Feature learning

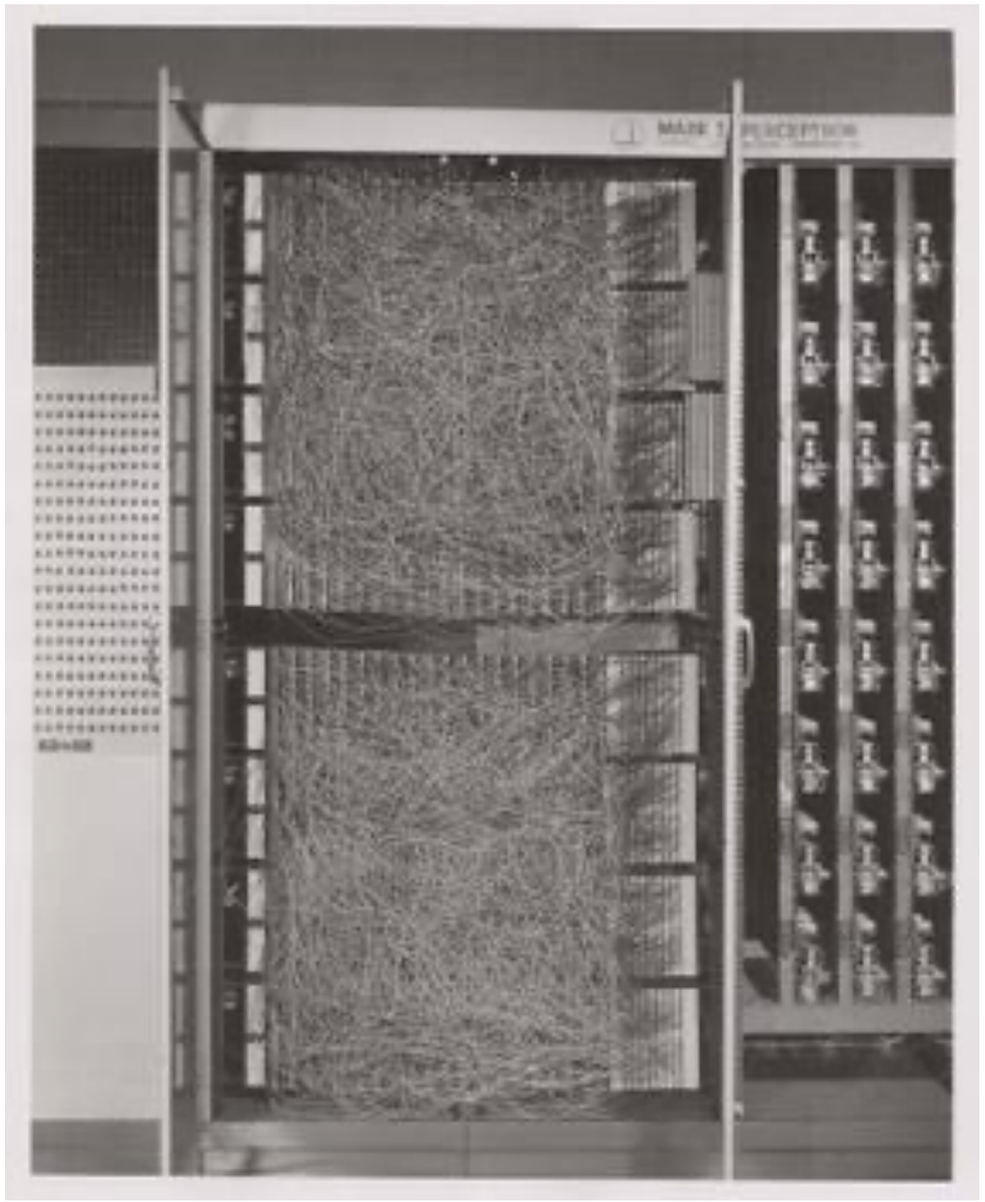
Key points:

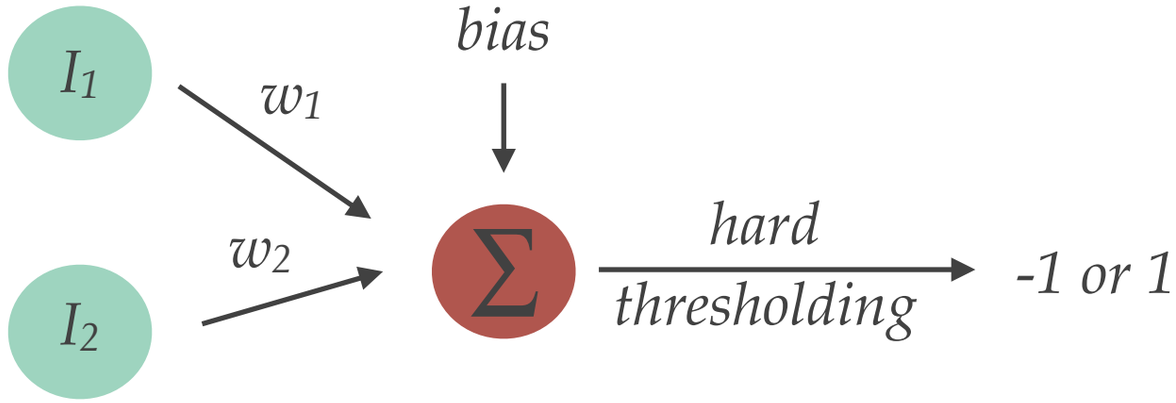
- What makes neural networks different from “classical” models
- What are message passing models, CNN and RNN?

Neural Networks: Perceptron (*"may eventually be able to learn, make decisions, and translate languages"*)

The Perceptron (Rosenblatt (1957))

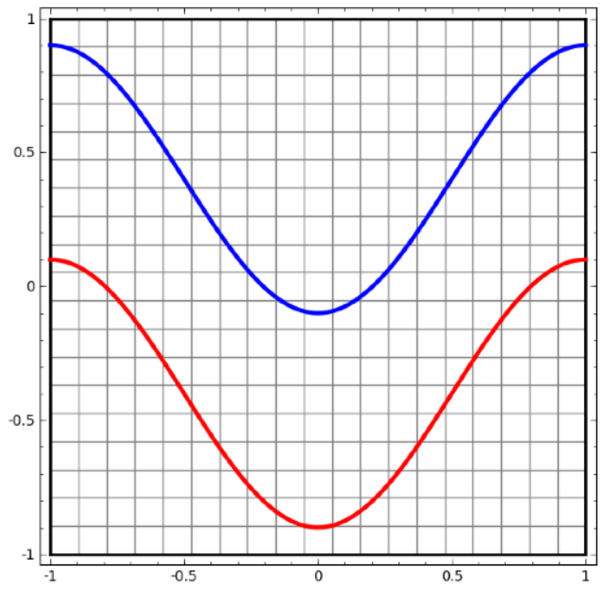
Mark 1 built for image recognition

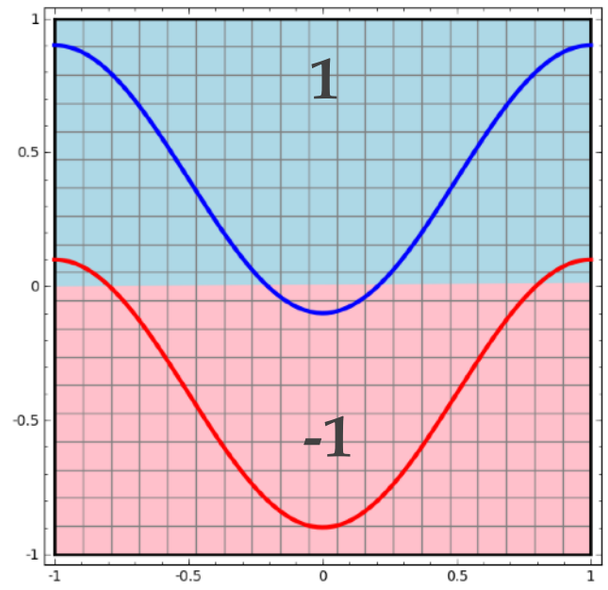




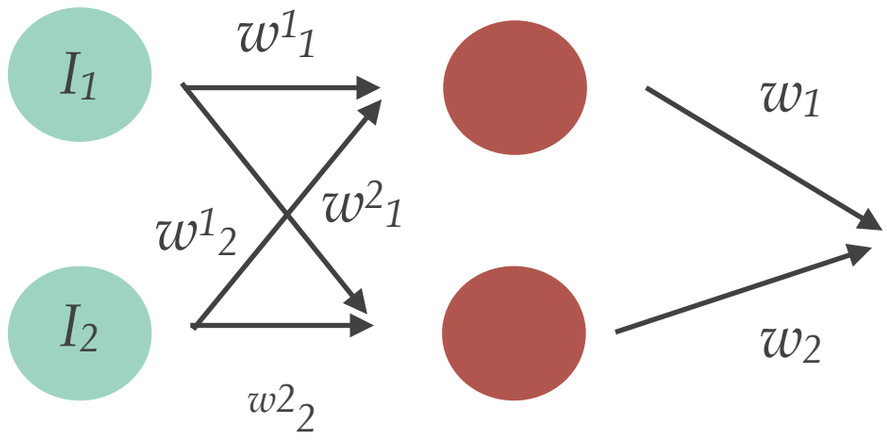
Try to classify which points belong to which curve.

Decision boundary: $w_1x_1 + w_2x_2 + b = 0$





Multilayer Perceptron: Representation Learning



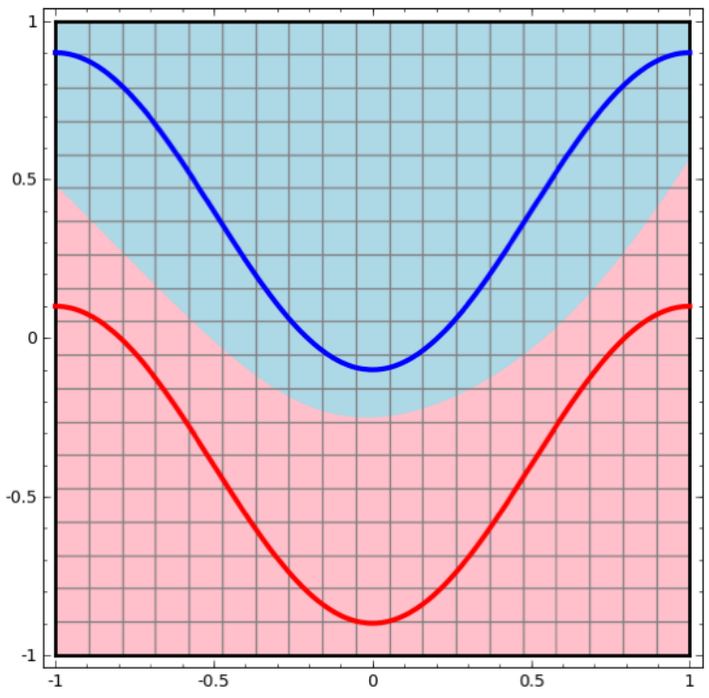
output

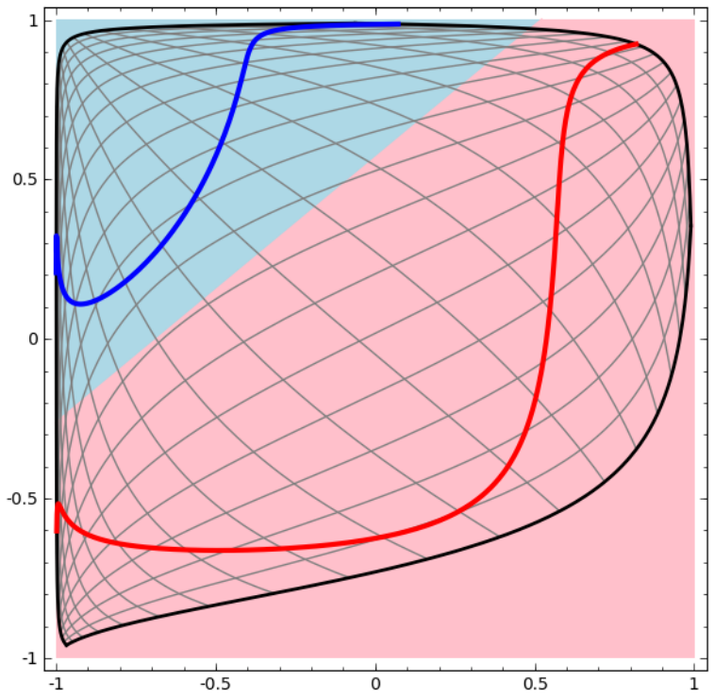
transform representation such that it is linearly separable

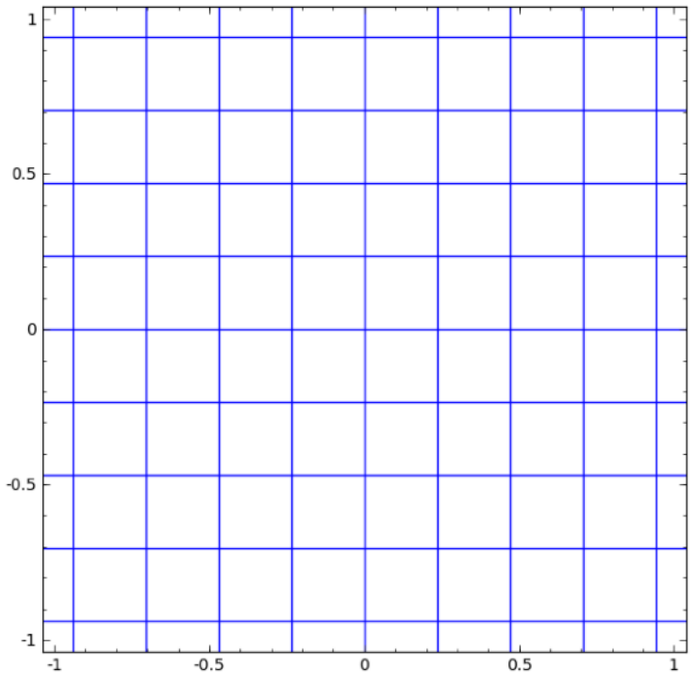
hidden layer, e.g. tanh

in tanh(**W**x+b):

- rotate (**W**)
- Translate (b)
- point-wise application of tanh



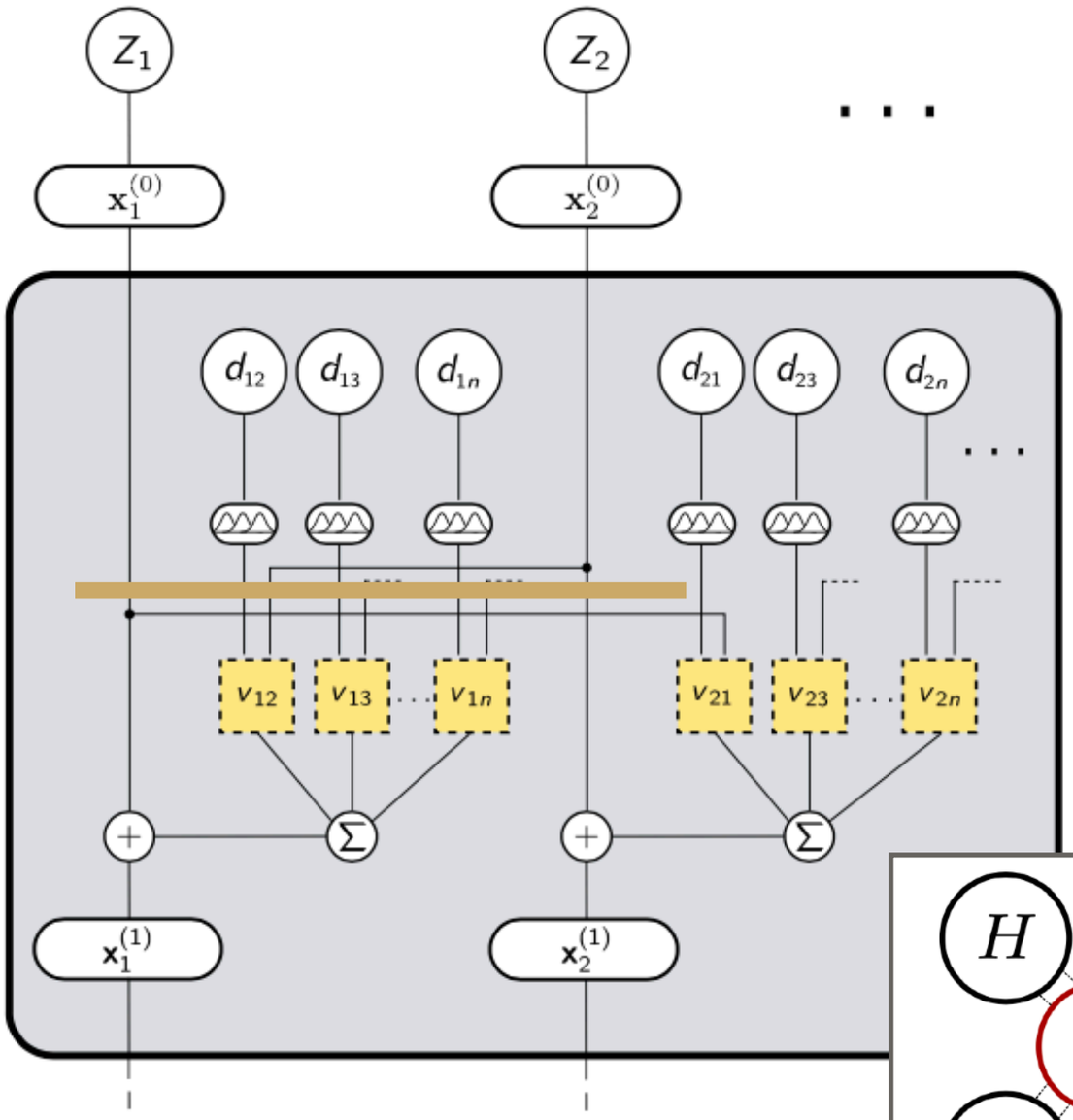




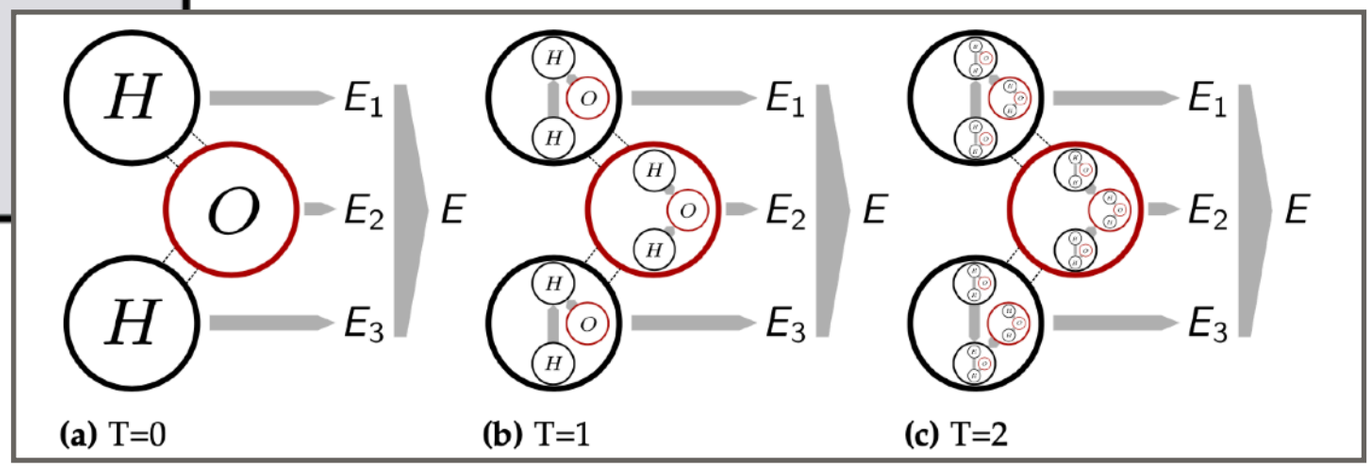
Goodfellow, I.; Bengio, Y.; Courville, A. *Deep Learning*. The MIT Press: Cambridge, Massachusetts, 2016.

LeCun, Y.; Bengio, Y.; Hinton, G. *Nature* **2015**, *521* (7553), 436–444.
http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

Message Passing Neural Networks



- Do not use highly engineered features, like symmetry function, but directly **Z** and ***r.***
- Transferable across **Z**

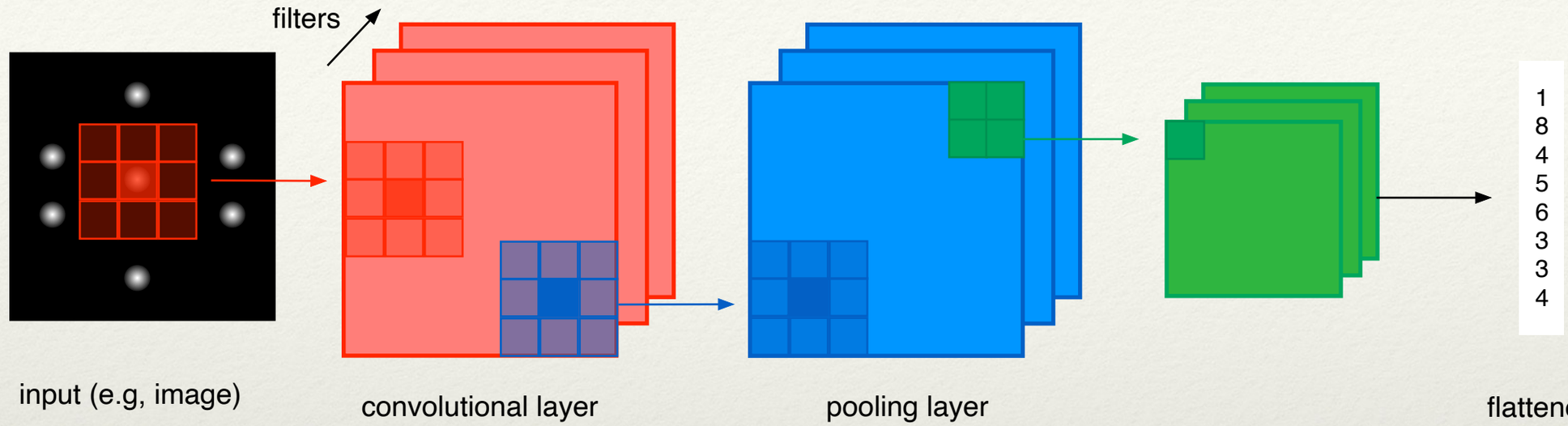


Schütt, K. Learning Representations of Atomistic Systems with Deep Neural Networks TU Berlin, 2018.

Gilmer, J.; Schoenholz, S. S.; Riley, P. F.; Vinyals, O.; Dahl, G. E.*arXiv:1704.01212 [cs]* **2017**.

Convolutional Neural Networks (CNN)

Weights shared in depth slice to reduce the number of parameters.



convolution operator

10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0
0	0	0	10	10	10
0	0	0	10	10	10
0	0	0	10	10	10

Image matrix

×

1	1	1
0	0	0
-1	-1	-1

Vertical sobel filter

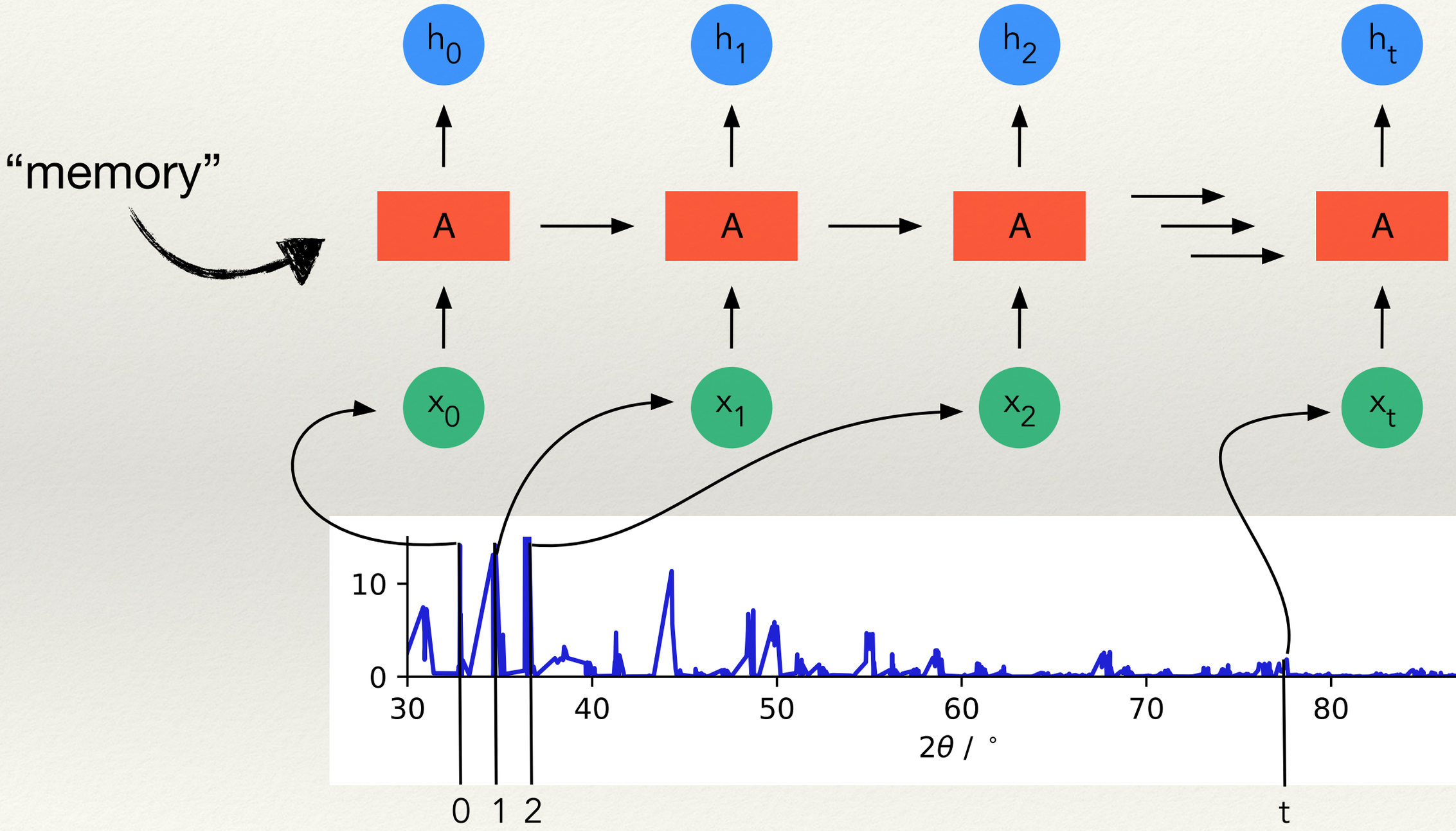
=

0	0	0	0
30	10	-10	-30
30	10	-10	-30
0	0	0	0

inner representation

Recurrent Neural Networks (RNN)

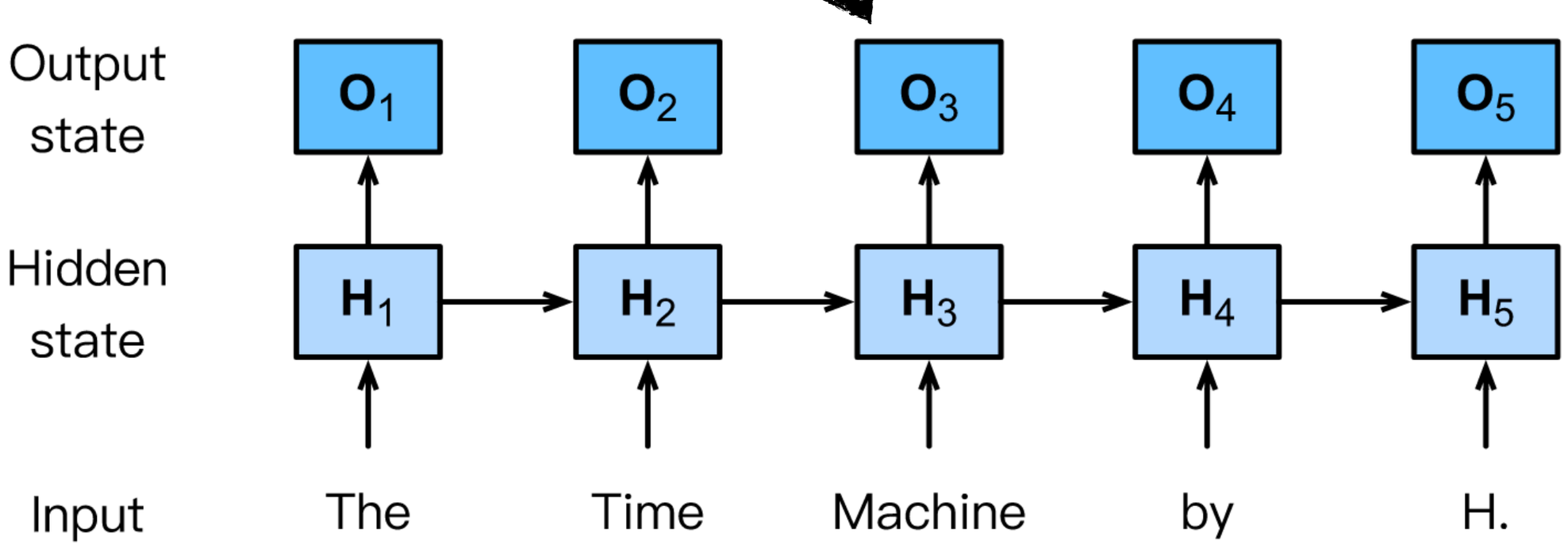
Weights shared between sequence points.



Training of RNN for language modeling

P(“The”, “Time”, “Machine” | “by)

Step	1	2	3	4	5
Output	Time	Machine	by	H.	G.



Feature learning

Key points:

- What makes neural networks different from “classical” models
  - Feature learning: Learning a inner representation
- What are message passing models, CNN and RNN?