# Artificial Intelligence

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## So far

- Simple Reflex, Random agents, Utility based, Goal based
- Improvement through Search Methods (uninformed (DFS, BFS), informed (BS, A$^*$)).
- Logical Reasoning, Propositional logic + First Order Logic, Inference
- Learning
  - Decision trees, regression, classification
  - Neural Networks
  - Parametric vs non parametric
  - Kernels and SVMs
  - Unsupervised and Clustering
  - Reinforcement learning

## Parametric vs Non Parametric

- Linear regression, logistic regression and neural networks use the training data to estimate a fixed set of parameters
- Those parameters define our hypothesis $h_{\boldsymbol{\beta}}(\boldsymbol{x})$. Once we have the hypothesis, we can just throw away the training data
- A learning model that summarizes data with a set of parameters of fixed size is called a parametric model
- No matter how much data you throw at a parametric model, it won't change its mind about how many parameters it needs
- A non parametric model is one that cannot be characterized by a bounded set of parameters

## Parametric vs Non Parametric

- A example of a non parametric model for classification is the K nearest neighbor (KNN) classifier
- Given a query $\boldsymbol{x}_q$, KNN works by first finding the $k$ examples that are the nearest to $\boldsymbol{x}_q$
- In classification, we then simply take the majority vote across the neighbors
- In regression, we can take the mean, or median of the neighbors, or solve a regression problem on the neighbors

## Parametric vs Non Parametric

- Another popular non parametric approach in classification are Support Vector Machines (or Max Margin Classifiers).
- SVMs is currently the most popular approach for 'off the shelf' supervised learning. If you don't have any specialized prior knowledge about a domain, the SVM is an excellent method to try first

## Parametric vs Non Parametric

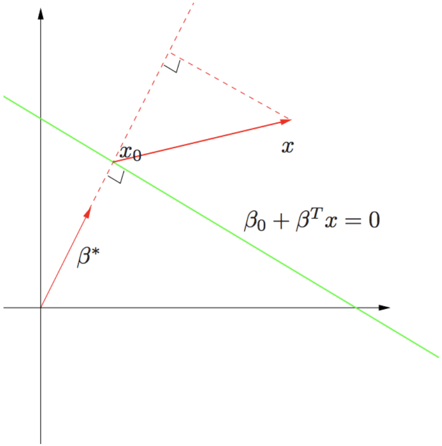
- There are three properties that make SVM attractive:
    - SVM constructs a maximum margin separator (decision boundary with the largest possible distance to example points)
    - SVM creates a linear separating plane but they have the ability to embed the data into a higher dimensional space using the so called kernel trick
    - SVM are a nonparametric method (they retain training examples and potentially need to store them all). However in practice they often end up retaining only a small fraction of the examples. Thus they combine the advantages of nonparametric and parametric models: they have the flexibility to represent complex functions but they are resistant to overfitting.

## Separating Hyperplanes (quick recap)

- Consider the separating hyperplane $\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}$
- $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ belong to the plane if they satisfy

$$\boxed{\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}_1 = \beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}_2}$$

- We thus have $\boldsymbol{\beta}^T(\boldsymbol{x}_1 - \boldsymbol{x}_2) = 0$ for all $\boldsymbol{x}_1, \boldsymbol{x}_2$ in the plane
- $\boldsymbol{\beta}$ ($\boldsymbol{\beta}^* = \boldsymbol{\beta}/\|\boldsymbol{\beta}\|$) is the vector normal to the hyperplane



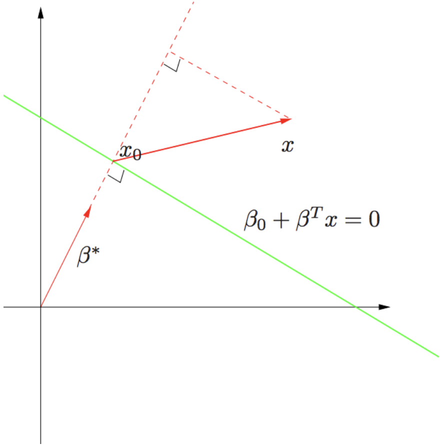
H,T,F, Elem. of Stat. Learn.

- The signed distance of a point $\boldsymbol{x}$ to the hyperplane is defined as

$$(\boldsymbol{\beta}^*)^T(\boldsymbol{x} - \boldsymbol{x}_0) = \frac{1}{\|\boldsymbol{\beta}\|}(\boldsymbol{\beta}^T\boldsymbol{x} + \beta_0)$$

- Points that are located above thus lead to positive values $\beta^T\boldsymbol{x} + \beta_0 > 0$

- Points that are located below lead to negative values $\beta^T\boldsymbol{x} + \beta_0 < 0$



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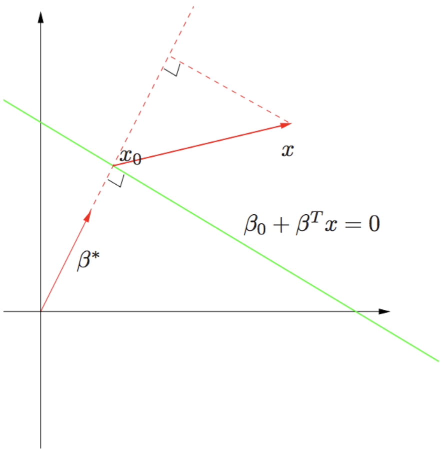
- A separating plane thus gives a natural way to associate positive or negative labels to points
- For a two class classification problem, we can look for the plane that gives positive labels to one class and negative labels to the other
- This idea leads to the perceptron algorithm of Rosenblatt



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## Support vector machines

- Linear models have interesting computational and anlytical properties but their practical applicability is limited by the curse of dimensionality
- Support vector machines are also called sparse vector machines
- SVM start by defining basis functions that are centered on the data and then select a subset of these during training

## Support vector machines

- Consider the linear regression model

$$y(\boldsymbol{x}) = \boldsymbol{\beta}^T \phi(\boldsymbol{x}) + \beta_0$$

- Assume we want to do classification so the labels are $t_n = \{\pm 1\}$
- We further assume that the dataset of linearly separable in feature space so that there exist at least one seprating hyperplane with $\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0 > 0$ for the $\boldsymbol{x}_n$ with $t_n > 0$ and $\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0 < 0$ otherwise
- When there are multiple choices we should choose the one that gives the smallest generalization error. SVM tries to achieves this through the notion of margin

## Support vector machines

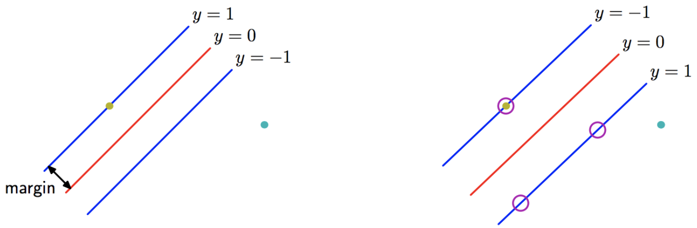

**Figure 7.1** The margin is defined as the perpendicular distance between the decision boundary and the closest of the data points, as shown on the left figure. Maximizing the margin leads to a particular choice of decision boundary, as shown on the right. The location of this boundary is determined by a subset of the data points, known as support vectors, which are indicated by the circles.

(Bishop, Pattern recognition and Machine Learning)

## SVM as Maximum Margin Classifier

- Recall from the geometry of separating hyperplanes that the distance of a point $\phi(\boldsymbol{x}_n)$ to the hyperplane $\boldsymbol{\beta}^T\boldsymbol{x} + \beta_0$ is defined as $|y(\boldsymbol{x})|/\|\boldsymbol{\beta}\|$

- When all the points are correctly classified, the sign of $t_n$ equals the sign of $\boldsymbol{y}_n = \boldsymbol{\beta}^T\phi(\boldsymbol{x}_n) + \beta_0$ and we can thus write the distance as

$$\frac{t_n y_n}{\|\boldsymbol{\beta}\|} = \frac{t_n(\boldsymbol{\beta}^T\phi(\boldsymbol{x}_n) + \beta_0)}{\|\boldsymbol{\beta}\|}$$

- The margin is the perpendicular distance of the closest point $\phi(\boldsymbol{x}_n)$ to the plane

## SVM as Maximum Margin Classifier

$$\frac{t_n y_n}{\|\boldsymbol{\beta}\|} = \frac{t_n(\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0)}{\|\boldsymbol{\beta}\|}$$

- The maximum margin solution is thus given by

$$\underset{\boldsymbol{\beta}, \beta_0}{\operatorname{argmax}} \left\{ \frac{1}{\|\boldsymbol{\beta}\|} \min_n \left[ t_n(\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0) \right] \right\}$$

- We don't want to solve this problem because deriving a direct solution in this framework would be difficult

## SVM as Maximum Margin Classifier

$$\underset{\boldsymbol{\beta},\beta_0}{\operatorname{argmax}} \left\{ \frac{1}{\|\boldsymbol{\beta}\|} \min_n \left[ t_n(\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0) \right] \right\}$$

- First note that for any rescaling $\boldsymbol{\beta} \leftarrow \alpha\boldsymbol{\beta}$, $\beta_0 \leftarrow \beta_0\alpha$, the objective $t_n(\boldsymbol{\beta}^T \boldsymbol{\phi}(\boldsymbol{x}_n) + \beta_0)/\|\boldsymbol{\beta}\|$ is unchanged
- We can thus focus on one of these solution (fix one particular scale for $[\boldsymbol{\beta}, \beta_0]$) as all the others give the same objective
- In particular we can choose to fix the scale by setting

  $$t_n(\boldsymbol{\beta}^T \boldsymbol{\phi}(\boldsymbol{x}_n) + \beta_0) = 1$$

  For the point that is the closest to the boundary.

## SVM as Maximum Margin Classifier

$$\underset{\boldsymbol{\beta},\beta_0}{\operatorname{argmax}} \left\{ \frac{1}{\|\boldsymbol{\beta}\|} \min_n \left[ t_n(\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0) \right] \right\}$$

- Now all the other points will necessarily satisfy

$$t_n(\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0) \geq 1$$

- Because we fixed the distance of the closest point to the plane the original optimization problem reduces to

$$\underset{\boldsymbol{\beta}}{\operatorname{argmin}} \frac{1}{2} \|\boldsymbol{\beta}\|^2$$

together with the constraint $t_n(\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0) \geq 1$

## SVM as Maximum Margin Classifier

$$\begin{aligned} \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \quad & \frac{1}{2}\|\boldsymbol{\beta}\|^2 \\ \text{subject to} \quad & t_n(\boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0) \geq 1 \end{aligned}$$

- This constrained optimization problem can be recast as an unconstrained problem by introducing multipliers $\lambda_n \geq 0$

$$L(\boldsymbol{\beta}, \beta_0, \boldsymbol{\lambda}) = \frac{1}{2}\|\boldsymbol{\beta}\|^2 - \sum_{n=1}^{N} \lambda_n \left\{ t_n \left( \boldsymbol{\beta}^T \boldsymbol{\phi}(\boldsymbol{x}_n) + \beta_0 \right) - 1 \right\}$$

(see for example Appendix E in Bishop, Pattern Recognition and Machine Learning)

## SVM as Maximum Margin Classifier

$$L(\boldsymbol{\beta}, \beta_0, \boldsymbol{\lambda}) = \frac{1}{2}\|\boldsymbol{\beta}\|^2 - \sum_{n=1}^{N} \lambda_n \left\{ t_n \left( \boldsymbol{\beta}^T \phi(\boldsymbol{x}_n) + \beta_0 \right) - 1 \right\}$$

- To find the minimum of this function, we set the derivatives with respect to $\boldsymbol{\beta}$ and $\beta_0$ to zero, getting

$$\boldsymbol{\beta} = \sum_{n=1}^{N} \lambda_n t_n \phi(\boldsymbol{x}_n)$$

$$0 = \sum_{n=1}^{N} t_n \lambda_n$$

- and maximize with respect to $\lambda_n$ (large $\lambda_n$ penalize the constraint a lot if it becomes negative)

## SVM as Maximum Margin Classifier

- Eliminating $\boldsymbol{\beta}$ and $\beta_0$ from $L(\boldsymbol{\beta}, \beta_0, \boldsymbol{\lambda})$, we get

$$L(\boldsymbol{\lambda}) = \sum_{n=1}^{N} \lambda_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m t_n t_m \phi(\boldsymbol{x}_n)^T \phi(\boldsymbol{x}_m)$$

- with the constraints

$$\sum_{n=1}^{N} \lambda_n t_n = 0$$

$$\lambda_n \geq 0$$

- Maximizing $L(\boldsymbol{\lambda})$ under the constraints above is a quadratic programming problem for which efficient techniques exist. Moreover when $\boldsymbol{\kappa}(\boldsymbol{x}_n, \boldsymbol{x}_m)$ is Mercer, there is a single solution

## SVM as Sparse Kernel Machines(I)

- Given the function $L(\boldsymbol{\beta}, \beta_0, \boldsymbol{\lambda})$, it is known (Karush-Kuhn-Tucker conditions) that any optimal solution must satisfy the follosing 3 conditions

$$\begin{aligned} \lambda_n &\geq 0 \\ t_n y(\boldsymbol{x}_n) - 1 &\geq 0 \\ \lambda_n \left\{ t_n y(\boldsymbol{x}_n) - 1 \right\} &= 0 \end{aligned}$$

- The last conditions have a very important consequence on SVM

- Either $\lambda_n = 0$ or $t_n y(\boldsymbol{x}_n) = 1$ (support vectors)

## SVM as Sparse Kernel Machines (II)

- Either $\lambda_n = 0$ or $t_n y(\boldsymbol{x}_n) = 1$ (support vectors)
- In particular many $\lambda_n$ will be zero
- Using $\boldsymbol{\beta} = \sum_{n=1}^{N} \lambda_n t_n \phi(\boldsymbol{x}_n)$, and substituting it in $y(\boldsymbol{x}) = \boldsymbol{\beta}^T \phi(\boldsymbol{x}) + \beta_0$, we get the prediction model

$$y(\boldsymbol{x}) = \sum_{n=1}^{N} \lambda_n t_n \phi(\boldsymbol{x})^T \phi(\boldsymbol{x}_n) + \beta_0$$

- Which is a combination of the $\lambda_n$ !

## SVM as Sparse Kernel Machines (III)

$$\text{(Karush-Kuhn-Tucker)} \quad \begin{cases} \lambda_n \geq 0 \\ t_n y(\boldsymbol{x}_n) - 1 \geq 0 \\ \lambda_n \left\{ t_n y(\boldsymbol{x}_n) - 1 \right\} = 0 \end{cases}$$

- Using the Karush-Kuhn-Tucker conditions, the SVM prediction model thus reduces to

$$y(\boldsymbol{x}) = \sum_{n \in \mathcal{S}} \lambda_n t_n \phi(\boldsymbol{x})^T \phi(\boldsymbol{x}_n) + \beta_0$$

Where $\mathcal{S}$ are the support vectors (all remaining $\lambda_n$'s are 0)

## SVM as Sparse Kernel Machines (IV)

- This sparsity property (i.e the need to only keep a small number of support vectors) is a key property of SVM
- It guarantees efficiency of the prediction step !
- Once you know the support vectors, $\beta$ and $\beta_0$ can be computed using $\boldsymbol{\beta} = \sum_{n=1}^{N} \lambda_n t_n \phi(\boldsymbol{x}_n)$, as well as the fact that at any of the support vectors we must have

$$t_n y_n = t_n \left( \sum_{m \in \mathcal{S}} \lambda_m t_m \kappa(\boldsymbol{x}_n, \boldsymbol{x}_m) + \beta_0 \right) = 1$$

- Sometimes we average the estimate for $\beta_0$ over the support vectors (here $n$) to get more stability

## Short summary

- General geometry of separating hyperplane, distance to hyperplane, perceptron
- Curse of dimensionality
- Kernels
  - As a way to encode similarity rather than features
  - As smooth interpolating functions
- SVM
  - Maximum Margin
  - Sparse Kernel machines $\Rightarrow$ efficient prediction

## Kernels

- In linear regression we have seen that we could generate higher dimensional feature vectors $\phi(\boldsymbol{x}^{(i)})$ to replace $\boldsymbol{x}^{(i)}$

- We can then substitute those vectors to get the expression

$$h(\boldsymbol{x}) = \text{sign}\left(\sum_{i\in\mathcal{D}} \alpha_i t^{(i)} \langle \phi(\boldsymbol{x}^{(i)}), \phi(\boldsymbol{x})\rangle - b\right)$$

- It turns out that the inner product $\langle \phi(\boldsymbol{x}^{(i)}), \phi(\boldsymbol{x})\rangle$ can often be derived without computing the feature vectors explicitely.

- Instead of thinking in terms of feature vectors, we can think in terms of similarity and replace the inner product by a similarity function which we call kernel

$$h(\boldsymbol{x}) = \text{sign}\left(\sum_{i\in\mathcal{D}} \alpha_i t^{(i)} \kappa(\boldsymbol{x}^{(i)}, \boldsymbol{x}) - b\right)$$

## Kernel

- The most popular example of such function is the Gaussian kernel

$$\kappa(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|^2}{\sigma})$$

- Just as the inner product, you see that $\kappa(\boldsymbol{x}, \boldsymbol{x}')$ will be larger when $\boldsymbol{x}$ is similar to $\boldsymbol{x}'$

- Learning a classifier with a Gaussian kernel corresponds to centering a Gaussian with a particular width around each sample, and weighting that Gaussian by the target

## Unsupervised Learning

- So far : predictions based on training samples for which joint values $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^N$ are known.
- Problem: costly. Most datasets are not labeled.
- Today: Unsupervised learning = learning without a teacher
- In unsupervised Learning we are given samples $(x_1, x_2, \ldots, x_N)$ from a distribution $P(X)$ and the goal is to infer the properties of the distribution without the help of the teacher.
- There are two main types of unsupervised learning approaches: (1) clustering the attribute vectors and (2) trying to find low dimensional representation of those attribute vectors such that $X = X(\boldsymbol{\theta})$ and $\boldsymbol{\theta}$ reveals meaningful information.

## Clustering: K-means

- The most popular clustering algorithms are combinatorial algorithms which assign every observation to a given cluster without regard to any predefined probabilistic model.
- The number of clusters $K$ is usually predefined
- One approach is to introduce a loss that will drive the assignment. If we let $\mathcal{C}_k$ to denote the $k^{th}$ cluster, we get

$$\ell(\mathcal{C}) = \frac{1}{2} \sum_{k=1}^{K} \sum_{i \in \mathcal{C}_k} \sum_{j \in \mathcal{C}_k} d(x_i, x_j)$$

## K-means

- When the dissimilarity is chosen to be the Euclidean distance,

$$d(x_i, x_i') = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = \|x_i - x_{i'}\|^2$$

- The loss then reads as

$$\boxed{\ell(\mathcal{C}) = \frac{1}{2} \sum_{k=1}^{K} \sum_{i \in \mathcal{C}_k} \sum_{j \in \mathcal{C}_k} \|x_i - x_j\|^2}$$

# K-means

- In particular, developing, we get

$$
\begin{aligned}
&\frac{1}{2}\sum_{k}\sum_{i\in\mathcal{C}_k}\sum_{j\in\mathcal{C}_k}\|x_i - x_j\|^2 \\
&= \frac{1}{2}\sum_{k}\sum_{i\in\mathcal{C}_k}\sum_{j\in\mathcal{C}_k}\langle x_i, x_i\rangle + \langle x_j, x_j\rangle - 2\langle x_i, x_j\rangle \\
&= \frac{1}{2}\sum_{k}\sum_{i\in\mathcal{C}_k}\langle x_i, x_i\rangle N_k - \frac{1}{2}\sum_{k}\sum_{i\in\mathcal{C}_k} 2\langle x_i, \sum_{j\in\mathcal{C}_k} x_j\rangle \\
&= \left(\sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\langle x_i, x_i\rangle - \sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\langle x_i, \sum_{j\in\mathcal{C}_k} x_j\rangle \frac{1}{N_k}\right)
\end{aligned}
$$

## K-means

$$\frac{1}{2}\sum_{k}\sum_{i\in\mathcal{C}_k}\sum_{j\in\mathcal{C}_k}\|x_i - x_j\|^2$$

$$= \left(\sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\langle x_i, x_i\rangle - \sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\langle x_i, \sum_{j\in\mathcal{C}_k} x_j\rangle \frac{1}{N_k}\right)$$

$$= \sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\left(\langle x_i, x_i\rangle - \langle x_i, \sum_{j\in\mathcal{C}_k} x_j\rangle \frac{1}{N_k}\right)$$

$$= \sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\left(\langle x_i, x_i\rangle - \langle x_i, \sum_{j\in\mathcal{C}_k} x_j\rangle \frac{1}{N_k} + \frac{1}{N_k^2}\langle \sum_{j\in\mathcal{C}_k} x_j, \sum_{j\in\mathcal{C}_k} x_j\rangle\right)$$

$$- \sum_{k=1}^{K}\sum_{i\in\mathcal{C}_k}\left(\frac{1}{N_k}\sum_{j\in\mathcal{C}_k}\langle x_j, x_i\rangle\right)$$

## K-means

$$\frac{1}{2}\sum_{k}\sum_{i\in\mathcal{C}_k}\sum_{j\in\mathcal{C}_k}\|x_i - x_j\|^2$$

$$= \sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\left(\langle x_i, x_i\rangle - \langle x_i, \sum_{j\in\mathcal{C}_k} x_j\rangle\frac{1}{N_k} + \frac{1}{N_k^2}\langle\sum_{j\in\mathcal{C}_k} x_j, \sum_{j\in\mathcal{C}_k} x_j\rangle\right)$$

$$- \sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\left(\frac{1}{N_k}\sum_{j\in\mathcal{C}_k}\langle x_j, x_i\rangle\right)$$

$$= \sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\left(\langle x_i, x_i\rangle - 2\langle x_i, \frac{1}{N_k}\sum_{j\in\mathcal{C}_k} x_j\rangle + \langle\frac{1}{N_k}\sum_{j\in\mathcal{C}_k} x_j, \frac{1}{N_k}\sum_{j\in\mathcal{C}_k} x_j\rangle\right)$$

$$= \boxed{\sum_{k=1}^{K} N_k \sum_{i\in\mathcal{C}_k}\|x_i - \frac{1}{N_k}\sum_{j\in\mathcal{C}_k} x_j\|^2}$$

## K-means

- In other words, when using the Euclidean distance, one can write the clustering objective/loss as

$$\ell(\mathcal{C}) = \sum_{k=1}^{K} N_k \sum_{i \in \mathcal{C}_k} \|x_i - \overline{x}^k\|^2$$

  Where $\overline{x}^k$ is the center of mass of the $k^{th}$ cluster.

- the optimal clustering in that framework is thus the clustering that minimizes the average dissimilarity

## K-means

- **1.** Update the assignement by setting

$$x_i \in \mathcal{C}_k \quad \text{if} \quad k = \operatorname*{argmin}_k \|x_i - m_k\|^2$$

- **2.** Given a cluster assignement $\mathcal{C}$, compute the center of mass of each cluster

$$\bar{x}_S = \operatorname*{argmin}_m \sum_{i \in S} \|x_i - m\|^2$$

- Repeat Steps 1 and 2 until the assignement does not change

## Reinforcement learning

- Reinforcement learning is learning what to do so as to maximize a numerical reward signal
- "The learner is not told which action to take but instead must discover which action yield the most reward by trying them"
- Ex.1.: "A chess player makes a move. The choice is informed by planning (anticipation of possible replies and counterreplies) and by immediate intuitive judgements of the desirability of possible positions and moves"
- Ex.2. "A mobile robot decides whether it should enter a room in search of a target or start to find its way back to its battery charging station"

source: R. Sutton, A.G. Barto, Reinforcement learning: An introduction

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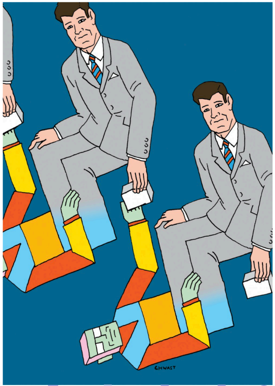
10 BREAKTHROUGH TECHNOLOGIES

## Reinforcement Learning

**By experimenting, computers are figuring out how to do things that no programmer could teach them.**

**Availability: 1 to 2 years**

by Will Knight



## Reinforcement learning

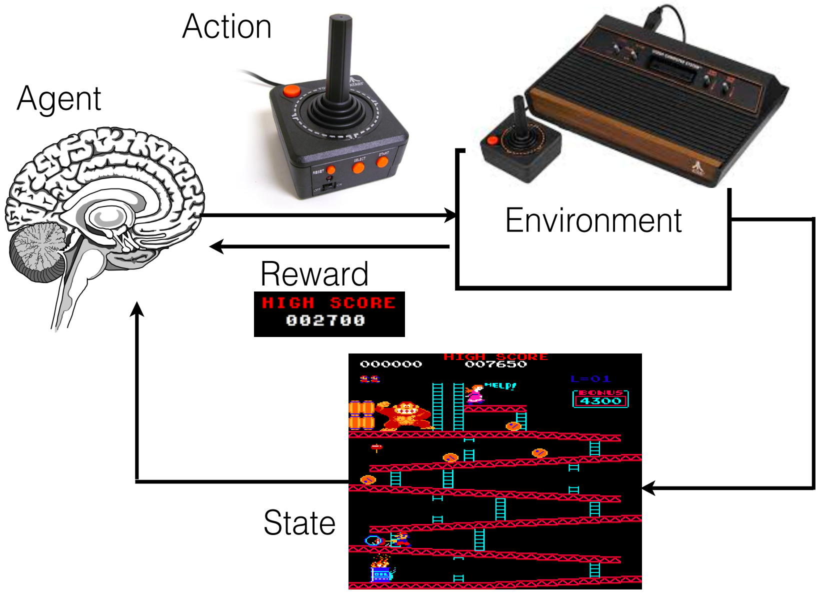
- The policy defines the learning agent's way of behaving at any given time
- On each time step, the evironment sends to the reinforcement learning agent a single number called the reward which specifies what are good and bad events in an immediate sense.
- To know what is good in the long run, we use a value function which is the total amount of reward the agent can expect to accumulate over the future, starting from that state.
- Finally, the last element is a model for the environment which enables inferences to be made on how the environment will react w.r.t a particular action. The role of the model is essentially to predict the next state and next reward given the current state and action.

source: R. Sutton, A.G. Barto, Reinforcement learning: An introduction

## Reinforcement learning

- Action are usually taken to maximize the value, not the reward, because high value actions are those that lead to the highest level of reward in the long run. Finding such actions is however hard as those have to be constantly re-estimated based on the decisions of the agent.
- An important instance of reinforcement learning in which there is a single state is the bandit problem

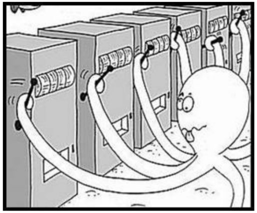
source: R. Sutton, A.G. Barto, Reinforcement learning: An introduction



Inspired from https://keon.io/deep-q-learning/, Deep Q-Learning with Keras and Gym

## Reinforcement learning

- The multi-armed bandit is a simplified version of non associative feedback problem
- In the k-armed bandit problem, you are faced repeatedly with a choice among *k* different possible options or actions. After each choice, you receive a numerical reward chosen from some stationnary probability distribution that depends on the action you selected.



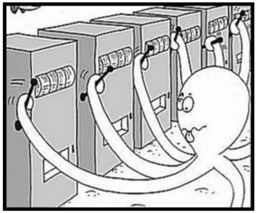
source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning

- You can think of the $k$-armed bandit problem as the problem of playing one of the $k$ levers of a slot machine. You choose which lever you play and the reward is the payoff for hitting the jackpot

- The value of an arbitrary action, $a$, which we denote $v(a)$ is the expected reward given that you selected $a$

$$v(a) = \mathbb{E}\{R_t | A_t = a\}$$



source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning

- We don't know the exact value $v^*(a)$ (because we don't know the distribution). So we would like an estimate $v_{\text{est},t}(a)$ (estimated value at time $t$) that would be as close as possible to $v^*(a)$
- When you keep track of the estimated action values through time, then at each time step, there is always at least one action whose estimated value is best. We call this greedy actions.
- When you select one of these actions, we say that you are exploiting your current knowledge of the values of the actions
- When you select one of the non greedy actions, then we say you are exploring. In particular, exploring enables you to improve your estimates of the non greedy action's values.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning

- Exploitation will maximize your expected reward on the one step but exploration may lead to greater total reward in the long run.
- Intuitively, if you have many time steps ahead, it may be better to explore.
- How do we balance exploration and exploitation when dealing with the $k$-armed bandit problem?

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Action value estimates

- The first thing we want to do is get an estimate of the value of an action at time $t$.
- The natural approach is to average over the rewards received in the past

$$v_{\text{est},t}(a) = \frac{\text{sum of rewards when } a \text{ taken}}{\text{number of times } a \text{ taken}} = \frac{\sum_{i=1}^{t-1} R_i \mathbb{1}_{A_i=a}}{\sum_{i=1}^{t} \mathbb{1}_{A_i=a}}$$

Here $\mathbb{1}_{\text{predicate}}$ is used to denote the indicator function for the predicate. $\mathbb{1}_p = 1$ if the predicate is verified and 0 otherwise.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Action value estimates

- Then the simplest action selection procedure (known as greedy action selection) is to select (one of) the action(s) with the highest estimated value,

$$A^* = \underset{a}{\operatorname{argmax}}\, v_{\mathrm{est},t}(a)$$

- Greedy action selection always exploits current knowledge to maximize immediate reward (i.e it does not spend time investigating inferior actions to see if they might be better)

- A group of alternative methods known as $\varepsilon$-greedy methods consist in behaving greedily most of the time, but once in a while (with probability $\varepsilon$) select an action randonly (with uniform probability) from the list of all possible actions.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Action value estimates

- $\varepsilon$-greedy methods ensure that every action is sampled an infinite number of times. Which in turns implies that the estimator $v_{\text{est}}(a)$ converges to the $v^*$ (the true expected value)

- To avoid keeping each reward in memory independently, typical implementations of greedy and $\varepsilon$-greedy only update the averaged reward (a.k.a value). If $Q_n$ is used to denote the value of a given action after the $n^{th}$ step,

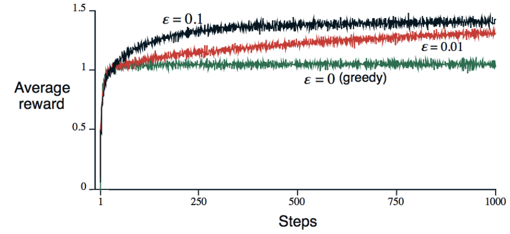
$$Q_n = \frac{R_1 + R_2 + \ldots R_{n-1}}{n-1}$$

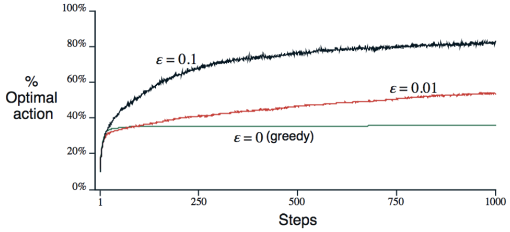
we compute $Q_{n+1}$ as

$$\begin{aligned} Q_{n+1} = \frac{1}{n}\sum_{i=1}^{n} R_i &= \frac{1}{n}\left(R_n + (n-1)\frac{1}{n-1}\sum_{i=1}^{n-1} R_i\right) \\ &= Q_n + \frac{1}{n}\left[R_n - Q_n\right] \end{aligned}$$

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: greedy vs $\varepsilon$-greedy





source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Simple Bandit algorithm

```
1. Initialize, for every action $a = 1$, to $k$
    1.1 $v(a) \leftarrow 0$
    1.2 $n(A) \leftarrow 0$ (number of times $A$ has been chosen)
2. Repeat
    2.1 $A \leftarrow \begin{cases} \operatorname{argmax}_a v(a) & \text{with probability } 1 - \varepsilon \\ \text{a random action} & \text{with probability } \varepsilon \end{cases}$
    2.2 $R \leftarrow \text{bandit}(a)$
    2.3 $n(A) \leftarrow n(A) + 1$
    2.4 $q(A) \leftarrow v(A) + \frac{1}{N(A)}[R - v(A)]$
```

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Simple Bandit algorithm

- So far we have focused on stationnary Bandit problems (Problems for which the reward probabilities do not change with time).

- When the problems are not stationnary, the choice of an action will depend on the instant at which the action is taken. In particular we will want to give more weight to the rewards associated to more recent actions. One way to achieve this is to add a weight in the update rule for the value $V_{n+1}$,

  $$v_{n+1} = v_n + \alpha(R_n - v_n)$$

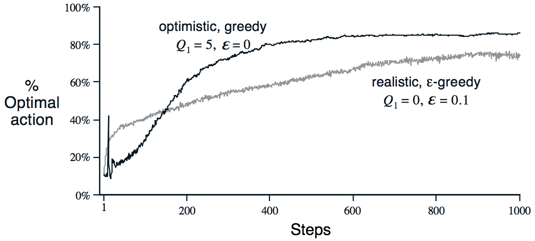
  Developing, we get

  $$v_{n+1} = (1-\alpha)^n v_1 + \sum_{i=1}^{n} \alpha(1-\alpha)^{n-i} R_i$$

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Simple Bandit algorithm

- If $\alpha = 1$, $1 - \alpha = 0$ and all the weight goes to the very last reward
- This idea of associating high initial values to every action in order to force an initial decrease of the greedy search method is known as optimistic initial values.



source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Policy gradient/gradient Bandit algorithm

- Instead of taking the action that maximizes the value at each step (as in the greedy approach), one can instead introduce policies (i.e. probability that one action is optimal against the others)

- In Gradient bandit algorithms, we define policies (and the corresponding preferences $H_t$) by means of a softmax distribution (equiv. Gibbs or Boltzmann distribution),

$$\pi_t(a) = \Pr\{A_t = a\} = \frac{e^{H_t(a)}}{\sum_{b=1}^{k} e^{H_t(b)}}$$

  here $\Pr\{A_t = a\}$ really means "the probability that the optimal action at time $t$ is $a$".

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Policy gradient/gradient Bandit algorithm

- Policy gradient algorithms then increase the preference of an action when the reward associated to this action is larger than a baseline ($\overline{R}_t$) which is the average of all previous rewards.
- All the other actions are updated in the opposite direction

$$
\begin{aligned}
H_{t+1}(A_t) &\leftarrow H_t(A_t) + \alpha(R_t - \overline{R}_t)(1 - \pi_t(A_t)) \\
H_{t+1}(a) &\leftarrow H_t(a) - \alpha(R_t - \overline{R}_t)\pi_t(a), \quad \text{for all } a \neq A_t
\end{aligned}
$$

- We compare the current reward for action $a$ to the average reward $\overline{R}_t(a)$. If $\overline{R}_t > R_t$, the agent interpret the action as being suboptimal compared to previous ones and hence reduces its weight more.
- The weighting by the policies $\pi_t$ has a similar interpretation.

sources: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Associative search (contextual bandit)

$$H_{t+1}(A_t) \leftarrow H_t(A_t) + \alpha(R_t - \overline{R}_t)(1 - \pi_t(A_t))$$
$$H_{t+1}(a) \leftarrow H_t(a) - \alpha(R_t - \overline{R}_t)\pi_t(a), \quad \text{for all } a \neq A_t$$

- When an action has a low probability of being selected, there is no need to decrease the weight of this action anymore as it cannot really be held responsible for the fact that the average reward is lower than the current reward.
- On the opposite, if one action $a$ has a relatively higher probability of being selected but is different from the current optimal action $A_t$, it probably contributed for most of the (underoptimal) average $\overline{R}_t$ and should be considered as suboptimal.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Bandit/Policy gradient as stochastic gradient ascent

- The Bandit gradient method or policy gradient method has an interpretation as stochastic gradient ascent
- To see this, note that to update the preferences, we will want to follow the direction that maximizes the average reward,

$$H_{t+1}(a) \leftarrow H_t(a) + \alpha \frac{\partial \mathbb{E}[R_t]}{\partial H_t(a)}$$

Here $\mathbb{E}\{R_t\}$ is viewed as a multivariate function in the preferences.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Bandit/Policy gradient as stochastic gradient ascent

- In practice, we do not know the population average $\mathbb{E}[R_t] = \sum_b \pi_t(b) v_*(b)$ but let us forget that for the moment

$$\begin{aligned}
\frac{\partial \mathbb{E}[R_t]}{\partial H_t(a)} &= \frac{\partial}{\partial H_t(a)} \left[ \sum_b \pi_t(b) v_*(b) \right] \\
&= \sum_b v_*(b) \frac{\partial \pi_t(b)}{\partial H_t(a)} \\
&= \sum_b (v_*(b) - X_t) \frac{\partial \pi_t(b)}{\partial H_t(a)}
\end{aligned}$$

  The last line follows from the definition of the policy and the fact that $\sum_b \frac{\partial \pi_t(b)}{\partial H_t(a)} = 0$

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Bandit/Policy gradient as stochastic gradient ascent

- Developing further, we get

$$\begin{aligned}
\frac{\partial \mathbb{E}\left[R_t\right]}{\partial H_t(a)} &= \frac{\partial}{\partial H_t(a)}\left[\sum_b \pi_t(b) v_*(b)\right] \\
&= \sum_b \pi_t(b)(v_*(b) - X_t)\frac{\partial \pi_t(b)}{\partial H_t(a)}/\pi_t(b) \\
&= \mathbb{E}_{A_t}\left\{(v_*(A_t) - X_t)\frac{\partial \pi_t(A_t)}{\partial H_t(a)}/\pi_t(A_t)\right\} \\
&= \mathbb{E}_{A_t}\left\{(R_t - \overline{R}_t)\frac{\partial \pi_t(A_t)}{\partial H_t(a)}/\pi_t(A_t)\right\}
\end{aligned}$$

The last line follows from the definition of the value $v_*(A_t)$ of an action $A_t$ as the average reward $\mathbb{E}[R_t]$.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Bandit/Policy gradient as stochastic gradient ascent

- If we assume for now that

$$\frac{\partial \pi_t(A_t)}{\partial H_t(a)} / \pi_t(A_t) = \pi_t(A_t)(\mathbb{1}_{a=A_t} - \pi_t(A_t)) \quad ,$$

we get

$$\begin{aligned} \frac{\partial \mathbb{E}\left[R_t\right]}{\partial H_t(a)} &= \mathbb{E}\left[(R_t - \overline{R}_t)\pi - t(A_t)(\mathbb{1}_{a=A_t} - \pi_t(a))/\pi_t(A_t)\right] \\ &= \mathbb{E}\left[(R_t - \overline{R}_t)(\mathbb{1}_{a=A_t} - \pi_t(a))\right] \end{aligned}$$

- Stochastic gradient is used to maximize (resp. minimize) a population average by replacing this population average with a sample average ($\mathbb{E}V \to \sum_i V_i$). In its most compressed version, it actually defines the iterates by taking one sample at a time.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Bandit/Policy gradient as stochastic gradient ascent

- In this framework, the gradient

$$\frac{\partial \mathbb{E}\left[R_t\right]}{\partial H_t(a)} = \mathbb{E}\left[(R_t - \overline{R}_t)(\mathbb{1}_{a=A_t} - \pi_t(a))\right]$$

is turned into the updates

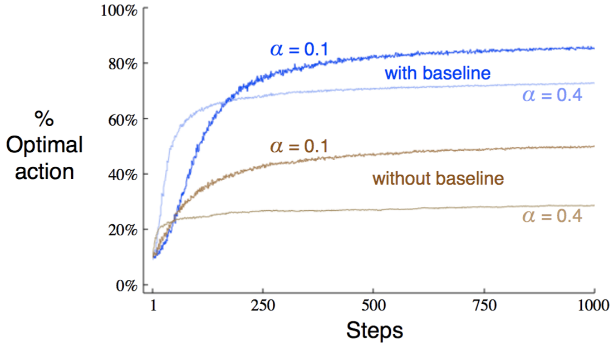
$$H_{t+1}(a) = H_t(a) + a(R_t - \overline{R}_t)(\mathbb{1}_{a=A_t} - \pi_t(a)), \quad \text{for all } a$$

source: Sutton & Barto, Reinforcement Learning: An Introduction.

- To conclude, use the quotient rule on derivatives to show the relation $\frac{\partial \pi_t(b)}{\partial H_t(a)} = \pi_t(b)$

$$\begin{aligned}
\frac{\partial \pi_t(b)}{\partial H_t(a)} &= \frac{\partial}{\partial H_t(a)} \left[ \frac{e^{H_t(b)}}{\sum_{c=1}^{k} e^{H_t(c)}} \right] \\
&= \frac{\frac{\partial e^{H_t(b)}}{\partial H_t(a)} \sum_{c=1}^{k} e^{H_t(c)} - e^{H_t(b)} \frac{\partial \sum_{c=1}^{k} e^{H_t(c)}}{\partial H_t(a)}}{\left(\sum_{c=1}^{k} e^{H_t(c)}\right)^2} \\
&= \frac{\mathbb{1}_{a=b} e^{H_t(b)} \sum_{c=1}^{k} e^{H_t(c)} - e^{H_t(b)} e^{h_t(a)}}{\left(\sum_{c=1}^{k} e^{H_t(c)}\right)^2} \\
&= \frac{\mathbb{1}_{a=b} e^{H_t(b)}}{\sum_{c=1}^{k} e^{H_t(c)}} - \frac{e^{H_t(b)} e^{H_t(a)}}{\left(\sum_{c=1}^{k} e^{H_t(c)}\right)^2} \\
&= \mathbb{1}_{a=b} \pi_t(b) - \pi - t(b) \pi_t(a) \\
&= \pi_t(b)(\mathbb{1}_{a=b} - \pi_t(a))
\end{aligned}$$

source: Sutton & Barto, Reinforcement Learning: An Introduction.



source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Upper Confidence Bound Action Selection

- A downside of the $\varepsilon$ greedy action selection approach is that when exploring, it does not discriminate between the actions.
- One possible improvement consists in selecting among the actions during the exploration step, according to their potential for being optimal (and not completely randomly)
- One approach is to rely on the following upper confidence bound (UCB)

$$A_t = \operatorname*{argmax}_a \left[ v_t(a) + c\sqrt{\frac{\ln(t)}{N_t(a)}} \right]$$

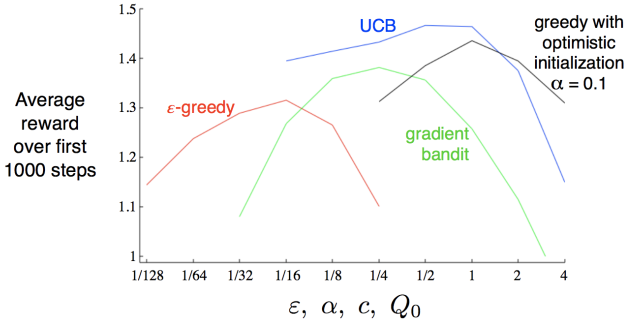
source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Upper Confidence Bound Action Selection

- The idea of the UCB selection approach is to add a term (the $\sqrt{\log(t)/N_t}$ term) that accounts for the uncertainty in the value of an action $a$
- The objective that is maximized can be viewed as an upper bound on the potential value of the action $a$
- When the action $a$ is visited, the number $N_t(a)$ increases. On the opposite, when $a$ is not selected, the numerator $t$ increases while the number $N_t(a)$ remain constant, thus making this action more likely to get selected in future steps.
- After an infinite number of iterations, as the function is unbounded, every action will be selected at least once.

source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning: Comparison of Bandit algorithms



source: Sutton & Barto, Reinforcement Learning: An Introduction.

## Reinforcement learning

- So far in this chapter we have considered only nonassociative tasks, in which there is no need to associate different actions with different situations
- In these tasks the learner either tries to find a single best action when the task is stationary, or tries to track the best action as it changes over time when the task is nonstationary
- The Multi-armed bandit problem is an instance of non associative learning.
- However, in a general reinforcement learning task there is more than one situation, and the goal is to learn a policy: a mapping from situations to the actions that are best in those situation

source: Barto, Sutton, and Brouwer, Biological Cybernetics, 1981.