RECITATION 3 CLASSIFICATION AND REGRESSION

10-301/10-601: Introduction to Machine Learning 06/02/2022

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.

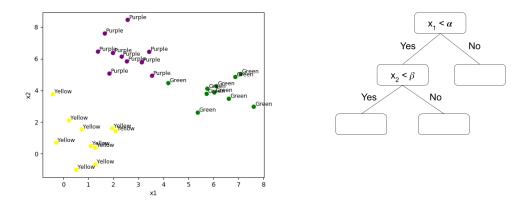


Figure 1: Classification of 2D points, with Decision Tree to fill in

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.

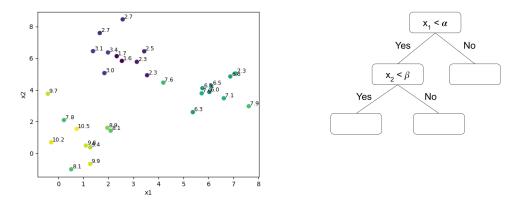


Figure 2: Regression on 2D points, with Decision Tree to fill in

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?

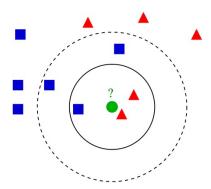
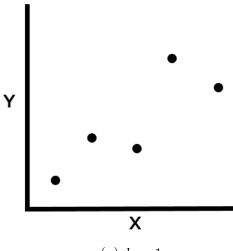


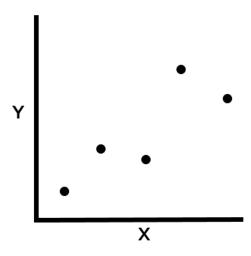
Figure 3: From wiki

2.2 k-NN for Regression

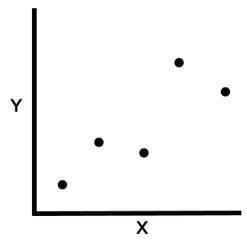
You want to predict a continuous variable Y with a continuous variable X. Having just learned k-NN, you are super eager to try it out for regression. Given the data below, draw the regression lines (what k-NN would predict Y to be for every X value if it was trained for the given data) for k-NN regression 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 $J(\theta)$ with respect to 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 γ and all points inside a ball of radius R, then the perceptron makes less than or equal to $(R/\gamma)^2$ mistakes.

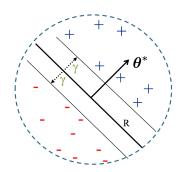


Figure 5: Perceptron Mistake Bound Setup

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 γ_w of a set of examples S wrt a linear separator w is the smallest margin over points $x \in S$.
- The margin γ of a set of examples S is the maximum γ_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.

Update Rule: When the k-th mistake is made on data point $\mathbf{x}^{(i)}$, the parameter update is

$$\boldsymbol{\theta}^{(k+1)} = \boldsymbol{\theta}^{(k)} + \mathbf{y}^{(i)} \mathbf{x}^{(i)}$$

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

4.3 Theorem: Block, Novikoff

Given dataset $\mathcal{D} = (x^{(i)}, y^{(i)})_{i=1}^N$, suppose:

- 1. Finite size inputs: $||x^{(i)}|| \le R$
- 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 k made by the perceptron algorithm on \mathcal{D} is bounded by $(R/\gamma)^2$.

Proof:

Part 1: For some $A, Ak \leq ||\boldsymbol{\theta}^{(k+1)}||$

Part 2: For some B, $||\boldsymbol{\theta}^{(k+1)}|| \leq B\sqrt{k}$

Part 3: Combine the bounds

Main Takeaway:

5 Summary

5.1 *k*-NN

Pros	Cons	Inductive bias	When to use
 No training of parameters Can apply to multi-class problems and use different metrics 	 Slow for large datasets Must select good k Imbalanced data and outliers can lead to misleading results 	 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 true relationship between the inputs and output is linear.	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 for online learning. Provable guarantees on mistakes made for linearly separable data. 	 No guarantees on finding best (maximum-margin) hyperplane. Output is sensitive to noise in the training data. 	• The binary classes are separable in the feature space by a line.	• Not used much anymore, but variants (kernel perceptron, structured perceptron) may have more success.