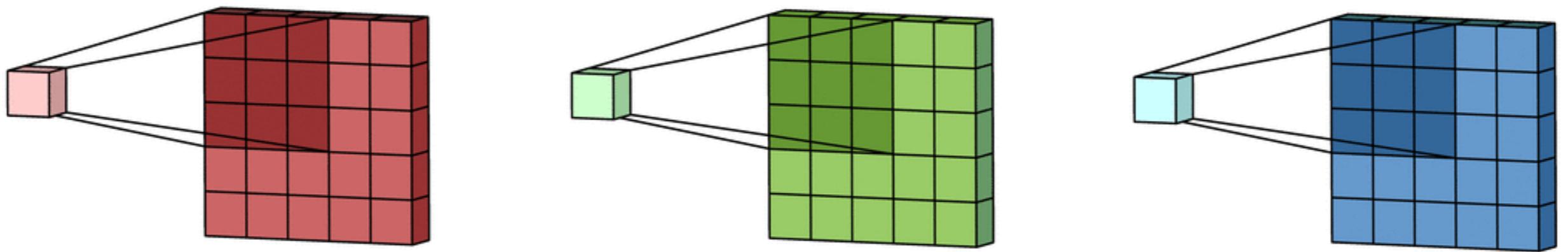
Many 2D images stacked on top of each others
— the third dimension is called “channel”

2D CNNs with multiple channels



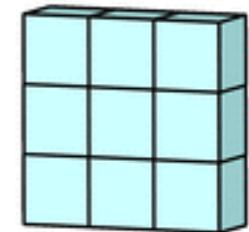
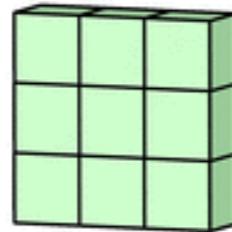
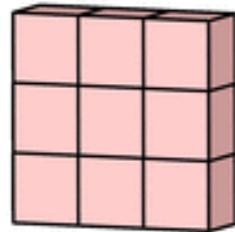
**The filter is decomposed in C filters of same size each
acting independently on each of the C channels**

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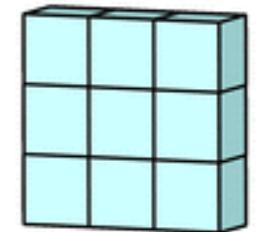
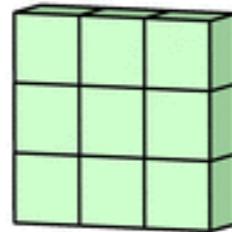
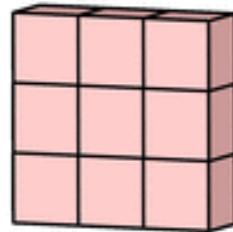
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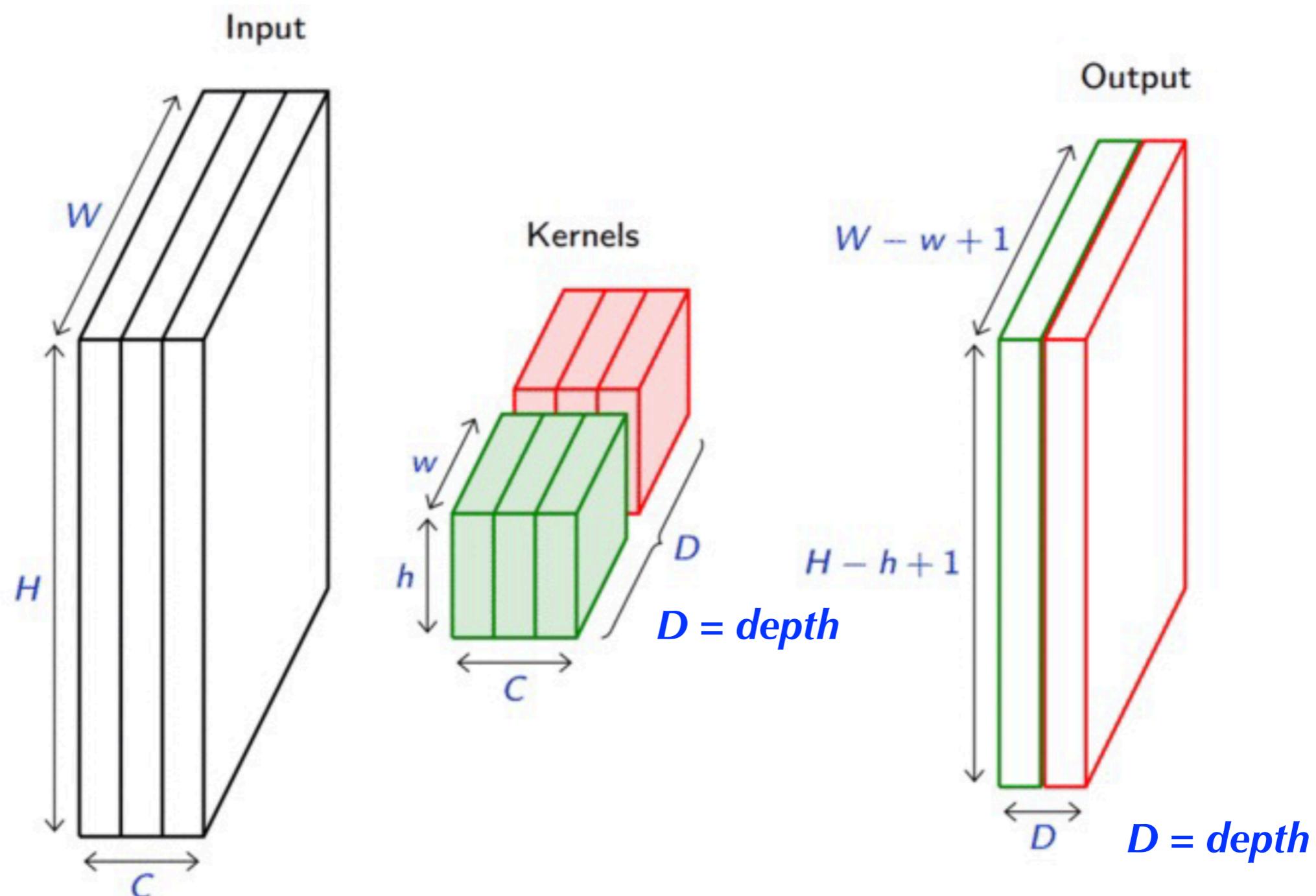
Each of the per-channel processed versions are then summed together to form *one* channel. Each sub-filter produces one processed version of each channel, and then the filter as a whole produces one overall output channel.

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2D CNNs with multiple channels



You can have more than one filter
→ each of them add one more dimension to the output

2D convolutional layers

- Input data is a tensor \mathbf{x} of size $C \times h \times w$

- Learnable filter \mathbf{u} of size $C \times h_k \times w_k$

- the size $h_k \times w_k$ is called the *receptive field*

- Through the convolution operation:

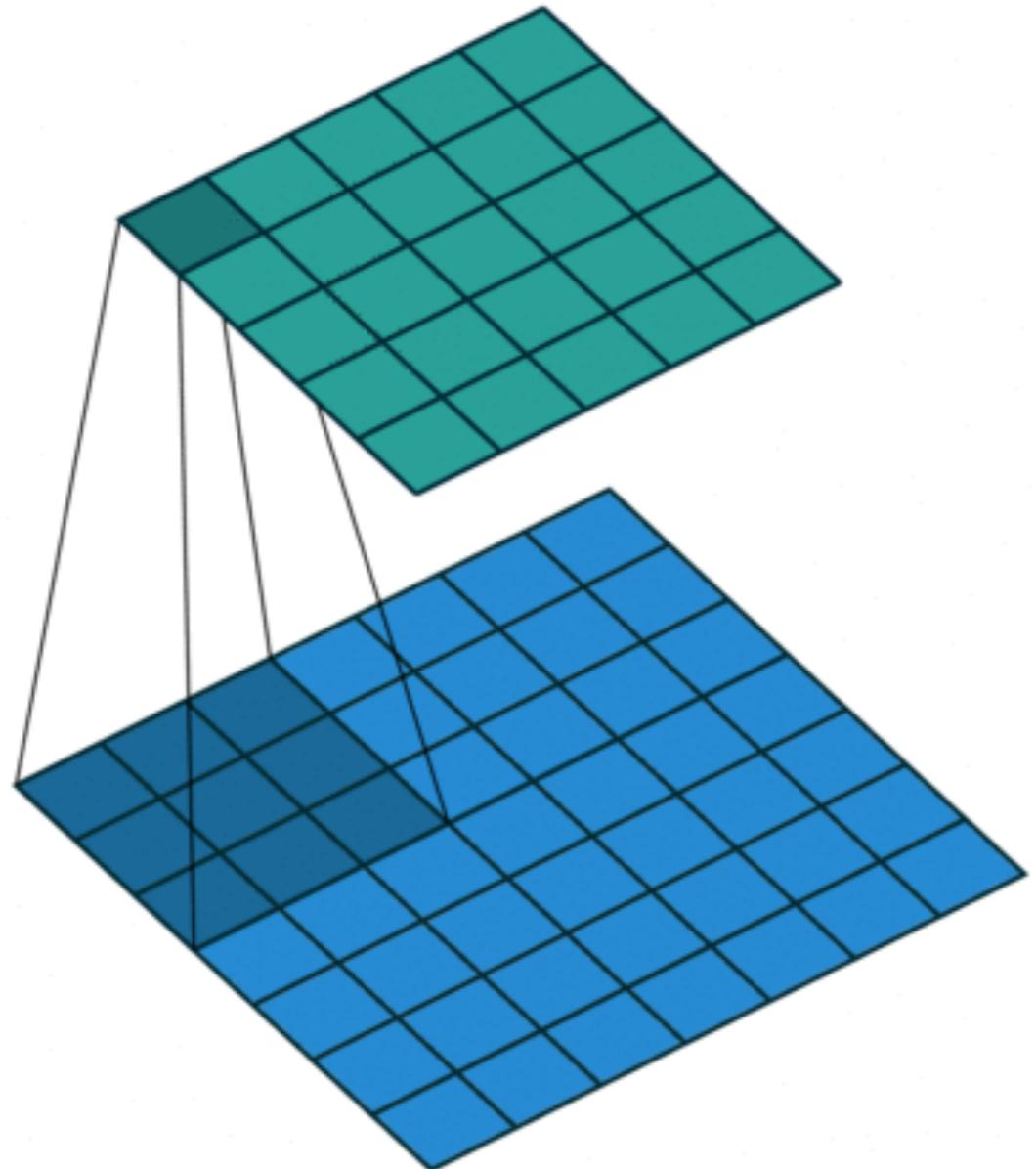
$$(\mathbf{x} \circledast \mathbf{u})_k = \sum_{c=0}^{C-1} (\mathbf{x}_c \circledast \mathbf{u}_c)_k = \sum_{c=0}^{C-1} \sum_{n=0}^{h_k-1} \sum_{m=0}^{w_k-1} x_{c,n+i,m+j} u_{c,n,m}$$

- Scan vector \mathbf{x} by iterating over i and j to get each output element k

- Output size is $(h - h_k + 1) \times (w - w_k + 1)$ for each filter

- often called *activation map* or *output feature map*

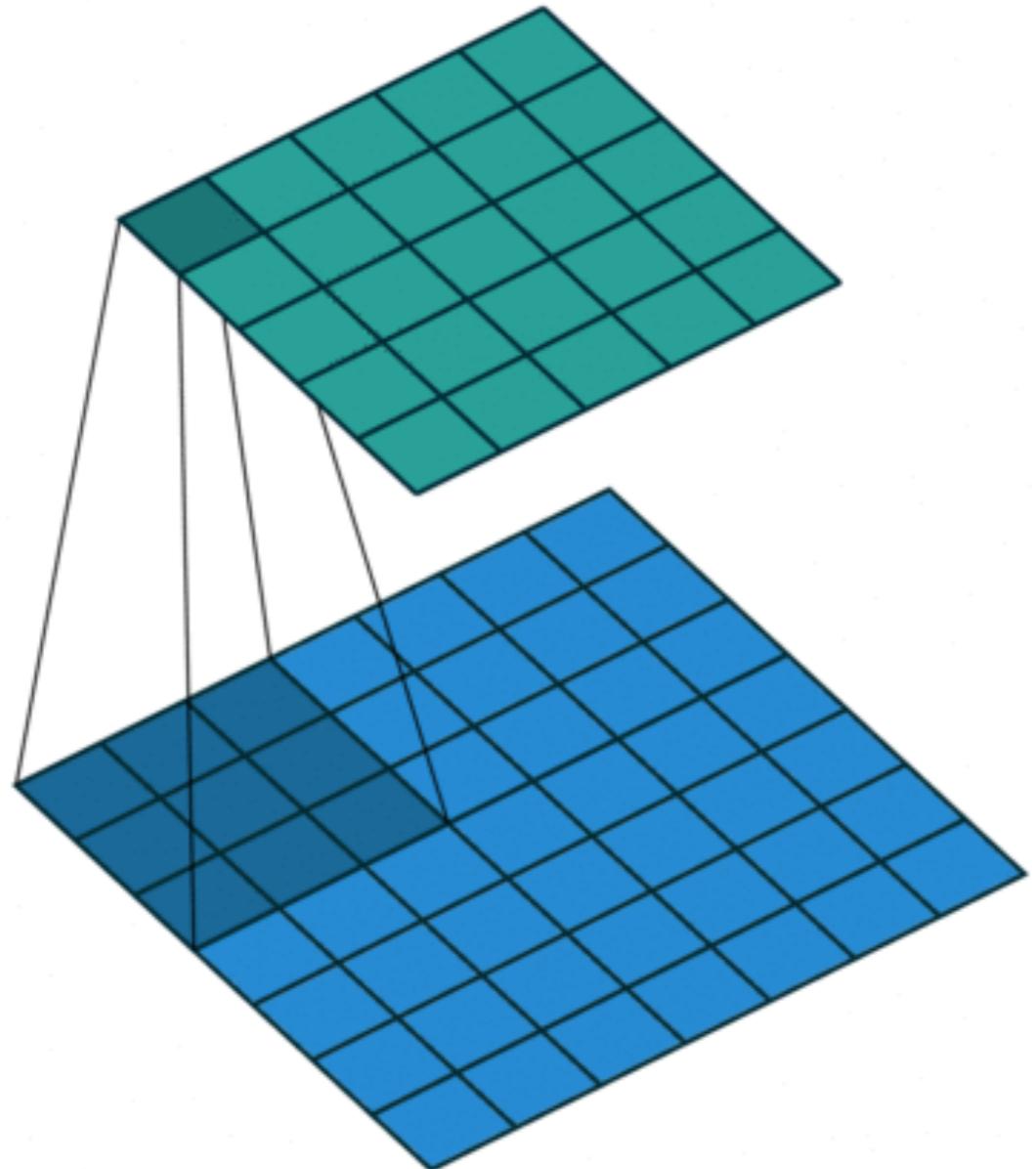
Hyperparameters: stride



**Of how many pixels to move the filter
– this case has stride one but could be larger**

**The stride basically defines how many times you see the same pixels
Caveat: even with stride 1 the corner pixels will be seen only once**

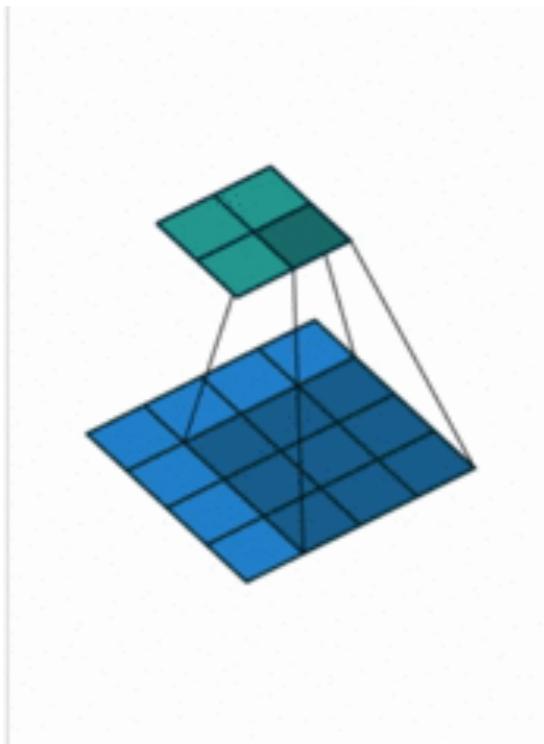
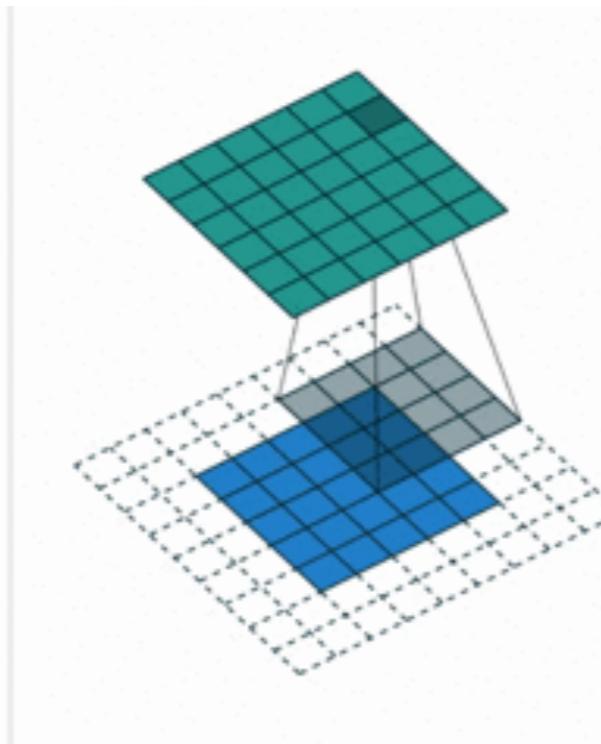
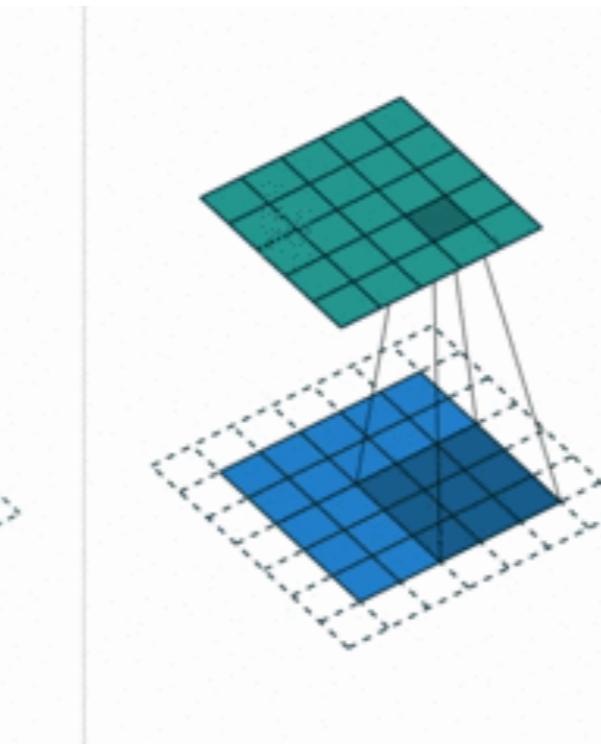
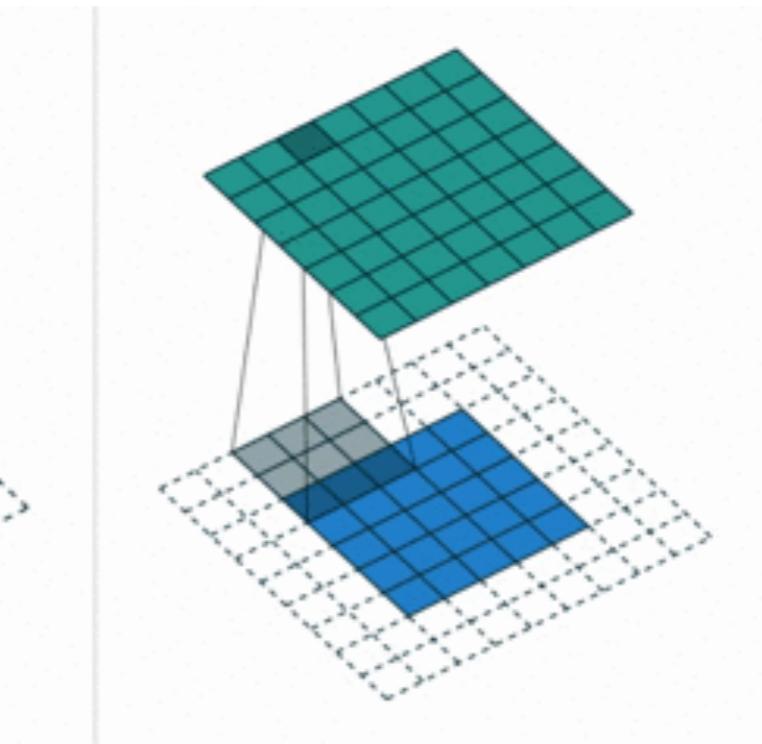
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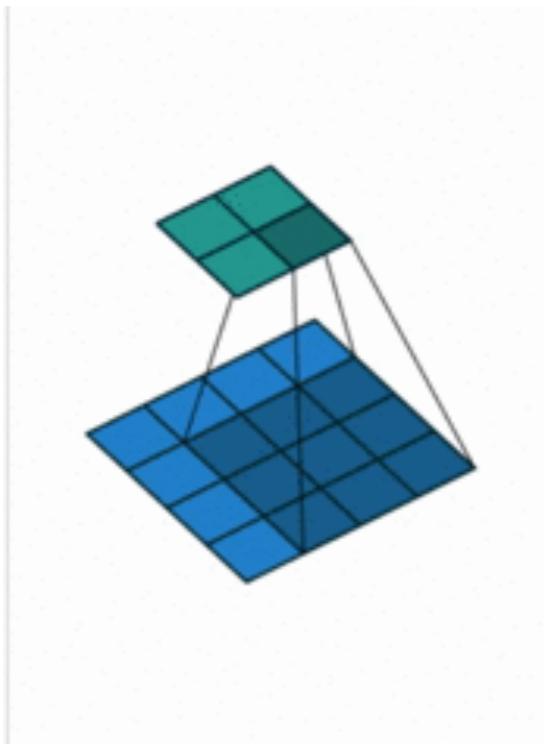
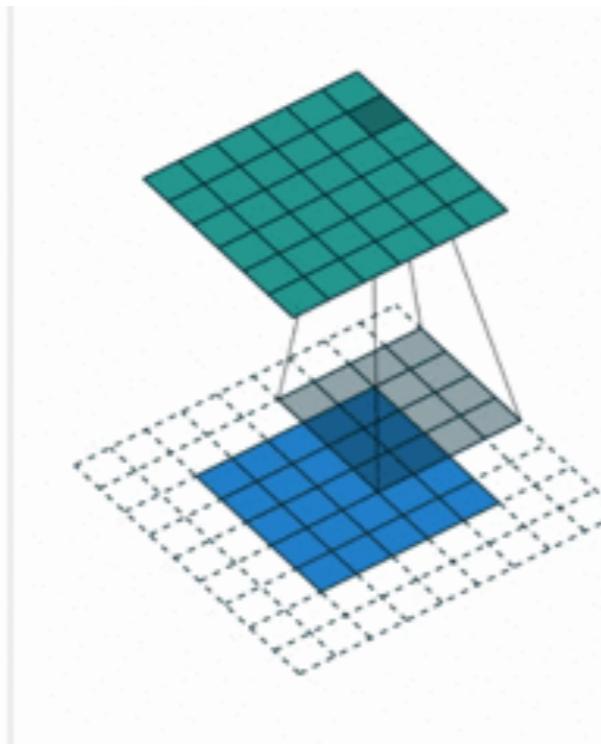
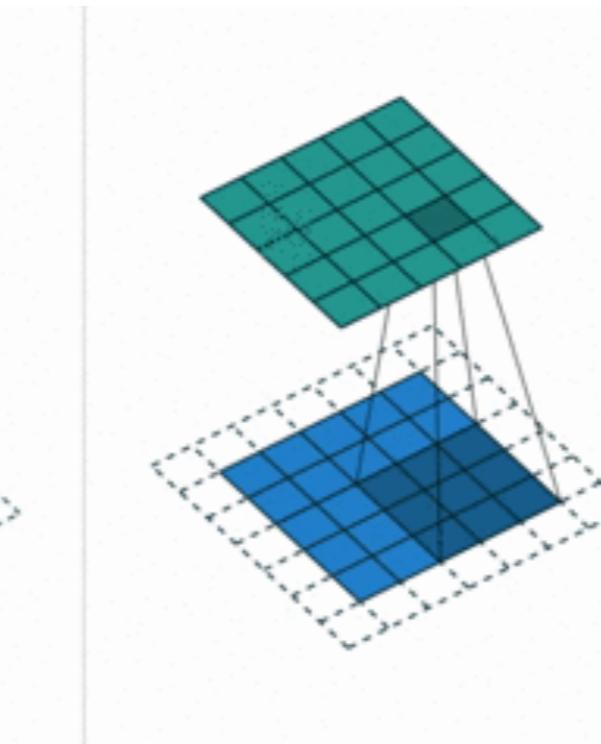
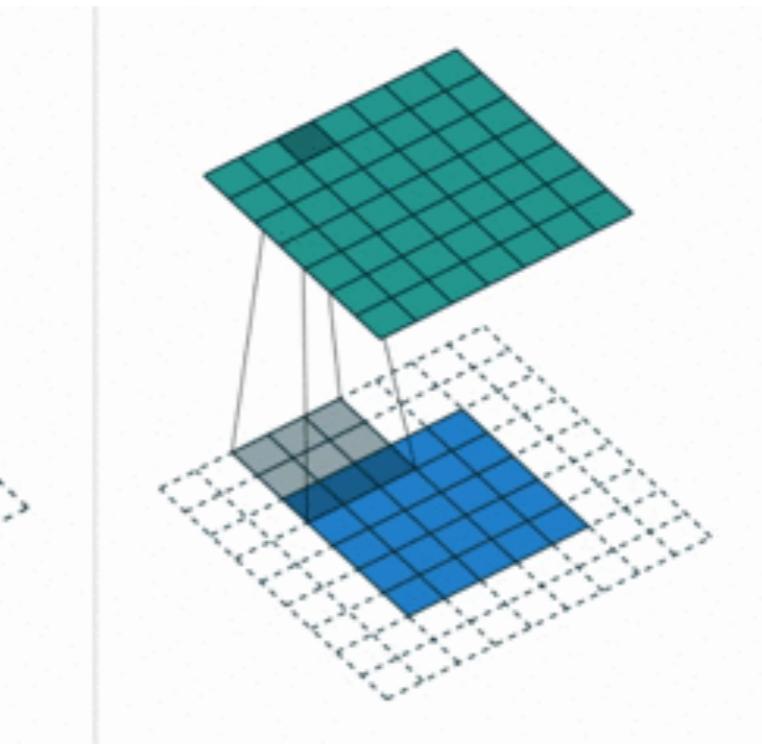
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How about adding zeros at the end so we can move the window and see every number exactly twice? The adding of zeros is called **padding**.

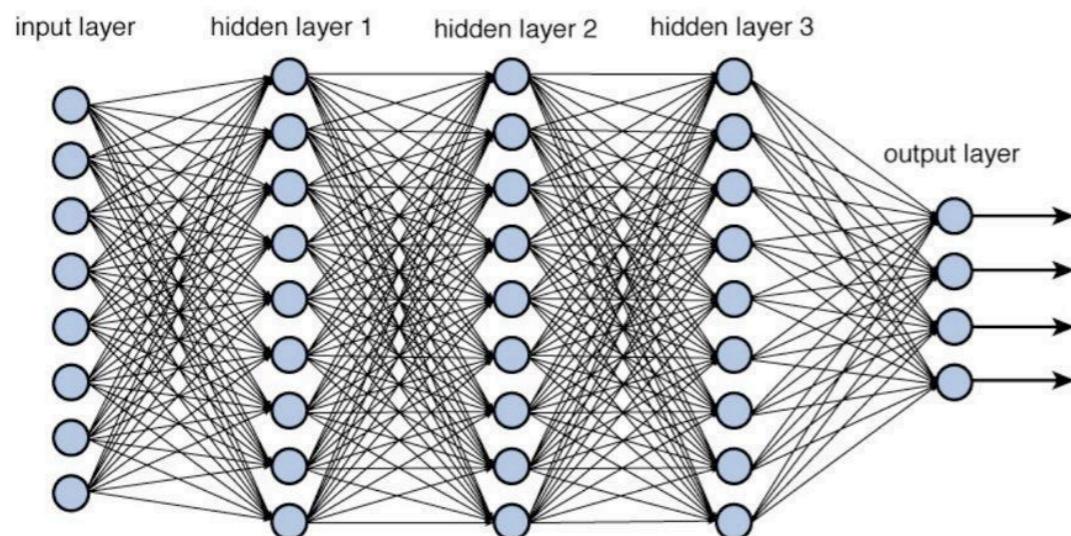
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- Parameters are shared by each neuron producing in the activation map
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 - Data: $256 \times 256 \times 3$ RGB image
 - Kernel: $3 \times 3 \times 3 \rightarrow 27$ weights
 - Fully connected layer: $256 \times 256 \times 3$ inputs $\rightarrow 256 \times 256 \times 3$ neurons $\rightarrow O(10^{10})$ weights
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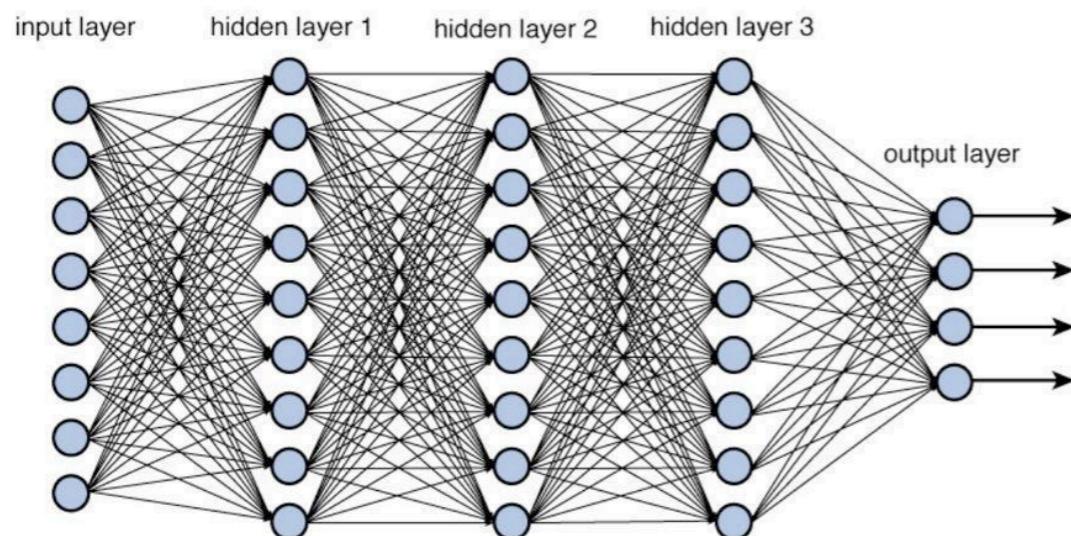


3_0	3_1	2_2	1	0
0_2	0_2	1_0	3	1
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Dimensionality reduction: pooling

- Its function is to progressively reduce the spatial size of the representation to reduce the amount of parameters and computation in the network
- It also makes processing independent to local features (distortion, translation)

- **MaxPooling:** given an image and a filter of size $h \times w$, scans the image and replaces each $h_p \times w_p$ patch with its maximum

0	3	5	6	2	4	5
7	4	7	3	6	3	4
9	1	2	1	9	6	0
9	2	1	1	7	3	5
8	0	4	7	6	8	0
8	3	4	5	5	3	4
7	9	4	6	5	2	6



9	7	9	9	9
9	7	9	9	9
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9	9	7	8	8

- **AveragePooling:** given an image and a filter of size $h \times w$, scans the image and replaces each $h_p \times w_p$ patch with its average

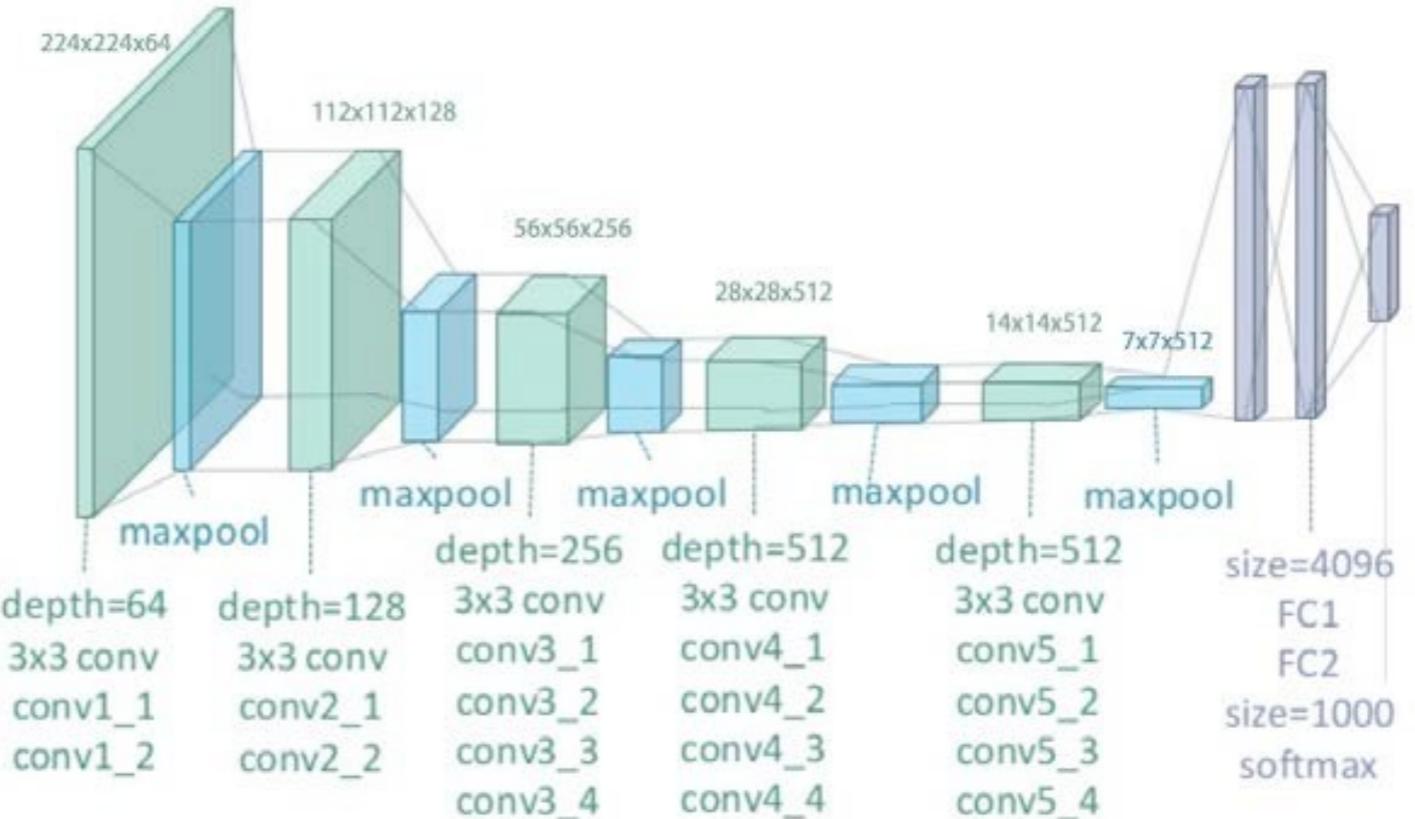
0	3	5	6	2	4	5
7	4	7	3	6	3	4
9	1	2	1	9	6	0
9	2	1	1	7	3	5
8	0	4	7	6	8	0
8	3	4	5	5	3	4
7	9	4	6	5	2	6



4.2
5.0

The final CNN model

- A full 2D CNN is a sequence of 2D CNN+Pooling layers
- The 2D CNN+Pooling layers reduces the 2D image representation
- The use of multiple filters on the image make the output grow on a third dimension
- Eventually, flattening occurs and the result is given to one or two MLP layers (e.g., for classification)



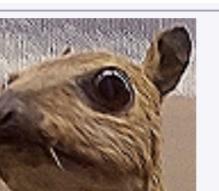
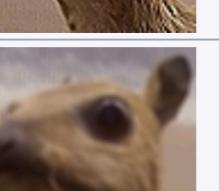
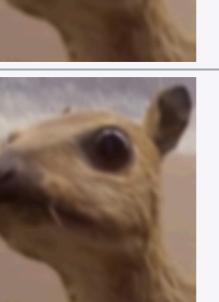
What does a CNN learn?

- Each filter alters the image in a different way, picking up different aspects of the image

- edges oriented in various ways
- enhancing / blurring of certain features

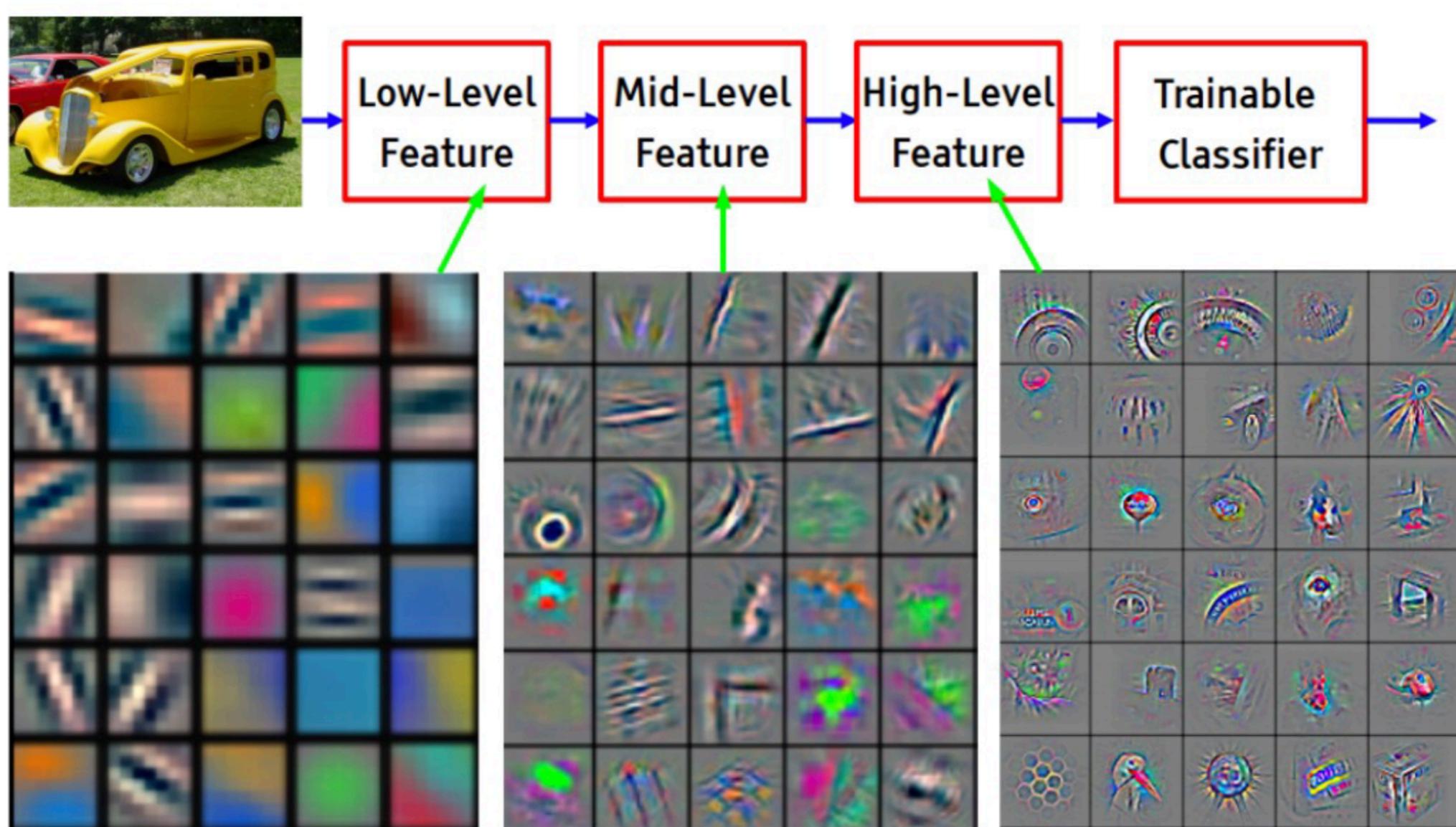
- In CNNs, filters are not defined: the value of each filter is learned during the training process.

- By being able to learn the values of different filters, CNNs can find more meaning from images that human designed filters might not be able to find

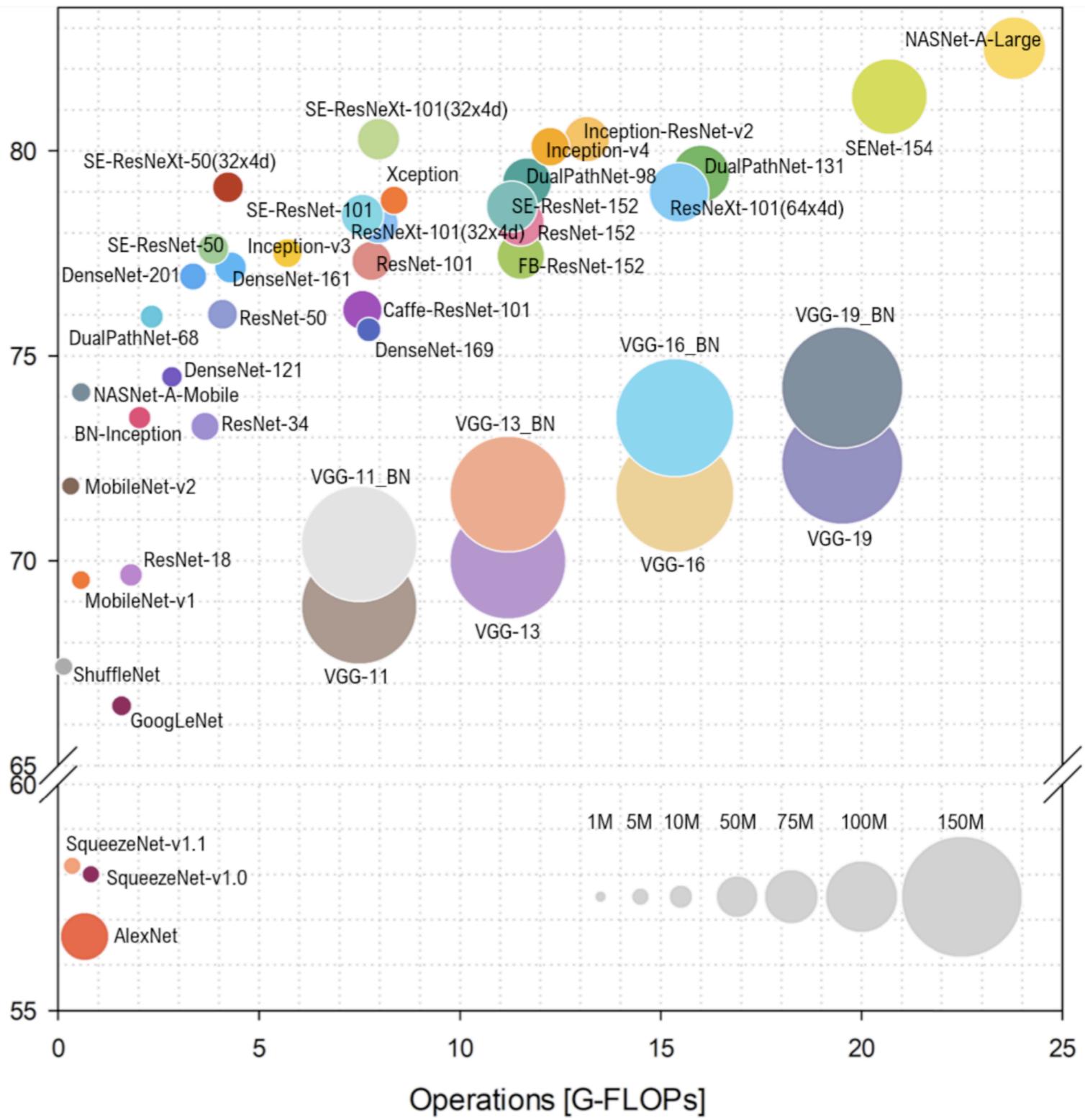
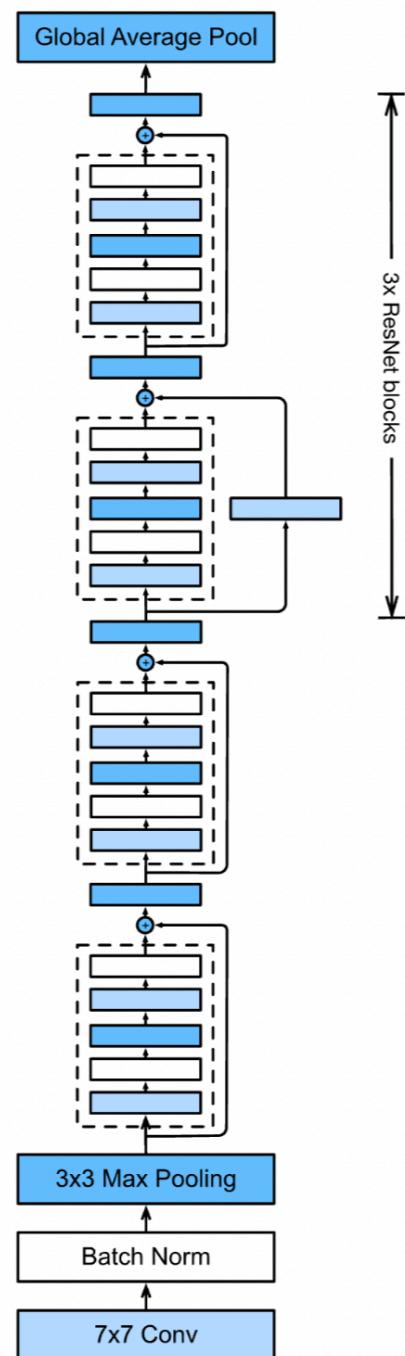
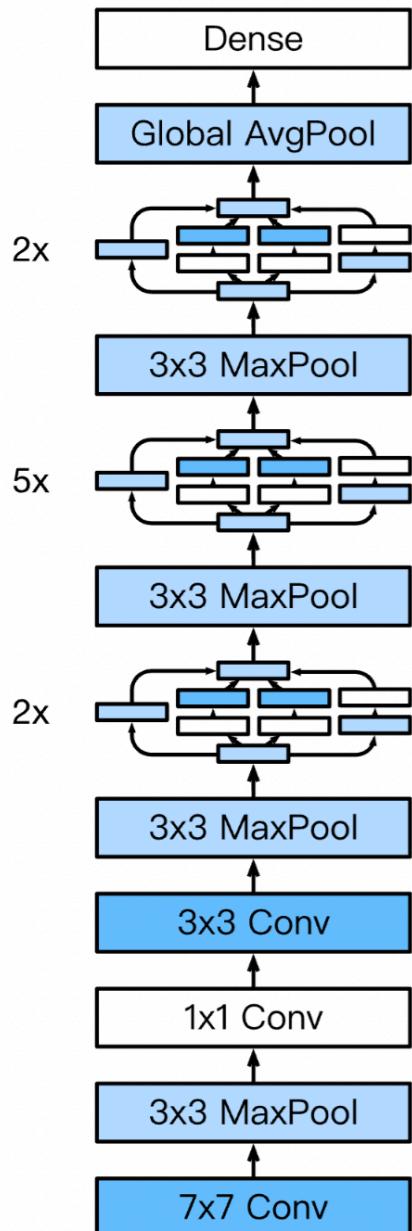
Operation	Kernel ω	Image result $g(x,y)$
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	
Edge detection	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Box blur (normalized)	$\frac{1}{9} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	
Gaussian blur 3×3 (approximation)	$\frac{1}{16} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	

What does a CNN learn?

- The 1st layers appear to encode direction and color
 - The direction and color filters get combined into grid and spot textures
 - These textures gradually get combined into increasingly complex patterns
- The network appears to learn a **hierarchical composition of patterns**



Deep CNNs



Residual connection

- Observation that deeper models leads to higher training errors → performance degradation problem due to vanishing gradient

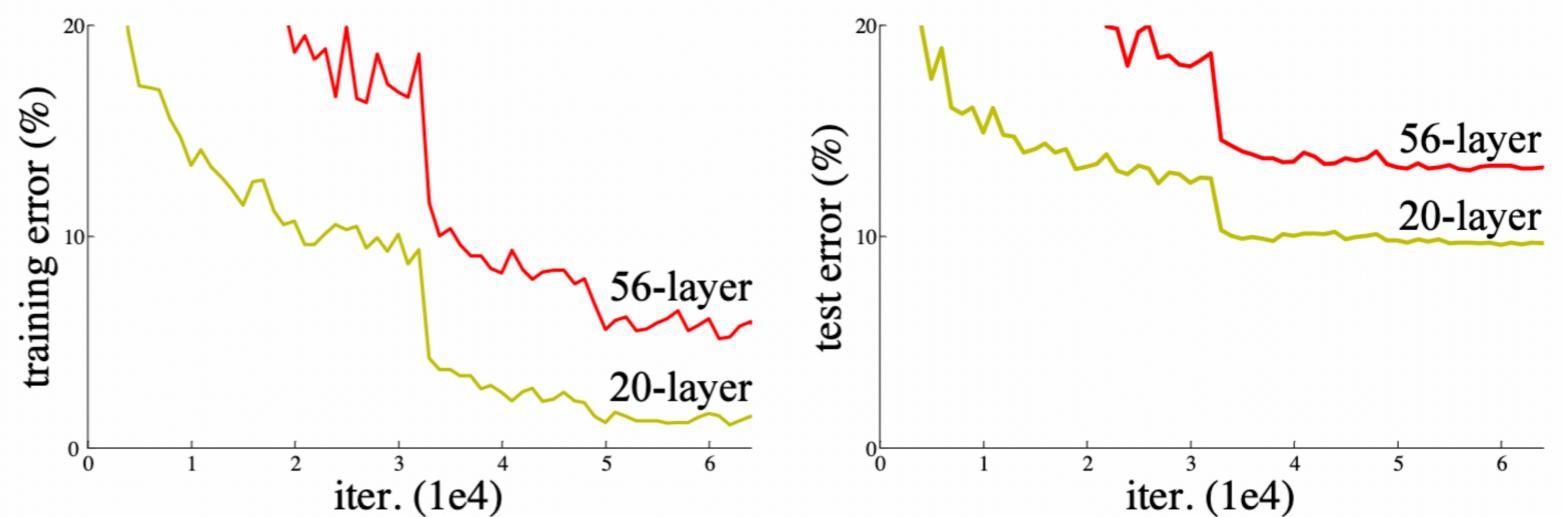
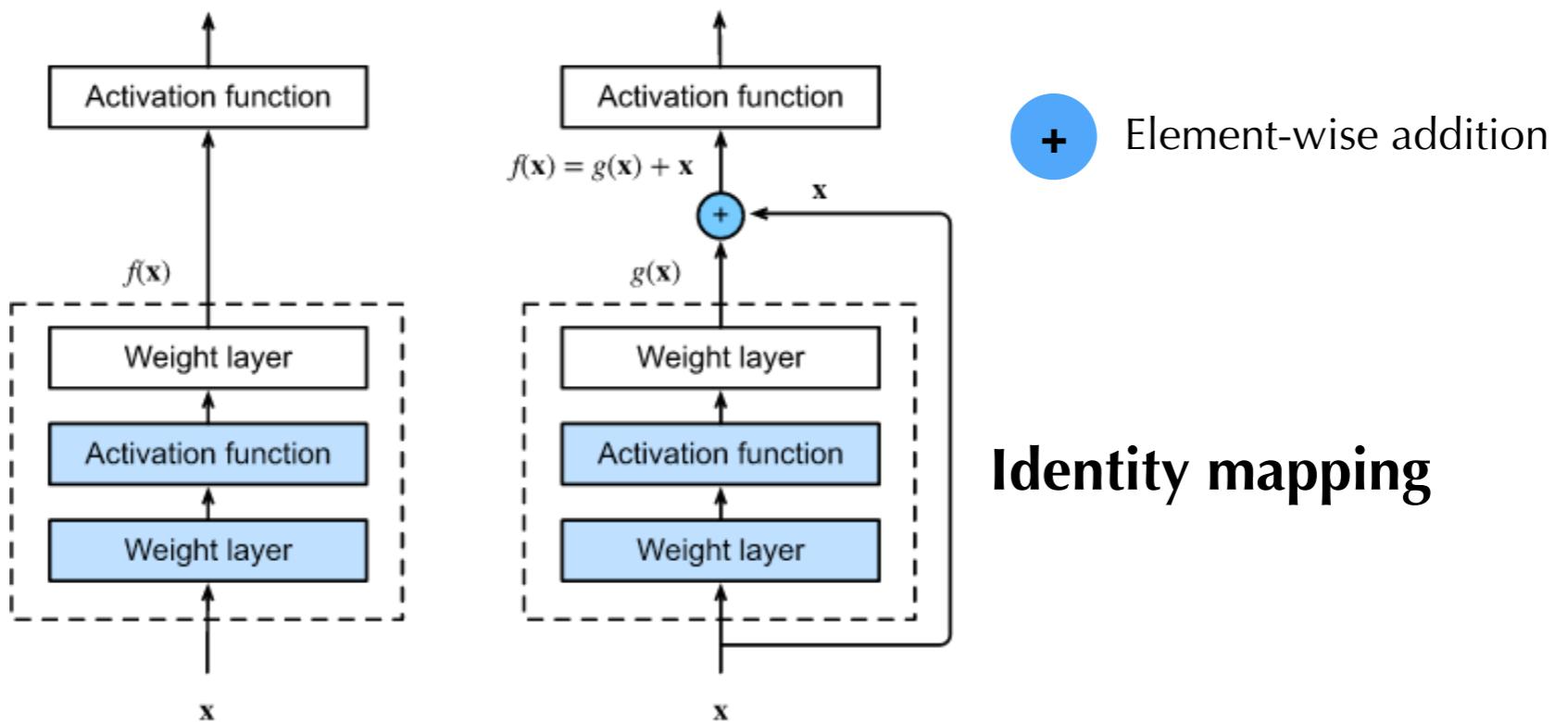


Figure 1. Training error (left) and test error (right) on CIFAR-10 with 20-layer and 56-layer “plain” networks. The deeper network has higher training error, and thus test error. Similar phenomena on ImageNet is presented in Fig. 4.

Residual connection

- Observation that deeper models leads to higher training errors → performance degradation problem due to vanishing gradient
- Breakthrough from Microsoft researchers was to introduced **residual connections** (also called *skip connections*):
 - instead of hoping that each stacked layer directly learn the underlying mapping $f(\mathbf{x})$ let them learn the residual mapping $g(\mathbf{x}) = f(\mathbf{x}) - \mathbf{x}$
 - intuition: if an identity mapping $f(\mathbf{x}) = \mathbf{x}$ were optimal, it would be easier to push the residual to zero than to fit an identity mapping by a stack of non-linear layers

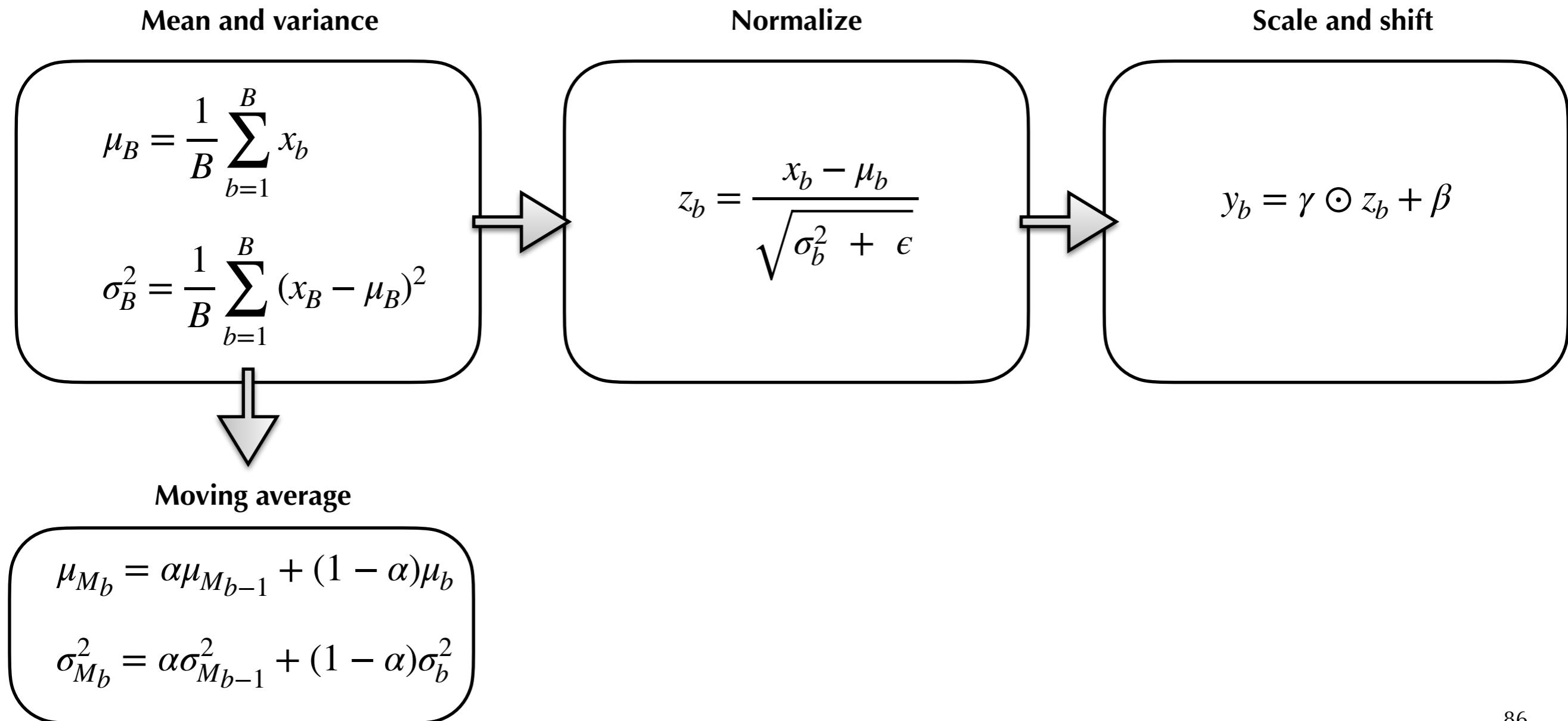


[Source]

Batch Normalization

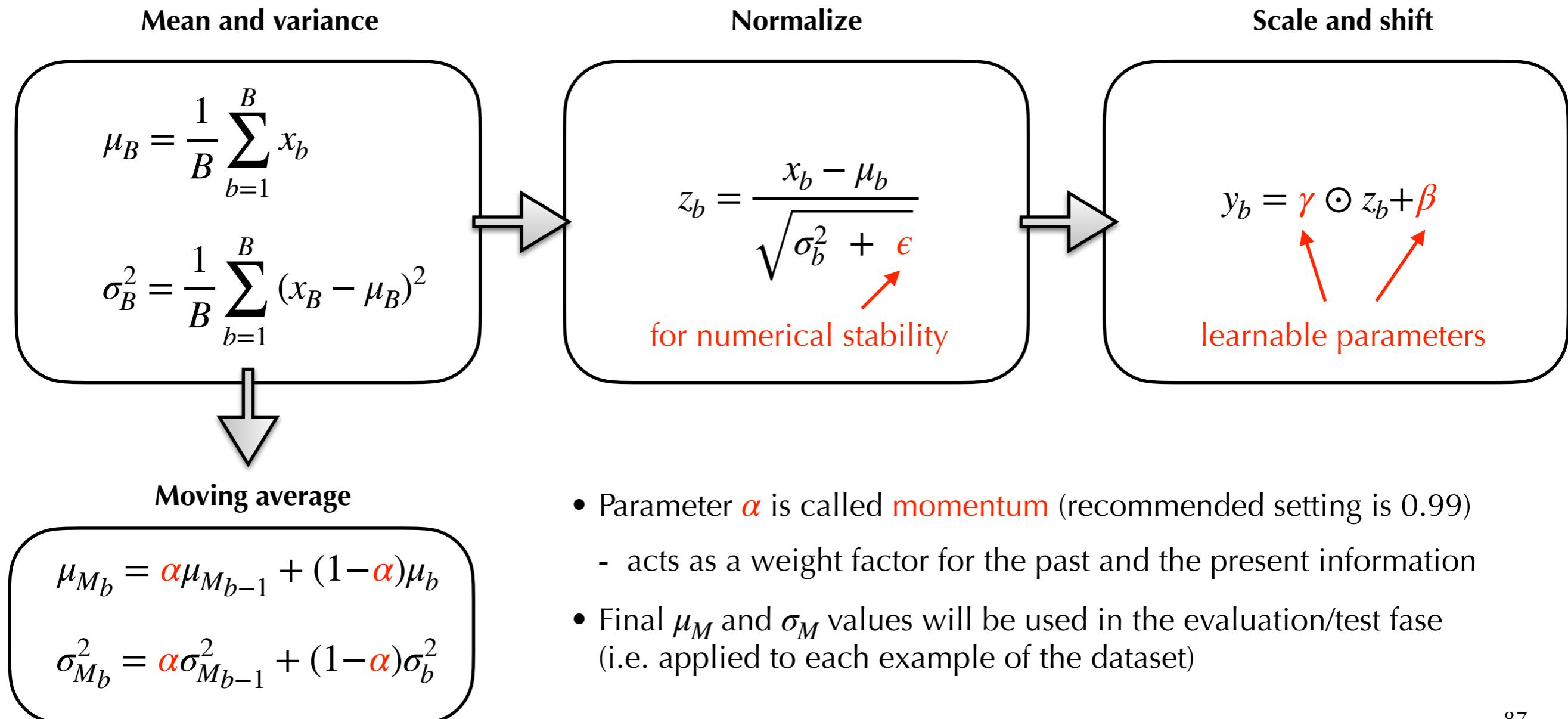
Batch Normalization

- Training deep NNs is also complicated by the fact that the distribution of each layer's inputs changes during training as the parameters of the previous layers change
- Solution: during training **batch normalization** shifts and rescales each layer output according to the mean and variance estimated on the batch



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Batch Normalization

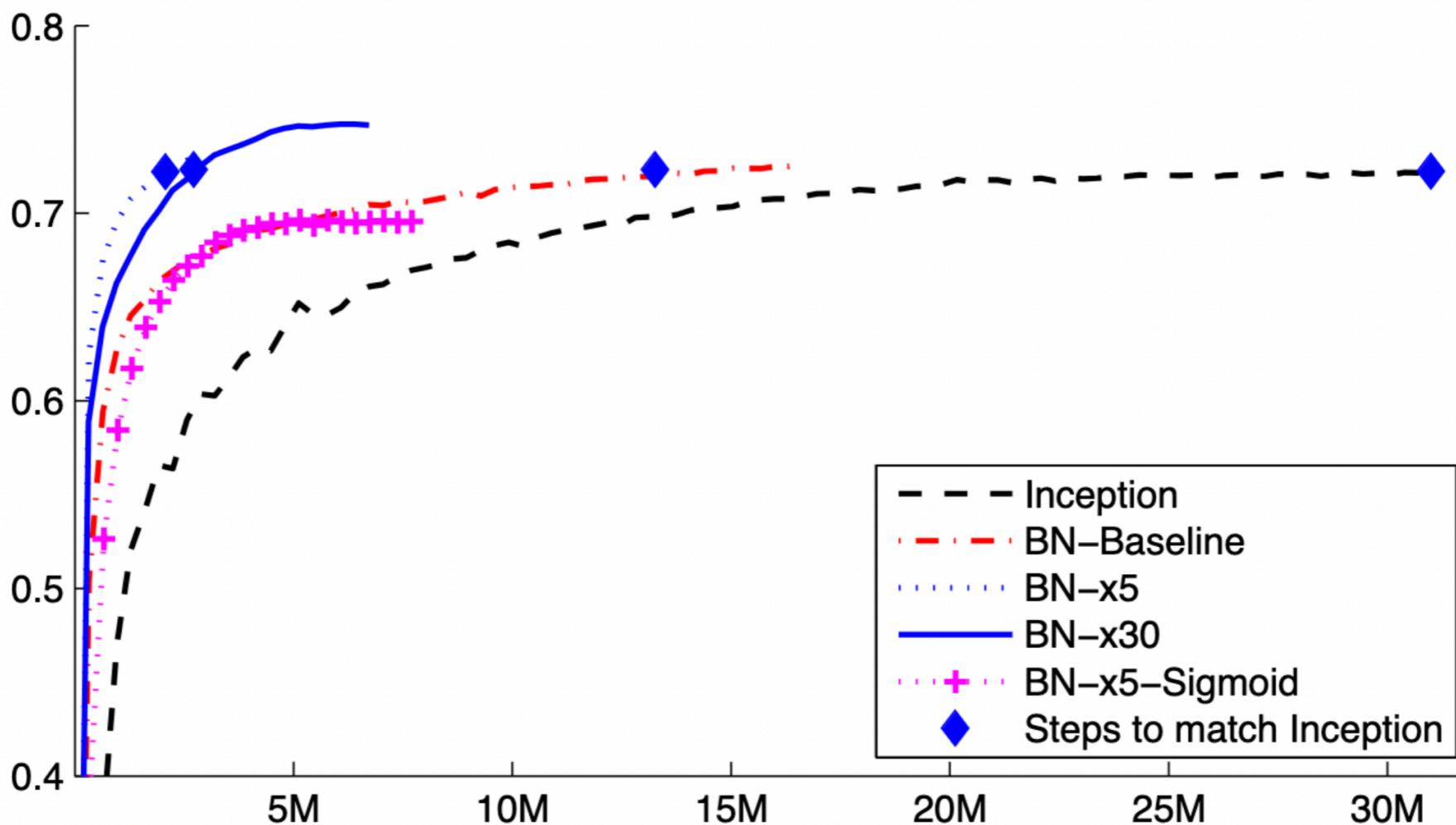


Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

[Source]

Summary lecture #2

- Today we discussed Neural Networks as a tool to model the data beyond linear correlations
- We have seen how Deep Neural Networks like Convolutional NN can extract useful representations for the task from raw-level data
- During the course we will see many other architectures and how they adapt to the data and task at hand
 - tomorrow: recurrent and graph neural networks
- This afternoon we will see a first implementation of deep neural networks using Keras for a typical task at LHC experiments