CSE 573 :
Artificial Intelligence

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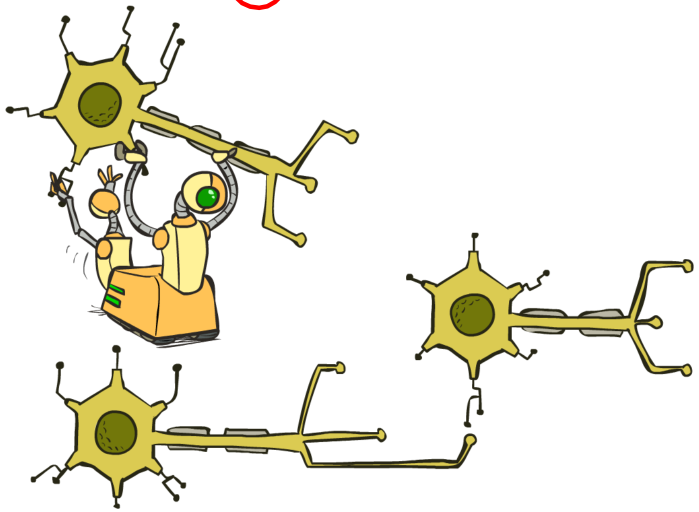
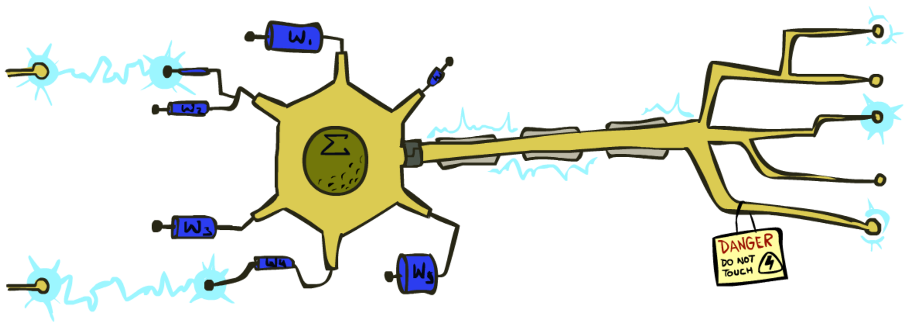
Neural Networks



slides adapted from
Dan Klein, Pieter Abbeel ai.berkeley.edu
And Dan Weld, Luke Zettlemoyer

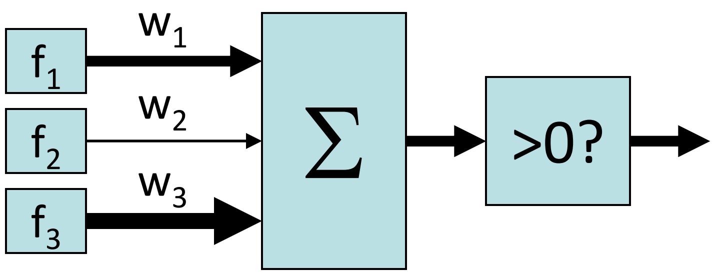
Reminder: Linear Classifiers

- Inputs are feature values
- Each feature has a weight
- Sum is the activation



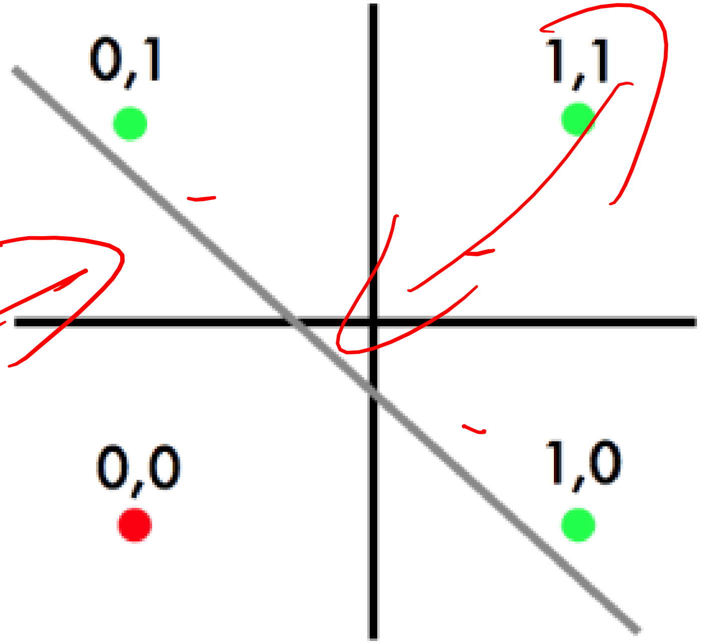
$$\text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$

- If the activation is:
  - Positive, output +1
  - Negative, output -1



Example

- Learning the OR function: 0, 1 inputs. 0, 1 outputs
- Draw a **straight** line separating the greens and reds (two classes)

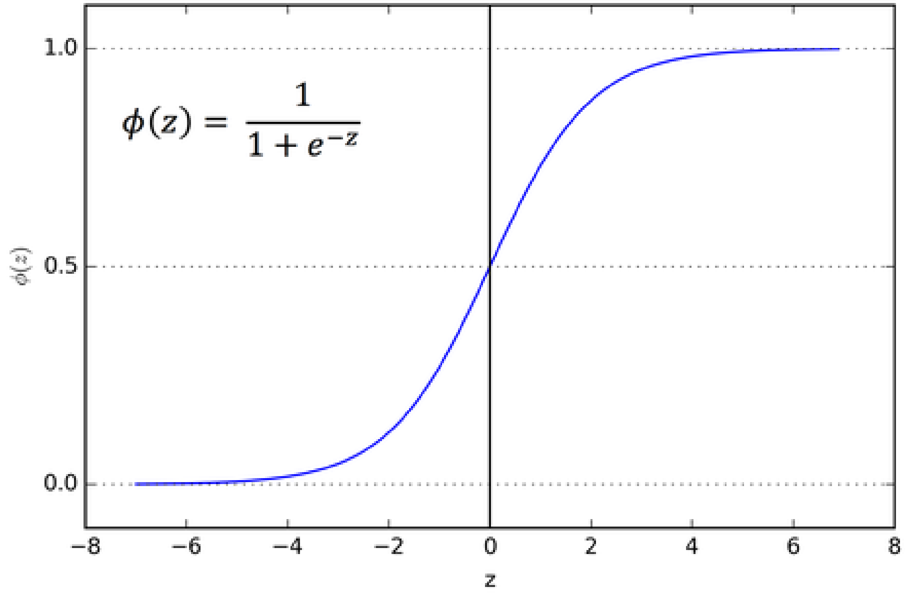


Recap: How to get probabilistic decisions?

- Activation: $z = w \cdot f(x)$
- If $z = w \cdot f(x)$ very positive → want probability going to 1
- If $z = w \cdot f(x)$ very negative → want probability going to 0

- Sigmoid function

$$\phi(z) = \frac{1}{1 + e^{-z}}$$



Best w?

- Maximum likelihood estimation:

$$\max_w \quad ll(w) = \max_w \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

with:

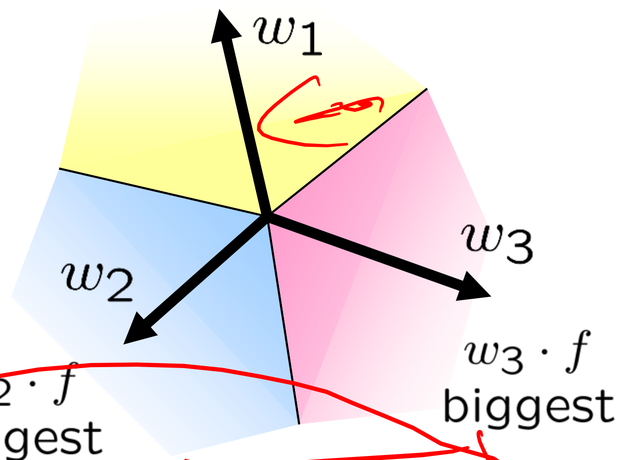
$$P(y^{(i)} = +1|x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

$$P(y^{(i)} = -1|x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

= Logistic Regression

Recap: Multiclass Logistic Regression

- Multi-class linear classification
  - A weight vector for each class: w_y
  - Score (activation) of a class y: $w_y \cdot f(x)$
  - Prediction w/highest score wins: $y = \arg\max_y \; w_y \cdot f(x)$



- How to make the scores into probabilities?

$$z_1, z_2, z_3 \rightarrow \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}, \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}}, \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

original activations — softmax activations

Best w?

- Maximum likelihood estimation:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

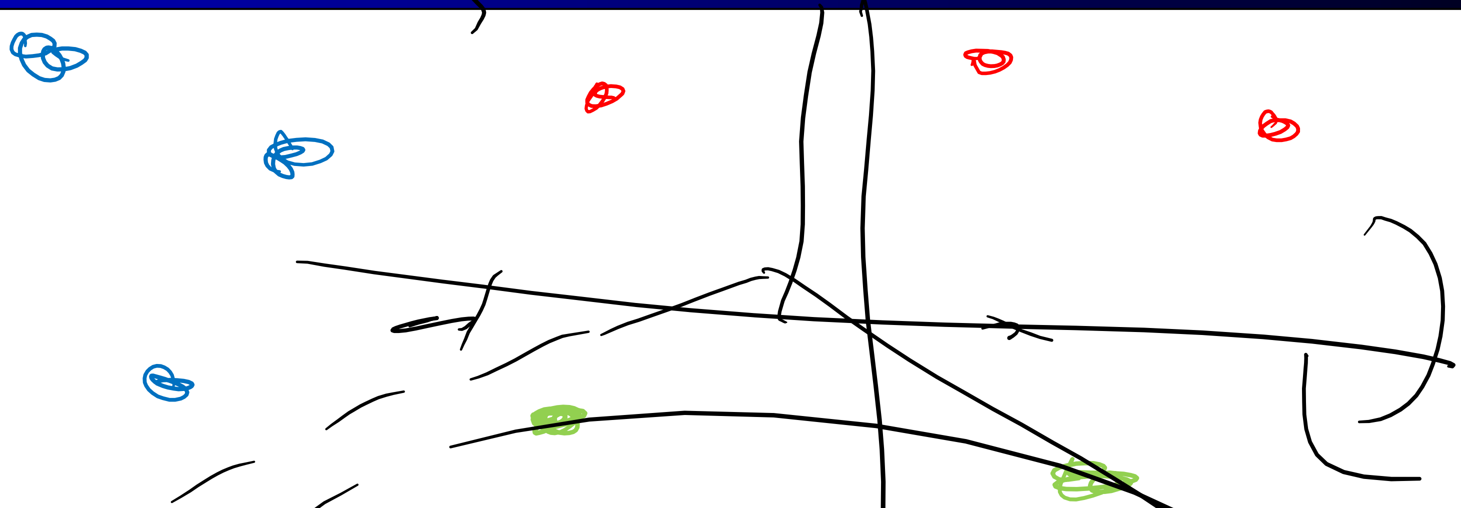
with:
$$P(y^{(i)}|x^{(i)}; w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_y e^{w_y \cdot f(x^{(i)})}}$$

softmax

$$\frac{1}{1+e^{w \cdot f(x^{(i)})}}$$

= Multi-Class Logistic Regression

Optimization



- Optimization
  - i.e., how do we solve:

$$\max_w \; ll(w) = \max_w \; \sum_i \log P(y^{(i)} | x^{(i)}; w)$$

Hill Climbing

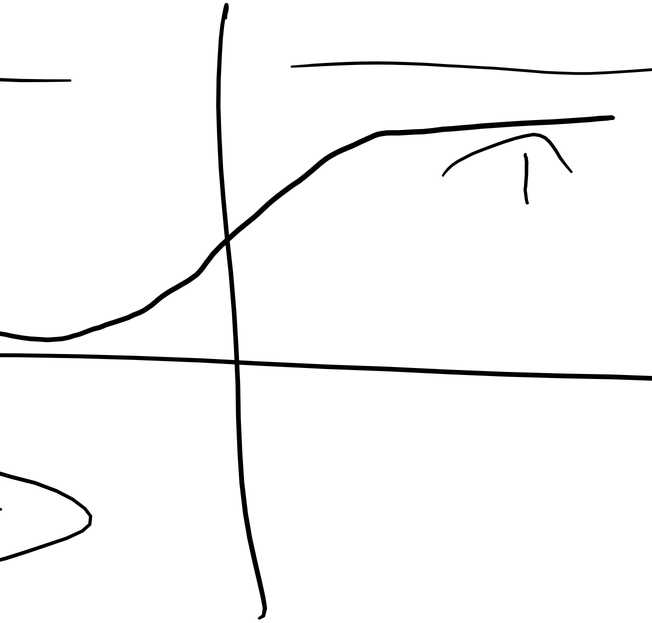
- simple, general idea
  - Start wherever
  - Repeat: move to the best neighboring state
  - If no neighbors better than current, quit

- What's particularly tricky when hill-climbing for multiclass logistic regression?
  - Optimization over a continuous space
    - Infinitely many neighbors!
    - How to do this efficiently?

Optimization Procedure: Gradient Ascent

```
▪ init w
▪ for iter = 1, 2, …
```

$$w \leftarrow w + \alpha * \nabla g(w)$$

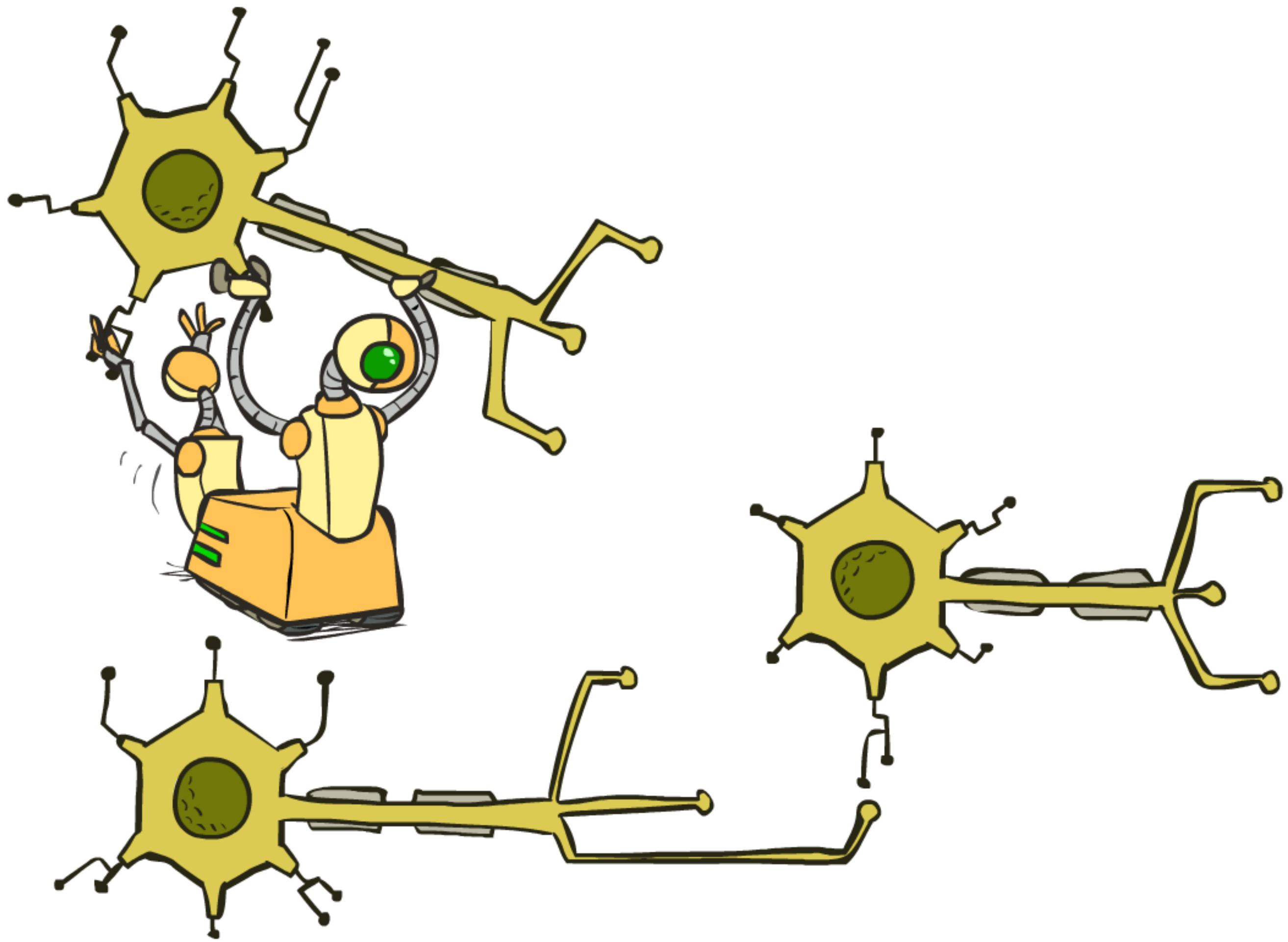


- α : learning rate --- tweaking parameter that needs to be chosen carefully
- How? Try multiple choices
  - Crude rule of thumb: update changes w about 0.1 – 1 %

How about computing all the derivatives?

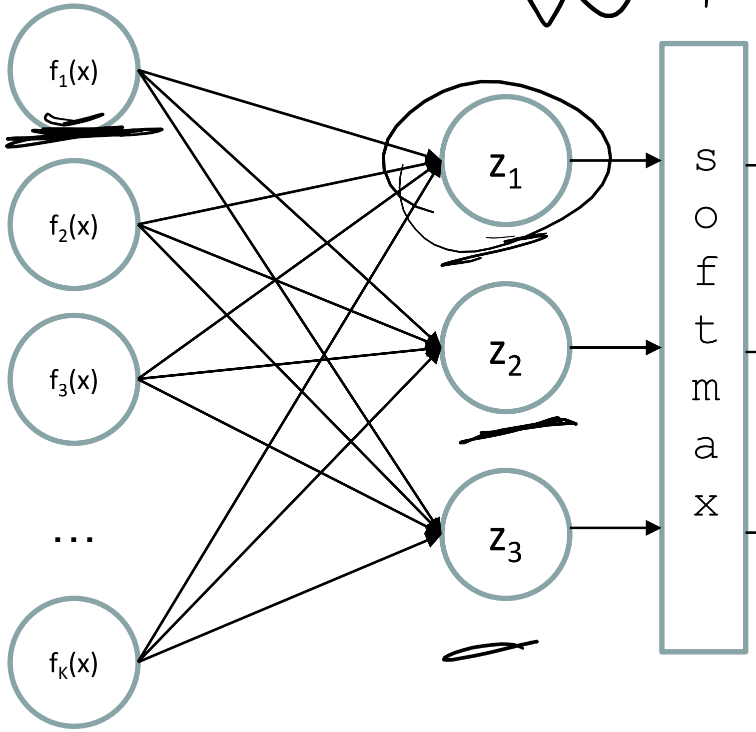
- We’ll talk about that once we covered neural networks, which are a generalization of logistic regression

Neural Networks



Multi-class Logistic Regression

- = special case of neural network

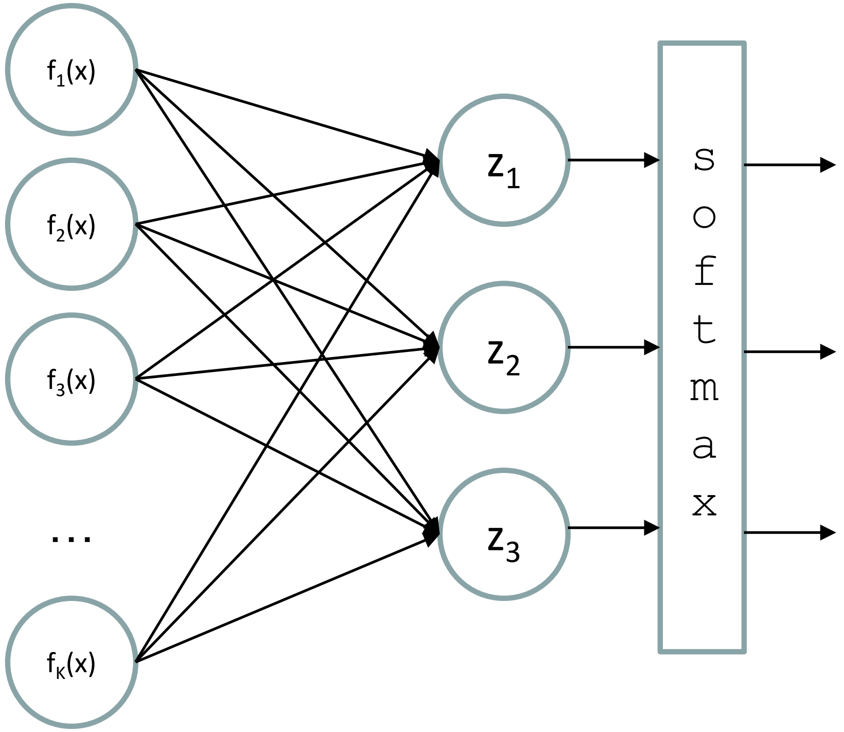


$$P(y_1|x;w) = \frac{e^{z_1}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_2|x;w) = \frac{e^{z_2}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

$$P(y_3|x;w) = \frac{e^{z_3}}{e^{z_1} + e^{z_2} + e^{z_3}}$$

Deep Neural Network = Also learn the features!



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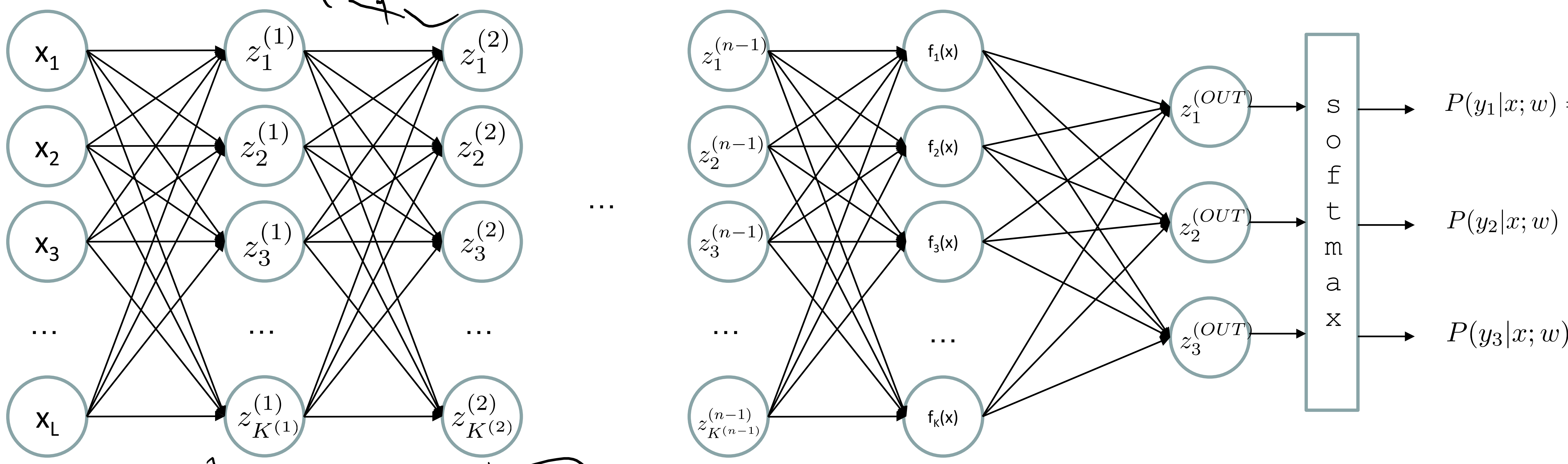
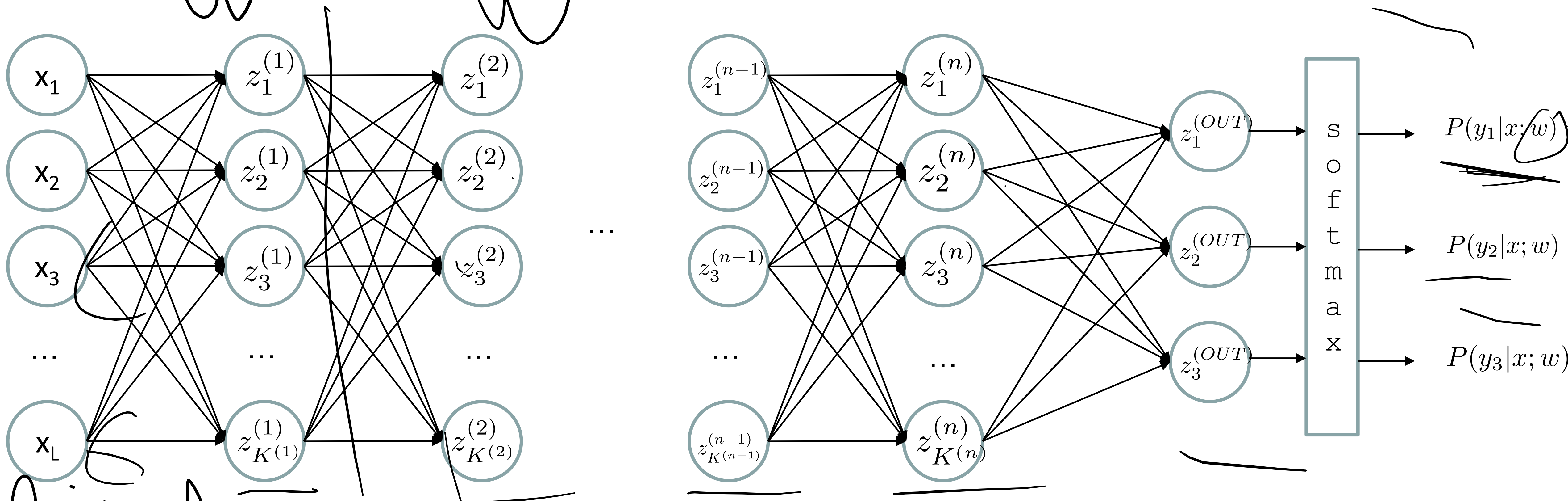


$$z_i^{(k)} = g\left(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)}\right)$$

g = nonlinear activation function

Deep Neural Network = Also learn the features!



$$z_i^{(k)} = g(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)})$$

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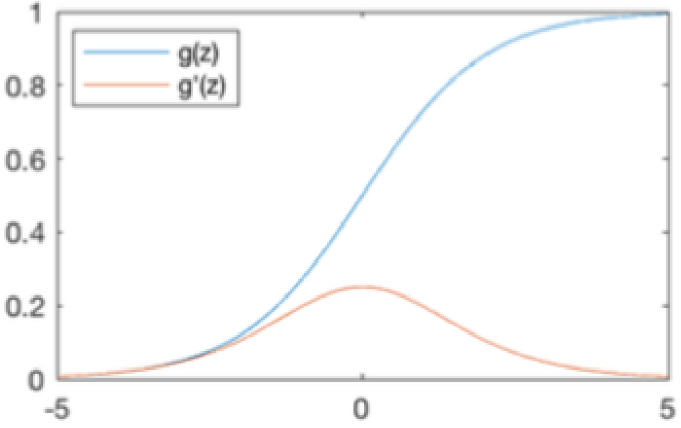
Common Activation Functions

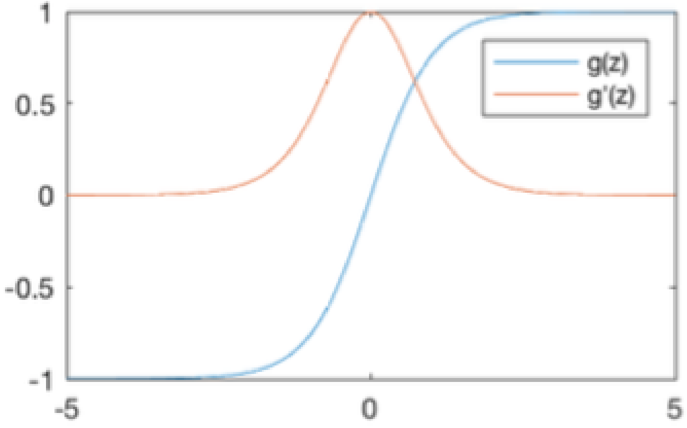
Sigmoid Function



$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

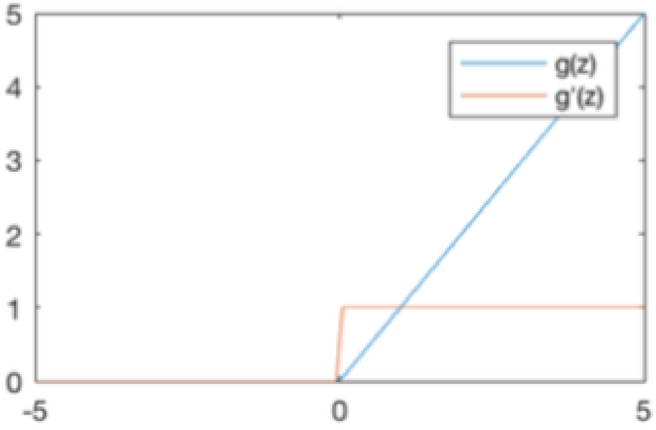
Hyperbolic Tangent



$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

Rectified Linear Unit (ReLU)



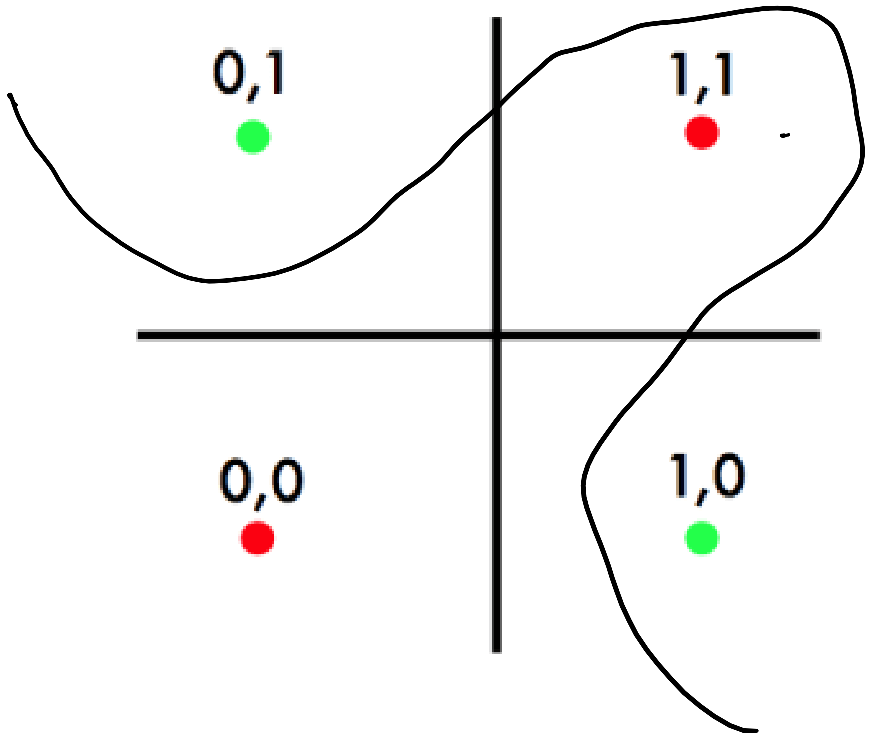
$$g(z) = \max(0, z)$$

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

[source: MIT 6.S191 introtodeeplearning.com]

Why non-linear activations?

- To understand, lets try to learn the XOR function
- Draw a **straight** line through the graph such that greens are on one side and reds are on another



Input 1	Input 2	Output
0	0	0
0	1	1
1	1	0
1	0	1

Deep Neural Network: Also Learn the Features!

- Training the deep neural network is just like logistic regression:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

just w tends to be a much, much larger vector ☺

→just run gradient ascent

+ stop when log likelihood of hold-out data starts to decrease

Neural Networks Properties

- Theorem (Universal Function Approximators). A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.

- Practical considerations
  - Can be seen as learning the features
  - Large number of neurons
    - Danger for overfitting
    - (hence early stopping!)

How about computing all the derivatives?

- But neural net f is never one of those?
  - No problem: CHAIN RULE:

If $$f(x) = g(h(x))$$

Then $$f'(x) = g'(h(x))h'(x)$$

→ **Derivatives can be computed by following well-defined procedures**

Automatic Differentiation

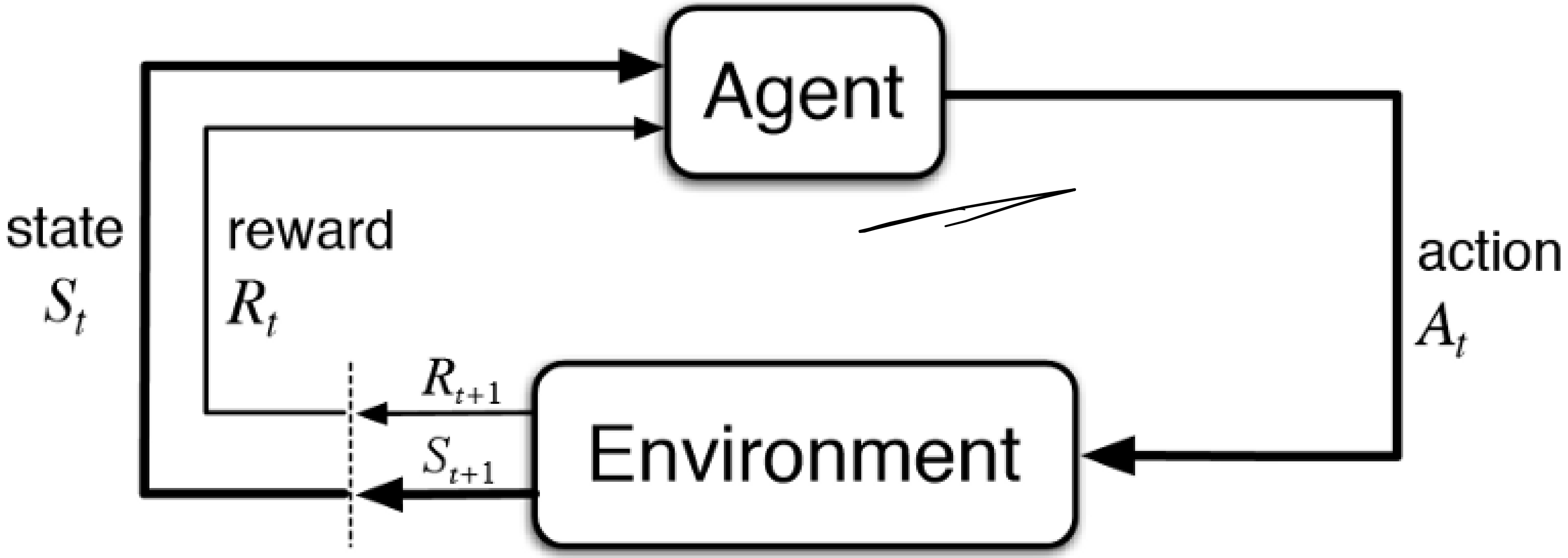
- Automatic differentiation software
  - e.g. Theano, TensorFlow, PyTorch, Chainer
  - Only need to program the function g(x,y,w)
  - Can automatically compute all derivatives w.r.t. all entries in w

- Need to know this exists
- How this is done? -- outside of scope of CSE573

Summary of Key Ideas

- Optimize probability of label given input $$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$
- Continuous optimization
  - Gradient ascent:
    - Compute steepest uphill direction = gradient (= just vector of partial derivatives)
    - Take step in the gradient direction
    - Repeat (until held-out data accuracy starts to drop = "early stopping")
- Deep neural nets
  - Last layer = still logistic regression
  - Now also many more layers before this last layer
    - = computing the features
    - → the features are learned rather than hand-designed
  - Automatic differentiation gives the derivatives efficiently (how? = outside of scope of 573)

Deep Reinforcement Learning



Reinforcement Learning
= Learning by Interaction

AGENT GOAL: FIND POLICY π: S → A
TO MAXIMIZE REWARD

Reinforcement Learning
= Learning by Interaction

Markov Decision Process

Mathematical formulation of the RL problem

Defined by: $(\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathbb{P}, \gamma)$

$\mathcal{S}$: set of possible states
$\mathcal{A}$: set of possible actions
$\mathcal{R}$: distribution of reward given (state, action) pair
$\mathbb{P}$: transition probability i.e. distribution over next state given (state, action) pair
γ : discount factor

Markov property: Current state completely characterizes the state of the world

$$p(r, s' | s, a) = Prob\left[R_{t+1} = r, S_{t+1} = s' \,\middle|\, S_t = s, A_t = a\right]$$

Recap: Solving for the optimal policy

Value iteration algorithm: Use Bellman equation as an iterative update

$$Q_{i+1}(s,a) = \mathbb{E}\left[r + \gamma \max_{a'} Q_i(s',a') | s,a\right]$$

Q_i will converge to Q^* as i -> infinity

Approximate MDP solvers

What's the problem with this?

1. Not scalable. Must compute Q(s,a) for every state-action pair. If state is e.g. current game state pixels, computationally infeasible to compute for entire state space!
2. Real problems do not give you transition matrix. Again, need to account for all possibilities.

Solution: use a function approximator to estimate Q(s,a). E.g. a neural network!

Deep Q-learning

Remember: want to find a Q-function that satisfies the Bellman Equation:

$$Q^*(s,a) = \mathbb{E}[r + \gamma \max_{a'} Q^*(s',a') \mid s,a]$$

Forward Pass

Loss function: $L_i(\theta_i) = \mathbb{E}\left[(y_i - Q(s,a;\theta_i))^2\right]$

where $y_i = \mathbb{E}[r + \gamma \max_{a'} Q^*(s',a') \mid s,a]$

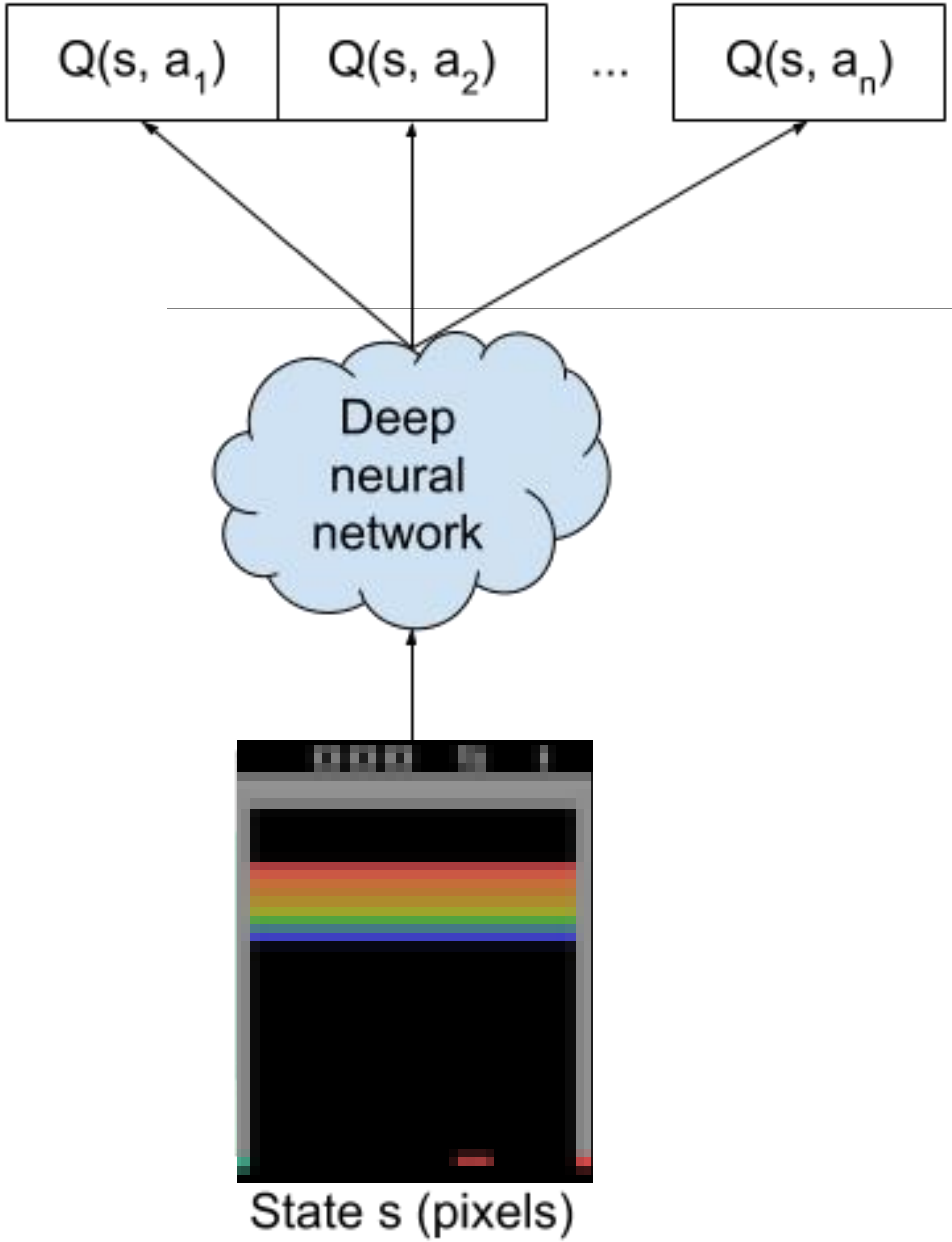
Backward Pass

Gradient update (with respect to Q-function parameters θ):

$$\nabla_{\theta_i} L_i(\theta_i) = \mathbb{E}\left[r + \gamma \max_{a'} Q(s',a';\theta_{i-1}) - Q(s,a;\theta_i))\nabla_{\theta_i} Q(s,a;\theta_i)\right]$$

Breakout as an MDP

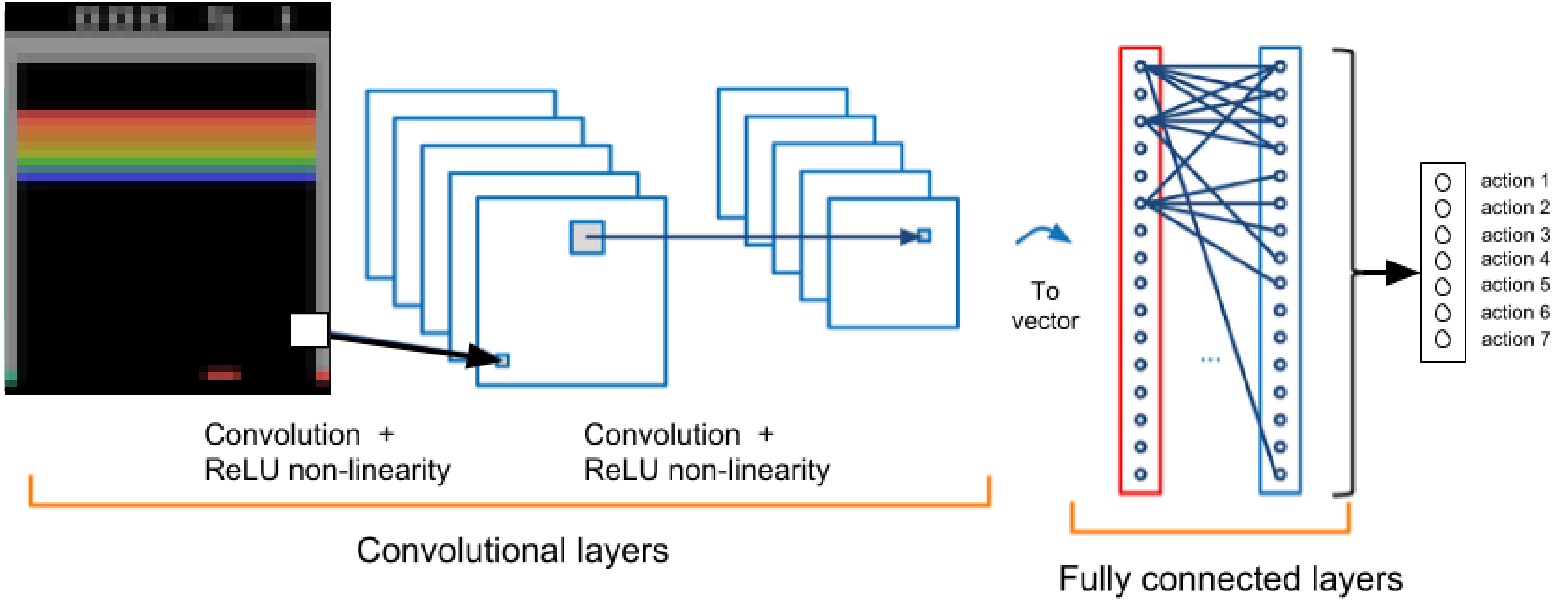
- **Objective**: Complete the game with the highest score
- **State:** Raw pixel inputs of the game state
- **Action:** Game controls e.g. Start, Left, Right, Stay
- **Reward:** Score increase/decrease at each time step



Deep Q-Learning for Breakout

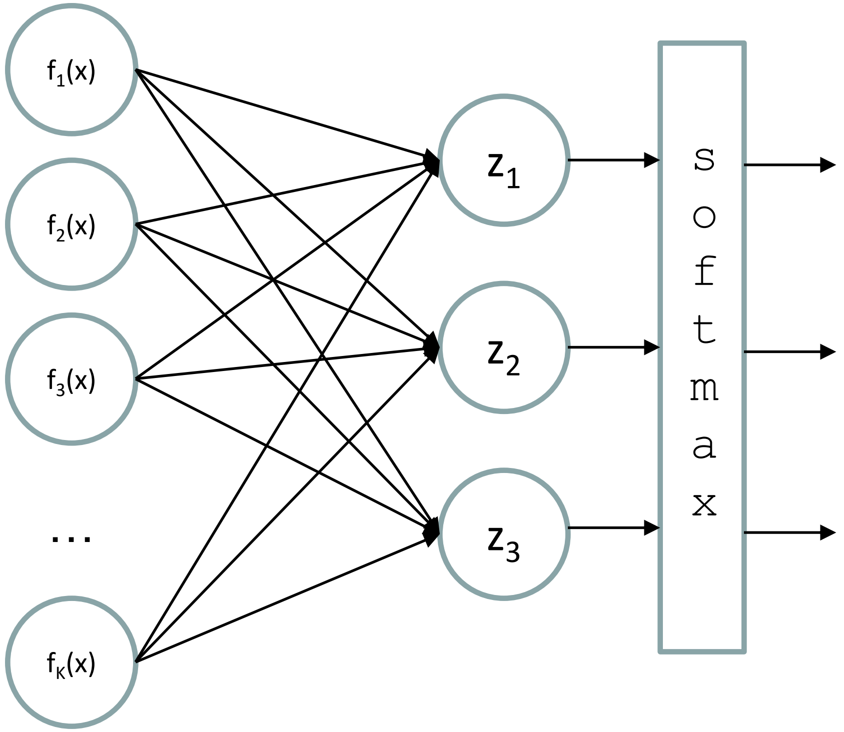
- $\pi(s) = argmax_a\ Q(s, a)$ once trained
- Next questions:
  - What is the structure of this network?
  - How do we train this network?

Network Structure



Multi-class Logistic Regression

- = special case of neural network



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Pytorch Demo! Open those Colab Notebooks if you want to follow along!

https://colab.research.google.com/drive/1PR8wBdglJ10yikyUkU8fmjl7-WviWC_W?usp=sharing

https://tinyurl.com/cse573-dqn

[Mnih et al. NIPS Workshop 2013; Nature 2015]

Training the Q-network: Experience Replay

Learning from batches of consecutive samples is problematic:

- Samples are correlated => inefficient learning
- Current Q-network parameters determines next training samples (e.g. if maximizing action is to move left, training samples will be dominated by samples from left-hand size) => can lead to bad feedback loops

Training the Q-network: Experience Replay

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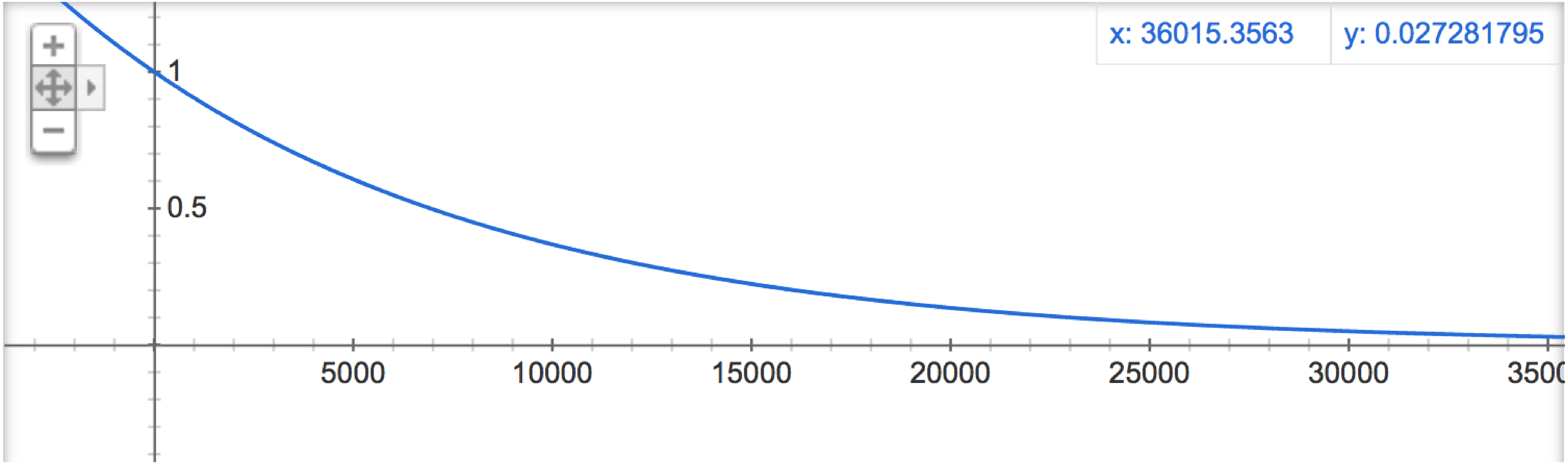
Address these problems using **experience replay**

- Continually update a **replay memory** table of transitions (s_t, a_t, r_t, s_{t+1}) as game (experience) episodes are played
- Train Q-network on random minibatches of transitions from the replay memory, instead of consecutive samples

Training the Q-network: Epsilon Greedy

- Epsilon is the term that decides how often the agent randomly picks an action



Algorithm 1: deep Q-learning with experience replay.

Initialize replay memory D to capacity N
Initialize action-value function Q with random weights θ
Initialize target action-value function $\hat{Q}$ with weights $\theta^- = \theta$
For episode = 1, M **do**
  Initialize sequence $s_1 = \{x_1\}$ and preprocessed sequence $\phi_1 = \phi(s_1)$
  For t = 1,T **do**
    With probability ε select a random action a_t
    otherwise select $a_t = \text{argmax}_a Q(\phi(s_t), a; \theta)$
    Execute action a_t in emulator and observe reward r_t and image x_{t+1}
    Set $s_{t+1} = s_t, a_t, x_{t+1}$ and preprocess $\phi_{t+1} = \phi(s_{t+1})$
    Store transition $(\phi_t, a_t, r_t, \phi_{t+1})$ in D
    Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from D
    Set $y_j = \begin{cases} r_j & \text{if episode terminates at step j+1} \\ r_j + \gamma \max_{a'} \hat{Q}(\phi_{j+1}, a'; \theta^-) & \text{otherwise} \end{cases}$
    Perform a gradient descent step on $\left(y_j - Q(\phi_j, a_j; \theta)\right)^2$ with respect to the network parameters θ
    Every C steps reset $\hat{Q} = Q$
  End For
End For