# Unsupervised Learning

## Clustering

- In *clustering*, the target feature is not given.
- Goal: Construct a natural classification that can be used to predict features of the data.
- The examples are partitioned in into *clusters* or *classes*.
- Each class predicts values of the features for the examples in the class.
- In *hard clustering*, each example is placed definitively in a class.
- In *soft clustering*, each example has a probability of belonging to each class.
- The best clustering minimizes an error measure.



## EM Algorithm

- The EM (Expectation Maximization) algorithm is not an algorithm, but is an algorithm design technique.
- Start with a hypothesis space for classifying the data and a random hypothesis.
- Repeat until convergence:
  - **E Step**. Classify the examples using the current hypothesis.
  - **M Step**. Learn a new hypothesis from the examples using their current classification.
- This can get stuck in local optima; different initializations can affect the result.





## $k$-Means Algorithm

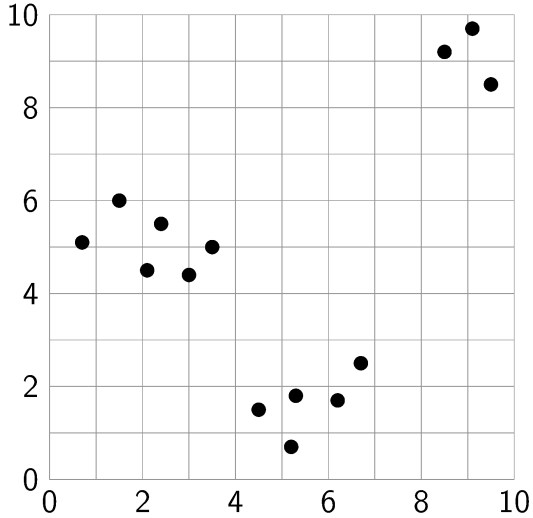
- The $k$-means algorithm is used for hard clustering.
- Inputs:
  - training examples
  - the number of classes/clusters, $k$
- Outputs:
  - Each example is assigned to one class.
  - The average/mean example of each class.
- If example $e = (x_1, \ldots, x_n)$ is assigned to class $i$ with mean $u_i = (u_{i1}, \ldots, u_{in})$, error is
  $\|e - u_i\|^2 = \sum_{j=1}^{n}(x_j - u_{ij})^2$



## $k$-Means Procedure

Procedure *K-Means*$(E, k)$
  Inputs: set of examples and number of classes
  Randomly assign each example to a class
  Let $E_i$ be the examples in class $i$
  Repeat
    M-Step:
      for each class $i$ from $1$ to $k$
        $u[i] \leftarrow \sum_{e \in E_i} e/|E_i|$
    E-Step:
      for each example $e$ in $E$
        put $e$ in class $\arg\min_i \|u[i] - e\|^2$
  until no changes in any $E_i$
  return $u$ and $E_i$ clusters

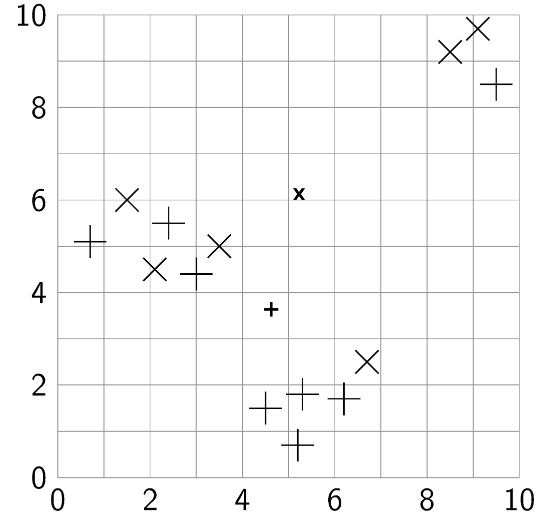
## Example Data



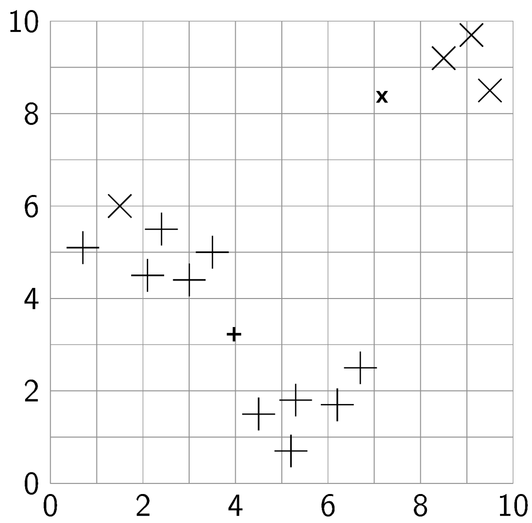





## Random Assignment to Classes

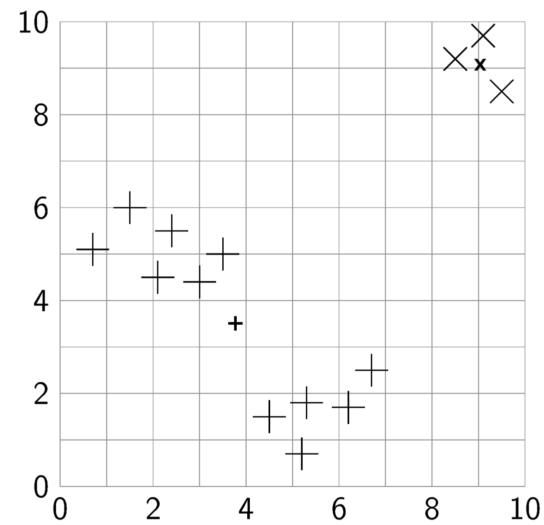


## Assign to Closest Mean






## Assign to Closest Mean Again






## Properties of $k$-Means

- An assignment of examples to classes is *stable* if running both the M step and the E step does not change the assignment.
- This algorithm will converge to a stable local minimum.
- It is not guaranteed to converge to a global minimum.
- It is sensitive to the relative scale of the dimensions.
- Increasing $k$ can always decrease error until $k$ is the number of different examples.

## Soft $k$-Means

- To illustrate soft clustering, consider a "soft" $k$-means algorithm.
- E-Step: For each example $e$, calculate probability distribution $P(\text{class } i \mid e)$

  $$P(c_i \mid e) \propto \exp\{-\|u_i - e\|^2\}$$

- M-Step: For each class $i$, determine mean probabilistically.

  $$u_i = \frac{\sum_{e \in E} P(c_i \mid e) * e}{\sum_{e \in E} P(c_i \mid e)}$$



## Soft $k$-Means Example

| $e$ | $P_0(C_x \mid e)$ | $P_1(C_x \mid e)$ | $P_2(C_x \mid e)$ |
|---|---|---|---|
| $(0.7, 5.1)$ | 0.0 | 0.013 | 0.0 |
| $(1.5, 6.0)$ | 1.0 | 0.764 | 0.0 |
| $(2.1, 4.5)$ | 1.0 | 0.004 | 0.0 |
| $(2.4, 5.5)$ | 0.0 | 0.453 | 0.0 |
| $(3.0, 4.4)$ | 0.0 | 0.007 | 0.0 |
| $(3.5, 5.0)$ | 1.0 | 0.215 | 0.0 |
| $(4.5, 1.5)$ | 0.0 | 0.000 | 0.0 |
| $(5.2, 0.7)$ | 0.0 | 0.000 | 0.0 |
| $(5.3, 1.8)$ | 0.0 | 0.000 | 0.0 |
| $(6.2, 1.7)$ | 0.0 | 0.000 | 0.0 |
| $(6.7, 2.5)$ | 1.0 | 0.000 | 0.0 |
| $(8.5, 9.2)$ | 1.0 | 1.000 | 1.0 |
| $(9.1, 9.7)$ | 1.0 | 1.000 | 1.0 |
| $(9.5, 8.5)$ | 0.0 | 1.000 | 1.0 |



## Properties of Soft Clustering

- Soft clustering often uses a parameterized probability model, e.g., means and standard deviations for normal distribution.
- Initially, assign random probabilities to the examples: prob. of class $i$ given example $e$.
- The M-step updates the values of the parameters from the probabilities.
- The E-step updates the probabilities of the examples from the probability model.
- Does not guarantee global minimum.



# Reinforcement Learning



## Reinforcement Learning

What should an agent do given:

- Prior knowledge: possible states of the world
  possible actions
- Observations: current state of world
  immediate reward/punishment
- Goal: act to maximize accumulated reward
- We assume there is a sequence of experiences:

  state, action, reward, state, action, reward, ...

- At any time agent must decide whether to
  *explore* to gain more knowledge, or
  *exploit* knowledge it has already discovered



## Why is reinforcement learning hard?

- What actions are responsible for a reward may have occurred a long time before the reward was received.
- The long-term effect of an action depends on what the agent will do in the future.
- The explore-exploit dilemma: at each time should the agent be greedy or inquisitive?
  - The $\epsilon$-greedy strategy is to select what looks like the best action $1 - \epsilon$ of the time, and to select a random action $\epsilon$ of the time.

## Temporal Differences

- Suppose we have a sequence of values $v_1, v_2, v_3, \ldots$
- Estimating the average with the first $k$ values:

  $$A_k = \frac{v_1 + \cdots + v_k}{k}$$
- Separating out $v_k$:

  $$A_k = (v_1 + \cdots + v_{k-1})/k + v_k/k$$
- Let $\alpha = 1/k$, then

  $$A_k = (1-\alpha)A_{k-1} + \alpha v_k = A_{k-1} + \alpha(v_k - A_{k-1})$$
- The TD update is: $A \leftarrow A + \alpha(v - A)$

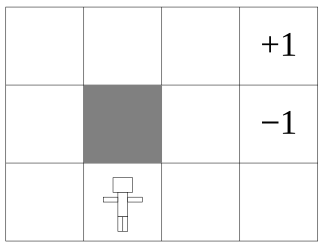


## Reinforcement Learning Example

Suppose a robot in this environment.

One terminal square has $+1$ reward (recharge station).

One terminal square has $-1$ reward (falling down stairs).




An action to stay put always succeeds.
An action to move to a neighbor square,
succeeds with probability 0.8,
stays in the same square with prob. 0.1,
goes to another neighbor with prob. 0.1
Should the robot try moving left or right?





## Review of Q Values

- A *policy* is a function from states to actions.
- For reward sequence $r_1, r_2, \ldots$, *discounted reward* is: $V = \sum_{i=1}^{\infty} \gamma^{i-1} r_i$ (discount $= \gamma$)
- $V(s)$ is expected value of state $s$.
- $Q(s,a)$ is value of action $a$ from $s$.
- For optimal policy:

  $V(s) = \max_a Q(s,a)$ (value of best action)

  $$Q(s,a) = \sum_{s'} P(s'|s,a)(R(s,a,s') + \gamma V(s')) = \sum_{s'} P(s'|s,a)(R(s,a,s') + \gamma \max'_a Q(s',a'))$$
- Learn optimal policy by learning $Q$ values.
  Use each experience $s, a, r, s'$ to update $Q[s,a]$.



## Q-Learning

Procedure Q-learning$(S, A, \gamma, \alpha, \epsilon)$
  Inputs: states, actions
      discount, step size, exploration factor
  Initialize $Q[S,A]$ to zeros
  Repeat for multiple episodes:
    $s \leftarrow$ initial state
    Repeat until end of episode:
      Select action $a$ using $\epsilon$-greedy strategy
      Do action $a$. Observe reward $r$ and state $s'$
      $Q[s,a] \leftarrow Q[s,a] +$
        $\alpha\,(r + \gamma \max_{a'} Q[s',a'] - Q[s,a])$
      $s \leftarrow s'$
  return $Q$

## Q-Learning Update

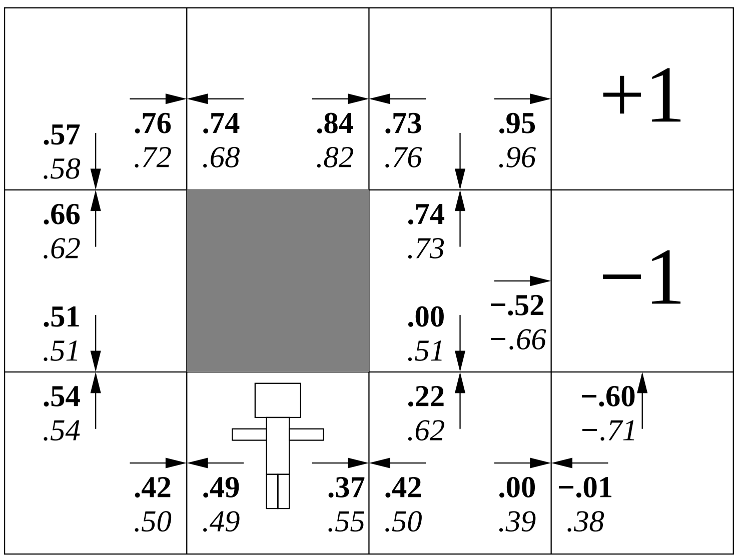
Unpacking the Q-Learning update:

$$Q[s,a] \leftarrow Q[s,a] + \\ \alpha\,(r + \gamma \max_{a'} Q[s',a'] - Q[s,a])$$

- $Q[s,a]$: Value of doing action $a$ from state $s$.
- $r, s'$: reward received and next state
- $\alpha, \gamma$: learning rate and discount factor
- $\max_{a'} Q[s',a']$: With current $Q$ values, the value of the optimal action from state $s'$.
- $r + \gamma \max_{a'} Q[s',a']$: With current $Q$ values, the discounted reward to be averaged in.



## Robot Q-Learner, $\gamma = 0.9$, $\alpha = \epsilon = 0.1$

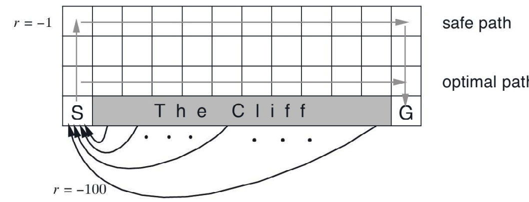







## Problems with Q-Learning

- Q-learning does off-policy learning: learns value of optimal policy, but does not follow it.
- This is bad if exploration is dangerous.
  Below, Q-learning walks off the cliff too much.



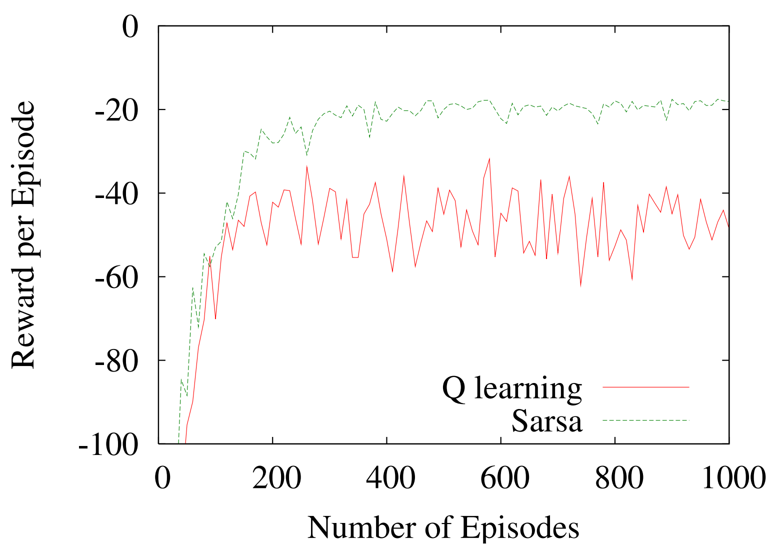

- On-policy learning learns the value of the policy being followed.
- SARSA uses the experience $s, a, r, s', a'$ to update $Q[s,a]$.



## SARSA Procedure

Procedure SARSA($S, A, \gamma, \alpha, \epsilon$)
  Initialize $Q[S,A]$ to zeros
  Repeat for multiple episodes:
    $s \leftarrow$ initial state
    Select action $a$ using $\epsilon$-greedy strategy
    Repeat until end of episode:
      Do action $a$. Observe reward $r$ and state $s'$
      Select action $a'$ for $s'$ using $\epsilon$-greedy
      $Q[s,a] \leftarrow Q[s,a] +$
        $\alpha\,(r + \gamma Q[s',a'] - Q[s,a])$
      $s \leftarrow s'$ and $a \leftarrow a'$
  return $Q$

## SARSA on the Cliff






## Reinforcement Learning with Features

- Often, we want to reason in terms of features.
- Want to take of advantage of similarities between states.
- Each assignment to the features is a state.
- Idea: Express $Q$ as a function of the features. Features encode state and action.

  $(s, a) = (x_1, x_2, x_3, \ldots)$

  $Q(s, a) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 + \ldots$

  $\delta = r + \gamma Q(s', a') - Q(s, a)$

  $w_i \leftarrow w_i + \alpha \delta x_i$



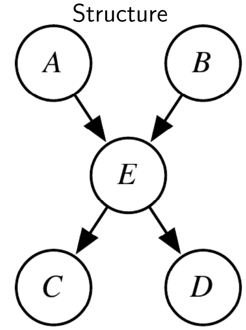


## Learning Bayesian Networks

Learn each probability separately, if you:

- know the structure of the network
- observe all the variables
- have many examples
- have no missing data

Structure Data Probababilities




| *A* | *B* | *C* | *D* | *E* |
|---|---|---|---|---|
| *t* | *f* | *t* | *t* | *f* |
| *f* | *t* | *t* | *t* | *t* |
| *t* | *t* | *f* | *t* | *f* |
| | | ... | | |

$P(A)$
$P(B)$
$P(E|A, B)$
$P(C|E)$
$P(D|E)$



## Learning Conditional Probabilities

- Use counts for each conditional probability. For example:

  $P(E = t \mid A = t \wedge B = f) =$

  $$\frac{\text{count}(E = t \wedge A = t \wedge B = f) + c_1}{\text{count}(A = t \wedge B = f) + c}$$

  $c_1$ and $c$ is prior (expert) knowledge ($c_1 \leq c$).
- When there are few examples or many parents to a node, there might be little data for probability estimates:
  - Use supervised learning or noisy ORs/ANDs.

## Unobserved Variables

- What if we had no observations of $E$?
- Use EM algorithm with probabilistic inference.
  - Randomly assign values to probability tables that include $E$.
  - Repeat:
  - E-step: Calculate $P(E \mid e)$ for each example $e$.
  - M-step: Update probabability tables using counts of $P(E \mid e)$.



## Learning Bayesian Network Structures

$$P(M \mid D) = \frac{P(D \mid M) * P(M)}{P(D)}$$

$$\log P(M \mid D) \propto \log P(D \mid M) + \log P(M)$$

- $M$ is a Bayesian network and $D$ is the data.
- Assume all variables are observed.
- A bigger network can have higher $P(M \mid D)$.
- $P(M)$ can help control the size. (e.g., using the description length).
- You can search over network structure looking for the most likely model.



## Algorithm I

- Search over total orderings of variables.
- For each total ordering $X_1, \ldots, X_n$ use supervised learning to learn $P(X_i | X_1 \ldots X_{i-1})$.
- Return the network model found with minimum: $-\log P(D \mid M) - \log P(M)$
  - $\log P(D \mid M)$ can be obtained by calculation.
  - Can approximate $\log P(M) \approx -m \log(d+1)$, where $m = \#$ of parameters in $M$ and $d = \#$ of examples.





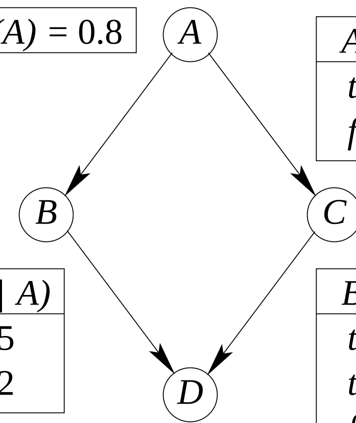
## Algorithm II

- Learn a tree-structured Bayesian network.
- Compute correlations between all pairs of variables.
- Do maximum spanning tree maximizing absolute values of correlations.
- Pick a variable to be root of the tree, then fill in probabilities using data.



## Example: Original Bayesian Network

$P(A) = 0.8$




| A | P(C \| A) |
|---|---|
| t | 0.2 |
| f | 0.5 |

| A | P(B \| A) |
|---|---|
| t | 0.5 |
| f | 0.2 |

| B | C | P(D \| B,C) |
|---|---|---|
| t | t | 0.5 |
| t | f | 0.8 |
| f | t | 0.2 |
| f | f | 0.4 |



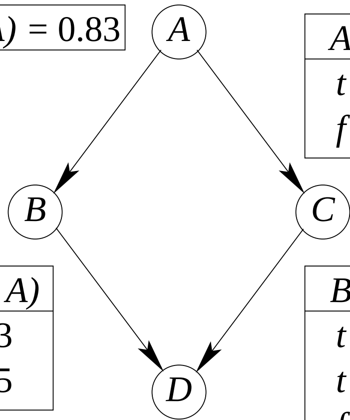
## Example: 1000 Examples

| $A$ | $B$ | $C$ | $D$ | Count |
|---|---|---|---|---|
| $T$ | $T$ | $T$ | $T$ | 39 |
| $T$ | $T$ | $T$ | $F$ | 37 |
| $T$ | $T$ | $F$ | $T$ | 300 |
| $T$ | $T$ | $F$ | $F$ | 69 |
| $T$ | $F$ | $T$ | $T$ | 15 |
| $T$ | $F$ | $T$ | $F$ | 67 |
| $T$ | $F$ | $F$ | $T$ | 117 |
| $T$ | $F$ | $F$ | $F$ | 189 |

| $A$ | $B$ | $C$ | $D$ | Count |
|---|---|---|---|---|
| $F$ | $T$ | $T$ | $T$ | 6 |
| $F$ | $T$ | $T$ | $F$ | 5 |
| $F$ | $T$ | $F$ | $T$ | 20 |
| $F$ | $T$ | $F$ | $F$ | 10 |
| $F$ | $F$ | $T$ | $T$ | 15 |
| $F$ | $F$ | $T$ | $F$ | 46 |
| $F$ | $F$ | $F$ | $T$ | 27 |
| $F$ | $F$ | $F$ | $F$ | 38 |

## Example: Learn Probabilities

$P(A) = 0.83$




| $A$ | $P(C \mid A)$ |
|---|---|
| $t$ | 0.19 |
| $f$ | 0.43 |

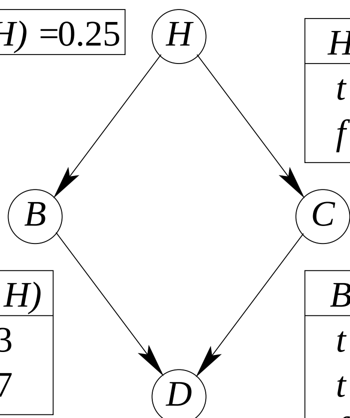
| $A$ | $P(B \mid A)$ |
|---|---|
| $t$ | 0.53 |
| $f$ | 0.25 |

| $B$ | $C$ | $P(D \mid B,C)$ |
|---|---|---|
| $t$ | $t$ | 0.52 |
| $t$ | $f$ | 0.80 |
| $f$ | $t$ | 0.21 |
| $f$ | $f$ | 0.39 |



## Example: EM for Hidden Variable

$P(H) = 0.25$




| $H$ | $P(C \mid H)$ |
|---|---|
| $t$ | 0.02 |
| $f$ | 0.30 |

| $H$ | $P(B \mid H)$ |
|---|---|
| $t$ | 0.83 |
| $f$ | 0.37 |

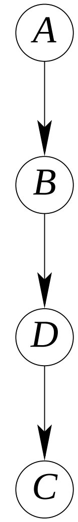
| $B$ | $C$ | $P(D \mid B,C)$ |
|---|---|---|
| $t$ | $t$ | 0.5 |
| $t$ | $f$ | 0.8 |
| $f$ | $t$ | 0.2 |
| $f$ | $f$ | 0.4 |



## Example: Learn Structure

Correlation Table

| | $B$ | $C$ | $D$ |
|---|---|---|---|
| $A$ | .22 | −.21 | .11 |
| $B$ | | −.12 | .41 |
| $C$ | | | −.23 |




$P(A) = 0.83$

| $A$ | $P(B \mid A)$ |
|---|---|
| $t$ | 0.53 |
| $f$ | 0.25 |

| $B$ | $P(D \mid B)$ |
|---|---|
| $t$ | 0.75 |
| $f$ | 0.34 |

| $D$ | $P(C \mid D)$ |
|---|---|
| $t$ | 0.14 |
| $f$ | 0.34 |