Recitation 3
Classification and Regression

10-301/10-601: Introduction to Machine Learning

02/09/2022

1 Decision Trees and Beyond

1. **Decision Tree Classification with Continuous Attributes**
Given the dataset $\mathcal{D}_1 = \{\mathbf{x}^{(i)}, y\}_{i=1}^N$ where $\mathbf{x}^{(i)} \in \mathbb{R}^2, y \in \{\text{Yellow}, \text{Purple}, \text{Green}\}$ as shown in Fig. 1, we wish to learn a decision tree for classifying such points. Provided with a possible tree structure in Fig. 1, what values of α, β and leaf node predictions could we use to perfectly classify the points? Now, draw the associated decision boundaries on the scatter plot.

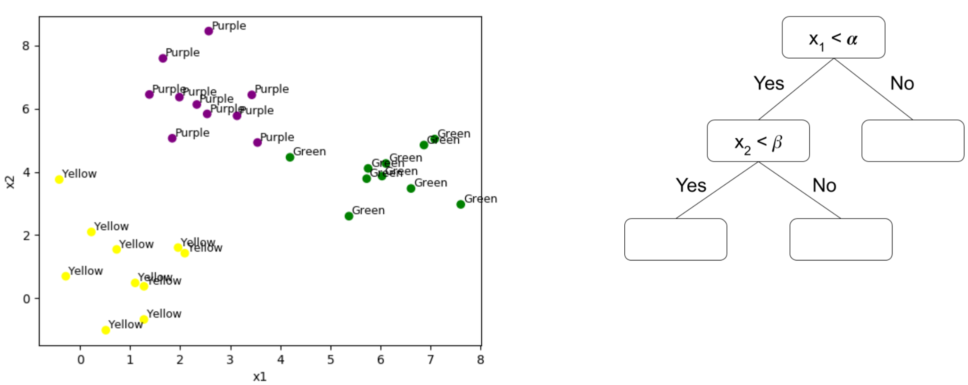


Figure 1: Classification of 2D points, with Decision Tree to fill in

Decision Tree Regression with Continuous Attributes

Now instead if we had dataset $\mathcal{D}_2 = \{\mathbf{x}^{(i)}, y\}_{i=1}^{N}$ where $\mathbf{x}^{(i)} \in \mathbb{R}^2, y \in \mathbb{R}$ as shown in Fig. 2, we wish to learn a decision tree for regression on such points. Using the same tree structure and values of α, β as before, what values should each leaf node predict to minimize the training Mean Squared Error (MSE) of our regression? Assume each leaf node just predicts a constant.

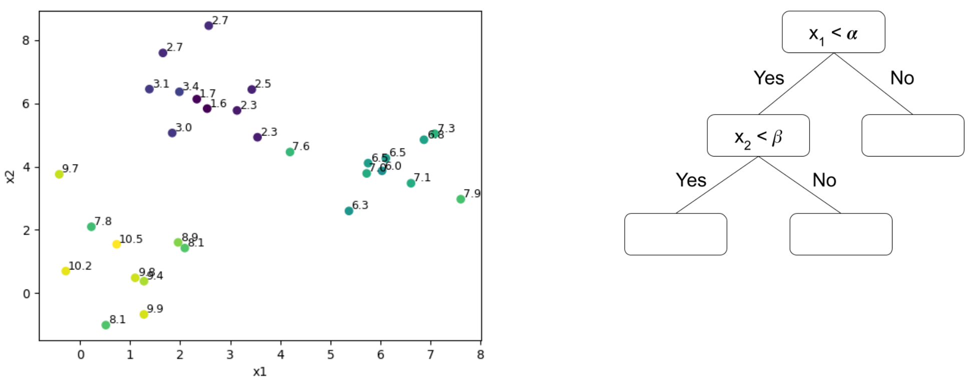


Figure 2: Regression on 2D points, with Decision Tree to fill in

2 k-NN

2.1 A Classification Example

Using the figure below, what would you categorize the green circle as with $k = 3$? $k = 5$?

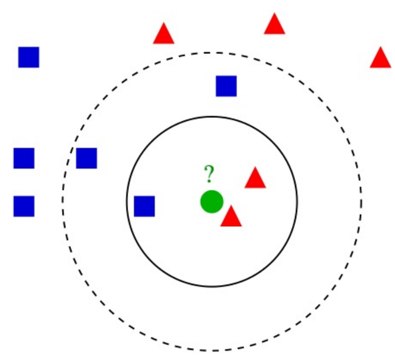
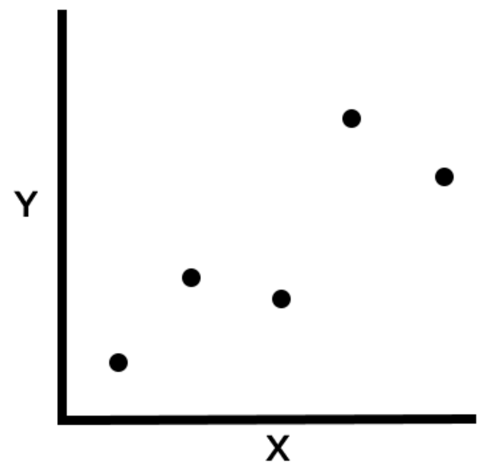


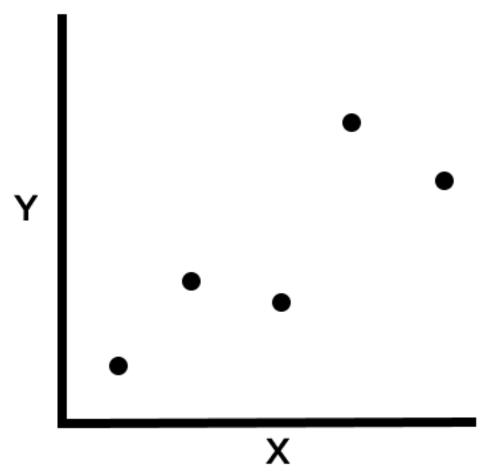
Figure 3: From wiki

2.2 k-NN for Regression

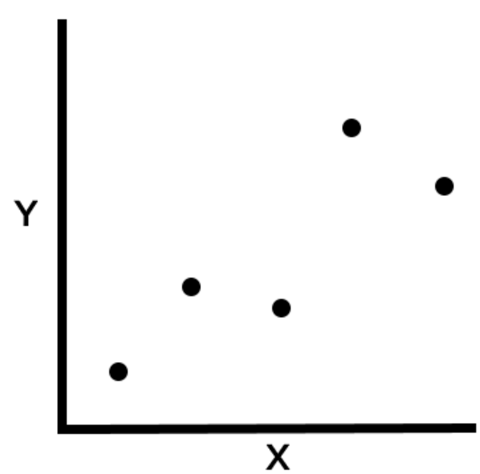
You want to predict a continuous variable Y with a continuous variable X. Having just learned k-NN, you are super eager to try it out for regression. Given the data below, draw the regression lines (what k-NN would predict Y to be for every X value if it was trained for the given data) for k-NN regression with $k = 1$, weighted $k = 2$, and unweighted $k = 2$. For weighted $k = 2$, take the weighted average of the two nearest points. For unweighted $k = 2$, take the unweighted average of the two nearest points. (Note: the points are equidistant along the x-axis)



(a) $k = 1$



(b) weighted $k = 2$



(c) unweighted $k = 2$

3 Linear Regression

3.1 Defining the Objective Function

1. What does an objective function $J(\theta)$ do ?

2. What are some properties of this function?

3. What are some examples?

3.2 Solving Linear Regression using Gradient Descent

	$\mathbf{x}^{(1)}$	$\mathbf{x}^{(2)}$	$\mathbf{x}^{(3)}$	$\mathbf{x}^{(4)}$	$\mathbf{x}^{(5)}$
x_1	1.0	2.0	3.0	4.0	5.0
x_2	-2.0	-5.0	-6.0	-8.0	-11.0
x_3	3.0	8.0	9.0	12.0	14.0
y	2.0	4.0	7.0	8.0	11.0

Now, we want to implement the gradient descent method.

Assuming that $\alpha = 0.1$ and w has been initialized to $[0, 0, 0]^T$, perform one iteration of gradient descent:

1. What is the gradient of the objective function , $J(\theta)$, w.r.t θ: $\nabla_\theta J(\theta)$

2. How do we carry out the update rule?

4 Perceptron

4.1 Perceptron Mistake Bound Guarantee

If a dataset has margin $\boldsymbol{\gamma}$ and all points inside a ball of radius R, then the perceptron makes less than or equal to $(R/\boldsymbol{\gamma})^2$ mistakes.

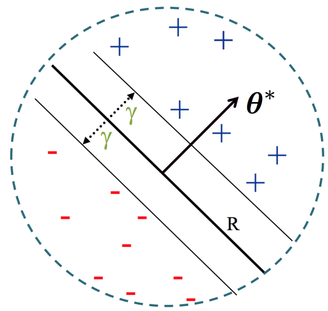


Figure 5: Perceptron Mistake Bound Setup

4.2 Definitions

Margin:

- The margin of example x wrt a linear separator w is the (absolute) distance from x to the plane $w \cdot x = 0$.
- The margin $\boldsymbol{\gamma}_w$ of a set of examples S wrt a linear separator w is the smallest margin over points $x \in S$.
- The margin $\boldsymbol{\gamma}$ of a set of examples S is the maximum $\boldsymbol{\gamma}_w$ over all linear separators w.

Linear Separability: For a binary classification problem, a set of examples S is linearly separable if there exists a linear decision boundary that can separate the points.

We say (batch) perceptron algorithm has converged when it stops making mistakes on the training data.

4.3 Theorem: Block, Novikoff

Given dataset $D = (x^{(i)}, y^{(i)})_{i=1}^N$. Suppose:

1. Finite size inputs: $||x^{(i)}|| \leq R$
2. Linearly separable data: $\exists \boldsymbol{\theta}^*$ and $\boldsymbol{\gamma} > 0$ s.t. $||\boldsymbol{\theta}^*|| = 1$ and $y^{(i)}(\boldsymbol{\theta}^* \cdot x^{(i)}) \geq \boldsymbol{\gamma}, \forall i$

Then, the number of mistakes made by the Perceptron algorithm on this dataset is $k \leq (R/\boldsymbol{\gamma})^2$

Proof:
Part 1: For some A, $Ak \leq ||\boldsymbol{\theta}^*||$

Part 2: For some B, $||\boldsymbol{\theta}^*|| \leq B\sqrt{k}$

Part 3: Combine the bounds

Main Takeaway:

5 Summary

5.1 k-NN

Pros	Cons	Inductive bias	When to use	
• Simple, minimal assumptions made about data distribution • No training of parameters • Can apply to multi-class problems and use different metrics	• Becomes slow as dataset grows • Requires homogeneous features • Selection of k is tricky • Imbalanced data can lead to misleading results • Sensitive to outliers	• Similar (i.e. nearby) points should have similar labels • All label dimensions are created equal	• Small dataset • Small dimensionality • Data is clean (no missing data) • Inductive bias is strong for dataset	

5.2 Linear regression

Pros	Cons	Inductive bias	When to use	
• Easy to understand and train • Closed form solution	• Sensitive to noise (other than zero-mean Gaussian noise)	• The relationship between the inputs x and output y is linear. i.e. hypothesis space is Linear Functions	• Most cases (can be extended by adding non-linear feature transformations)	

5.3 Decision Tree

Pros	Cons	Inductive bias	When to use	
• Easy to understand and interpret • Very fast for inference	• Tree may grow very large and tend to overfit. • Greedy behaviour may be sub-optimal	• Prefer the smallest tree consistent w/ the training data (i.e. 0 error rate)	• Most cases. Random forests are widely used in industry.	

5.4 Perceptron

Pros	**Cons**	**Inductive bias**	**When to use**	
• Easy to understand and works in an online learning setting. • Provable guarantees on mistakes made if the data is known to be linearly separable (perceptron mistake-bound).	• No guarantees on finding maximum-margin hyperplane (like in SVM), only that you will find **a** separating hyperplane. • Output is sensitive to noise in the training data.	• The binary classes are separable in the feature space by a line.	• The basic perceptron algorithm is not used much anymore, but other variants mentioned in class such as kernel perceptron or structured perceptron may have more success.	