



Machine Learning

ITAM



Menu

- Instance based learning
 - K-nearest neighbors



Instance based learning

- Well, really all methods use instances to learn
- The difference is that methods in this category **store** a subset of the training data rather than deriving an explicit representation of the objective function
 - Linear function, decision tree, neural net,...



Instance based learning

- This technique memorizes some examples and postpones generalization to the last moment. At prediction time
 - They are known as lazy methods or CS since they leave the heavy computation until the last moment
- One advantage is that they can locally approximate an objective function
 - Useful when the global target can be properly approximated with a set of local approximations



Instance based learning

- Algunas características
 - Son técnicas de aprendizaje supervisado i.e., los ejemplos con los que se entrena tiene asociado un valor de la función de evaluación
 - Estas técnicas funcionan bien tanto para problemas de regresión como de clasificación
 - Desventajas
 - Costo computacional en línea
 - Desempeño degradado si las instancias tienen muchos atributos irrelevantes (más sobre esto después)



k-Nearest Neighbors

- We will see one algorithm from this family k-nearest neighbors
 - Basic version
 - Distance weighed version



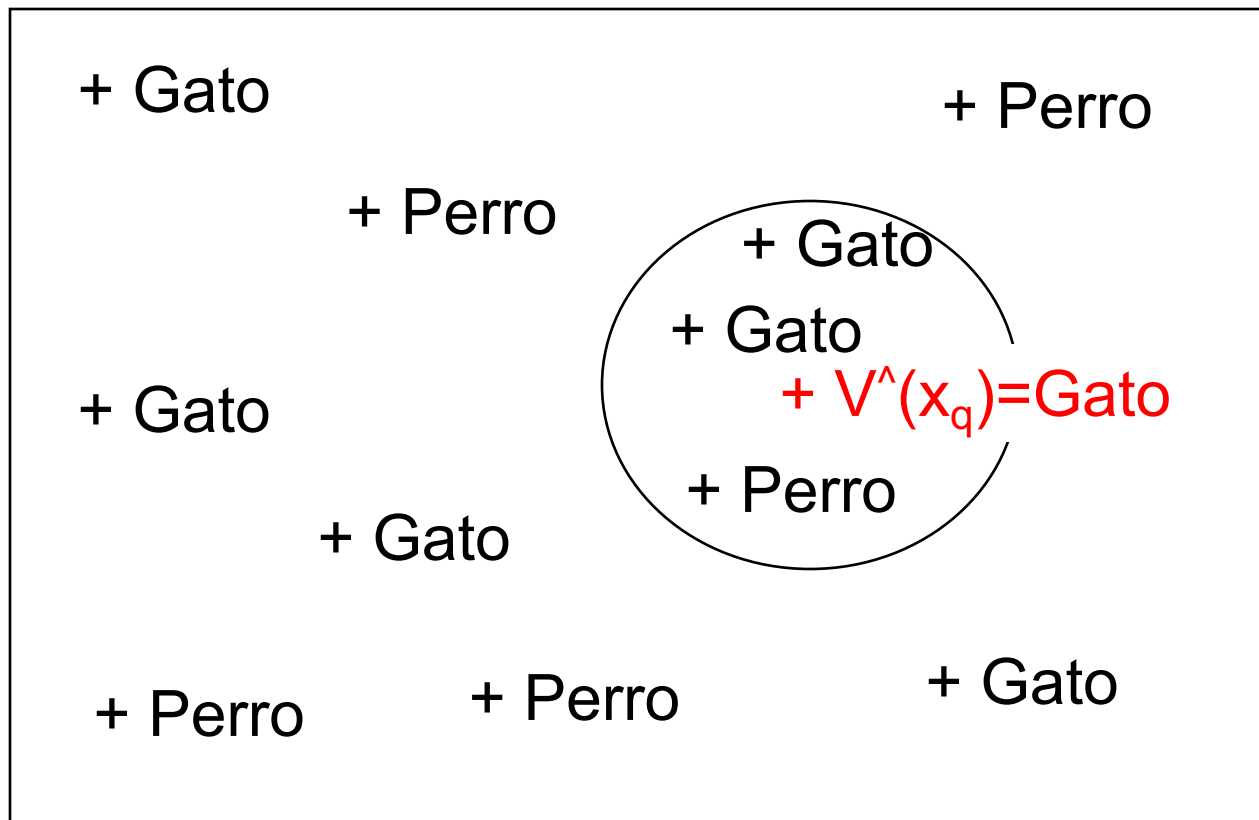
k-Nearest Neighbors

Basic version

- Each instance is considered as a point in n-dimensional space \mathcal{X}^n , where n is the number of attributes in each instance
- The objective function can be discrete or continuous (classification or regression)
- In **discrete** case, to classify instance x_q the algorithm selects its k nearest instances (which it saved during training) and assigns the most common class amongst them
 - $x_q = \langle 1, 0, 0, 1, 1 \rangle$
 - Suppose the $k=3$ nearest neighbors are:
 - $(\langle 1, 1, 0, 1, 1 \rangle, \text{Gato})$
 - $(\langle 1, 0, 0, 0, 1 \rangle, \text{Perro})$
 - $(\langle 0, 0, 0, 1, 1 \rangle, \text{Gato})$
 - The classification for $x_q \langle 1, 0, 0, 1, 1 \rangle$ will be Gato

Example

Classify x_q , with $k=3$



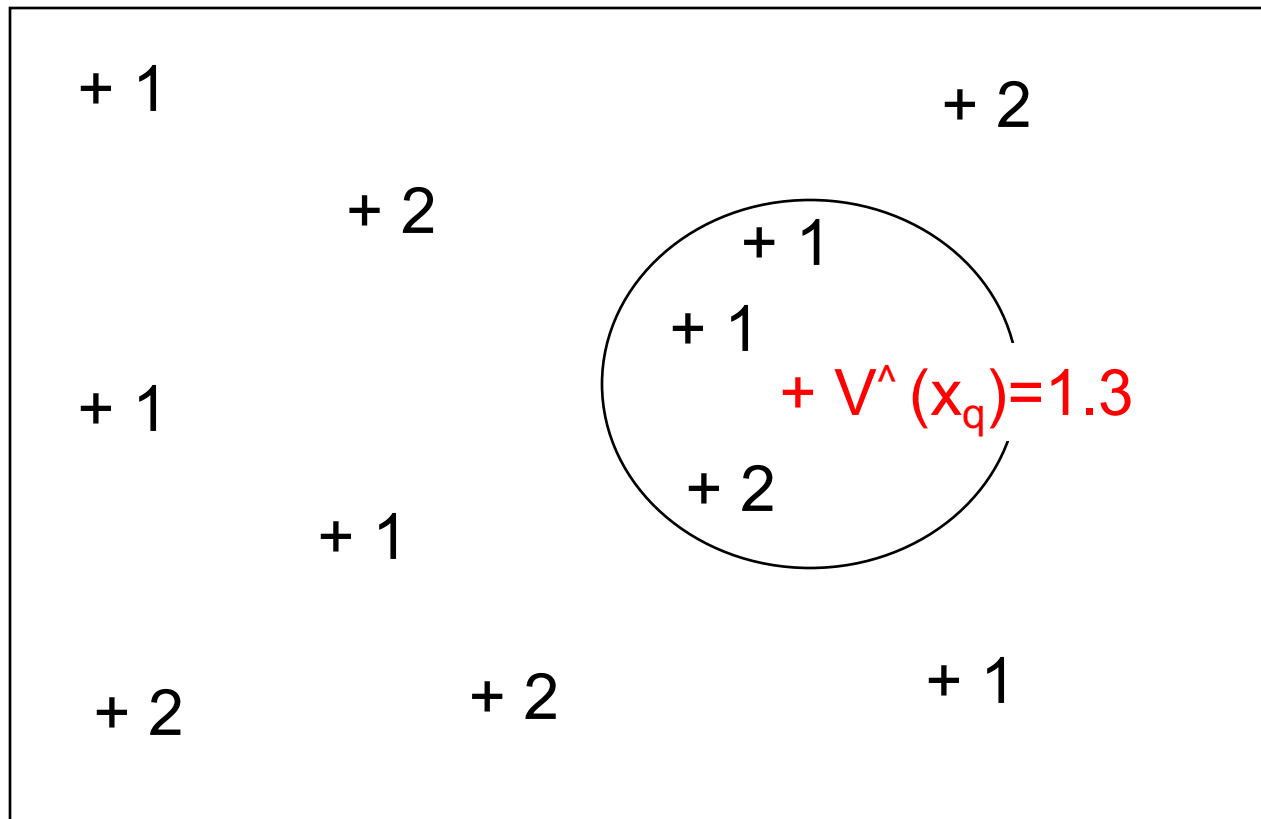
k-Nearest Neighbors

Basic version

- In the **continuous** case, the average of the objective function values of x_q 's k nearest instances are computed. For example, given
 - $x_q = \langle 1, 0, 0, 1, 1 \rangle$
 - Assume the $k=3$ nearest neighbors are:
 - $(\langle 1, 1, 0, 1, 1 \rangle, 1)$
 - $(\langle 1, 0, 0, 0, 1 \rangle, 2)$
 - $(\langle 0, 0, 0, 1, 1 \rangle, 1)$
 - The output for $\langle 1, 0, 0, 1, 1 \rangle$ will be $4/3=1.3$

Example

x_q with $k=3$



k-Nearest Neighbors

Basic version

- How close instances are is computed using some distance metric; for example Euclidean distance
 - The Euclidean distance between x_q and x_j is:
$$\text{distance}(x_q, x_j) = \sqrt{\sum_{r=1, n} (a_r(x_q) - a_r(x_j))^2}$$

-where $a_r(x_q)$ is the value of attribute r of instance x_q . The sum is over all n attributes



k-Nearest Neighbors Algorithm

- Training :
 - Store every instance $(x, f(x))$
 - (some implementations might choose representatives)
- Test:
 - Given x_q as input
 - Compute the distance between x_q and every stored instance
 - Classification:
 - Let $x_1 \dots x_k$ be the k nearest neighbors to x_q
 - $V^{\wedge}(x_q) \leftarrow$ Most common from $\{f(x_1), f(x_2) \dots f(x_k)\}$
 - Regression:
 - $V^{\wedge}(x_q) \leftarrow 1/k \sum_{i=1, k} f(x_i)$
 - The average value of the k nearest neighbors
 - Some implementations might use the median....



k-Nearest Neighbors

Classification example

■ Data

Calif. Mate	Calif. Bio	Estudiante	dist. a X_q
8	8	Bueno	1
9	8	Bueno	1.41421356
7	9	Bueno	2.23606798
9	5	Malo	2.23606798
6	7	Malo	2
7	7	Malo	1

■ Classification $x_q = (\text{Calif.Mate}=8, \text{Calif.Bio}=7)$

3-mas cercanos		
8	8	Bueno
7	7	Malo
9	8	Bueno

x_q is classified as Bueno



k-Nearest Neighbors Regression

■ Datos

Calif. Mate	Calif. Bio	Estudiante	dist. a X_q
8	8	2	1
9	8	2	1.41421356
7	9	2	2.23606798
9	5	1	2.23606798
6	7	1	2
7	7	1	1

■ Clasificación $x_q=(\text{Calif.Mate}=8, \text{Calif.Bio}=7)$

3-mas cercanos		Estudiante
8	8	2
7	7	1
9	8	2

x_q tests as $5/3=1.6$



k-Nearest Neighbors

Weighed version

- One extension of the algorithm is to weigh the contributions of each neighbor by how close they are to x_q
 - The further away from x_q the less its influence
 - One possibility is to use the inverse squared distance to make the influence fall off quickly



k-Nearest Neighbors

Weighed version

- We just need to modify the last line of the algorithm
- Classification
 - $f(x_q) \leftarrow$ Most common element of $\{w_1 f(x_1), w_2 f(x_2), \dots, w_k f(x_k)\}$
where $w_i = 1/\text{distance}(x_q, x_i)^2$. Note that to determine the most common element all the w_i associated with the same $f(x_i)$ must be added
- Regression
 - $f(x_q) \leftarrow 1/r \sum_{i=1,k} w_i f(x_i)$
where $r = \sum_{i=1,k} w_i$
- Note: If the distance between x_q y x_i is zero x_q is assigned the value of $f(x_i)$

k-Nearest Neighbors

Example

- Data

Calif. Mate	Calif. Bio	Estudiante	dist. a X_q
8	8	Bueno	2.01246118
9	8	Bueno	1.80277564
7	9	Bueno	3.38378486
9	5	Malo	1.20415946
6	7	Malo	3.00832179
7	7	Malo	2.06155281

- Clasificación $x_q = (\text{Calif.Mate}=8.9, \text{Calif.Bio}=6.2)$

3-mas cercanos		dist. A X_q	w_i	
8	8	2.012	0.24702679	bueno
9	8	1.802	0.30795725	bueno
9	5	1.204	0.68983786	malo

=	0.54(bueno)
	0.68(malo)

x_q es clasificado como malo



k-Nearest Neighbors

- Some characteristics
 - Robust to noisy data (with a large k)
 - Needs a lot of data
 - Slow to predict
 - Uses all attributes
 - This in contrast to decision trees
 - Problem: the curse of dimensionality



k-Nearest Neighbors

Example of the curse

- Data

Distancia	c3 de lluvia	Temp	Calif. Mate	Calif. Bio	Estudiante	dist. a Xq
500	50	25	8	8	Bueno	600.087494
1000	150	23	9	8	Bueno	148.667414
300	60	21	7	9	Bueno	800.255584
600	50	25	9	5	Malo	500.108988
300	100	23	6	7	Malo	802.249338
1500	40	21	7	7	Malo	400.00625

- Classification $x_q=(1100,40,23,8,7)$

3-mas cercanos					
1000	150	23	9	8	Bueno
1500	40	21	7	7	Malo
600	50	25	9	5	Malo

x_q is classified as Malo due to the new, irrelevant attributes
(used to be classified as Bueno)

There is also a problem of scale. What to do?



k-Nearest Neighbors

Curse of dimensionality

- Some possible solutions
 - Choose relevant attributes
 - “Subset selection”
 - “Principal components”: Find a linear combination of the attributes
 - Information Gain: Similar to what we did for the tree
 - “Correlation Based Feature Selection” : Determine correlation among attributes and between attributes and dependent variable s
 - Factor analysis,....many more



Exercise

- Generate a data set with many circles distributed in a plane. The points inside the circles belong to category “in” and the point outside to category “out”
- Compare with an SVM or Neural net (choose one)
 - Please not all of you SVM