Please pick up an anonymous evaluation sheet

Homework 3 Questions

1 K-means

Run examples 1 through 3 in the attached code. Each example displays a different result of running the k-means clustering algorithm on the iris data set. Which result do you think is the best, and why do the other runs of k-means fail?

2 PCA

How many principal components (PCs) could possibly be in the iris data set?

Run example 4 in the attached code. How much of the variance in the data set is explained by the first PC?

Run example 5 in the attached code. Does including another component improve the results? Why or why not?

Question 1: When doing PCA, using a higher number of PCs to create the final reduced representation of the data would __________ overfitting.

a. increase

b. decrease

Question 2: CCA can be used to find the linear transformations of more than 2 data sets that are most correlated.

a. true

b. false

Question 3: You want to perform k-means 2 separate times. You have asked for 2 clusters. The data also has labels, though note that k-means is still unsupervised (i.e. does not make use of the labels). After completing the first k-means with k-means++ initialization, you observe that all data from class 1 is in cluster 1. Now, you run k-means a second time, but you specify the means of the clusters to be the means of the clusters obtained after the first run of k-means. Do you expect that all data points from class 1 will again be in cluster 1?

a. yes

b. no

Question 4: Now, instead of running a second k-means with the cluster means initialized to be the cluster means from the first run, you run a second k-means with k-means++ initialization. Do you expect that all data points from class 1 will again be in cluster 1?

a. yes

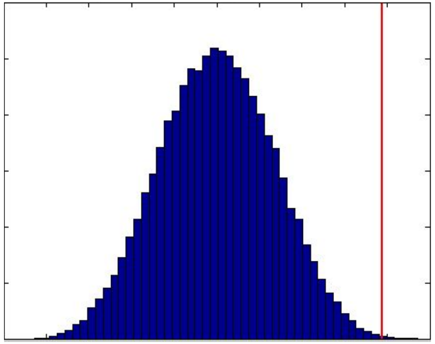
b. no

Advanced topics:
latent variable models, deep learning, and reinforcement learning

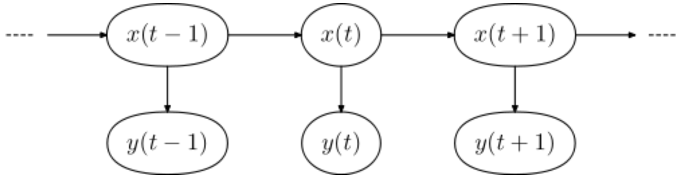
06/24/2016
Mariya Toneva
mariya@cmu.edu

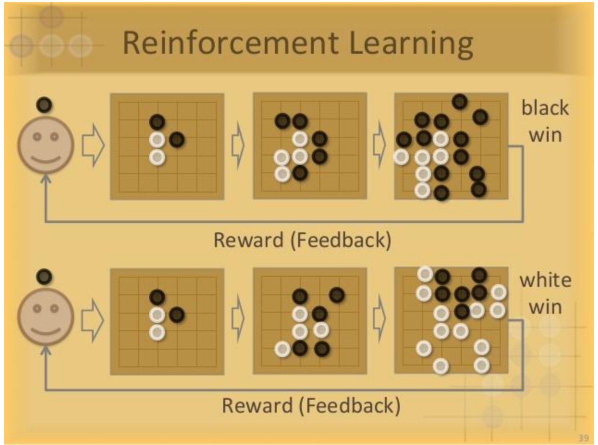
Some figures derived from slides by Tom Mitchell, Aarti Singh, Barnabás Póczos

How can ML help neuroscientists?



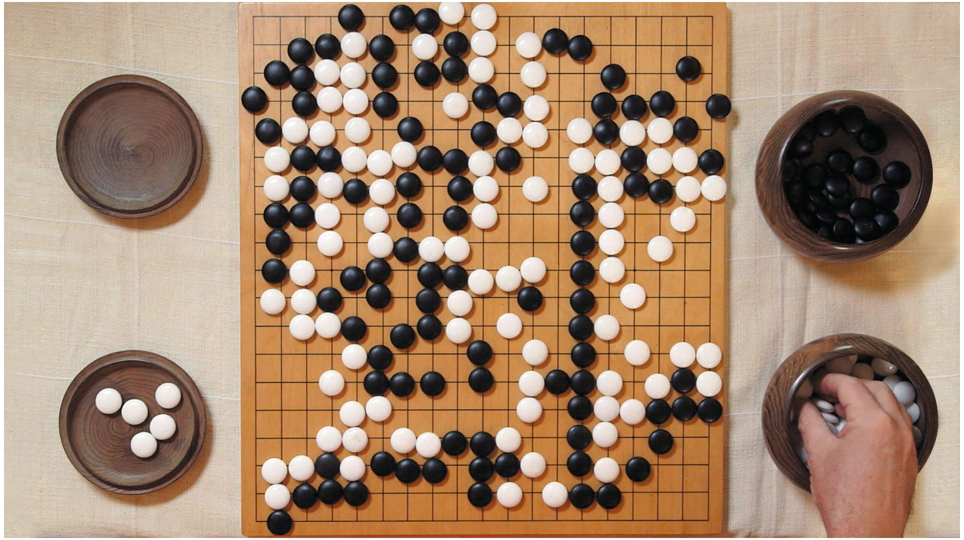
- ❏ Evaluate results
  - ❏ cross validation (how generalizable are our results?)
  - ❏ nearly assumption-free significance testing (are the results different from chance?)
- ❏ **Complex data-driven hypotheses of brain processing**
  - ❏ **advanced topics: latent variable models, reinforcement learning, deep learning**





Look ahead to end of lecture: understanding the most recent AI feat of beating Go world champion

Mnih et al., 2013



Silver et al., 2016 Nature

Today: advanced topics!

- Latent variable models
  - Hidden Markov models
- Reinforcement learning
- Deep learning
  - Neural networks
    - Recurrent NNs
      - Long short-term memory networks
  - Deep belief networks
  - Convolutional neural networks
- AlphaGo: RL + deep learning!

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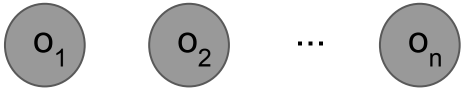

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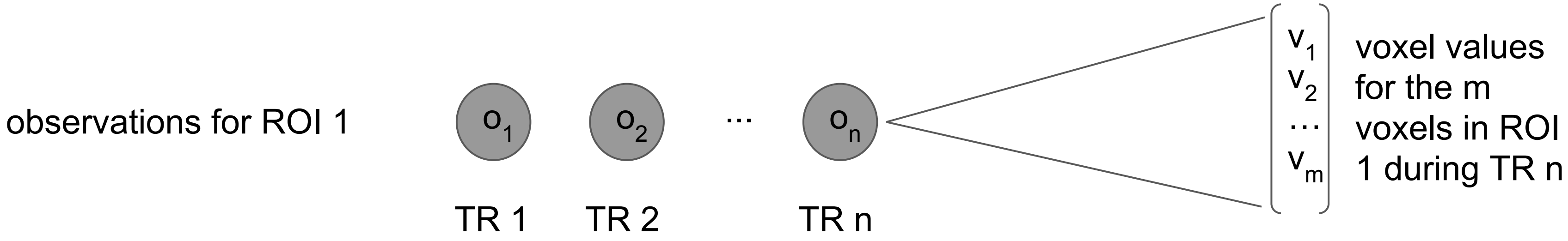

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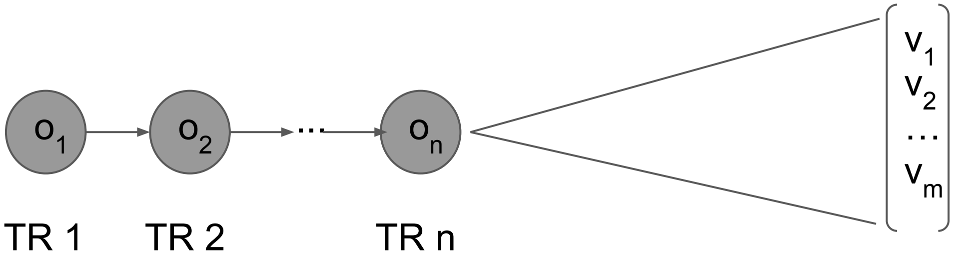
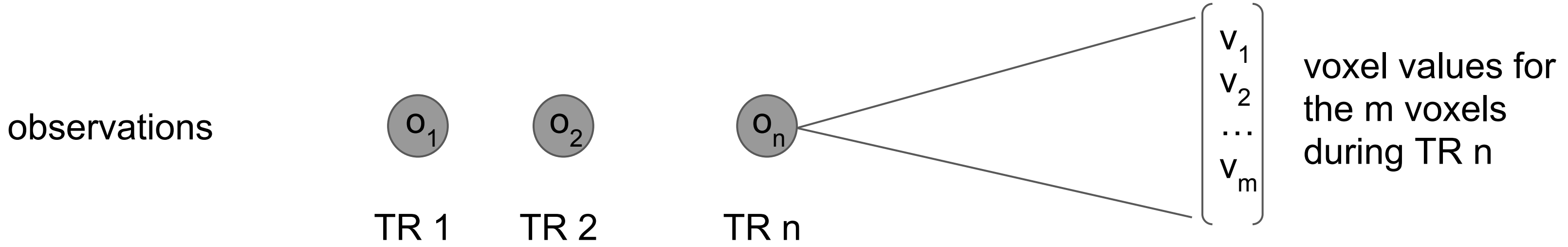
observations for ROI 1



voxel values for the m voxels in ROI 1 during TR n

What if there are latent processes?

- ❑ Dependence in observations may be due to dependence in latent states



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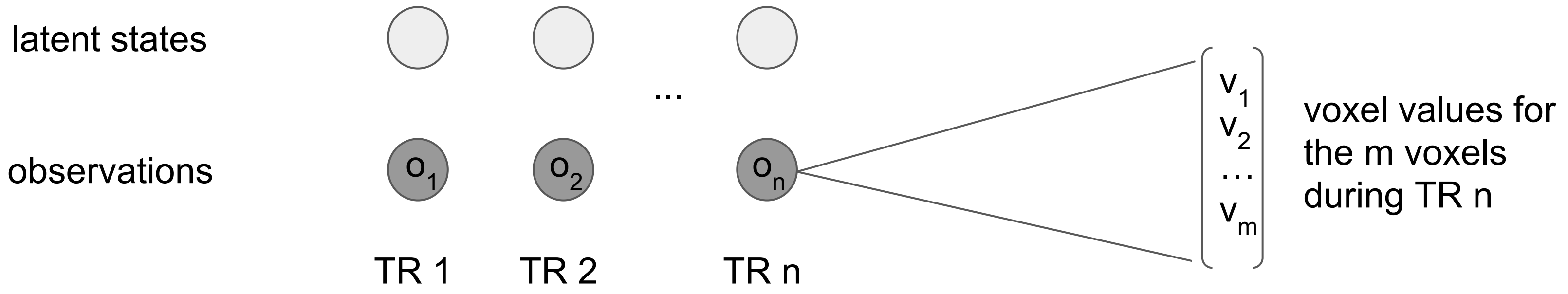

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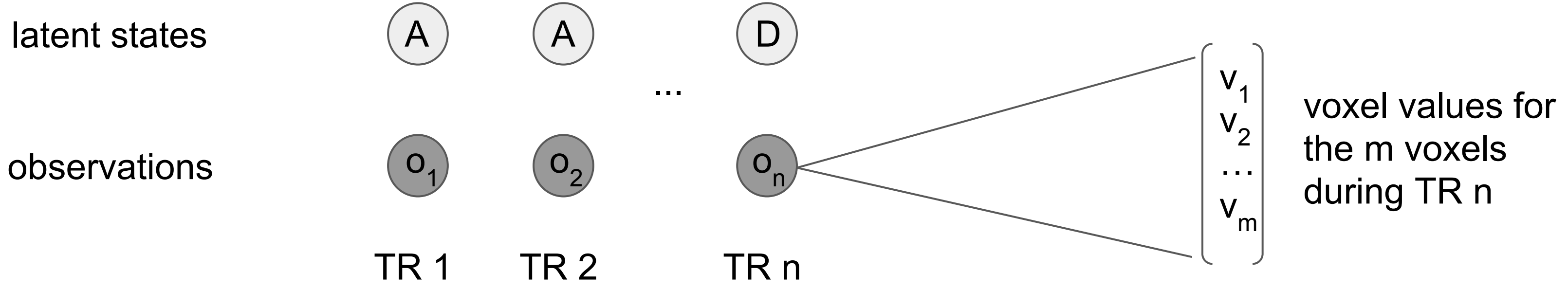

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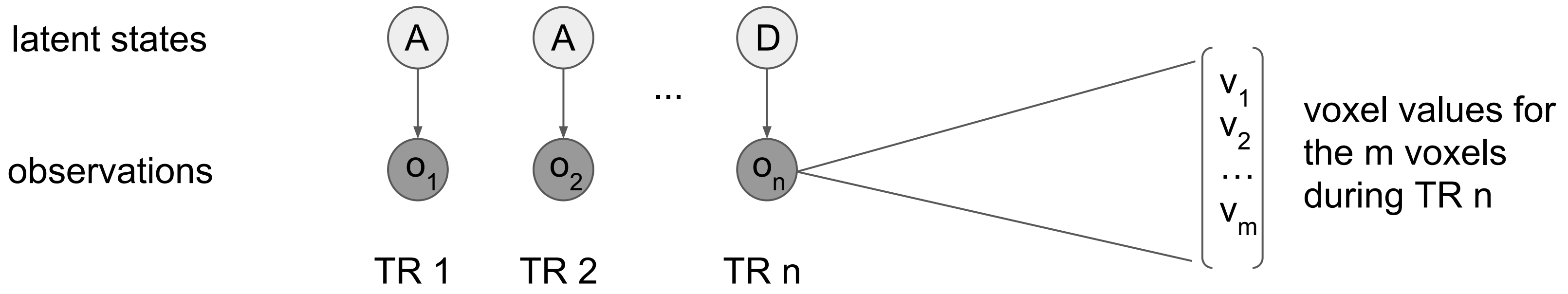

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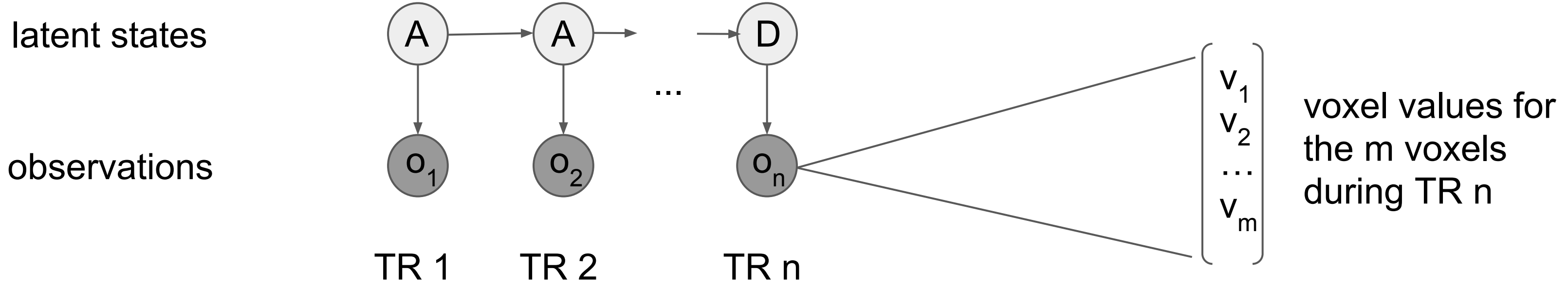
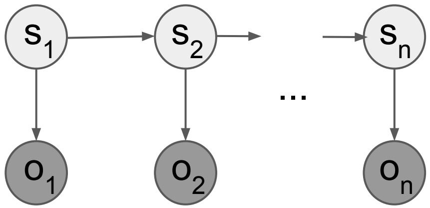
        - transitioning between states may help predict voxel values during next TR



Hidden Markov model (HMM)



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  - can be discrete or real-valued
  - example: voxel values for ROI 1 during one TR

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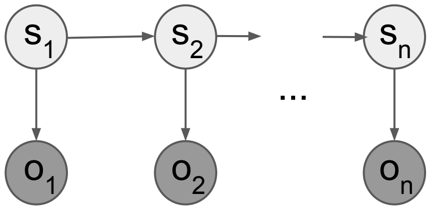

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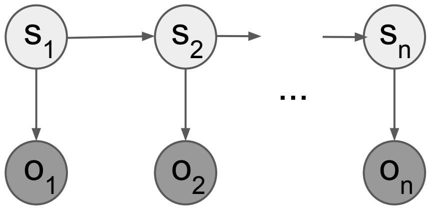

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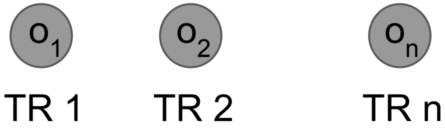
- Observed states are usually shaded

What can we use HMMs for?



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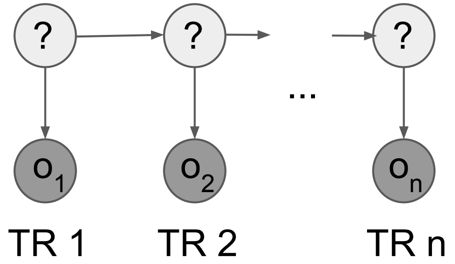

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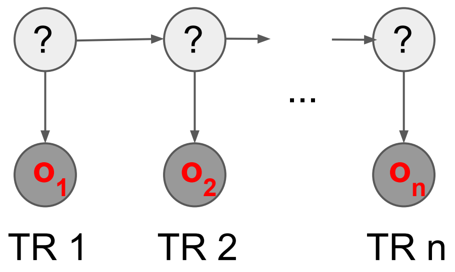

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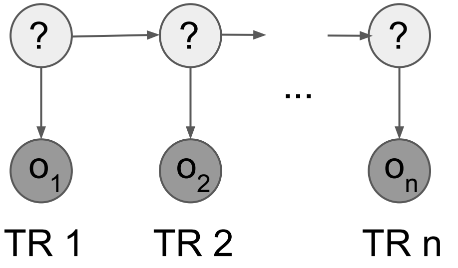

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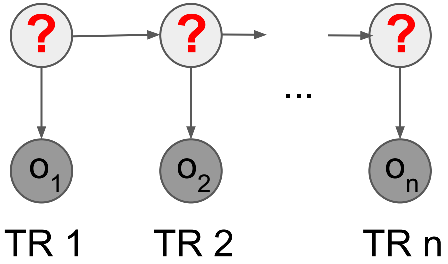

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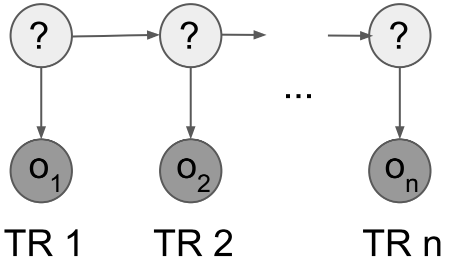

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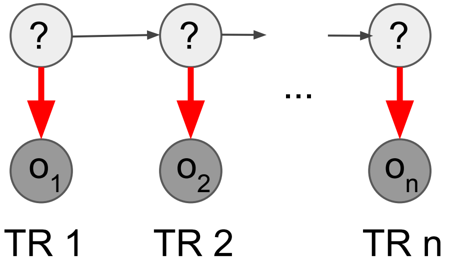

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  - Learn how the observed voxel values for a TR are related to the current brain state

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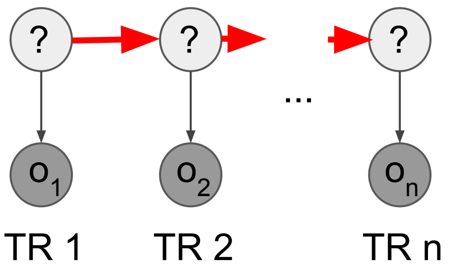

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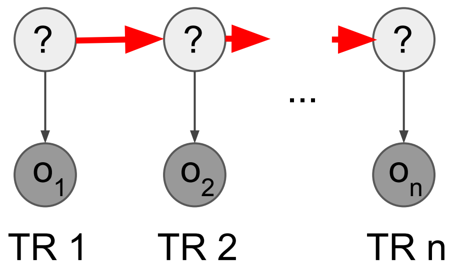

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  - Inferring what brain state the subject was in during each TR **Viterbi algorithm**
- How are observations emitted from the hidden states? How does the model transition from one hidden state to another? **Expectation-Maximization (EM)**
  - Learn how the observed voxel values for a TR are related to the current brain state
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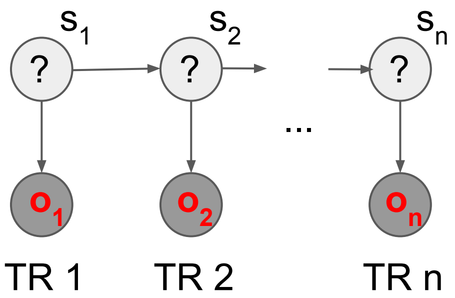

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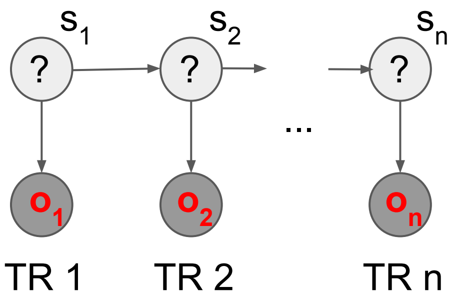

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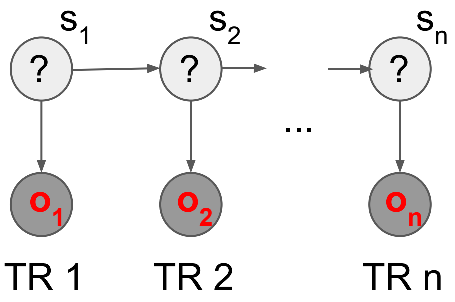

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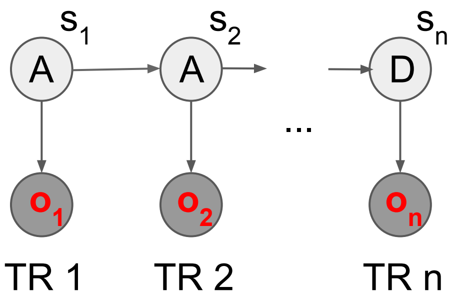
- ❑ If we know what the values of $s_1,...,s_n$ are, we quickly evaluate $P(o_1,...,o_n)$
  - ❑ example: if s_1= A, s_2= A,...,s_3= D



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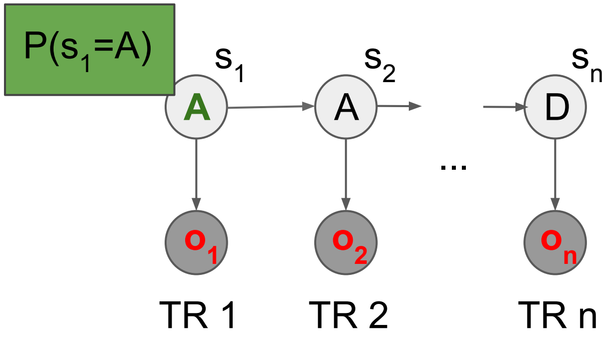

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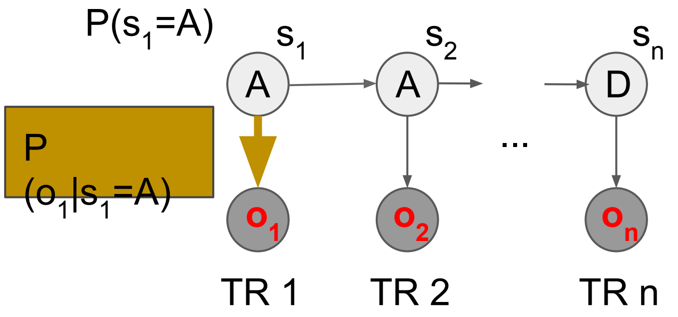

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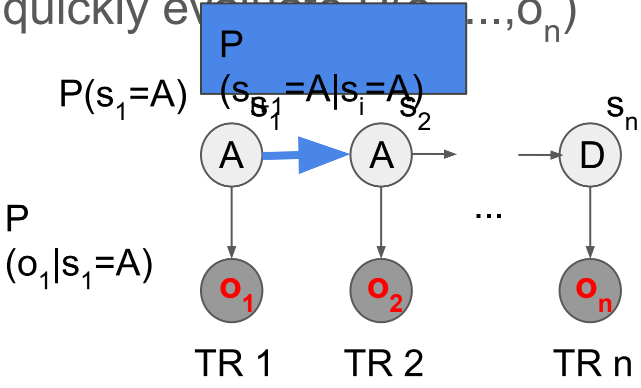

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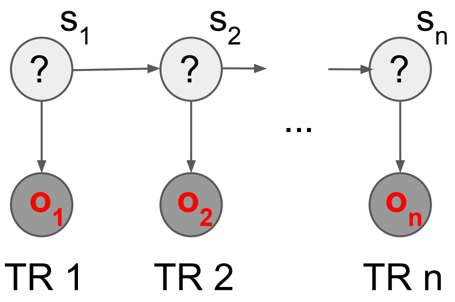

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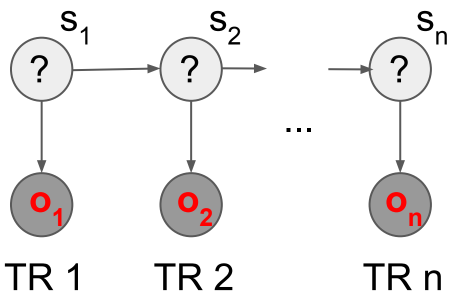

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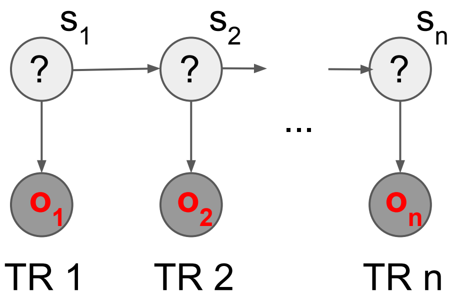

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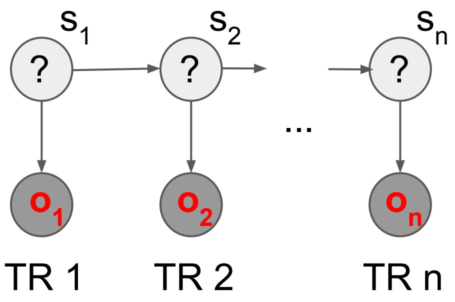

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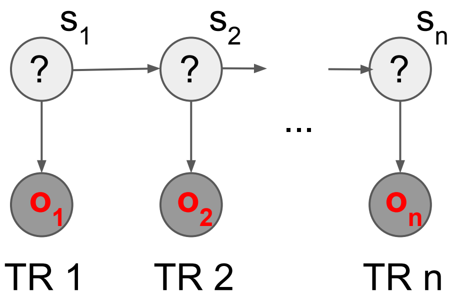

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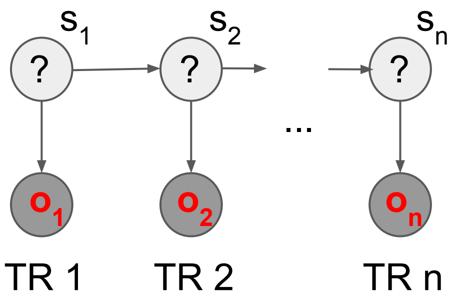
  - forward algorithm is a clever way to do this



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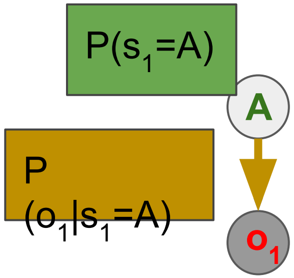

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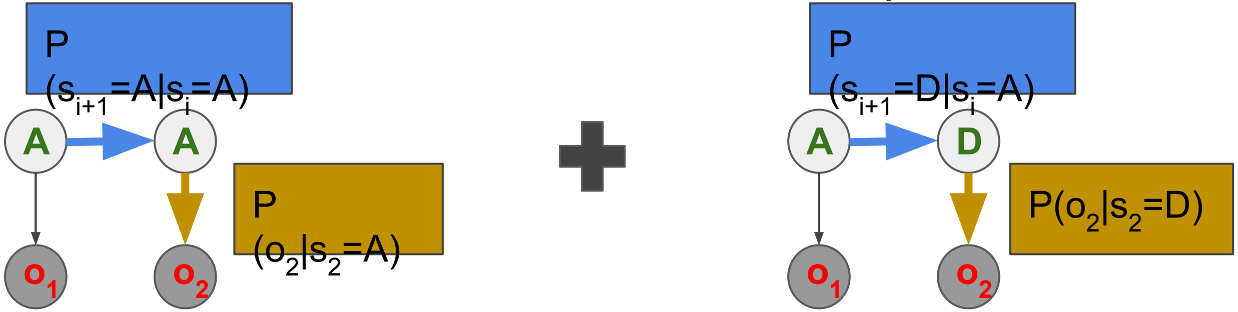
- All further subunits: sum of **emission** x **transition** x previous subunit



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- Viterbi algorithm: also relies on recursive computation using subunits
- Starting with the second hidden state, for each hidden state until the last one, we calculate the probability of the most likely path that ends in this hidden state
- For each of these probabilities, we record the previous hidden state in the most likely sequence => this enables us to follow the most probable path backwards once we're at the end of the sequence

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- Very general algorithm for learning parameters in models with latent variables

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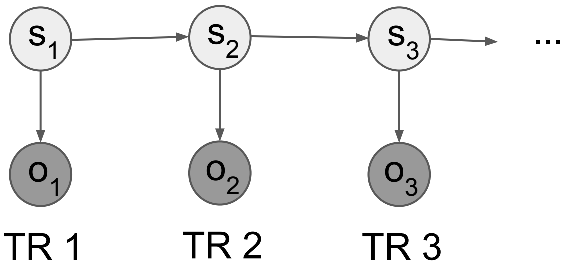
- SSM (state-space model) is another type of latent variable model that accounts for continuous hidden states

Can we model human learning with an HMM?

- To learn, we need some teaching, or reward, signal



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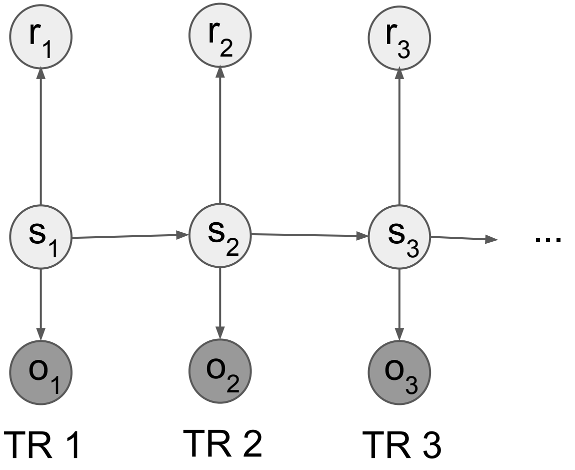

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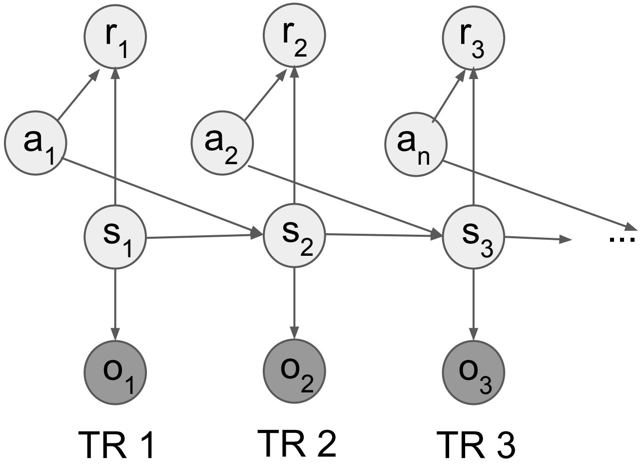

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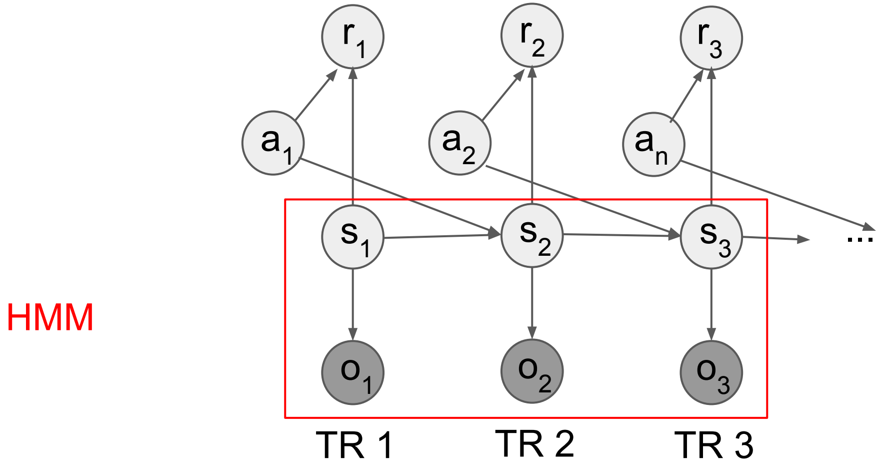

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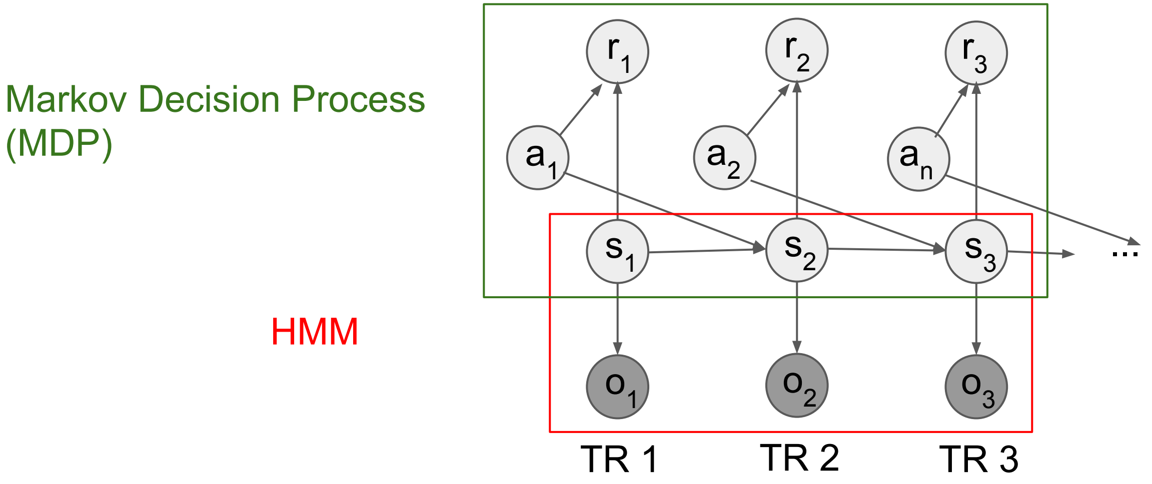

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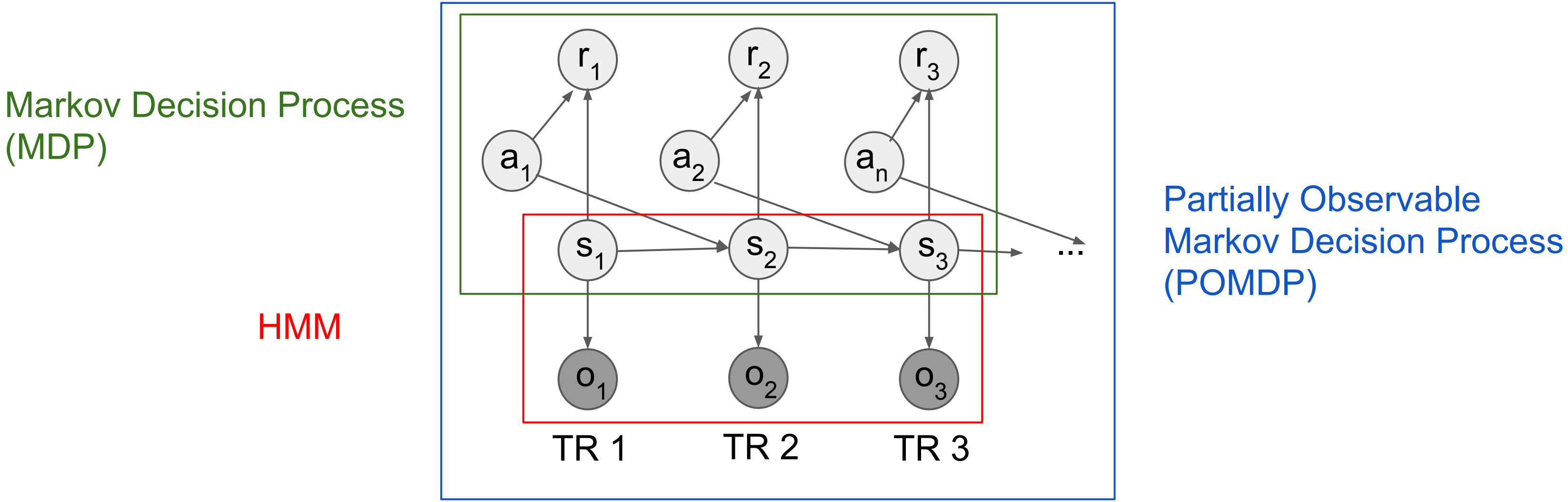
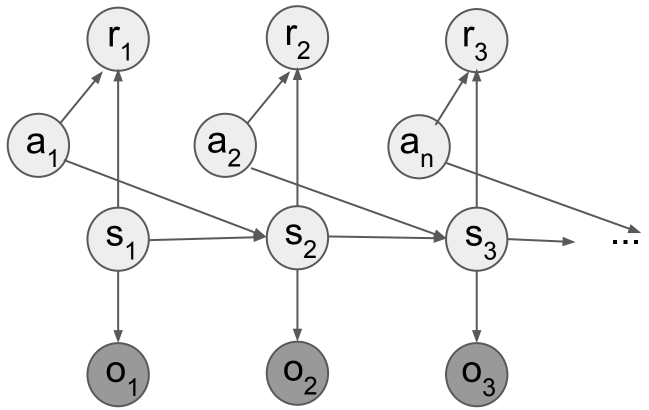


Reinforcement learning (RL): learning how to take the best actions to maximize expected future reward

- ❑ Delayed reward vs immediate reward



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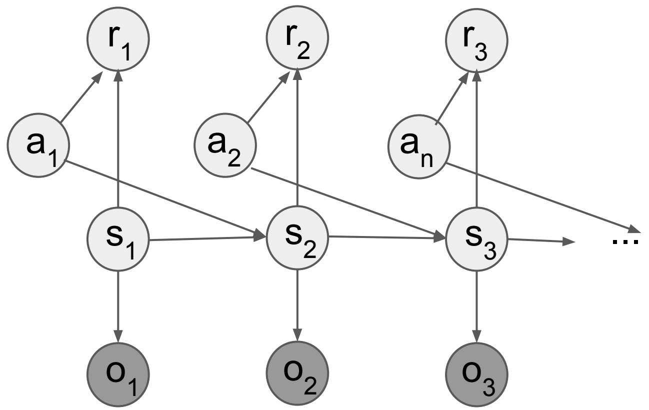

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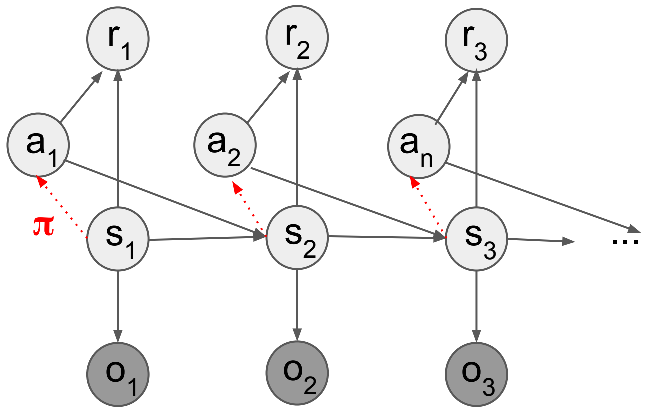

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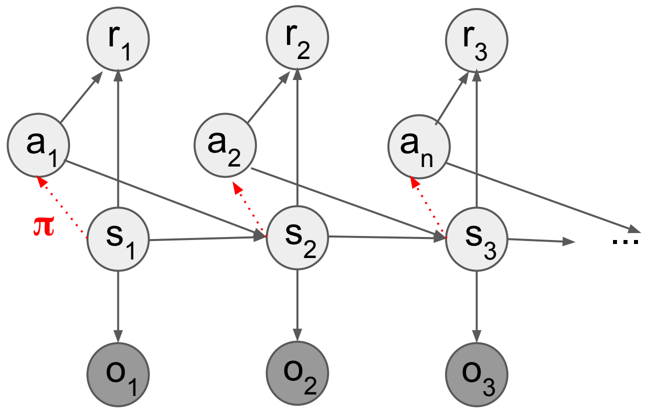

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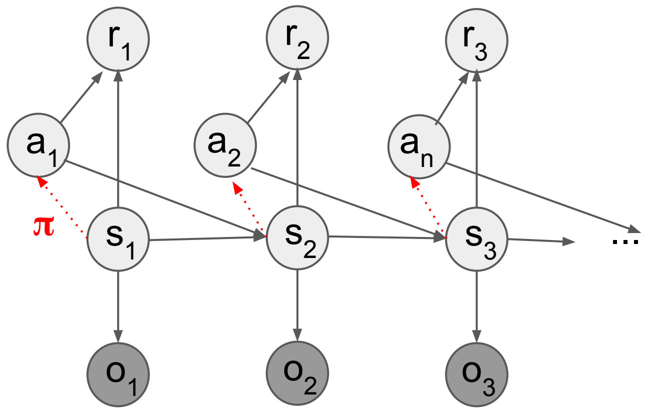

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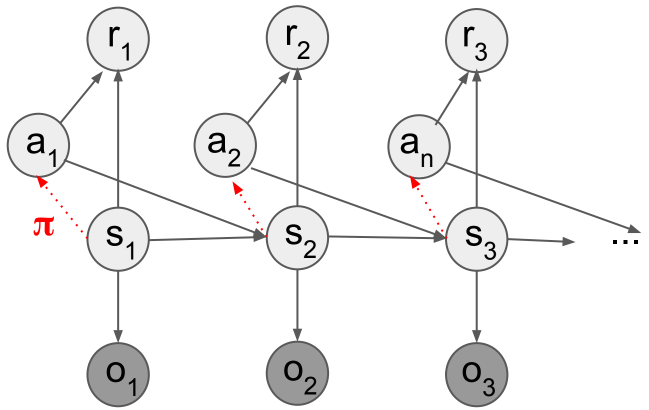

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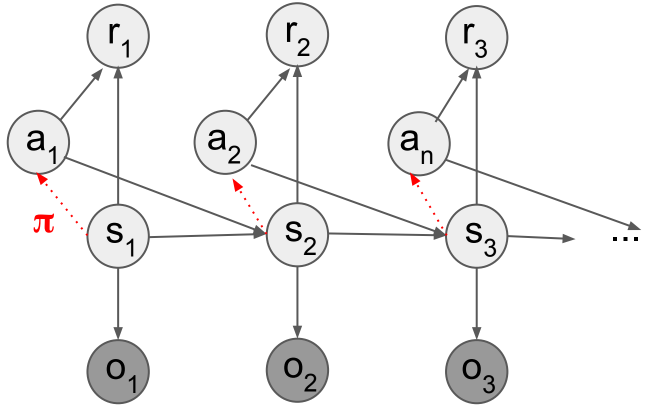

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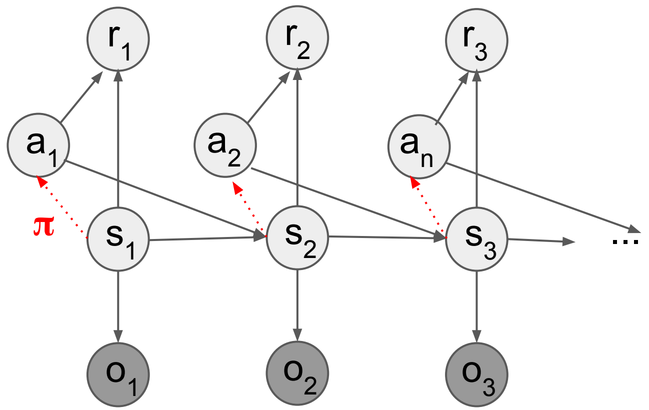

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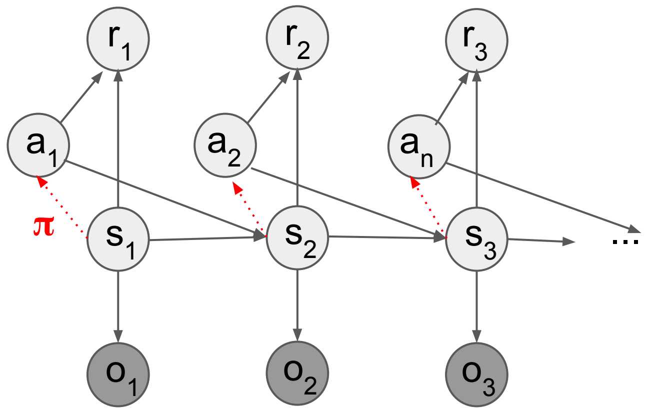

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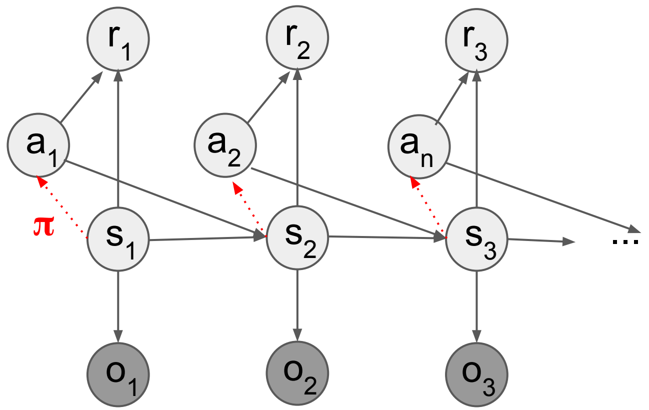

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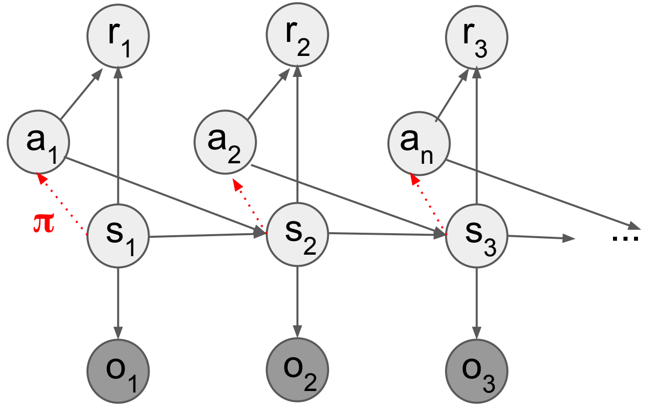
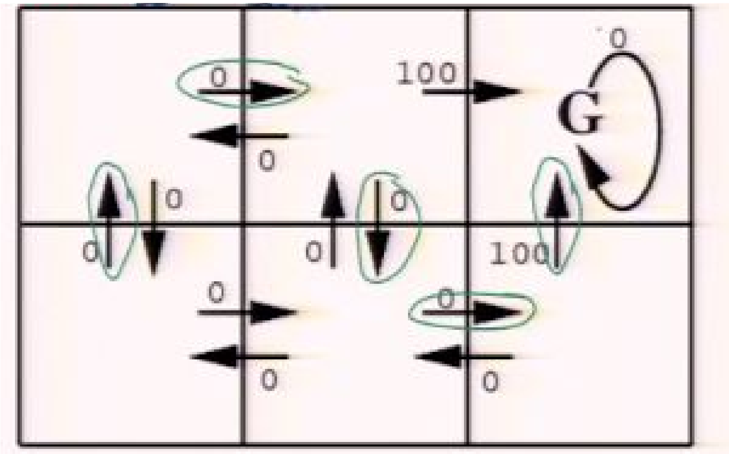
$$\pi^* = \arg\max_{\pi} V^{\pi}(s), \quad (\forall s)$$



Example: what are the $V^{\pi}(s)$ values?

- Image there is a robot that needs to get to the goal state G
- Each square is a state
- Circled arrows show the policy **π**
- Let γ = 0.9



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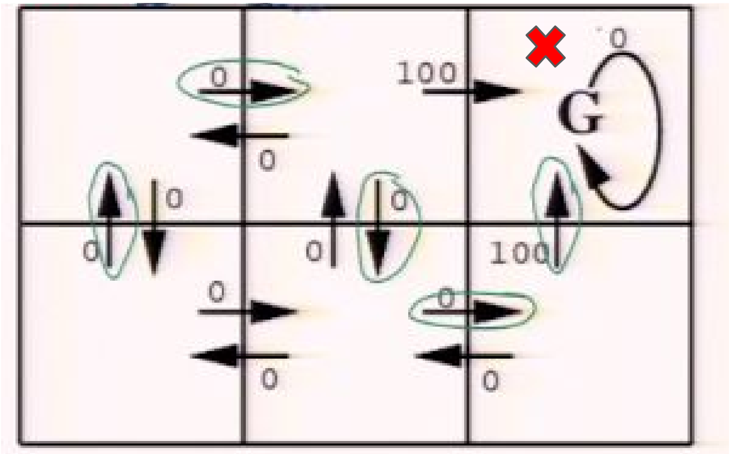

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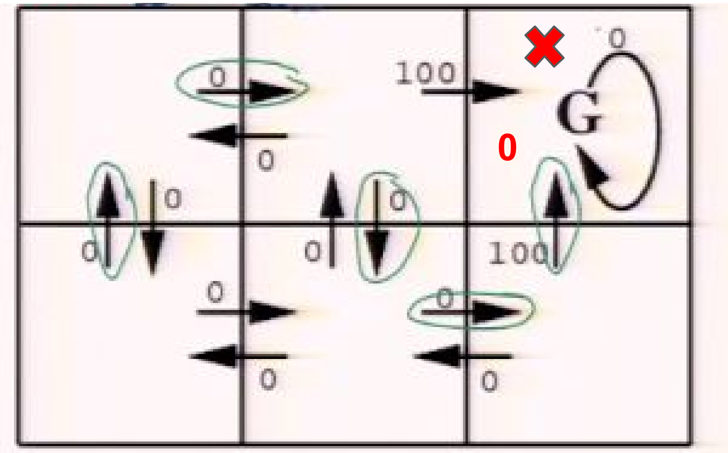

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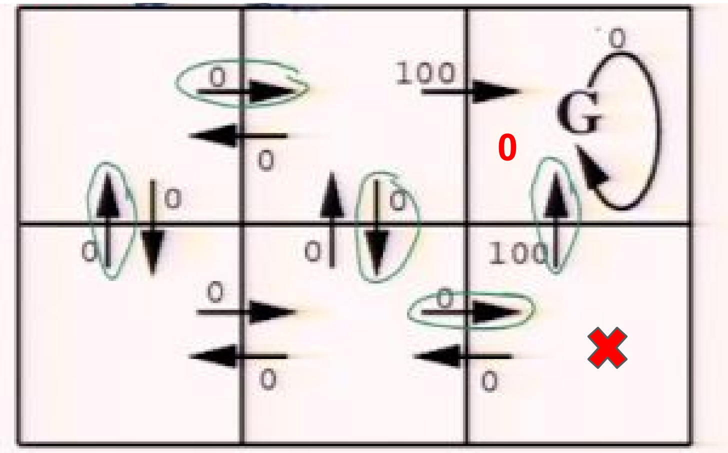

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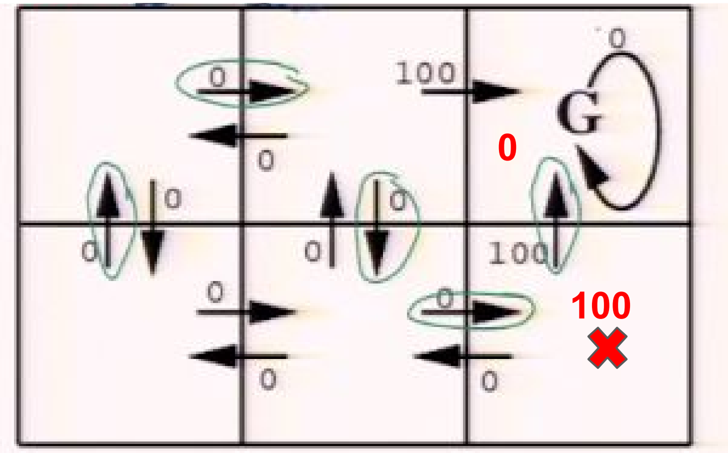

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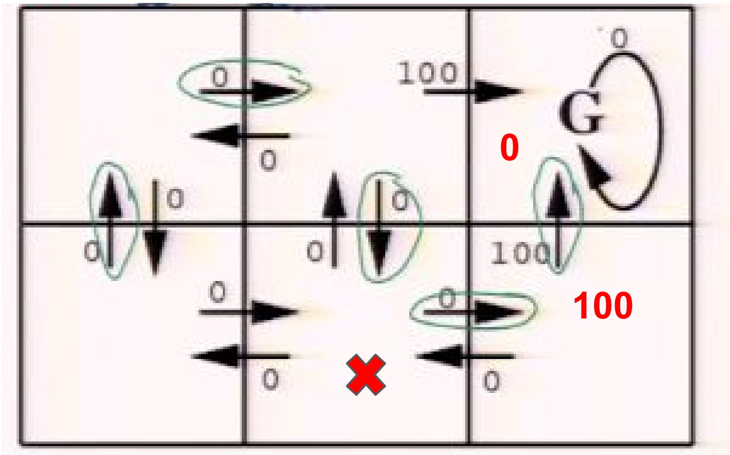

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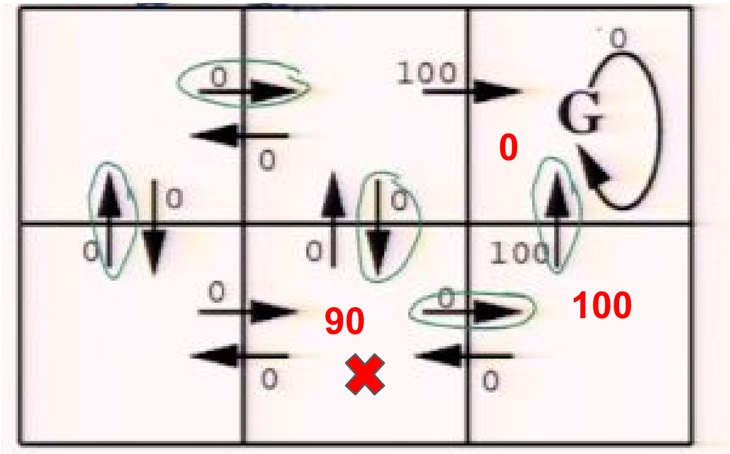
What is V^{π}(**x**)? 0.9 x100 = 90



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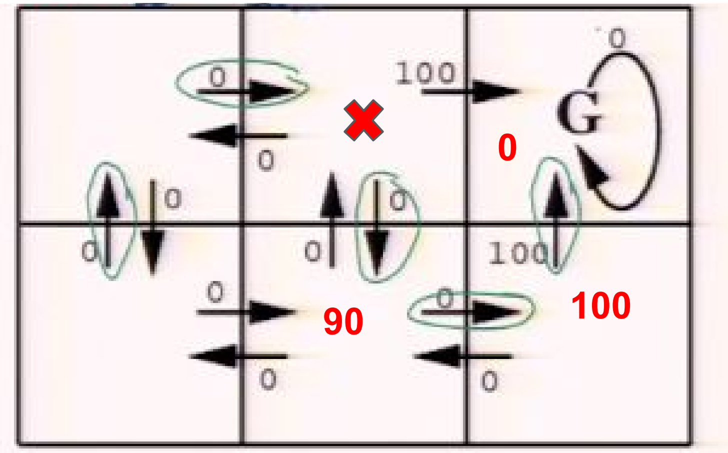

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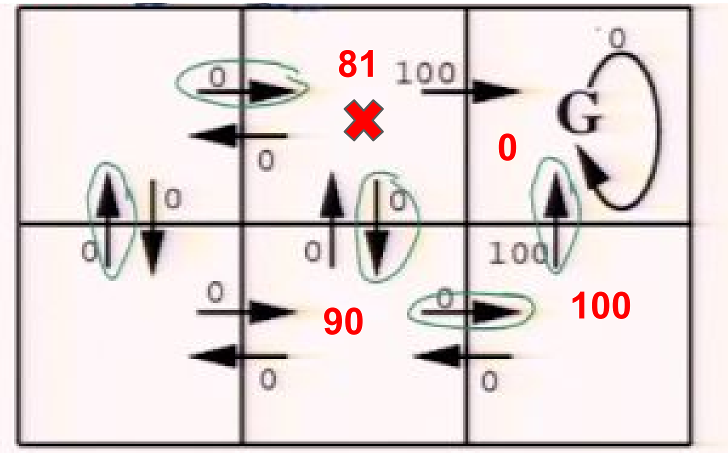

What is V^{π}(x)? 0.9x0.
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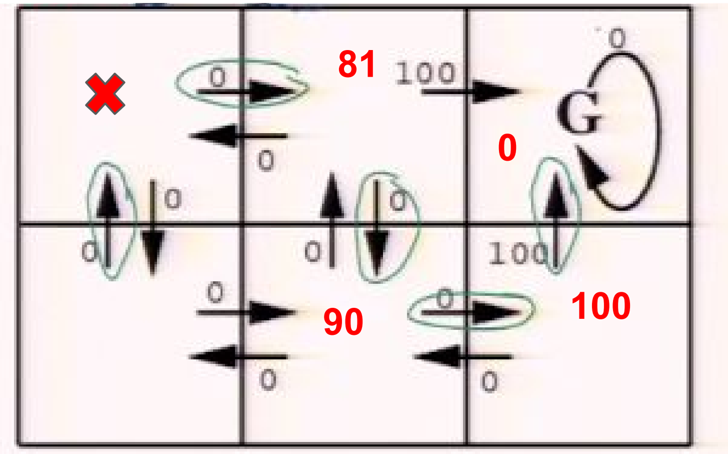

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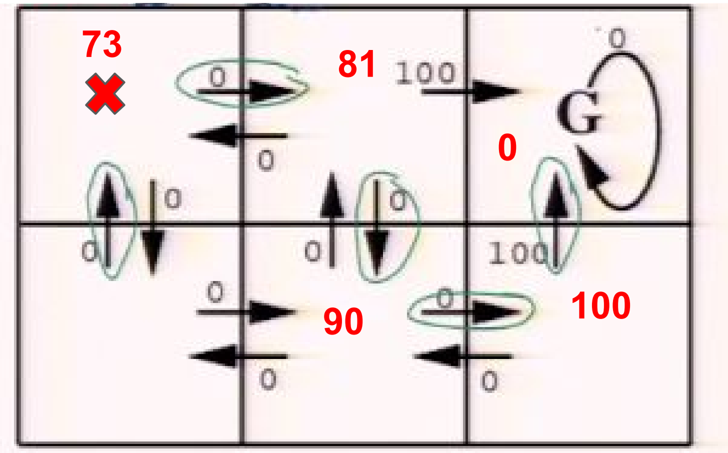

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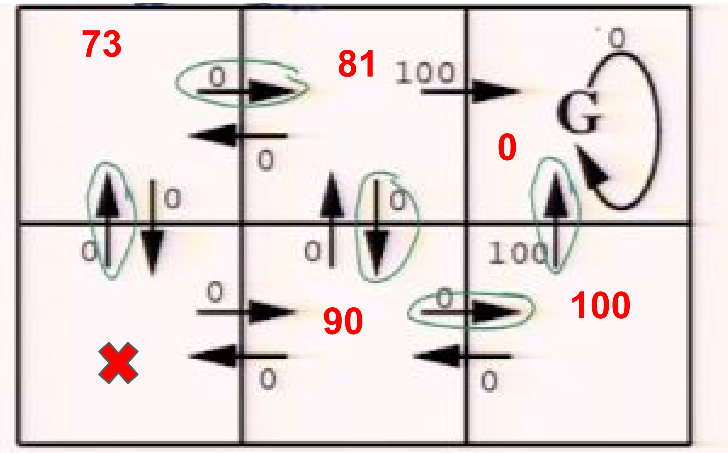

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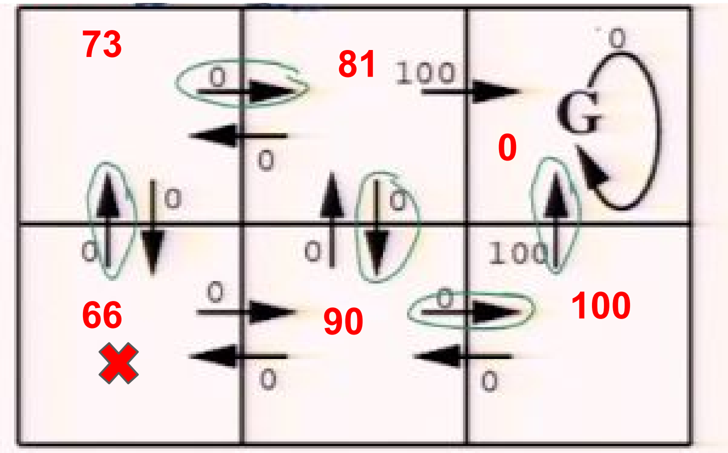

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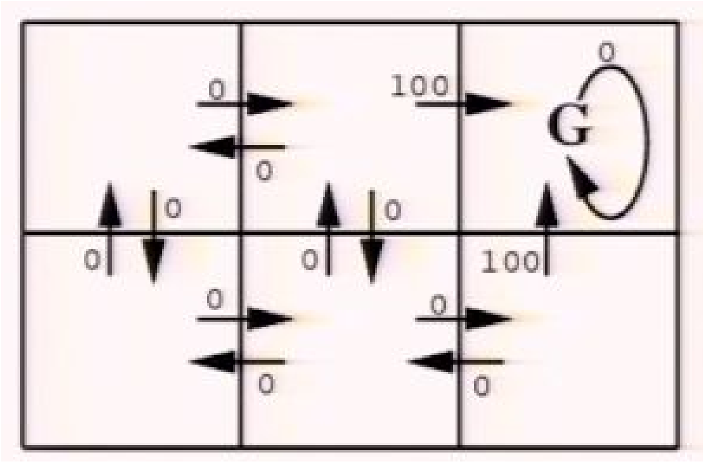

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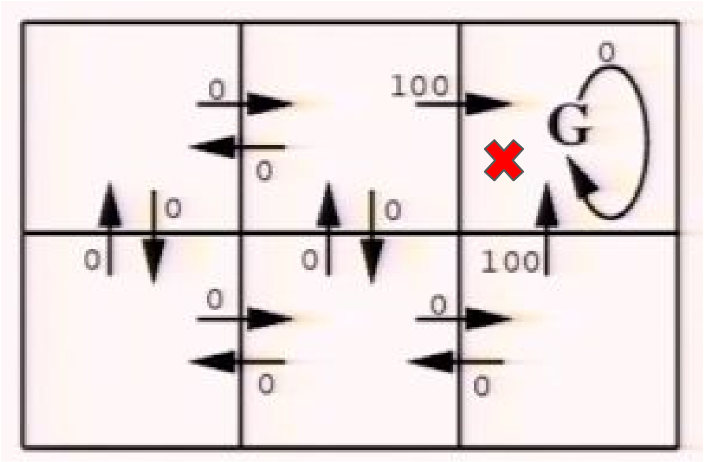

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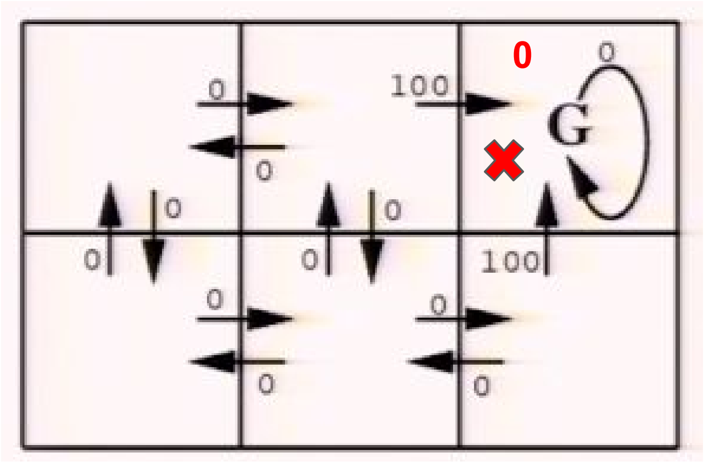

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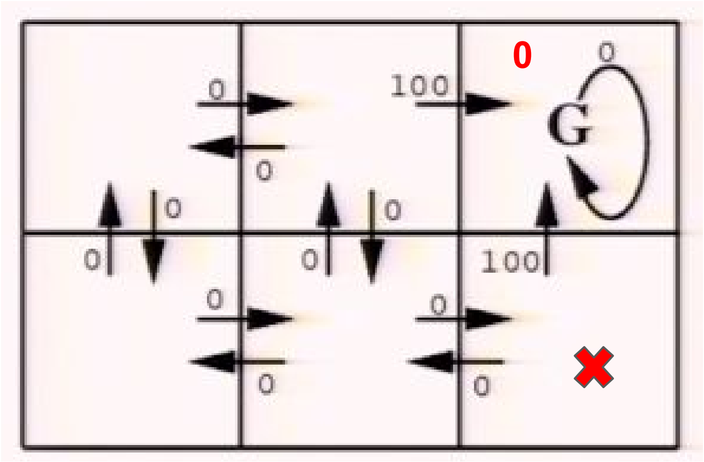

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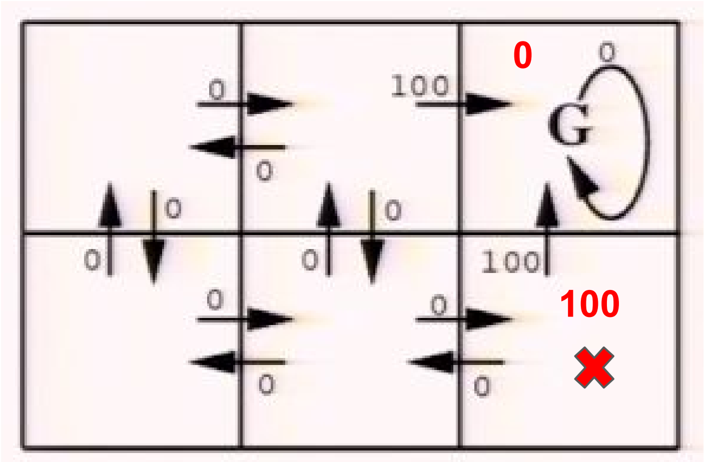

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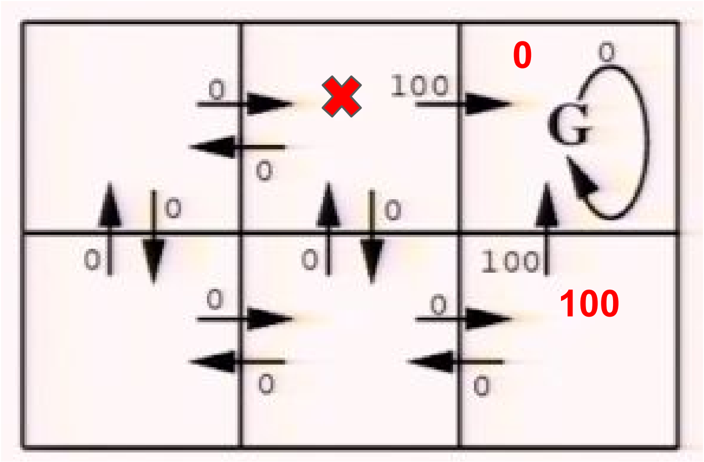

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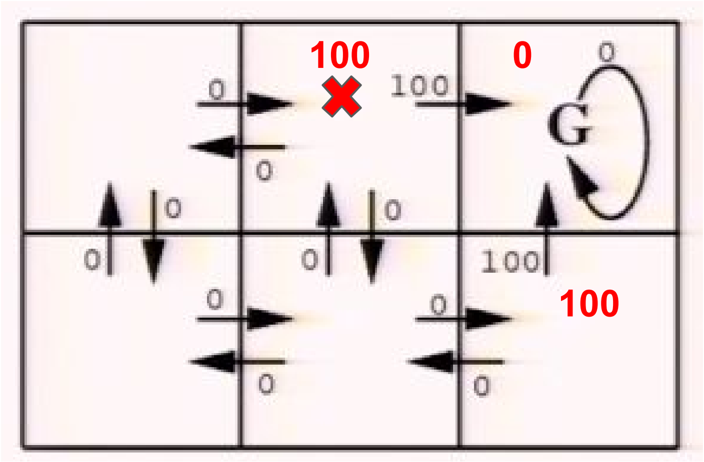

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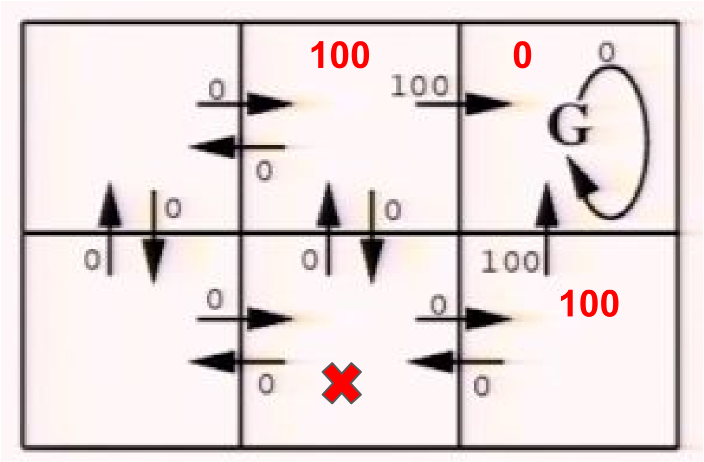

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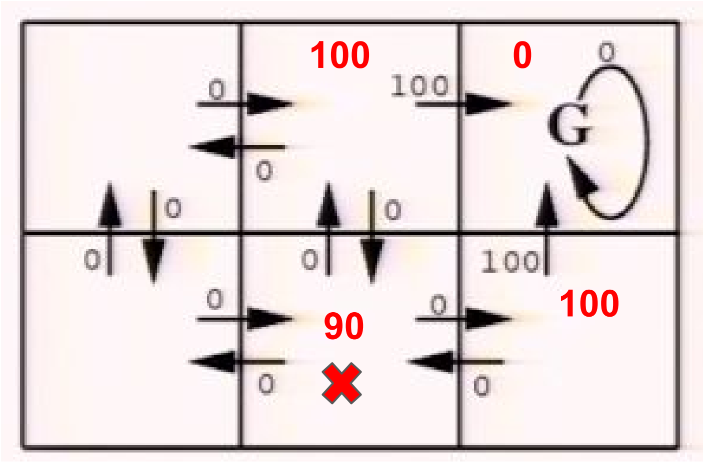

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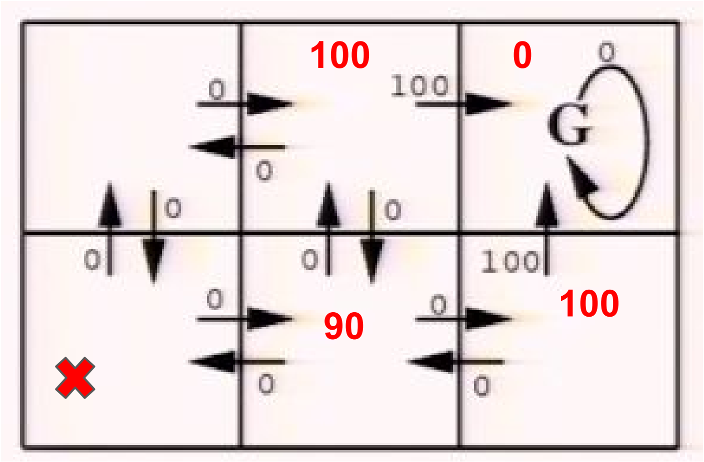

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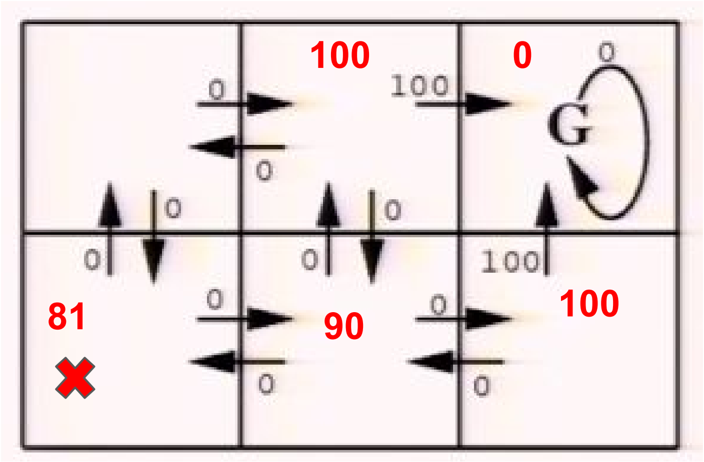

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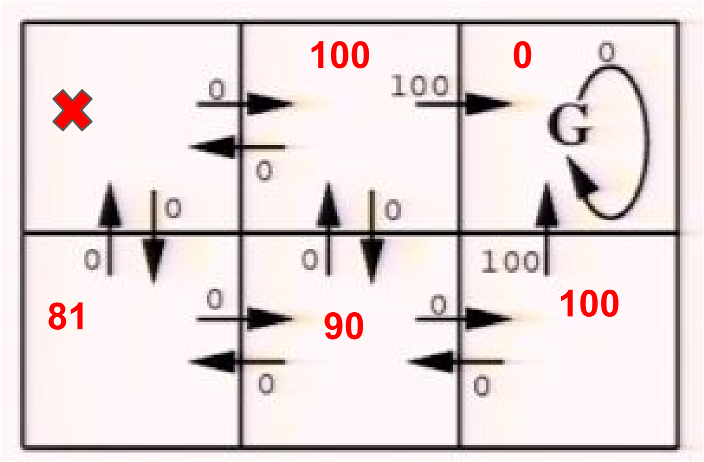

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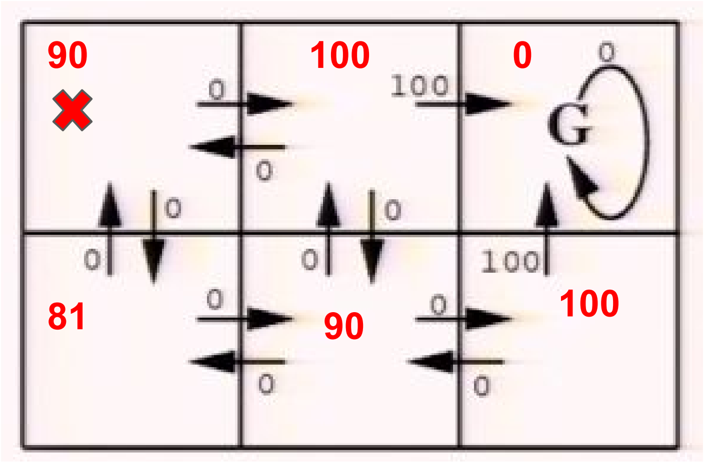

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- Recent advances in RL: combining it with deep learning!
  - learning deep policy and value networks

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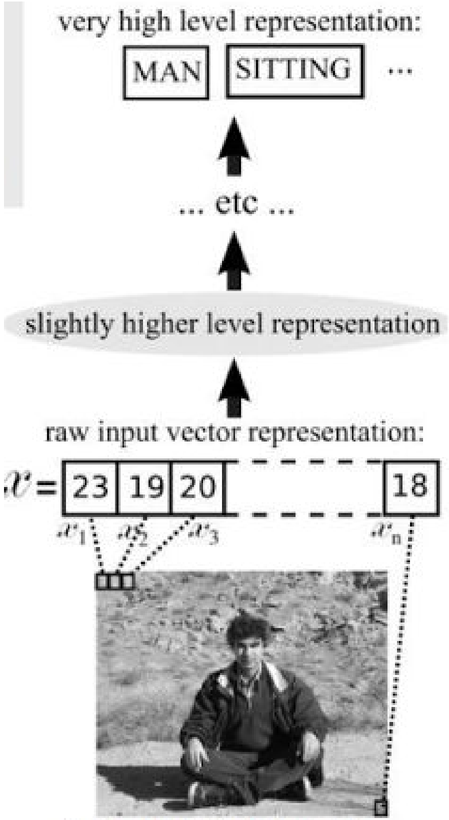

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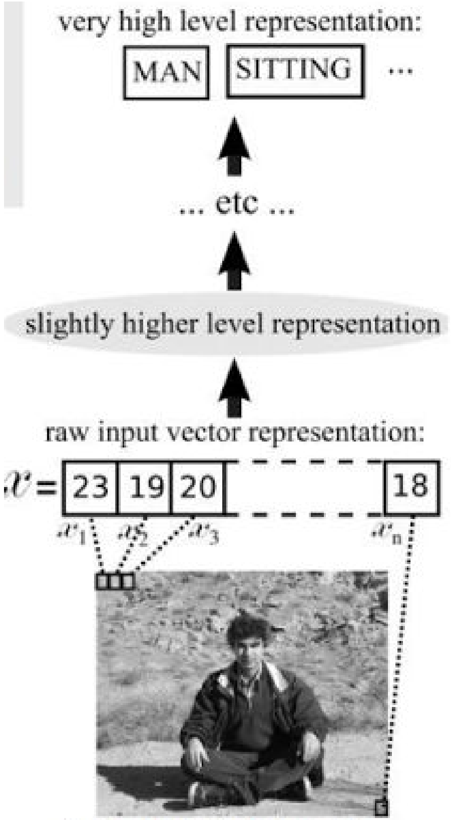

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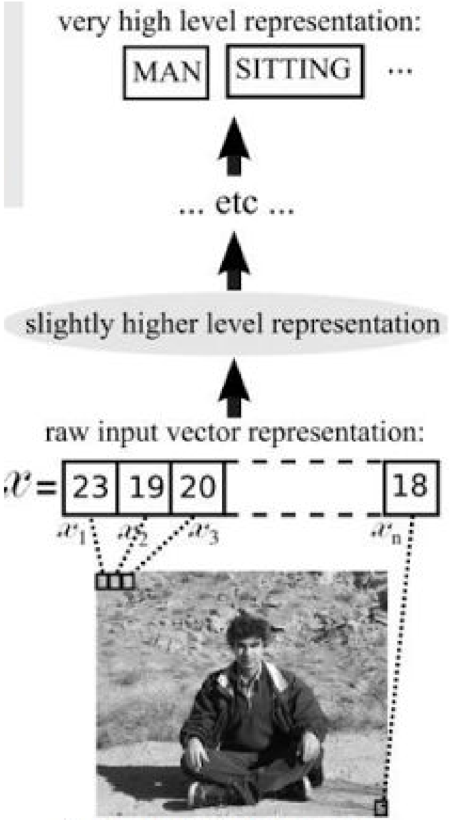

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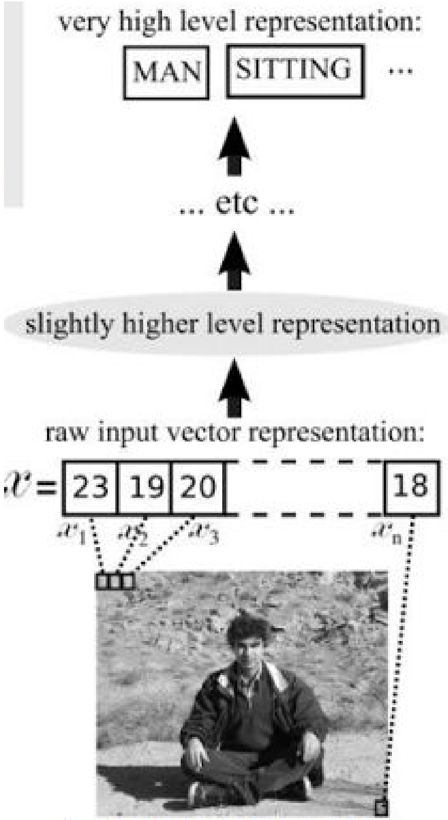
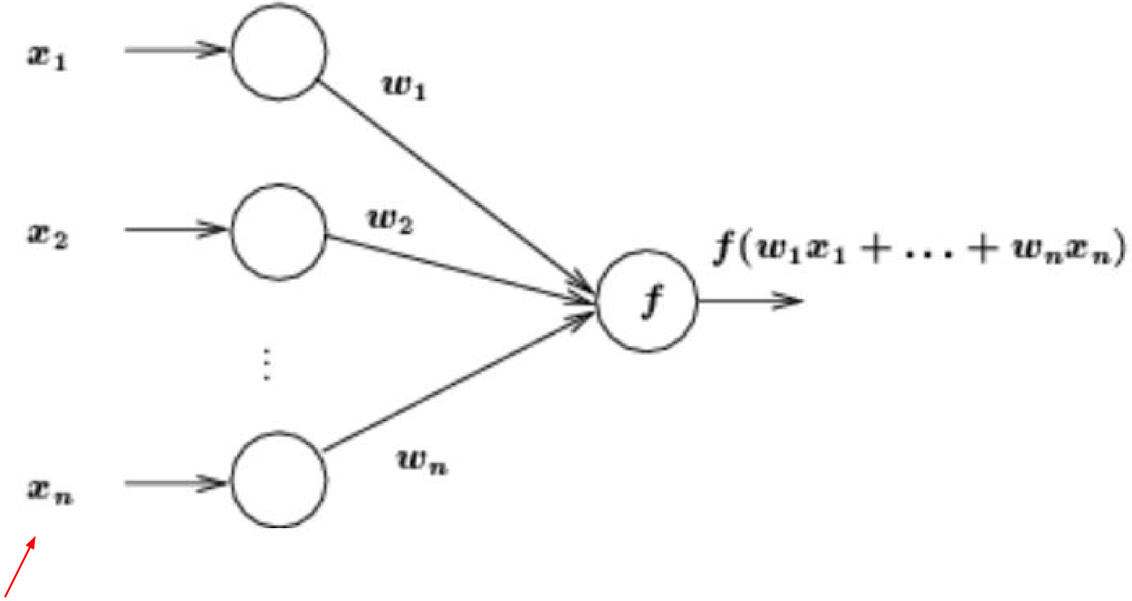
- There are a few important types:
  - Neural networks
  - Recurrent neural networks (RNNs)
    - Long short-term memory network (LSTM)
  - Deep belief networks (DBNs)
  - Convolutional neural networks (CNNs)



Artificial neural networks are inspired by connections between real neurons



data instance (like dendritic input)

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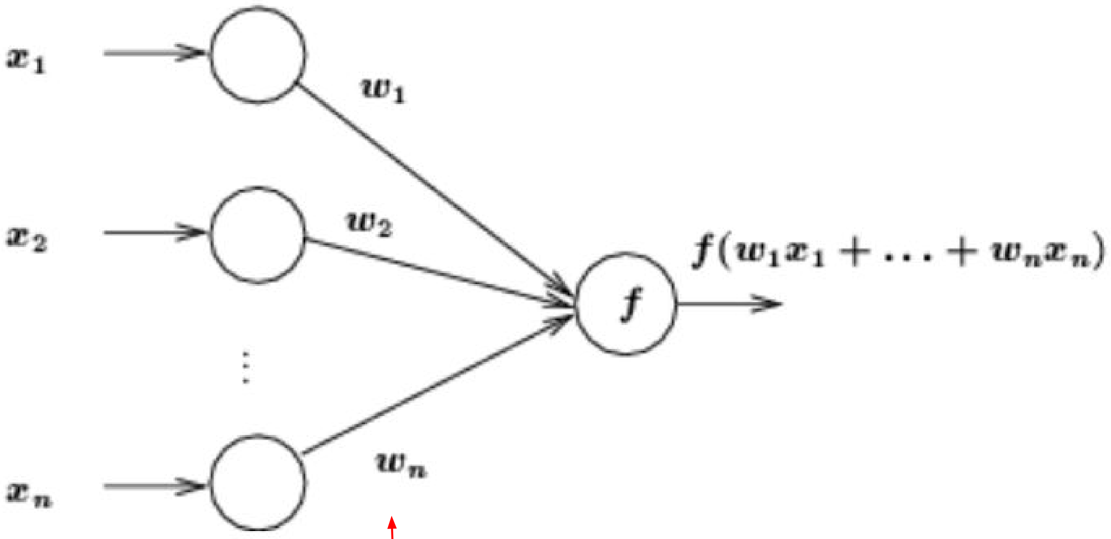

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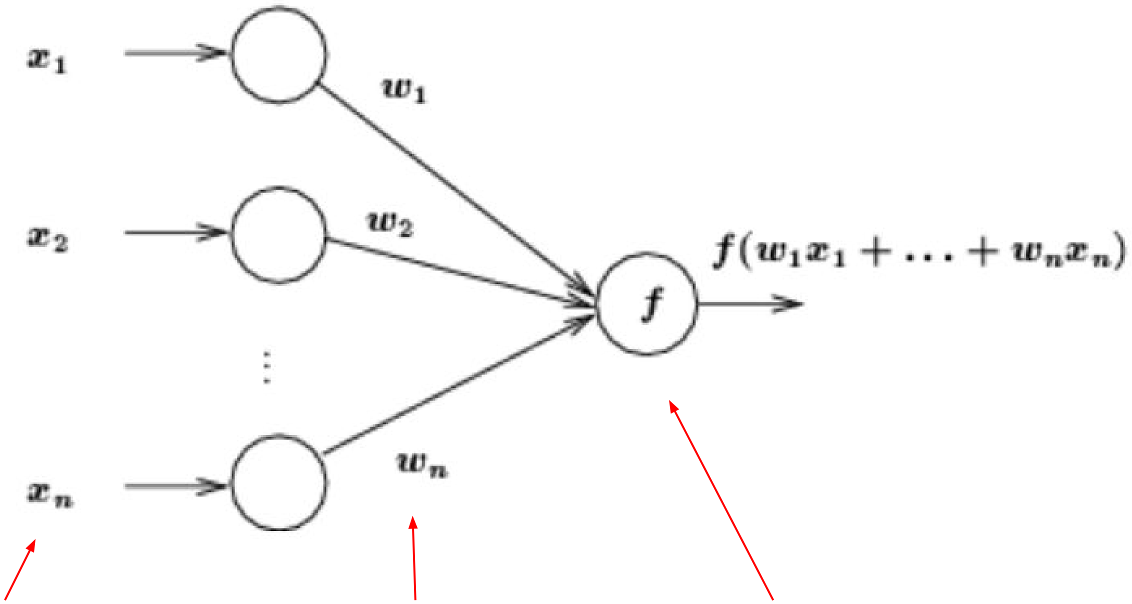
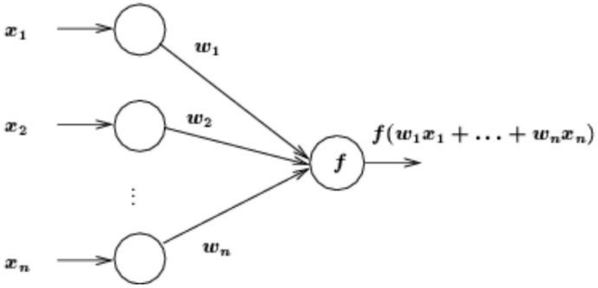


data instance (like dendritic input)

learned weights (like synaptic weights)

activation function (like firing threshold in neurons)

What is a good activation function f?



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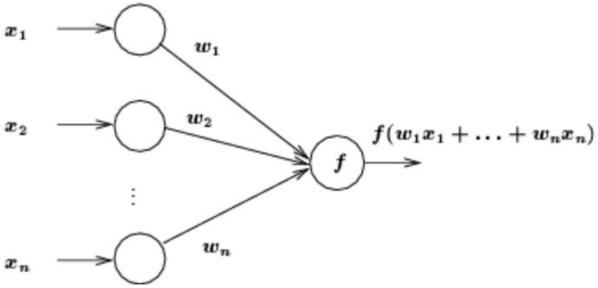


- Want non-linear f
- Some typical examples:
  - logistic (or sigmoid) function

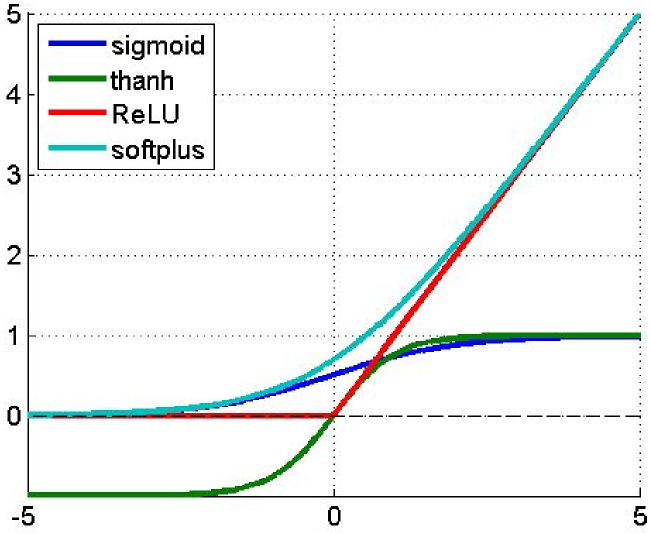
    $$f(x) = (1 + e^{-x})^{-1}$$

  - hyperbolic tangent function

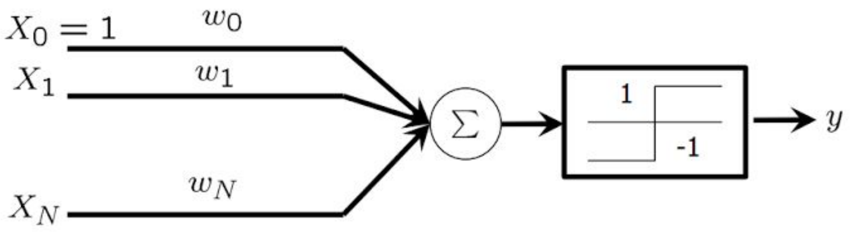
    $$f(x) = \tanh(x)$$

  - rectified linear function

    $$f(x) = \max(0, x)$$



Perceptron: simplest neural network



$$y = sgn(\mathbf{w}^T \mathbf{x})$$

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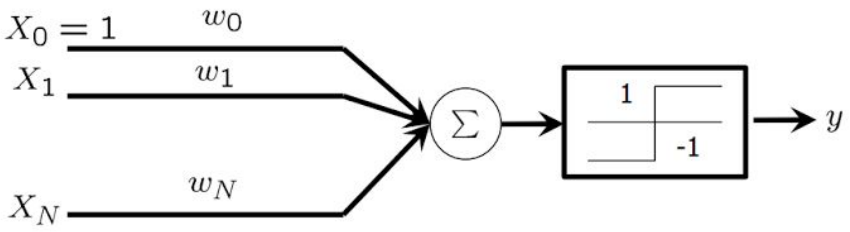

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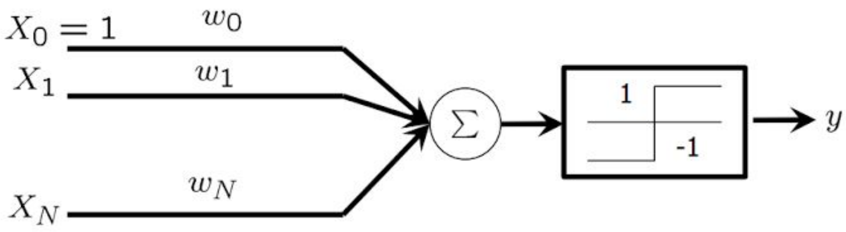

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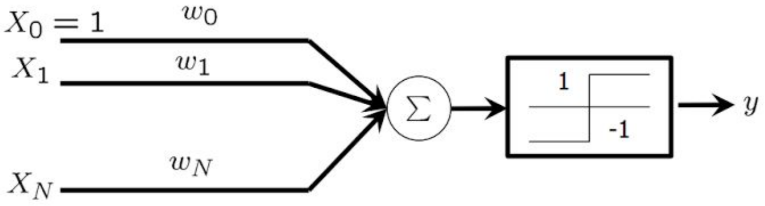
- activation function is just a threshold at 0 (checks for the sign of the weighted input sum)
- no hidden layer
- goal: given the input x and label y, find weights w such that y = sgn(w^Tx)

How do we learn the weights in the perceptron?

- Key idea: find classification error and update weights to reduce this error



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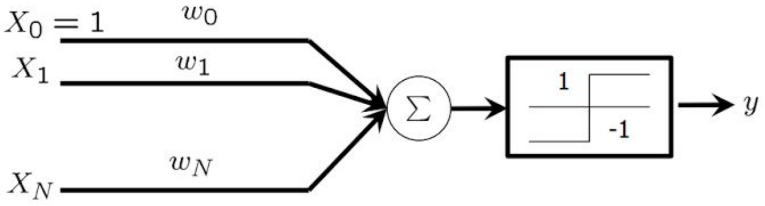

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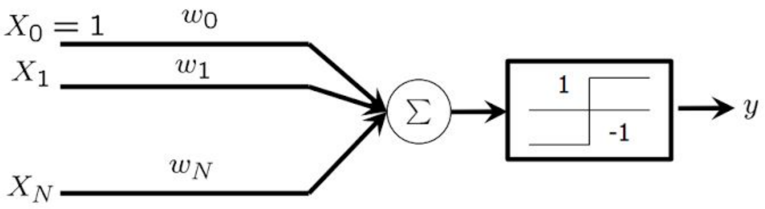

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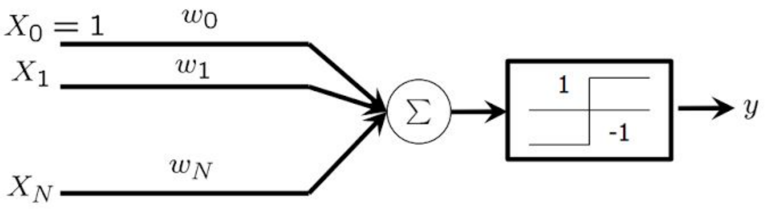

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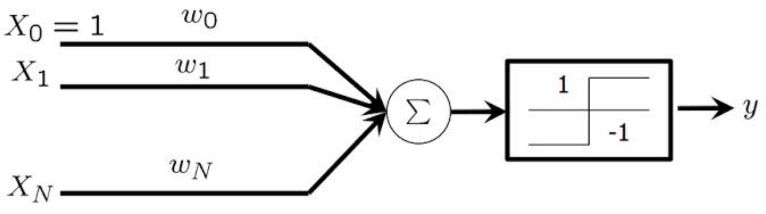

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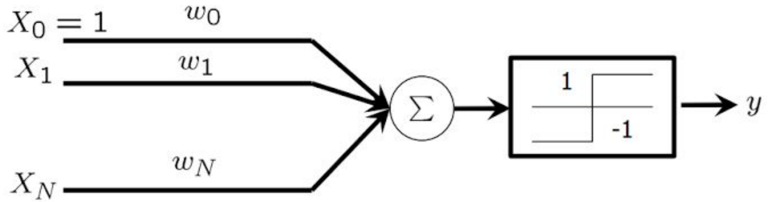

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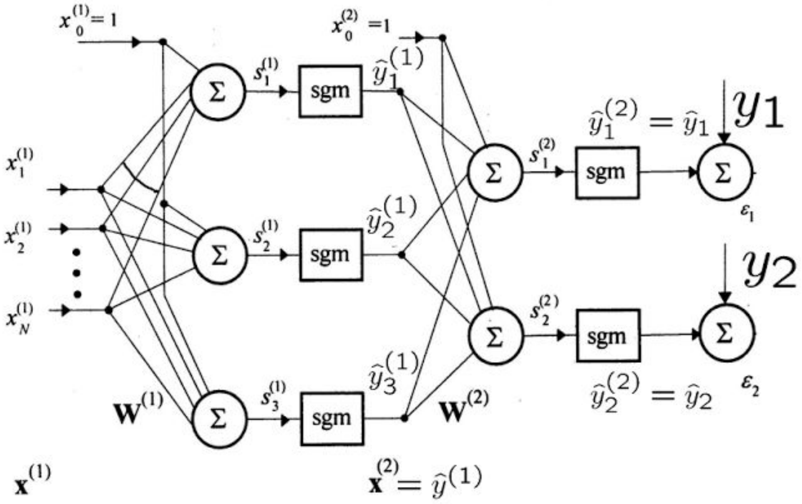
- step 5: t = t+1, end when there are no misclassifications

We add more layers => multilayer perceptron (MLP)

- Additional layers (not input or output) are called “hidden” layers



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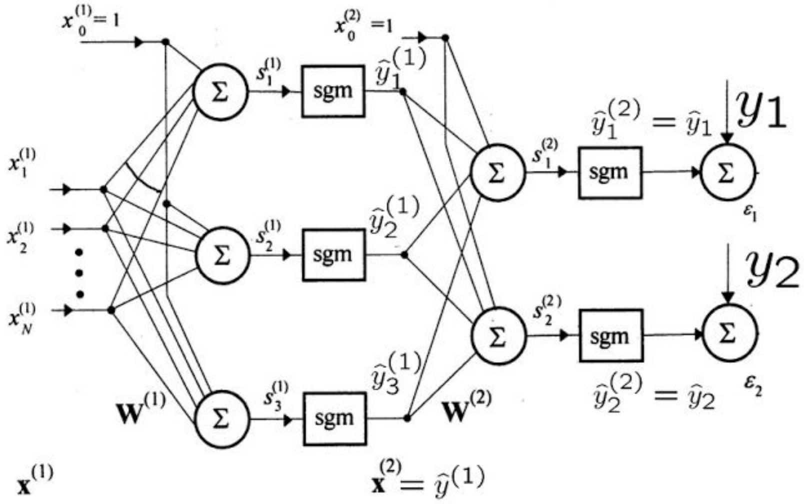

- Still need to learn weights W, but now we have multiple layers

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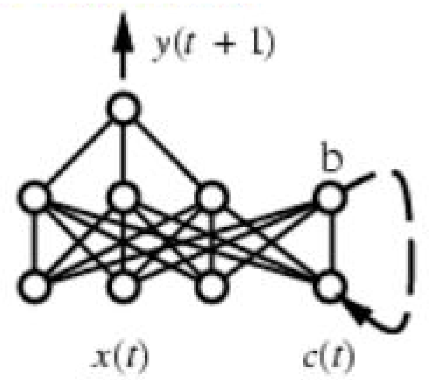
- Update weights according to the error

Neural networks for sequential data: recurrent NNs

- In sequential data, history can help predict the future



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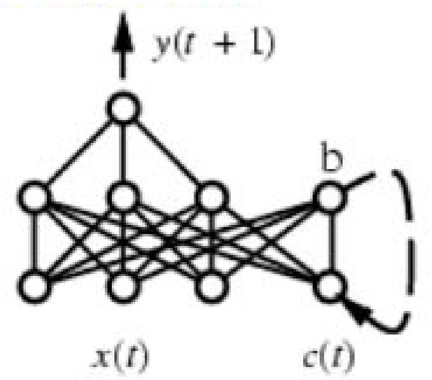

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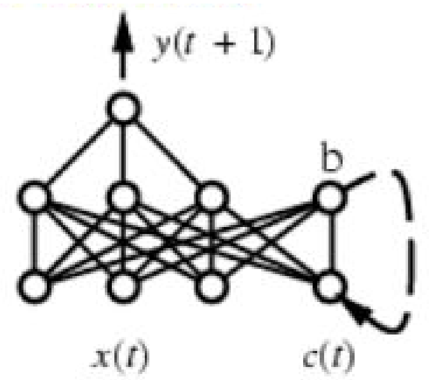

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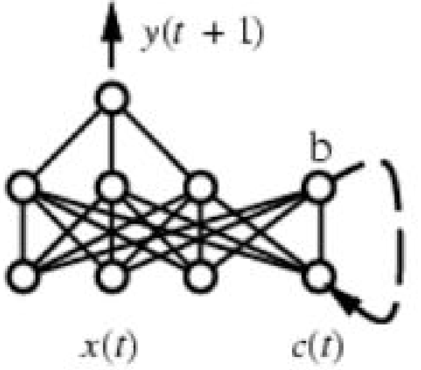

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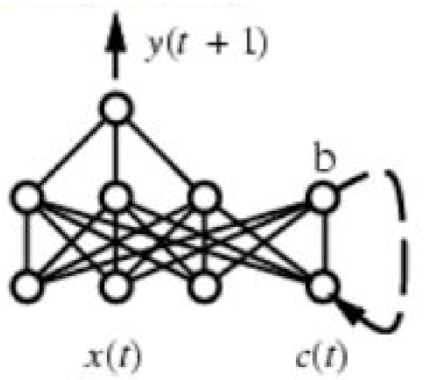

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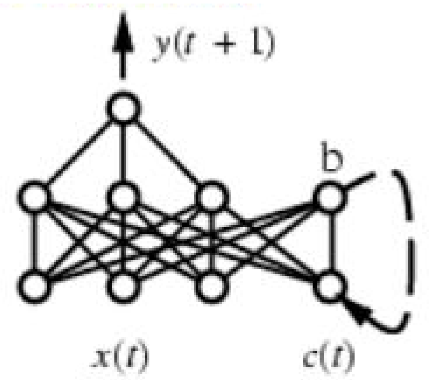

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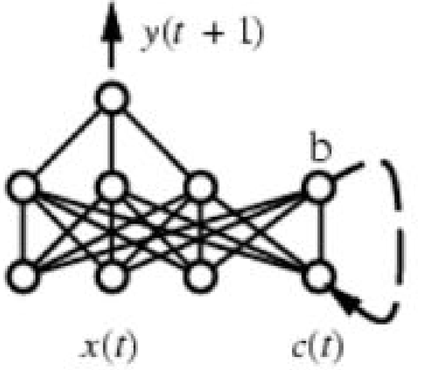

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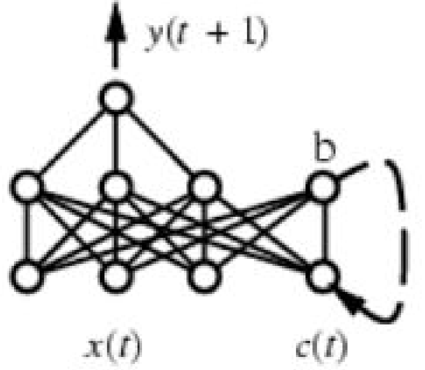

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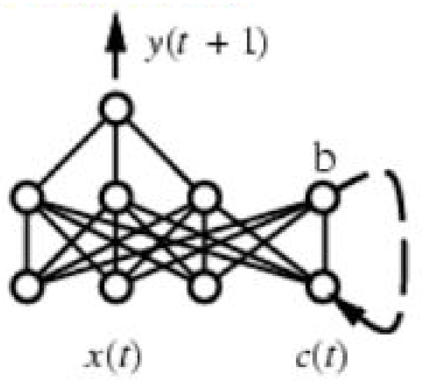

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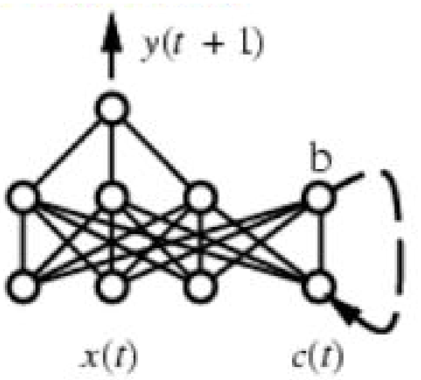

LSTMs: remembering values for arbitrary length of time

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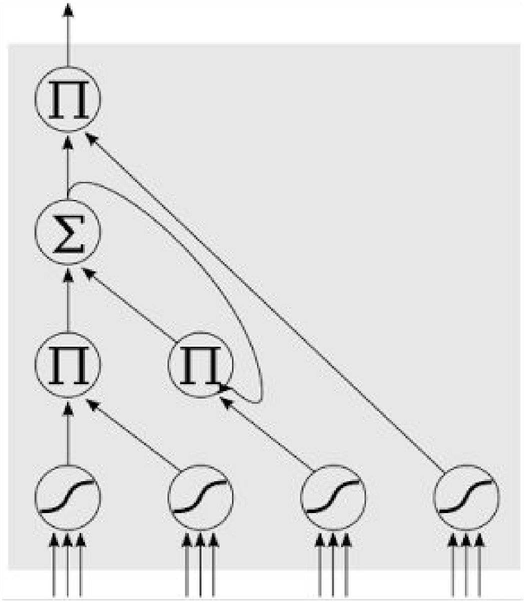

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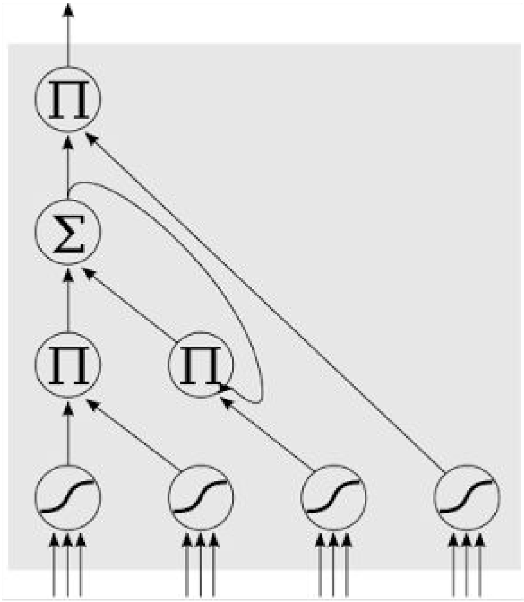

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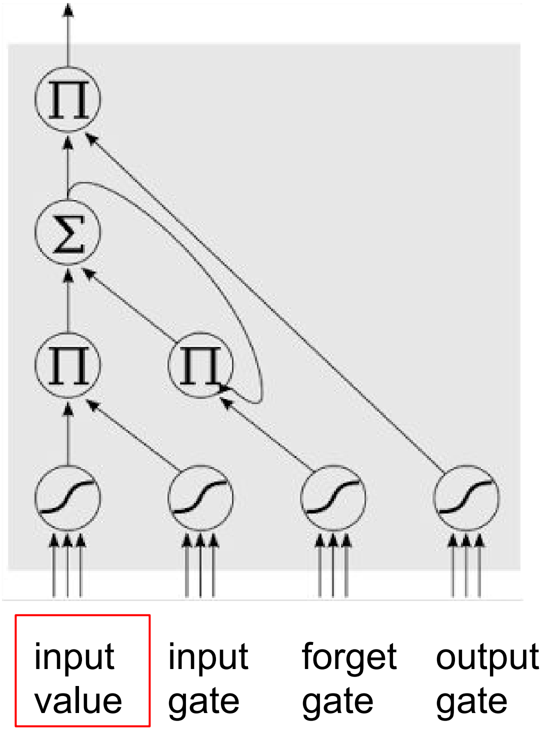

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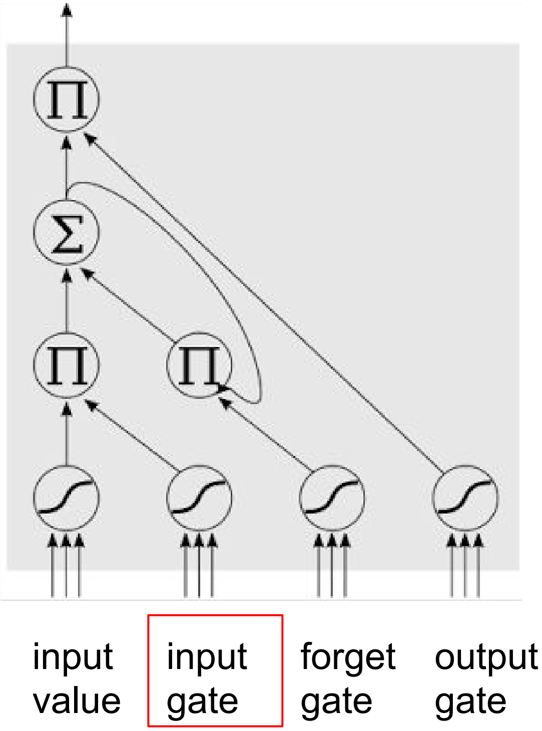

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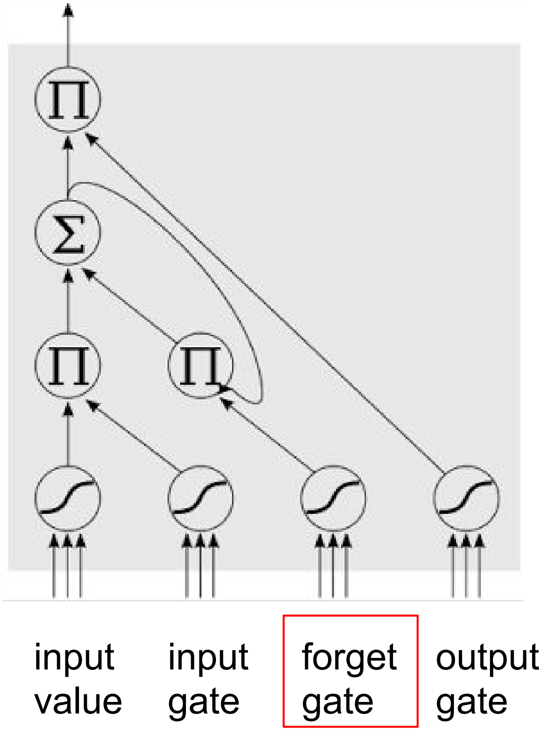

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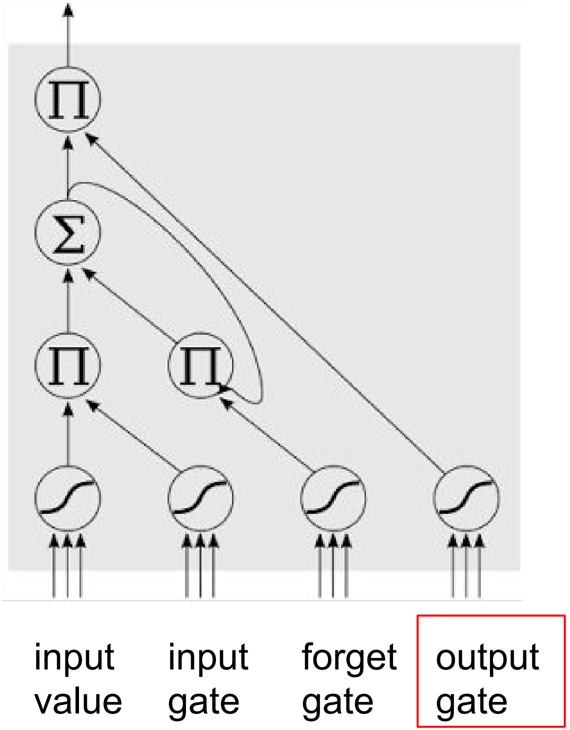

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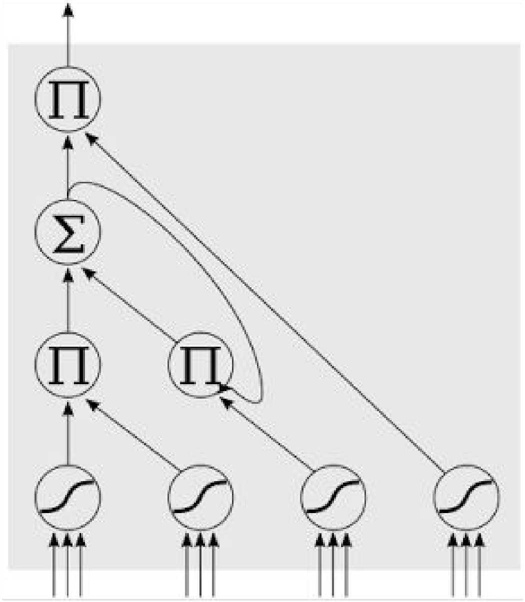

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- Problem 3: need a lot of data for good estimates of weights when we start from random initializations and to calculate classification error, we need labels => need a lot of labeled data, which is often scarce

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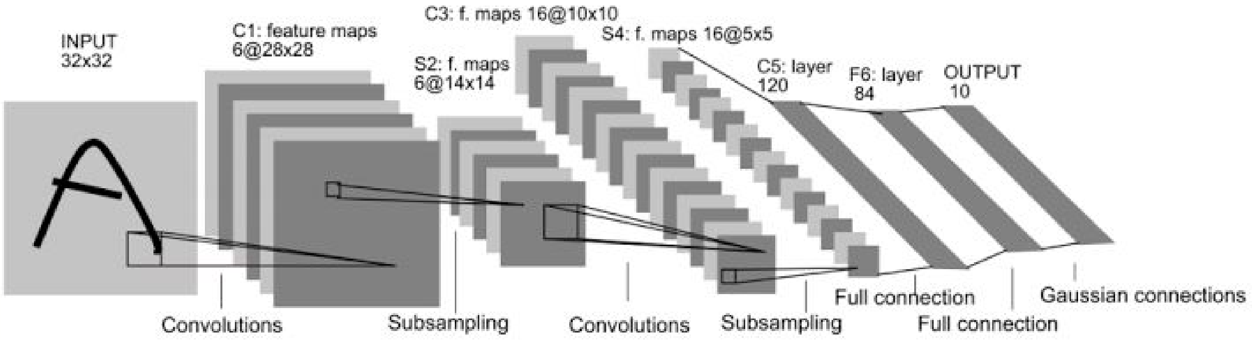
CNN: alternating convolutional and downsampling layers



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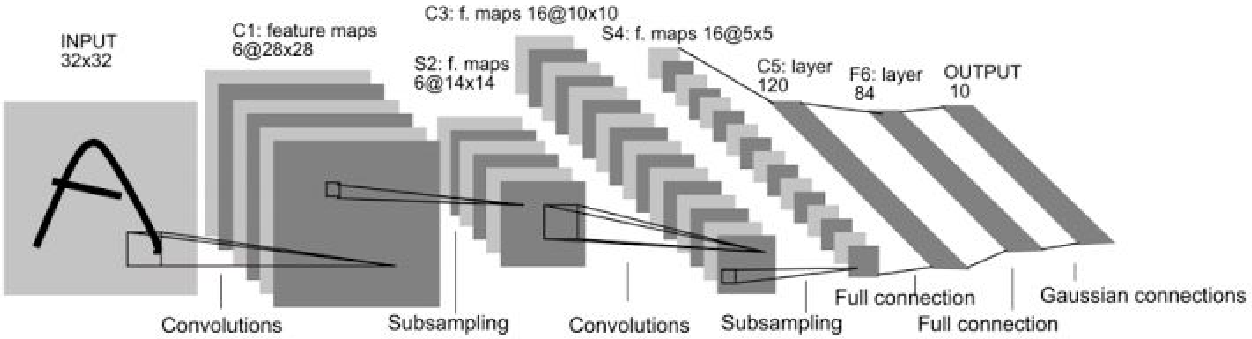

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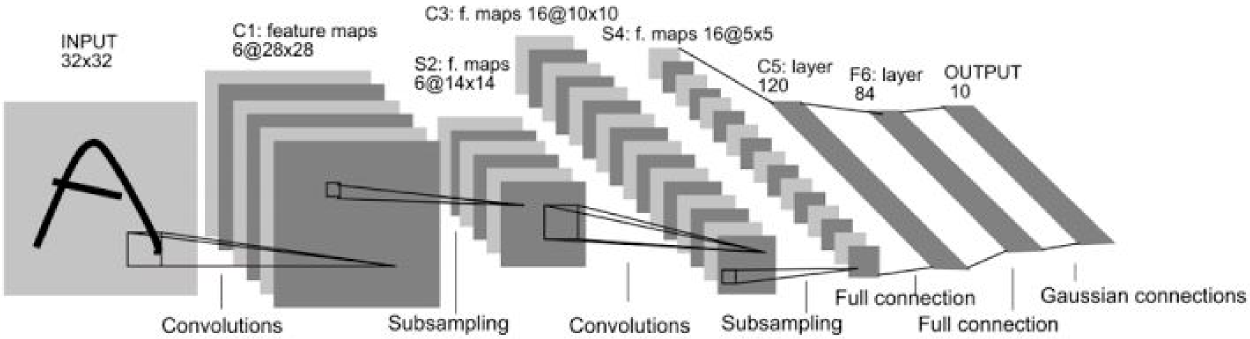

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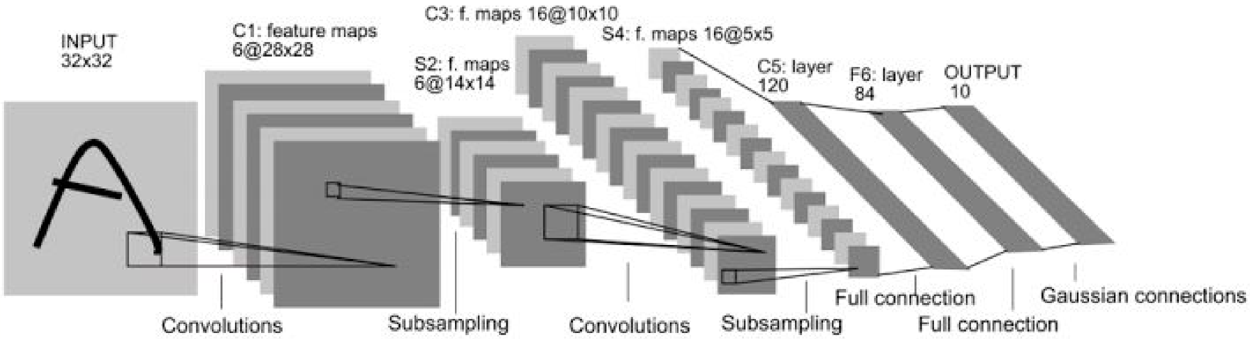

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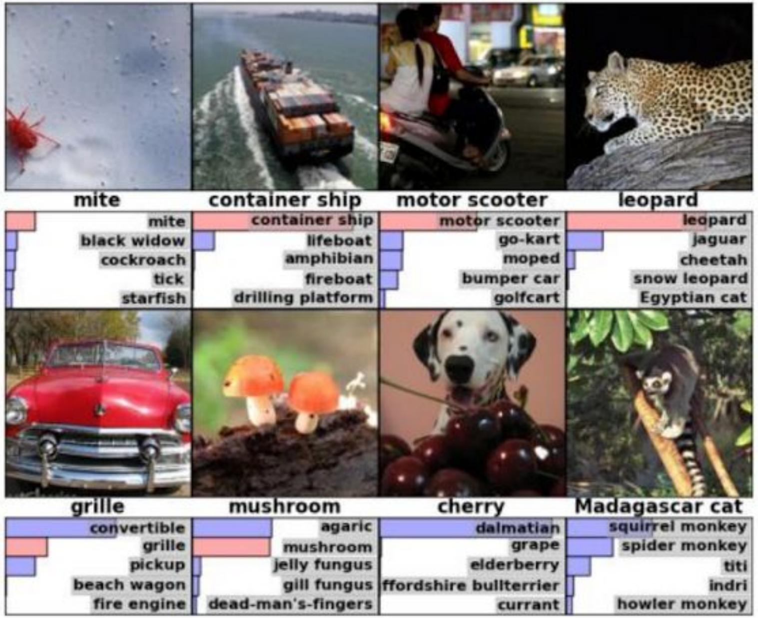
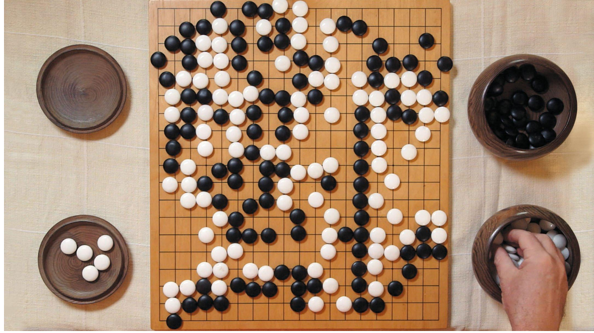


CNN also used in AlphaGo



- ❑ First off, why is Go so hard?

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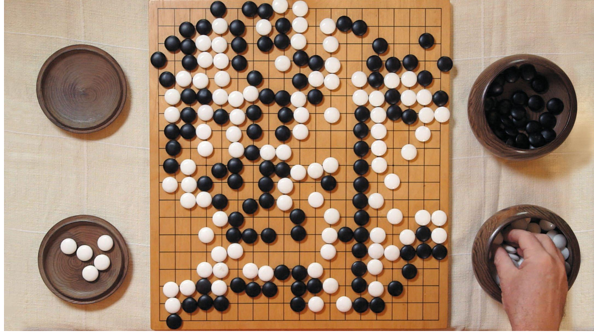

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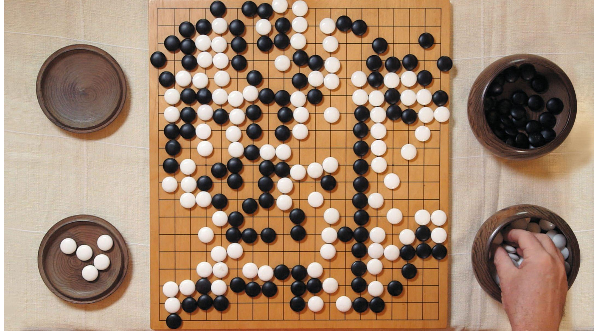

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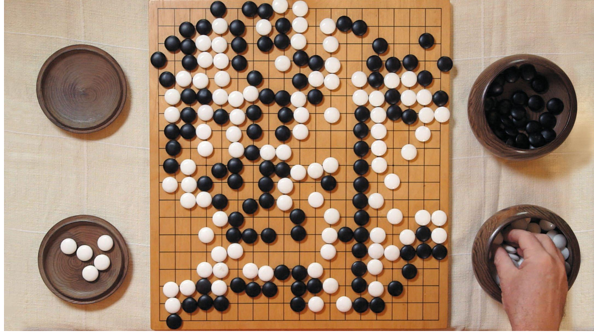

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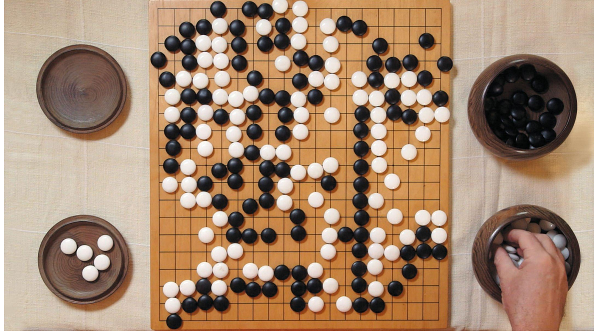

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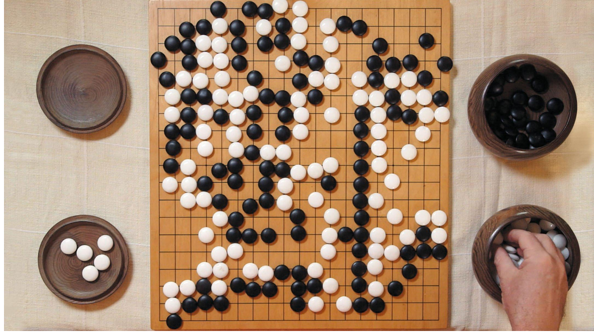

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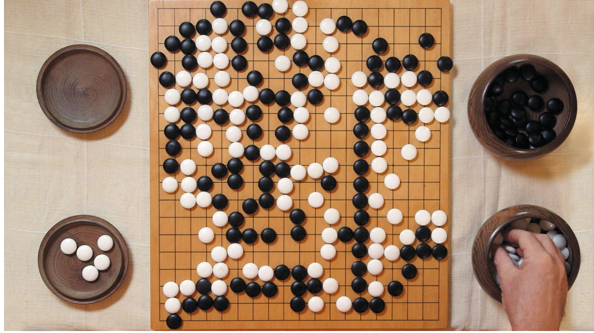

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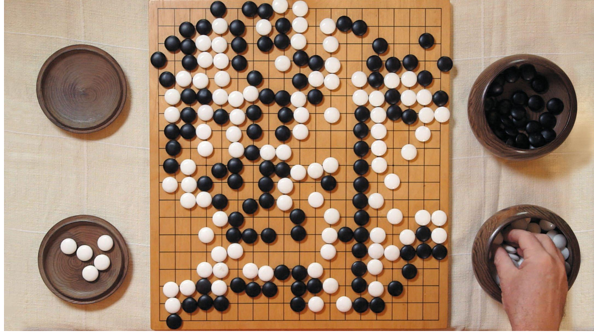

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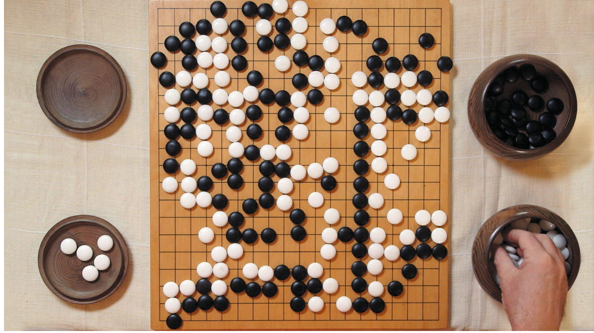

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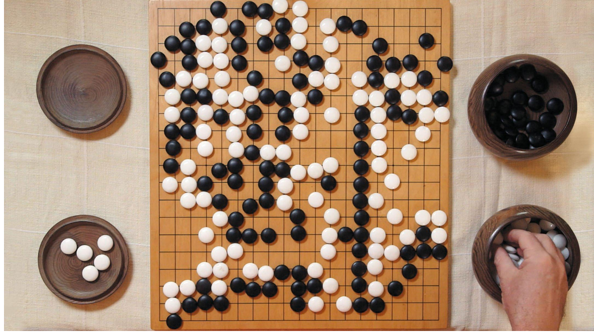

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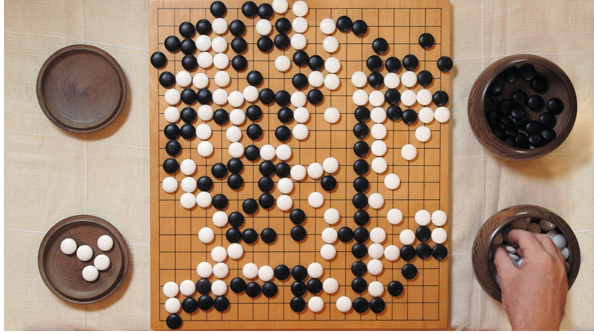

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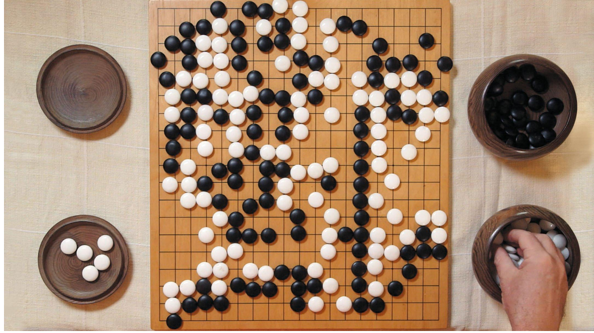

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  - "Weak amateur level play"
- AlphaGo combines tree search with RL executed with policy and value CNN networks
  - Won 4 out of 5 games against Lee Sedol, second best player of Go in the world (by # of won

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- Finally, use the value and policy networks to reduce depth breadth of search

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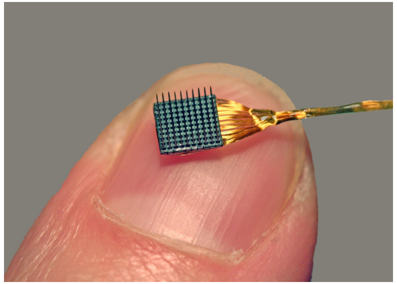
    - Written in python, compatible with GPUs
  - TensorFlow
    - Similar to Theano but arguably more intuitive
    - https://www.tensorflow.org/

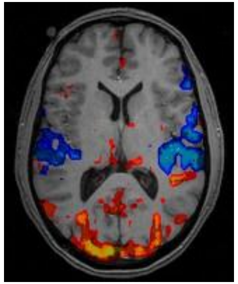
Main takeaways

- Considering the sequential nature of time series data is important
- Ways to account for this time dependence is through models, such as hidden Markov models, Markov decision processes, and long short-term memory neural networks
- We don’t know why exactly deep learning works *yet*, but it’s increasingly more popular, both in industry and academia
    - deep learning course at CMU taught by Ruslan Salakhutdinov in the Fall!

How can ML help neuroscientists?

- Deal with large number of sensors/recording sites





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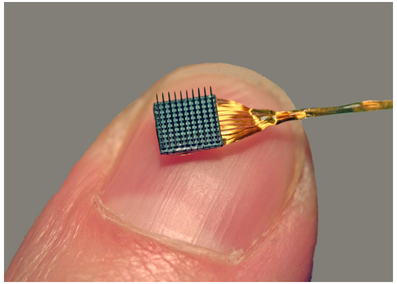

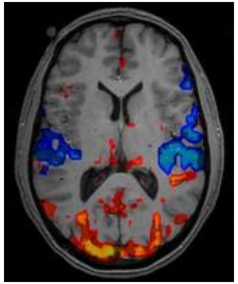

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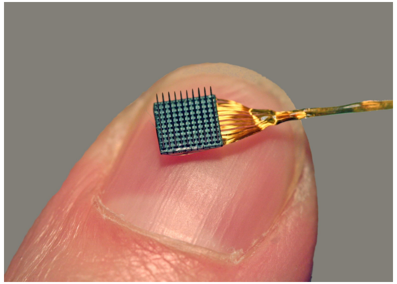
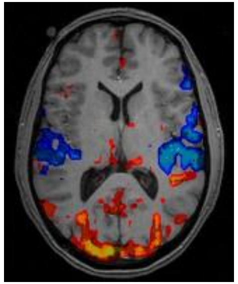

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 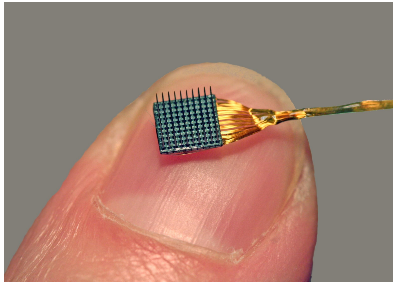 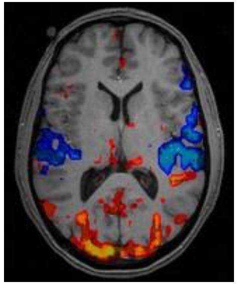

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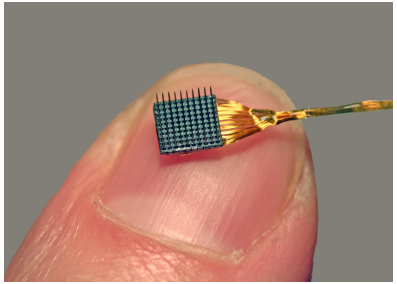

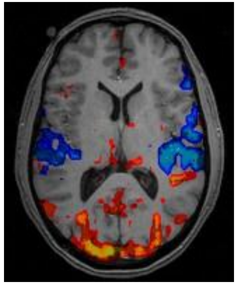

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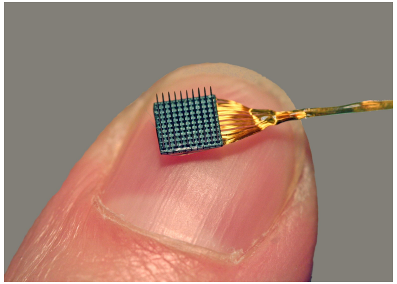
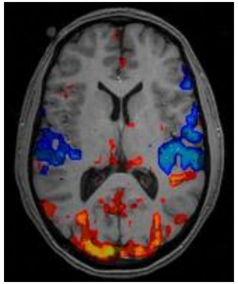

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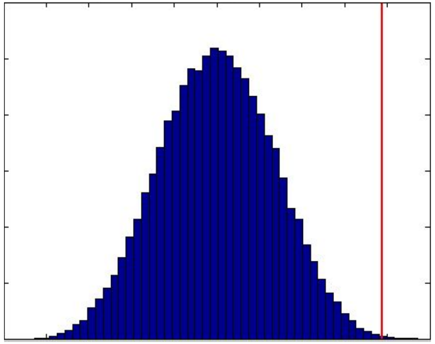

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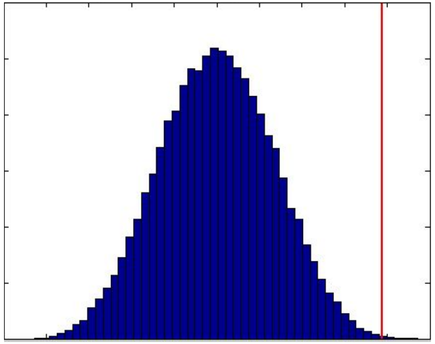

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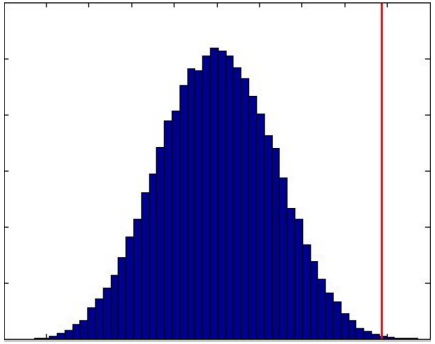

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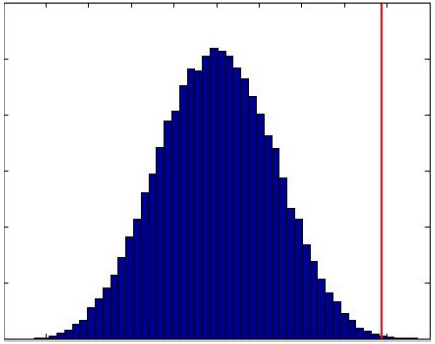

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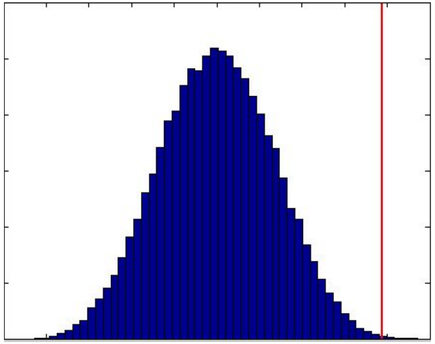

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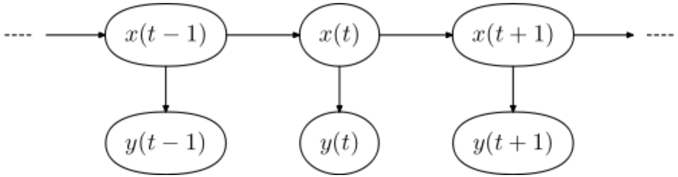
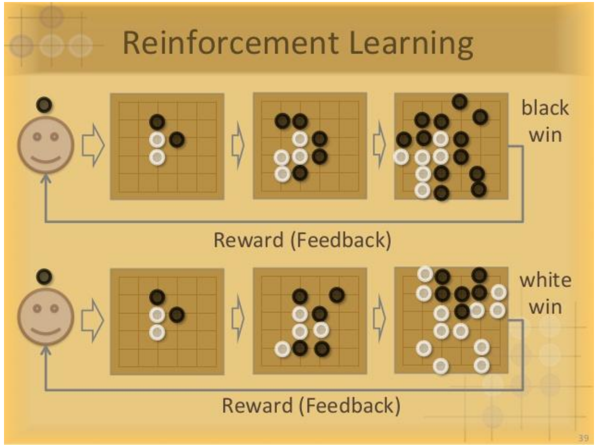
- ❑ Complex data-driven hypotheses of brain processing
  - ❑ advanced topics: latent variable models, reinforcement learning, deep learning





Thank you for your attention!

Please fill out the anonymous evaluation sheet -- your feedback is very important!

Looking forward to questions or follow-ups:

mariya@cmu.edu