Dive into Deep Learning

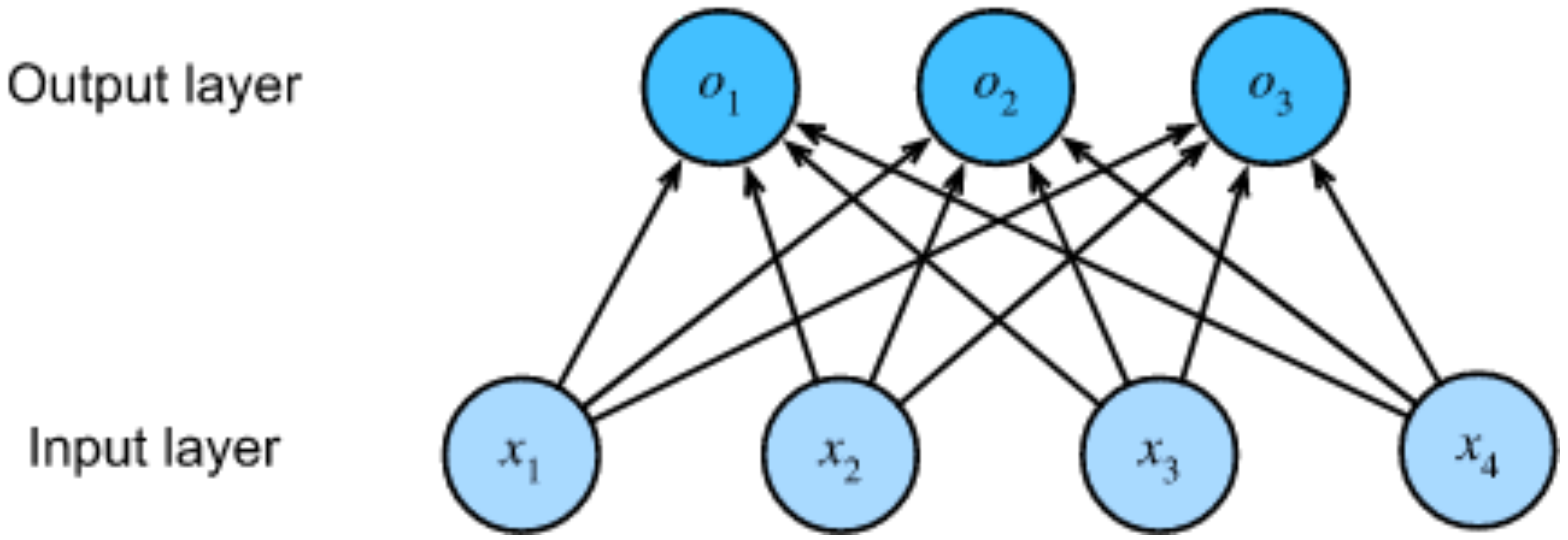
Chapter 4. Multilayer Perceptrons

Wayne L, Oct 18, 2020

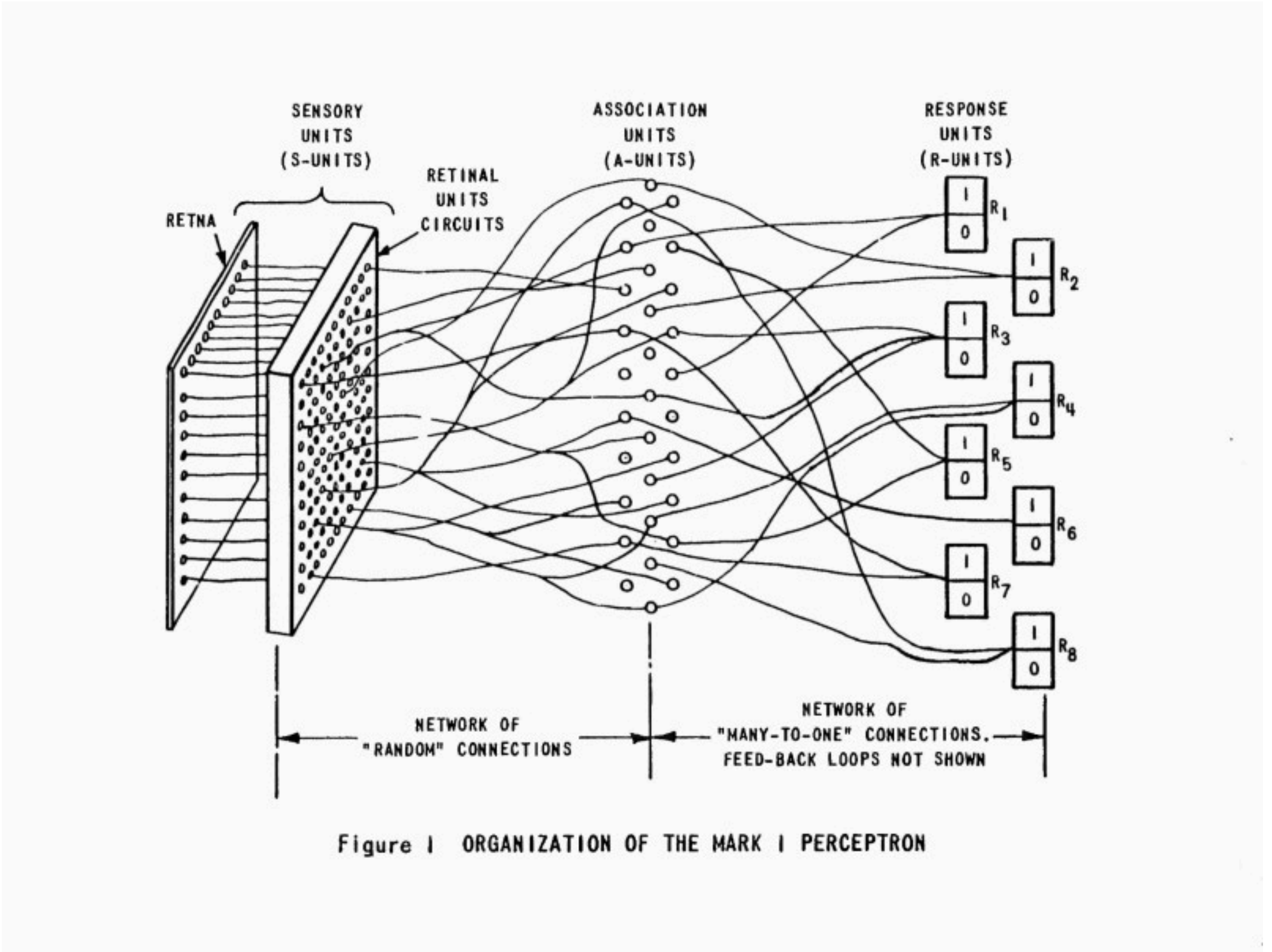
Previously

Perceptron (Linear = Single = Simple = Feedforward)

- This model mapped our inputs directly to our outputs via single affine transformation, followed by a softmax operation.



$$y = \mathbf{wx} + b$$

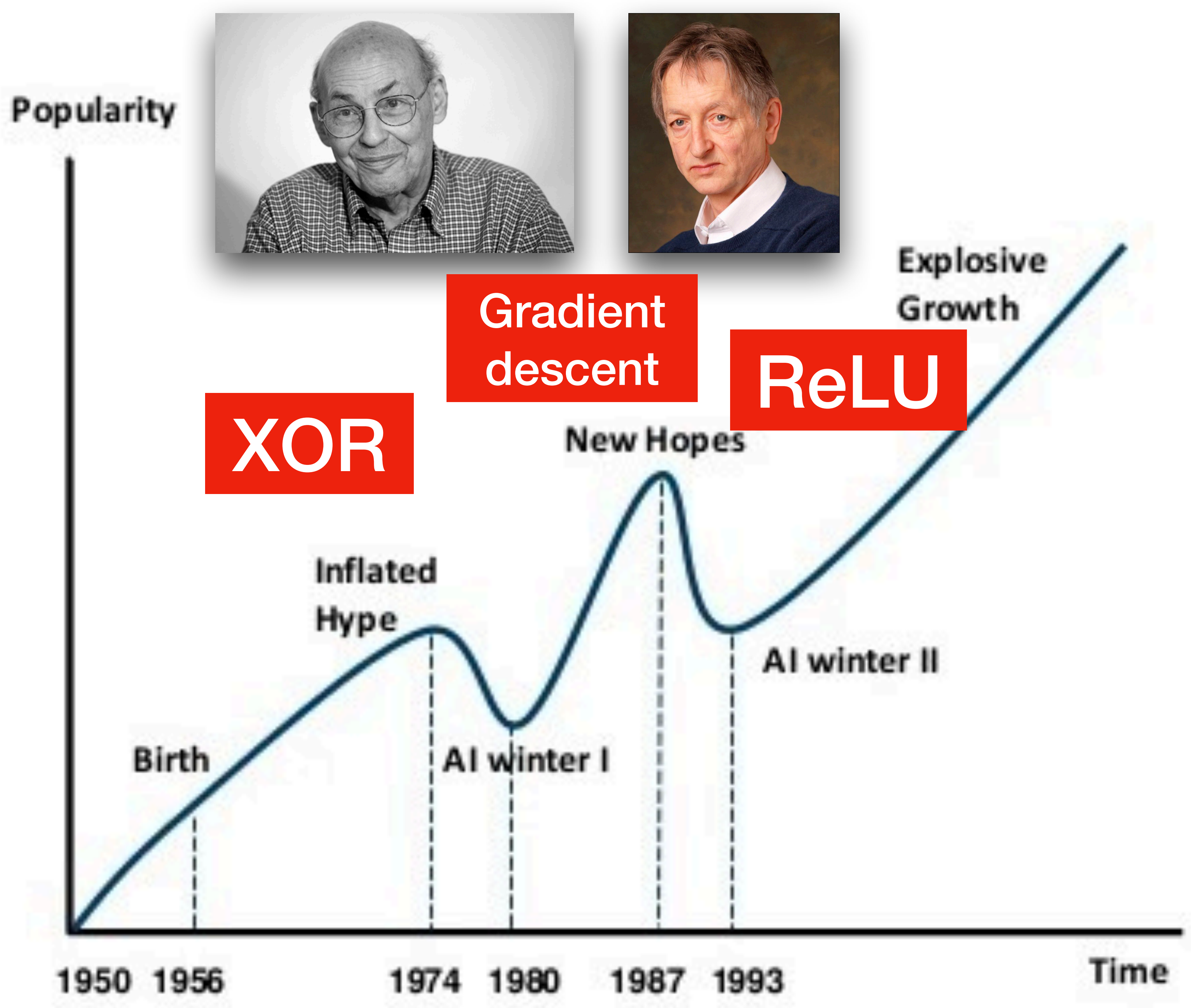


Mark 1 Perceptron (1959), Frank Rosenblatt

Previously

AI History

AI HAS A LONG HISTORY OF BEING "THE NEXT BIG THING"...

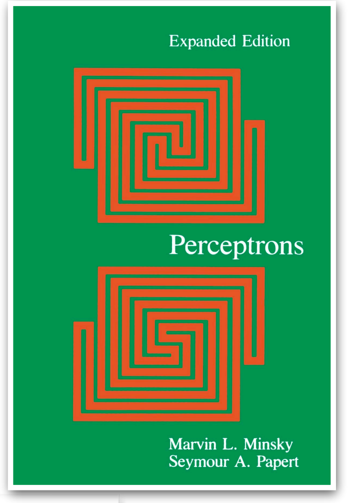


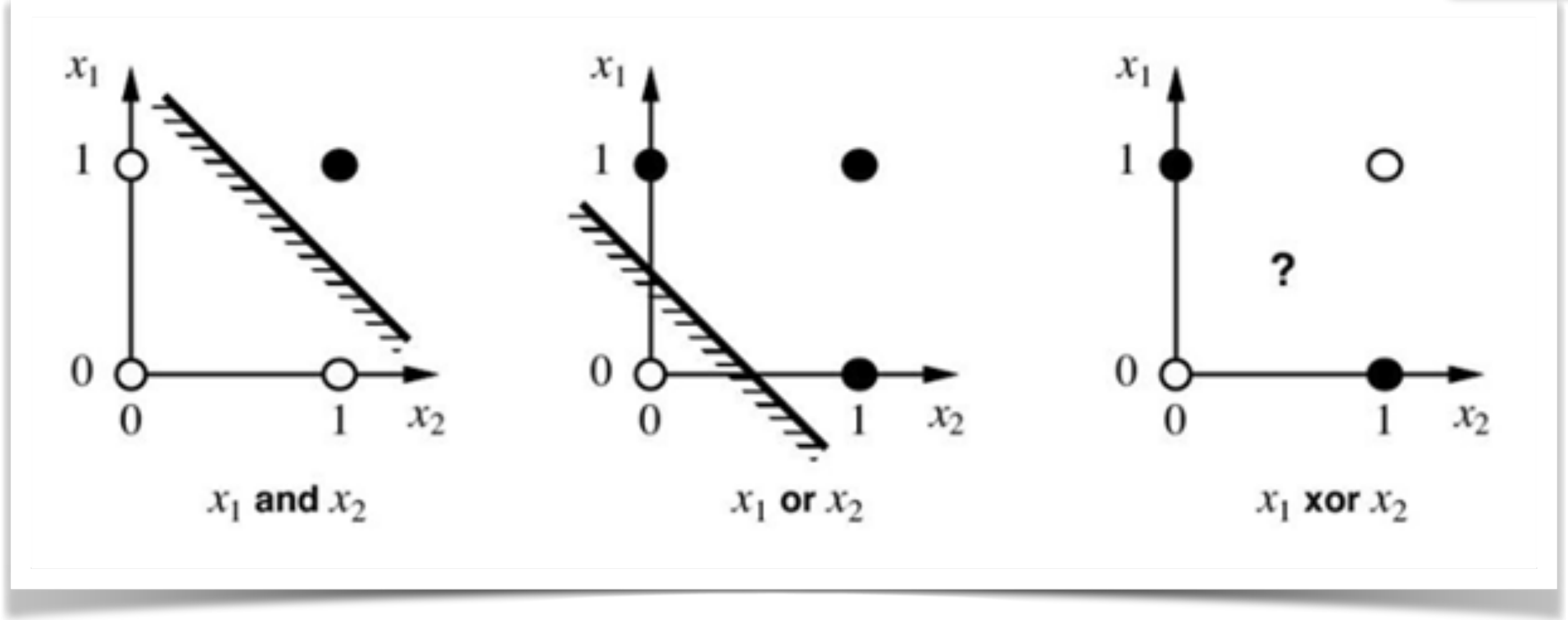
Timeline of AI Development

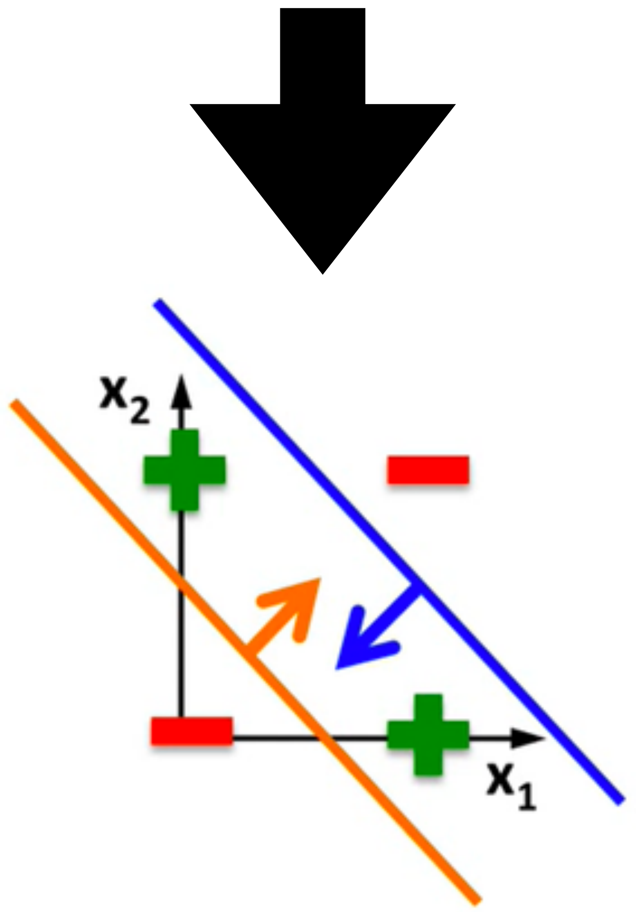
- **1950s-1960s**: First AI boom - the age of reasoning, prototype AI developed
- **1970s**: AI winter I
- **1980s-1990s**: Second AI boom: the age of Knowledge representation (appearance of expert systems capable of reproducing human decision-making)
- **1990s**: AI winter II
- **1997**: Deep Blue beats Gary Kasparov
- **2006**: University of Toronto develops Deep Learning
- **2011**: IBM's Watson won Jeopardy
- **2016**: Go software based on Deep Learning beats world's champions

XOR

Perceptrons (1969), Marvin minsky







No one on earth had found a viable way to train

Multilayer Perceptrons

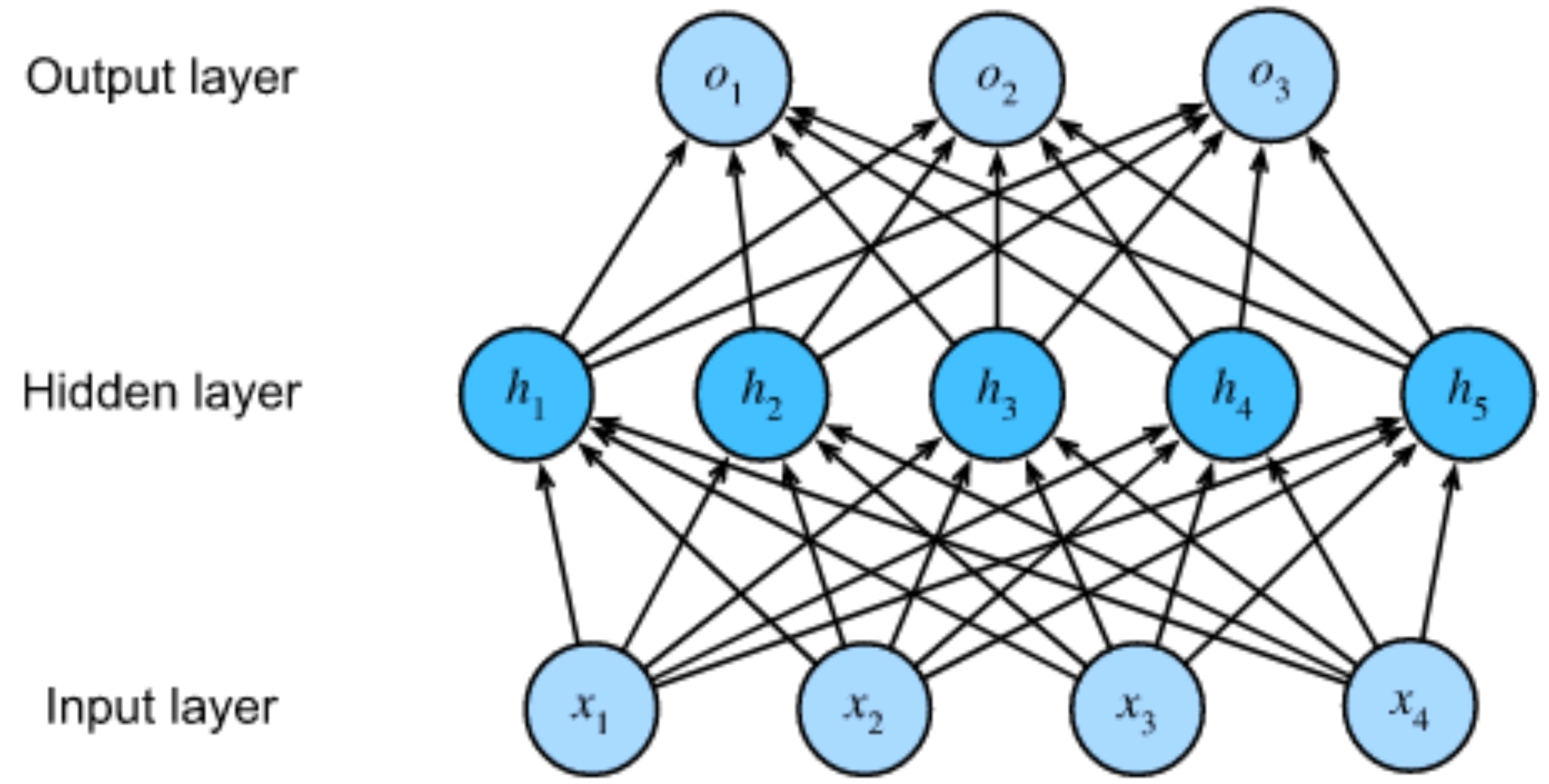
Perceptrons (Multi = Deep feedforward)

- The goal of a feedforward network is to approximate some function f^*.

- For example, for a classifier, $y = f^*(x)$ maps an input x to a category y.
  A feedforward network defines a mapping $\mathbf{y} = f(x; \theta)$ and learns the value of the parameters θ that result in the best function approximation.

- ***Universal approximation theorem*** means that regardless of what function we are trying to learn, we know that a large MLP will be able to represent this function.

$$f(x) = f^*(x) \approx y$$



$$\mathbf{O} = \mathbf{H}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}$$

$$\mathbf{H} = \mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)}$$

$$\mathbf{W} = \mathbf{W}^{(1)}\mathbf{W}^{(2)}$$
$$\mathbf{b} = \mathbf{b}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}$$

$$\mathbf{O} = (\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)})\mathbf{W}^{(2)} + \mathbf{b}^{(2)} = \mathbf{X}\mathbf{W}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)} = \mathbf{X}\mathbf{W} + \mathbf{b}$$

Even though MLP is going deeper, it can be equivalent with single-layer model !

Multilayer Perceptrons

From Linear to Nonlinear

- In order to realize the potential of multilayer architectures, we need one more key ingredient: a nonlinear *activation function* σ to be more ***expressive***.
- MLPs are ***universal approximators***, however, it doe not mean that we can solve all of problems with MLPs. In fact, we can approximate many functions much more compactly by using deeper (or wider) networks.
- Each neuron acts as a ***linear SVM***, however, …
  - its output is not interpreted immediately,
  - but it becomes a new feature,
  - to be forwarded to the next layer for further analysis **#SVMcascade**

$$\mathbf{H}^{(1)} = \sigma_1(\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)})$$

$$\mathbf{H}^{(2)} = \sigma_2(\mathbf{H}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)})$$

Multilayer Perceptrons

Activation function

- ***Activation function*** decide whether a neuron should be activated or not by calculating the weighted sum and further adding bias with it.
- They are ***differentiable*** operators to transform input signal to outputs, while most of them add non-linearity.

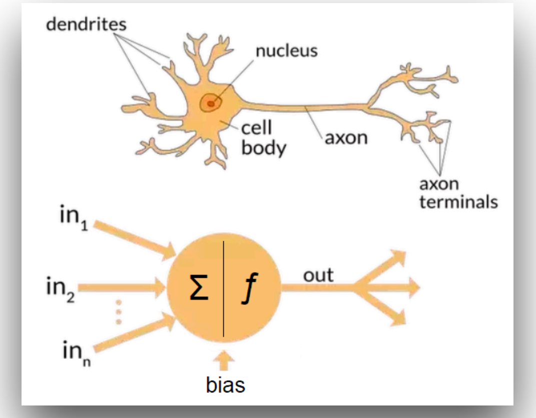
`nn.ELU`	Applies the element-wise function:
`nn.Hardshrink`	Applies the hard shrinkage function element-wise:
`nn.Hardsigmoid`	Applies the element-wise function:
`nn.Hardtanh`	Applies the HardTanh function element-wise
`nn.Hardswish`	Applies the hardswish function, element-wise, as described in the paper:
`nn.LeakyReLU`	Applies the element-wise function:
`nn.LogSigmoid`	Applies the element-wise function:
`nn.MultiheadAttention`	Allows the model to jointly attend to information from different representation subspaces.
`nn.PReLU`	Applies the element-wise function:
`nn.ReLU`	Applies the rectified linear unit function element-wise:
`nn.ReLU6`	Applies the element-wise function:
`nn.RReLU`	Applies the randomized leaky rectified liner unit function, element-wise, as described in the paper:
`nn.SELU`	Applied element-wise, as:
`nn.CELU`	Applies the element-wise function:
`nn.GELU`	Applies the Gaussian Error Linear Units function:
`nn.Sigmoid`	Applies the element-wise function:
`nn.Softplus`	Applies the element-wise function:
`nn.Softshrink`	Applies the soft shrinkage function elementwise:
`nn.Softsign`	Applies the element-wise function:
`nn.Tanh`	Applies the element-wise function:
`nn.Tanhshrink`	Applies the element-wise function:
`nn.Threshold`	Thresholds each element of the input Tensor.

https://pytorch.org/docs/stable/nn.html#non-linear-activations-weighted-sum-nonlinearity

Multilayer Perceptrons

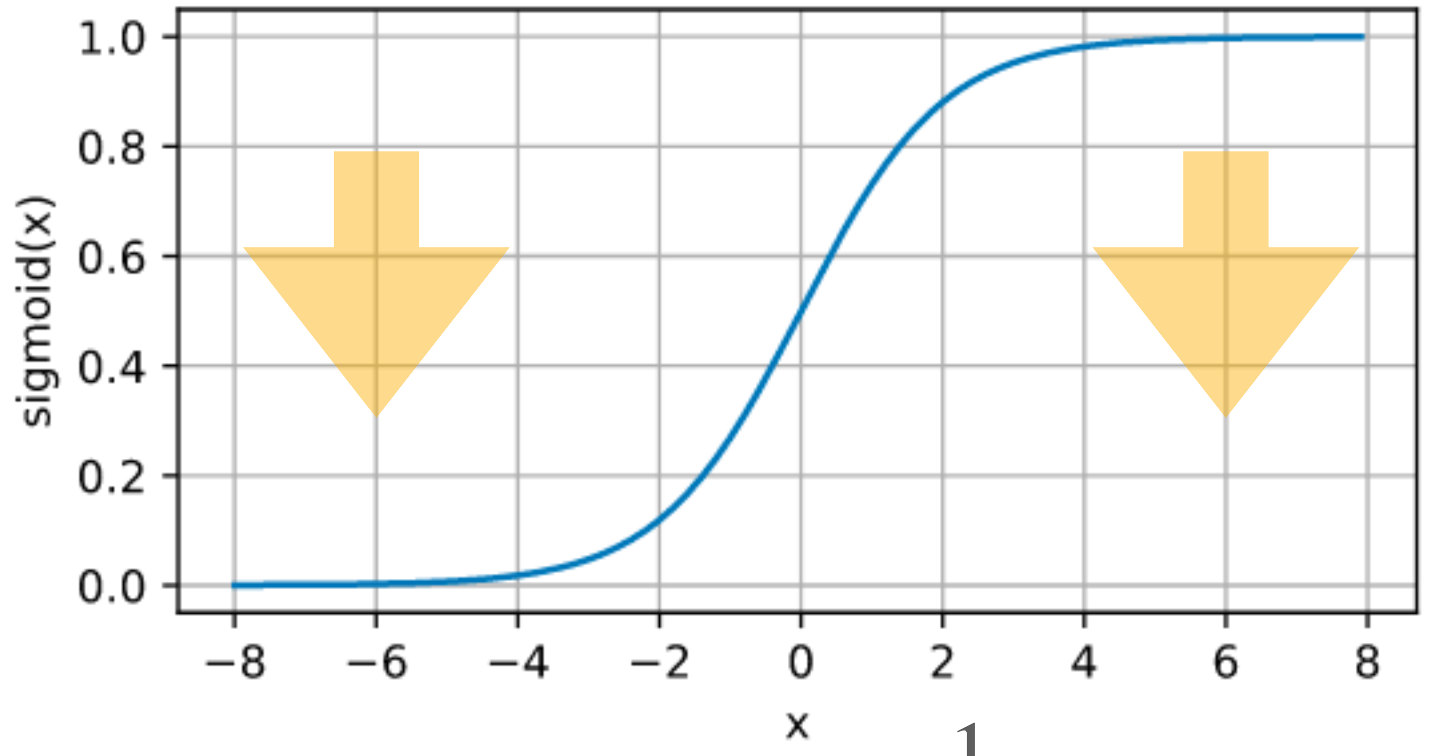
Sigmoid

- In the earliest neural networks, scientists were interested in modeling biological neurons which either fire or do not fire.

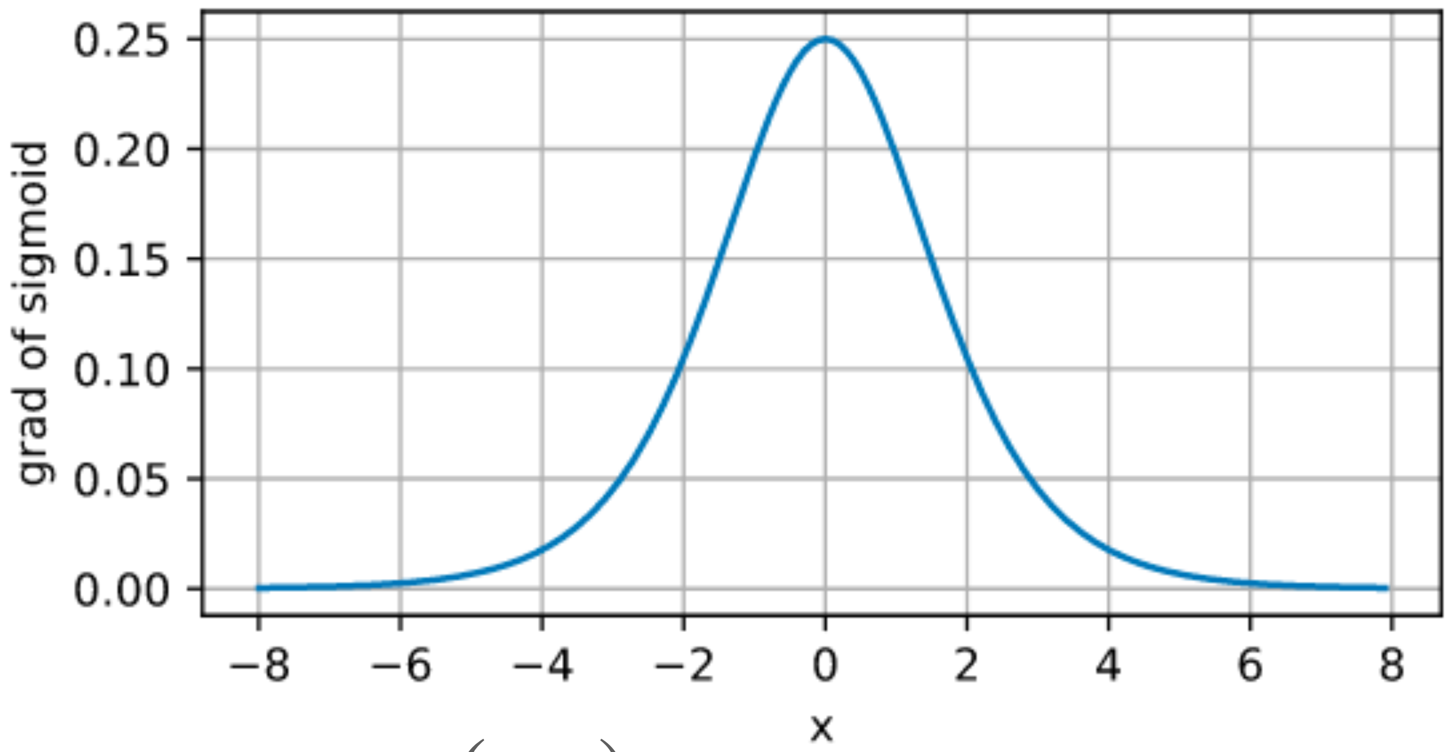


- When attention shifted to gradient based learning, the sigmoid funciton was a natural choice because it is a smooth, differentiable approximation to a thresholding unit.

- widely used as activation functions on the output units, when we want to interpret the outputs as probabilities for binary classification problems (special case of the softmax).



$$sigmoid(x) = \frac{1}{1 + exp(-x)}$$



vanishing gradient

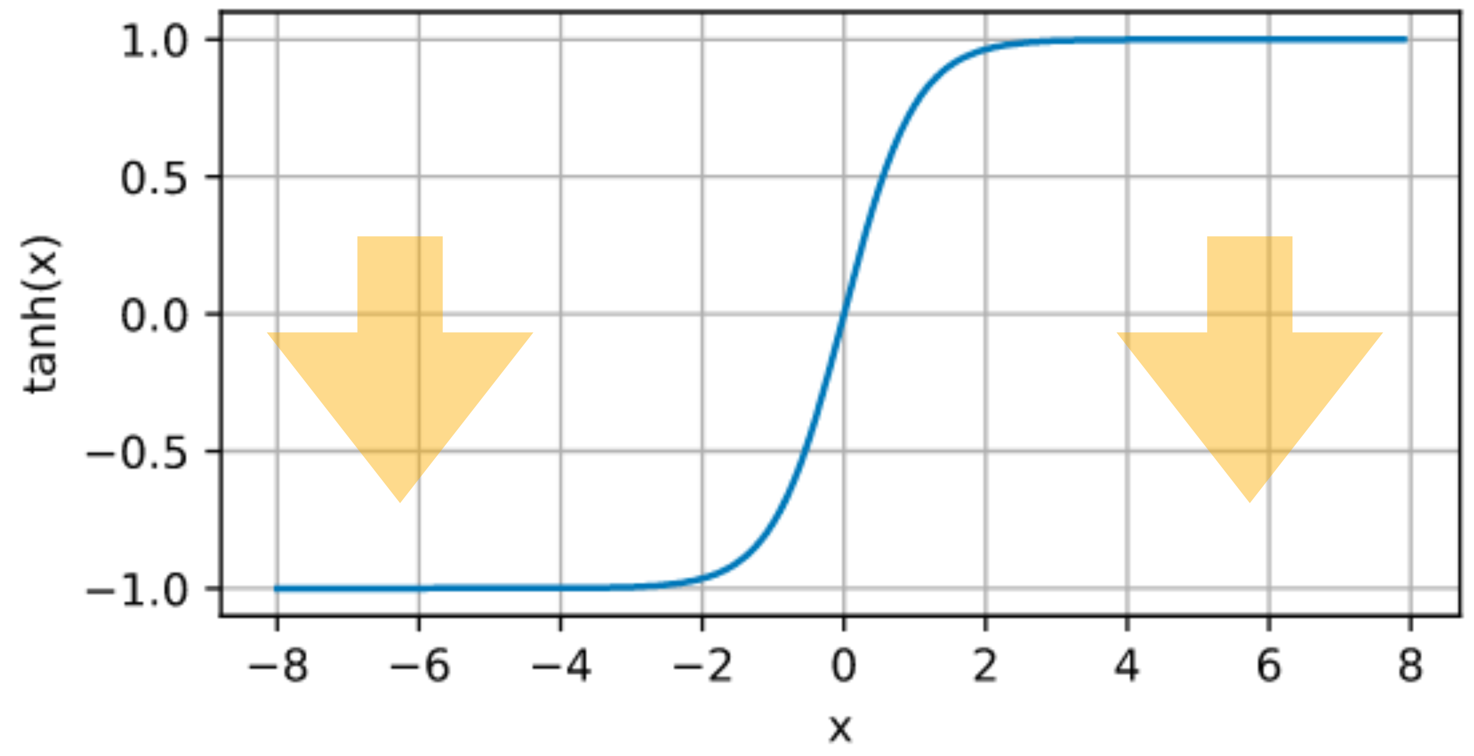
$$\frac{d}{dx} sigmoid(x) = \frac{exp(-x)}{(1 + exp(-x))^2} = sigmoid(x)(1 - sigmoid(x))$$

Multilayer Perceptrons

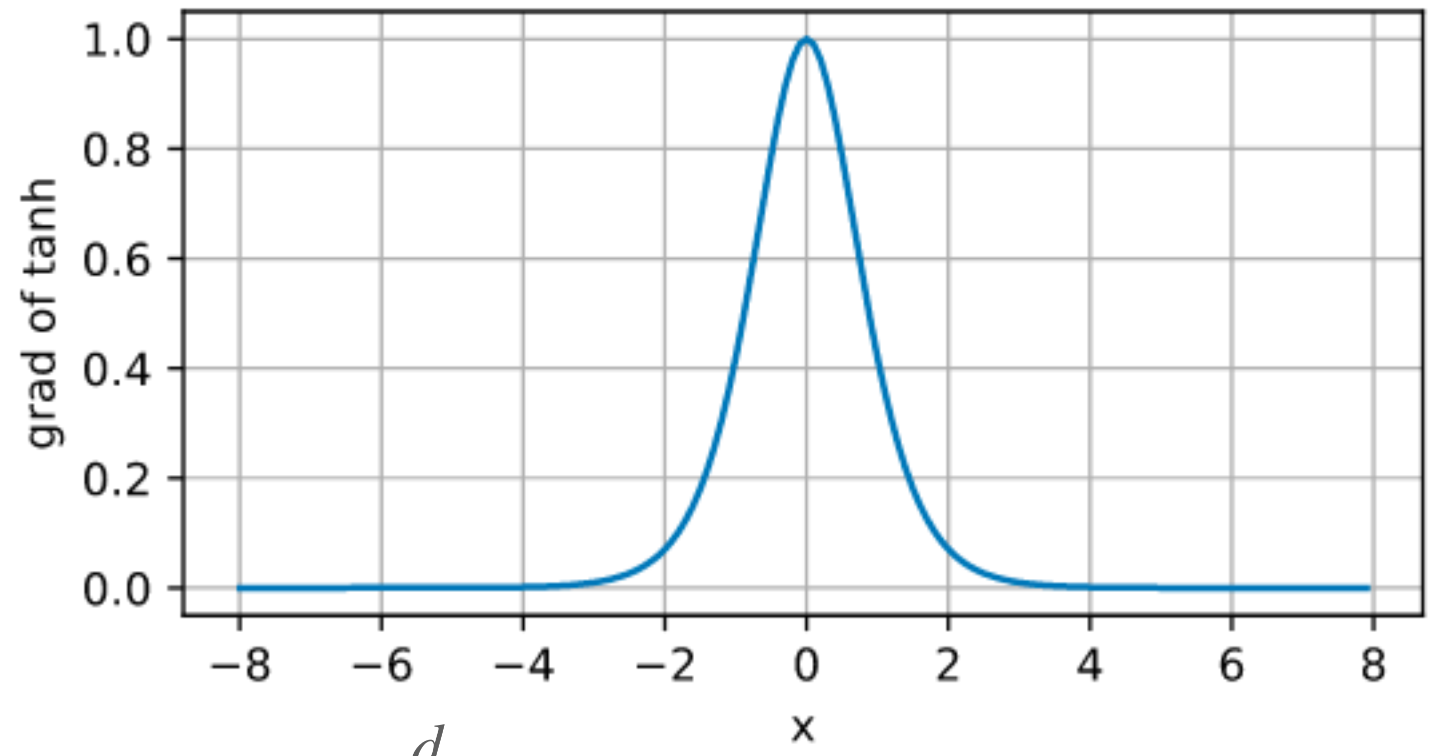
Tanh (hyperbolic tangent)

- Like the sigmoid function, the tanh function also squashes its inputs, transforming them into elements on the interval between -1 and 1.

- Although the shape of the function is similar to that of the sigmoid function, the tanh function exhibits point symmetry about the origin of the coordinate system.



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



$$\frac{d}{dx} tanh(x) = 1 - tanh^2(x)$$

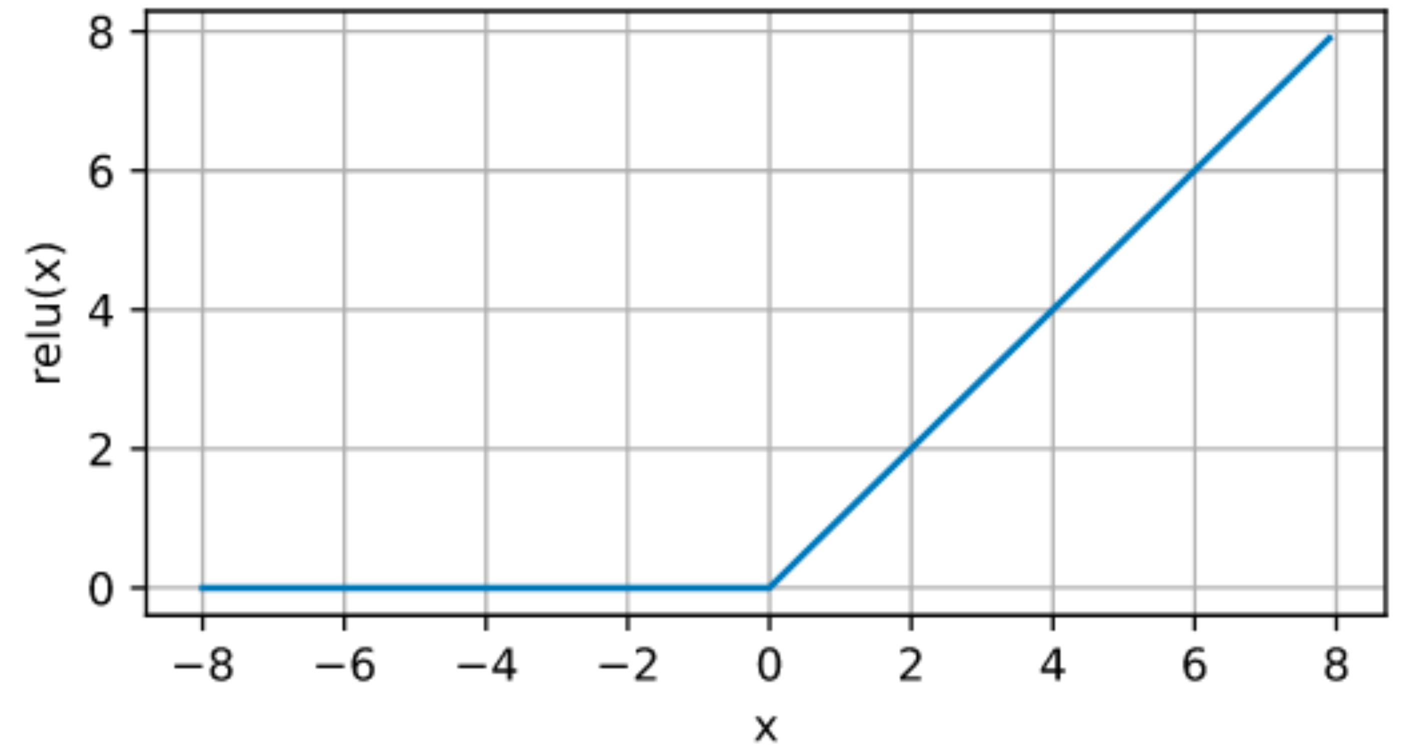
vanishing gradient

Multilayer Perceptrons

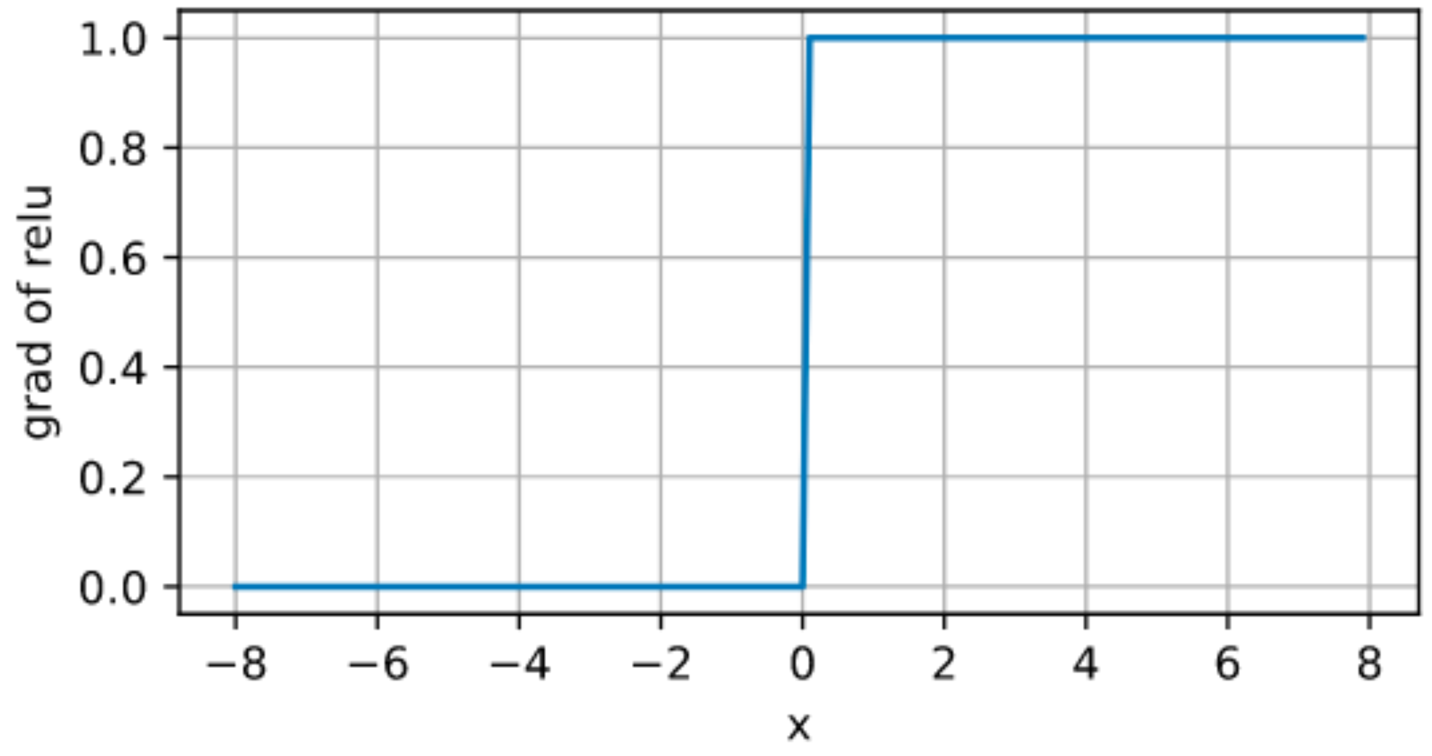
ReLU (rectified linear unit)

- The reason for using ReLU is that its derivates are particularly well behaved: either they vanish or they just let the argument through.
- This makes optimization better behaved and it mitigated the well-documented problem of vanishing gradients that plagued previous versions of neural networks.

$$pReLU(x) = max(0,x) + \alpha min(0,x)$$



$$ReLU(x) = max(x,0)$$



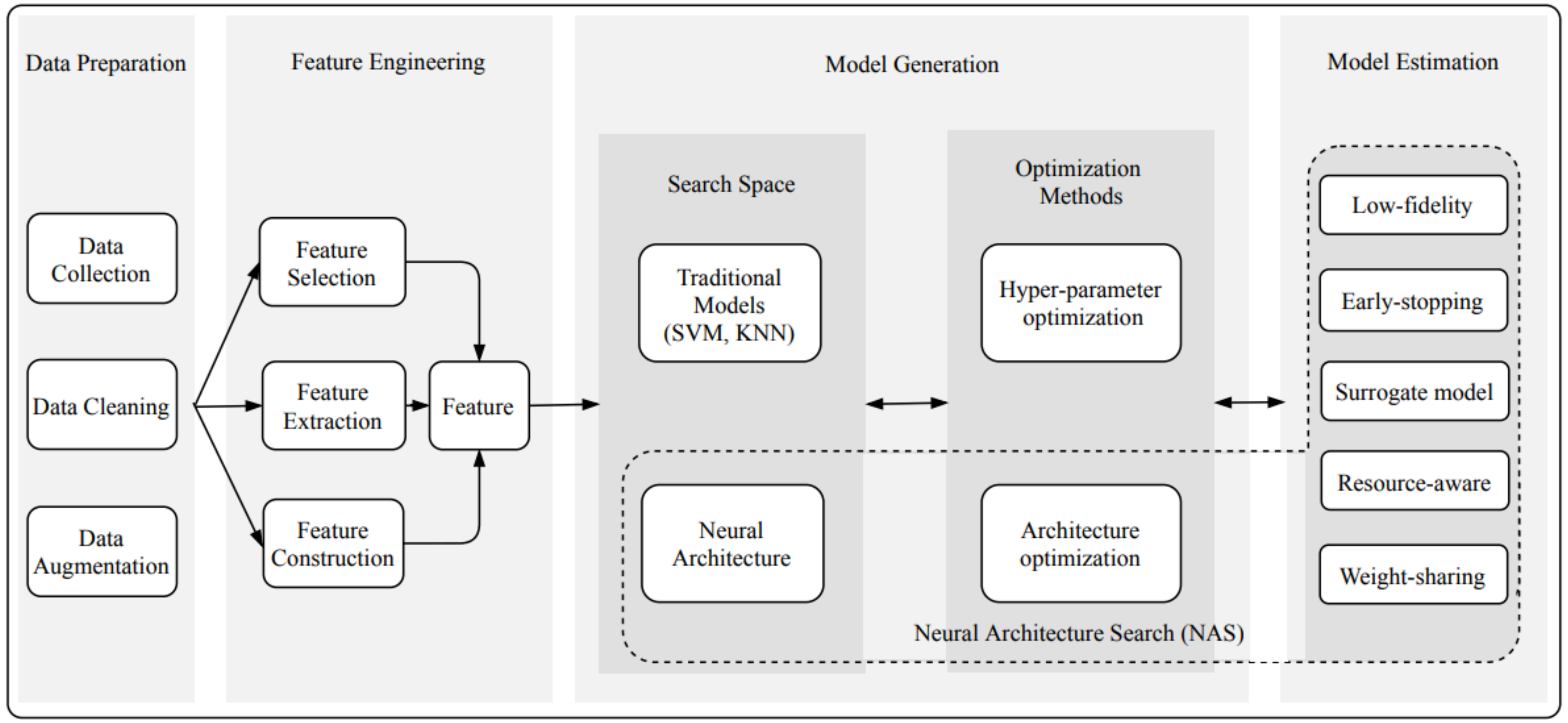
Predicting in advance which will work best is usually impossible.

“Predicting in advance which will work best is usually impossible.”

Deep Learning (Chapter 6) , Ian Goodfellow et al.

Auto ML

#AutoML: automated machine learning
#NAS: neural architecture search
#HPO: hyper-parameter optimization



(1) https://github.com/microsoft/nni
(2) https://github.com/automl/auto-sklearn
(3) https://github.com/google/automl

CIFAR 10 (https://www.cs.toronto.edu/~kriz/cifar.html)

Reference	Published in	#Params (Millions)	Top-1 Acc(%)	GPU Days	#GPUs	AO
ResNet-110 [2]	ECCV16	1.7	93.57	-	-	Maunally
PyramidNet [205]	CVPR17	26	96.69	-	-	designed
DenseNet [124]	CVPR17	25.6	96.54	-	-	
GeNet#2 (G-50) [30]	ICCV17	-	92.9	17	-	
Large-scale ensemble [25]	ICML17	40.4	95.6	2,500	250	
Hierarchical-EAS [19]	ICLR18	15.7	96.25	300	200	
CGP-ResSet [28]	IJCAI18	6.4	94.02	27.4	2	
AmoebaNet-B (N=6, F=128)+c/o [26]	AAAI19	34.9	97.87	3,150	450 K40	EA
AmoebaNet-B (N=6, F=36)+c/o [26]	AAAI19	2.8	97.45	3,150	450 K40	
Lemonade [27]	ICLR19	3.4	97.6	56	8 Titan	
EENA [146]	ICCV19	8.47	97.44	0.65	1 Titan Xp	
EENA (more channels)[146]	ICCV19	54.14	97.79	0.65	1 Titan Xp	
NASv3[12]	ICLR17	7.1	95.53	22,400	800 K40	
NASv3+more filters [12]	ICLR17	37.4	96.35	22,400	800 K40	
MetaQNN [23]	ICLR17	-	93.08	100	10	
NASNet-A (7 @ 2304)+c/o [15]	CVPR18	87.6	97.60	2,000	500 P100	
NASNet-A (6 @ 768)+c/o [15]	CVPR18	3.3	97.35	2,000	500 P100	
Block-QNN-Connection more filter [16]	CVPR18	33.3	97.65	96	32 1080Ti	
Block-QNN-Depthwise, N=3 [16]	CVPR18	3.3	97.42	96	32 1080Ti	RL
ENAS+macro [13]	ICML18	38.0	96.13	0.32	1	
ENAS+micro+c/o [13]	ICML18	4.6	97.11	0.45	1	
Path-level EAS [136]	ICML18	5.7	97.01	200	-	
Path-level EAS+c/o [136]	ICML18	5.7	97.51	200	-	
ProxylessNAS-RL+c/o[129]	ICLR19	5.8	97.70	-	-	
FPNAS[206]	ICCV19	5.76	96.99	-	-	
DARTS(first order)+c/o[17]	ICLR19	3.3	97.00	1.5	4 1080Ti	
DARTS(second order)+c/o[17]	ICLR19	3.3	97.23	4	4 1080Ti	
sharpDARTS [175]	ArXiv19	3.6	98.07	0.8	1 2080Ti	
P-DARTS+c/o[125]	ICCV19	3.4	97.50	0.3	-	
P-DARTS(large)+c/o[125]	ICCV19	10.5	97.75	0.3	-	
SETN[207]	ICCV19	4.6	97.31	1.8	-	
GDAS+c/o [151]	CVPR19	2.5	97.18	0.17	1	GD
SNAS+moderate constraint+c/o [152]	ICLR19	2.8	97.15	1.5	1	
BayesNAS[208]	ICML19	3.4	97.59	0.1	1	
ProxylessNAS-GD+c/o[129]	ICLR19	5.7	97.92	-	-	
PC-DARTS+c/o [209]	CVPR20	3.6	97.43	0.1	1 1080Ti	
MiLeNAS[150]	CVPR20	3.87	97.66	0.3	-	
SGAS[210]	CVPR20	3.8	97.61	0.25	1 1080Ti	
GDAS-NSAS[211]	CVPR20	3.54	97.27	0.4	-	
NASBOT[157]	NeurIPS18	-	91.31	1.7	-	
PNAS [18]	ECCV18	3.2	96.59	225	-	SMBO
EPNAS[163]	BMVC18	6.6	96.29	1.8	1	
GHN[212]	ICLR19	5.7	97.16	0.84	-	
NAO+random+c/o[166]	NeurIPS18	10.6	97.52	200	200 V100	
SMASH [14]	ICLR18	16	95.97	1.5	-	
Hierarchical-random [19]	ICLR18	15.7	96.09	8	200	RS
RandomNAS [177]	UAI19	4.3	97.15	2.7	-	
DARTS - random+c/o [17]	ICLR19	3.2	96.71	4	1	
RandomNAS-NSAS[211]	CVPR20	3.08	97.36	0.7	-	
NAO+weight sharing+c/o [166]	NeurIPS18	2.5	97.07	0.3	1 V100	GD+SMBO
RENASNet+c/o[42]	CVPR19	3.5	91.12	1.5	4	EA+RL
CARS[40]	CVPR20	3.6	97.38	0.4	-	EA+GD

https://arxiv.org/pdf/1908.00709.pdf