CS-UY 4563: Lecture 24
Reinforcement Learning

NYU Tandon School of Engineering, Prof. Christopher Musco

Supervised learning:

- **Decision trees.** Very effective model for problems with few features. Difficult to train, but heuristics work well in practice.
- **Boosting.** Approach for combining several "weak" models to obtain better overall accuracy than any one model alone.

Unsupervised learning:

- **Adversarial models.** Modern alternative to auto-encoders that performs very well for lots of interesting problems, especially in generative ML.
- **Clustering.** Hugely important for data exploration and visualization.

DATA CLUSTERING

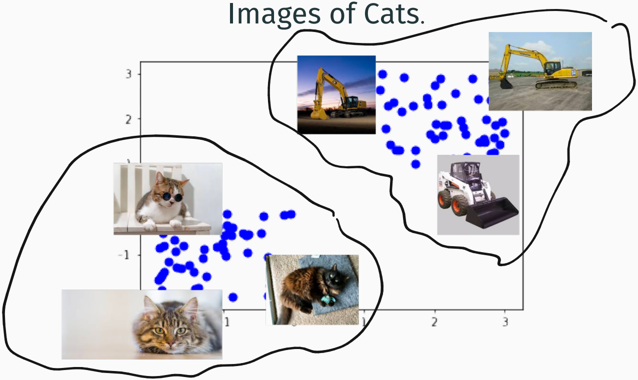
Important unsupervised learning task:

Separate unlabeled data into natural clusters.

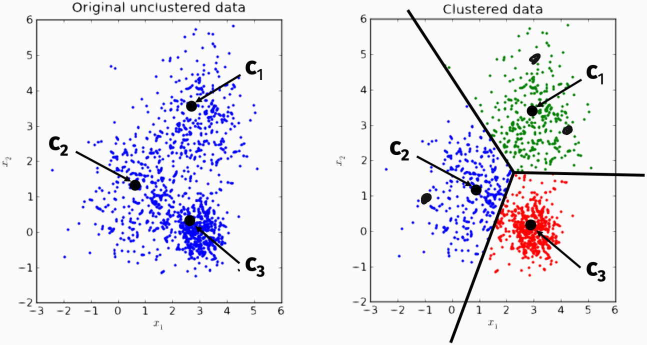
- Exploratory data analysis.
- Categorizing and grouping data.
- Visualizing data.

Example application:

Images of Cats.



Find sub-classes in your data which you did not know about.
Helps you decide how to adjust features or improve data set for a supervised application.



$K = 3$

k-center clustering:

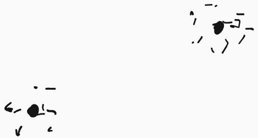
- Choose centers $\vec{c}_1, \ldots, \vec{c}_k \in \mathbb{R}^d$.
- Assign data point $\vec{x}$ to cluster i if $\vec{c}_i$ is the "nearest" center.
- Can use any distance metric.

$\in \mathbb{R}^d$

Given data points $\vec{x}_1, \ldots, \vec{x}_n$ and distance metric $\Delta(\vec{x}, \vec{c}) \rightarrow \mathbb{R}$, choose $\vec{c}_1, \ldots, \vec{c}_k$ to minimize:

$$Cost(\vec{c}_1, \ldots, \vec{c}_k) = \sum_{i=1}^{n} \min_j \Delta(\vec{x}_i, \vec{c}_j).$$

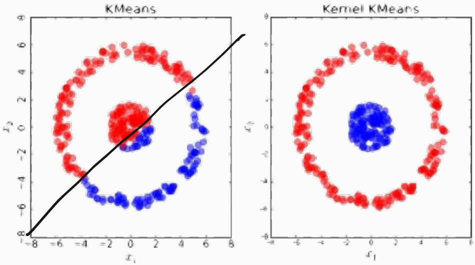
In general this could be a hard optimization problem.



K-MEANS CLUSTERING

Common choice: Use Euclidean distance. I.e. set $\Delta(\vec{x}, \vec{c}) = \|\vec{x} - \vec{c}\|_2^2$.

- If $k = 1$, optimal choice for c_1 is the centroid $\frac{1}{n}\sum_{i=1}^{n} \vec{x}_n$. For larger k the problem is NP-hard.
- Can be solved efficiently in practice using optimization techniques known as **alternating minimization**. Called "Llyod's algorithm" when applied to k-means clustering.
- Euclidean k-means can only identify linearly separable clusters.



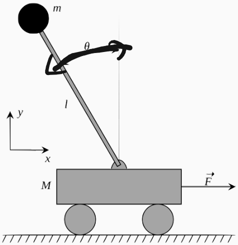
Today: Give flavor of the area and insight into one algorithm (Q-learning) which has been successful in recent years.

Basic setup:[1]

- **Agent** interacts with **environment** over time $1, \ldots, t$.
- Takes repeated sequence of **actions**, $a_1, \ldots, a_t$ which effect the environment.
- **State** of the environment over time denoted $s_1, \ldots, s_t$.
- Earn **rewards** $r_1, \ldots, r_t$ depending on actions taken and states reached.
- Goal is to maximize reward over time.

[1] Slide content adapted from: `http://cs231n.stanford.edu/`

Classic inverted pendulum problem:



$r_t = 1$

$r_t = 0$

- **Agent:** Cart/software controlling cart.
- **State:** Position of the car, pendulum head, etc.
- **Actions:** Move cart left or move right.
- **Reward:** 1 for every time step that $|\theta| < 90°$ (pendulum is upright). 0 when $|\theta| = 90°$

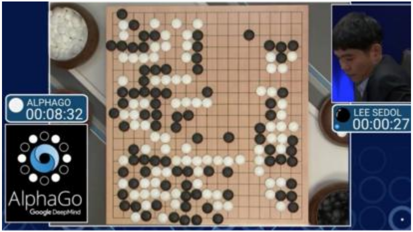
This problem has a long history in Control Theory. Other applications of classical control:

- Semi-autonomous vehicles (airplanes, helicopters, rockets, etc.)
- Industrial processes (e.g. controlling large chemical reactions)
- Robotics

Boston Dynamics

control theory : reinforcement learning :: stats : machine learning

Strategy games, like Go: 0 0 0 0 0 0 0 1



$r_t = 0$

- **State:** Position of all pieces on board.
- **Actions:** Place new piece.
- **Reward:** 1 if in winning position at time t. 0 otherwise.

This is a <u>sparse reward problem</u>. Payoff only comes after many times steps, which makes the problem very challenging.

Video games, like classic Atari games:

- **State:** Raw pixels on the screen (sometimes there is also hidden state which can't be observed by the player).
- **Actions:** Actuate controller (up,down,left,right,click).
- **Reward:** 1 if point scored at time t.

Model problem as a **Markov Decision Process (MDP)**:

- $\mathcal{S}$: Set of all possible states. $|\mathcal{S}| = n$.
- $\mathcal{A}$: Set of all possible actions. $|\mathcal{A}| = k$.
- **Reward function**
  $R(s, a) : \mathcal{S} \times \mathcal{A} \rightarrow$ probability distribution over $\mathbb{R}$. $r_t \sim R(s_t, a_t)$.
- **State transition function**
  $P(s, a) : \mathcal{S} \times \mathcal{A} \rightarrow$ probability distribution over $\mathcal{S}$. $s_{t+1} \sim P(s_t, a_t)$.

Why is this called a Markov decision process? What does the term Markov refer to?

Goal: Learn a **policy** $\Pi : \mathcal{S} \to \mathcal{A}$ from states to actions which maximized expected cumulative reward.

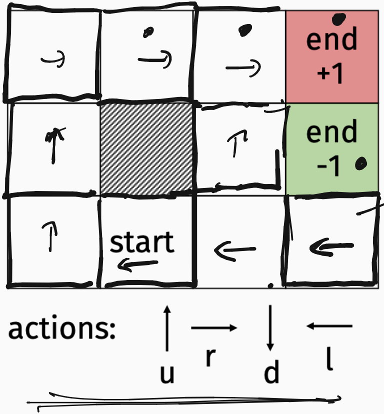
- Start is state s_0.
- For $t = 0 \ldots, T$
  - $r_t \sim R(s_t, \Pi(s_t))$.
  - $s_{t+1} \sim P(s_t, \Pi(s_t))$.

The **time horizon** T could be finite (game with fixed number of steps) or infinite (stock investing). Goal is to maximize:

$$reward(\Pi) = \mathbb{E} \sum_{t=0}^{T} r_t$$

$[s_0, a_0, r_0], [s_1, a_1, r_1], \ldots, [s_t, a_t, r_t]$ is called a **trajectory** of the MDP under policy Π.

$\pi(s) \to a$

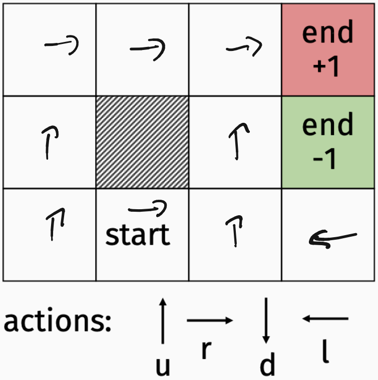


$\to s_1\ \pi(s_1)$

arrows indicate π^*

- $r_t = -.01$ if not at an end position. ± 1 if at end position.
- $P(s_t, a)$: 60% of the time move in the direction indicated by a. 40% of the time move in a random direction.

What is the optimal policy Π?



- $r_t = -.5$ if not at an end position. ± 1 if at end position.
- $P(s_t, a)$: 60% of the time move in the direction indicated by a. 40% of the time move in a random direction.

What is the optimal policy Π?

DISCOUNT FACTOR

For infinite or very long times horizon games (large T), we often introduce a **discount factor** γ and seek instead to find a policy Π which minimizes:

$\gamma \in (0, 1]$

$$\mathbb{E}\sum_{t=0}^{T} \gamma^t r_t$$

$$\sum_{t \geq 0}$$

where $r_t \sim R(s_t, \Pi(s_t))$ and $s_{t+1} \sim P(s_t, \Pi(s_t))$ as before.

From now on assume $T = \infty$. We can do this without loss of generality by adding a time parameter to state and moving into an "end state" with no additional rewards once the time hits T.

Two important definitions.

- **Value function:** $V^{\Pi}(s) = \mathbb{E}_{\Pi, s_0 = s} \sum_{t \geq 0} \gamma^t r_t$. Measures the expected return if we start in state s and follow policy Π.
- *Q*-**function:** $Q^{\Pi}(s, a) = \mathbb{E}_{\Pi, s_0 = s, a_0 = a} \sum_{t \geq 0} \gamma^t r_t$. Measures the expected return if we start in state s, play action a, and then follow policy Π.

$r_0 + \sum_{t \geq 0} \gamma^t r_t$

$\mathbb{E} r_0 = \mathbb{E}(R(s,a))$

$$\boxed{Q^*(s, a)} = \max_{\Pi} \mathbb{E}_{\Pi, s_0 = s, a_0 = a} \sum_{t \geq 0} \gamma^t r_t.$$

If we knew the function Q^*, we would immediately know an optimal policy. Whenever we're in state s, we should always play action $a^* = \arg\max_a \cancel{Q^*(s, a)}$. $Q^*(s, a)$

BELLMAN EQUATION

Q^* satisfies what's known as a Bellman equation:

$$Q^*(s,a) = \mathbb{E}_{s' \sim P(s,a)} \left[R(s,a) + \gamma \max_{a'} Q^*(s',a') \right].$$

Value Iteration: Used fixed point iteration to find Q^*:

- Initialize Q^0 (e.g. randomly).
- For $i = 1, \ldots, z$:
  - $Q^i_{(s,a)} = \mathbb{E}_{s' \sim P(s,a)} \left[R(s,a) + \gamma \max_{a'} Q^{i-1}(s',a') \right]$

guess at previous

Possible to prove that $Q^i \to Q^*$ as $i \to \infty$.

Note that many details are involved in this computation.

Need to handle the expectations on the right hand side by randomly sampling trajectories from the MDP.

20,000

Bigger issue: Even writing down Q^* is intractable... This is a function over $\cancel{|\mathcal{S}|^{|\mathcal{A}|}}$ possible inputs. Even for relatively simple games, $|\mathcal{S}|$ is gigantic... $|S| \cdot |A|$

Back of the envelope calculations:

- **Tic-tac-toe:** $3^{(3\times3)} \approx 20,000$
- **Chess:** $\approx 10^{43}$ (due to Claude Shannon).
- **Go:** $3^{(19\times19)} \approx 10^{171}$. $= |S|$
- **Atari:** $128^{(210\times160)} \approx 10^{71,000}$.

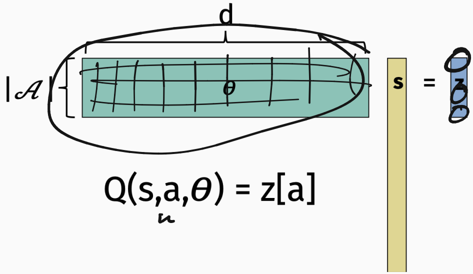
Number of atoms in the universe: $\approx 10^{82}$.

Learn a **simpler** function $Q(s, a, \theta) \approx Q^*(s, a)$ parameterized by a small number of parameters θ.

Example: Suppose our state can be represented by a vector in $\mathbb{R}^d$ and our action a by an integer in $1, \ldots, |\mathcal{A}|$. We could use a linear function where θ is a small matrix:

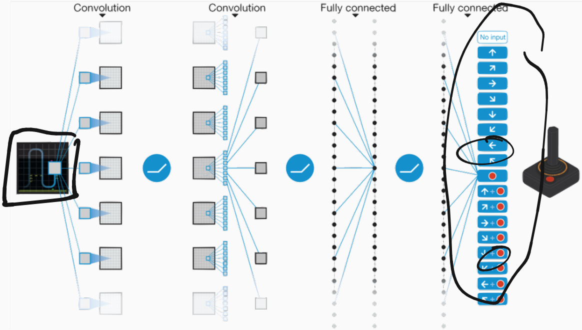
$|S| \cdot |A|$

$\log(|S|)$



Learn a **simpler** function $Q(s, a, \theta) \approx Q^*(s, a)$ parameterized by a small number of parameters θ.

Example: Could also use a (deep) neural network.



DeepMind: "Human-level control through deep reinforcement learning", Nature 2015.

If $Q(s, a, \theta)$ is a good approximation to $Q^*(s, a)$ then we have an approximately optimal policy: $\tilde{\Pi}^*(s) = \arg\max_a Q(s, a, \theta)$.

- Start in state s_0.
- For $t = 1, 2, \ldots$
    - $a^* = \arg\max_a Q(s, a, \theta)$
    - $s_t \sim P(s_{t-1}, a^*)$

How do we find an optimal θ? If we knew $Q^*(s, a)$ could use supervised learning, but the true Q function is infeasible to compute.

Find θ which satisfies the Bellman equation:

$$Q^*(s,a) = \mathbb{E}_{s' \sim P(s,a)} \left[R(s,a) + \gamma \max_{a'} Q^*(s',a') \right]$$

$$Q(s,a,\theta) \approx \mathbb{E}_{s' \sim P(s,a)} \left[R(s,a) + \gamma \max_{a'} Q(s,a,\theta) \right].$$

Should be true for all a, s. Should also be true for $a, s \sim \mathcal{D}$ for any distribution $\mathcal{D}$:

$$\mathbb{E}_{s,a \sim \mathcal{D}} Q(s,a,\theta) \approx \mathbb{E}_{s,a \sim \mathcal{D}} \mathbb{E}_{s' \sim P(s,a)} \left[R(s,a) + \gamma \max_{a'} Q(s,a,\theta) \right].$$

Loss function:

$$L(\theta) = \mathbb{E}_{s,a \sim \mathcal{D}} \left(y - Q(s,a,\theta) \right)^2$$

where $y = \mathbb{E}_{s' \sim P(s,a)} \left[R(s,a) + \gamma \max_{a'} Q(s',a',\theta) \right]$.

Q-LEARNING W/ FUNCTION APPROXIMATION

Minimize loss with **gradient descent**:

$$\nabla L(\theta) = -2 \cdot \mathbb{E}_{s,a\sim\mathcal{D}} \nabla Q(s,a,\theta) \cdot \left[R(s,a) + \gamma \max_{a'} Q(s',a',\theta) - Q(s,a,\theta) \right]$$

In practice use stochastic gradient:

$$\nabla L(\theta, s, a) = -2 \cdot \nabla Q(s,a,\theta) \cdot \left[R(s,a) + \gamma \max_{a'} Q(s',a',\theta) - Q(s,a,\theta) \right]$$

- Initialize θ_0
- For $i = 0, 1, 2, \ldots$
    - Choose random $s, a \sim \mathcal{D}$.
    - Set $\theta_{i+1} = \theta_i - \eta \cdot \nabla L(\theta_i, s, a)$

where η is a learning rate parameter.

- Initialize θ_0
- For $i = 0, 1, 2, \ldots$
    - Choose random $s, a \sim \mathcal{D}$.
    - Set $\theta_{i+1} = \theta_i - \nabla L(\theta_i, s, a)$.

What is the distribution $\mathcal{D}$?

- **Random play**: Choose uniformly over reachable states + actions.

Wasteful: Seeks to approximate Q^* well in parts of the state-action space that don't actually matter for optimal play. Would require a ton of samples.

More common approach: Play according to current guess for optimal policy, with some random "off-policy" exploration. The $\mathcal{D}$ is the distribution over states/actions results form this play. Note that $\mathcal{D}$ changes over time...

ϵ-greedy approach:

- Initialize s_0.
- For $t = 0, 1, 2, \ldots,$
  - $a_i = \begin{cases} \arg\max_a Q(s_t, a, \theta_{curr}) & \text{with probabilty } (1-\epsilon) \\ \text{random action} & \text{with probabilty } \epsilon \end{cases}$

Exploration-exploitation tradeoff. Increasing ϵ = more **exploration**.

REFERENCES

Lots of other details we don't have time for! References:

- Original DeepMind Atari paper: `https://www.cs.toronto.edu/~vmnih/docs/dqn.pdf`, which is very readable.
- Stanford lecture video: `https://www.youtube.com/watch?v=lvoHnicueoE` and slides: `http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture14.pdf`

Important concept we did not cover: **experience replay**.

ATARI DEMO

https://www.youtube.com/watch?v=V1eYniJ0Rnk