$\begin{array}{c} {\bf IAML-INFR10069~(LEVEL~10):} \\ {\bf Assignment~\#1} \end{array}$

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Question 1: (22 total points) Linear Regression

In this question we will fit linear regression models to data.

(a) (3 points) Describe the main properties of the data, focusing on the size, data ranges, and data types.

Data properties of the 'regression part1.csv' dataset:

Dataset size: 50 records Dataset shape: (50, 2)

Data types: all attribute values of type float64

2 ATTRIBUTES:

revision time (in hours)

Possible data range: $0 \le \mathbf{x}_i \le \alpha$, where α represents the available hours of study

Dataset data range: $2.723 \le x_i \le 48.011$

Mean: $\mu_x = 22.220019999999998$

Standard deviation: $\sigma_x = 13.986112431936743$

exam_score (in %)

Possible data range: $0 \le \mathbf{y}_i \le 100$

Dataset data range: $14.731 \le y_i \le 94.945$

Mean: $\mu_{\rm v} = 49.91986$

Standard deviation: $\sigma_y = 20.92559441626157$

(b) (3 points) Fit a linear model to the data so that we can predict exam_score from revision_time. Report the estimated model parameters w. Describe what the parameters represent for this 1D data. For this part, you should use the sklearn implementation of Linear Regression.

Hint: By default in sklearn $fit_intercept = True$. Instead, set $fit_intercept = False$ and pre-pend 1 to each value of x_i yourself to create $\phi(x_i) = [1, x_i]$.

Fitting a linear model to predict exam_score from revision time

Linear model:

Coefficient = 1.44114091Intercept = 17.89768025835017

Therefore:

 $w \approx [17.898, 1.441]$

Representation of w:

 w_0 represents the y-intercept of the model and thus denotes the minimum estimated possible exam score.

 w_1 represents the gradient of the model and thus quantifies the direct proportionality between the student's hours of study and their exam score.

(c) (3 points) Display the fitted linear model and the input data on the same plot.



(d) (3 points) Instead of using sklearn, implement the closed-form solution for fitting a linear regression model yourself using numpy array operations. Report your code in the answer box. It should only take a few lines (i.e. <5).

Hint: Only report the relevant lines for estimating \mathbf{w} e.g. we do not need to see the data loading code. You can write the code in the answer box directly or paste in an image of it.

Closed-form solution for fitting a linear regression model with numpy

Given our analytical solution for calculating ŵ:

$$\hat{\mathbf{w}} = (\mathbf{\Phi^T} \cdot \mathbf{\Phi})^{-1} \cdot \mathbf{\Phi^T} \cdot \mathbf{Y}$$

where $(\mathbf{\Phi}^{\mathbf{T}} \cdot \mathbf{\Phi})^{-1} \cdot \mathbf{\Phi}^{\mathbf{T}}$ is the pseudo-inverse of $\mathbf{\Phi}$

We can easily transfer this into code:

```
pseudoInversePhi = np.matmul(np.matrix(np.matmul(phi.transpose(), phi)).I, phi.transpose())
w_hat = np.matmul(pseudoInversePhi, Y)
print(w_hat)
[[17.89768026]
```

[17.89768026] [1.44114091]] (e) (3 points) Mean Squared Error (MSE) is a common metric used for evaluating the performance of regression models. Write out the expression for MSE and list one of its limitations.

Hint: For notation, you can use y for the ground truth quantity and \hat{y} ($\hbar t\{y\}$) in latex) in place of the model prediction.

Limitations of the Mean Squared Error (MSE) metric

$$MSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2}$$

One of the disadvantages of the MSE metric is that it is very sensitive to outliers. This is evident in the equation as shown above, where for each value of x_i the error value (difference in the predicted and actual value) of y_i is squared and the average error value is calculated. This squaring of error values ultimately magnifies the large errors (caused by outliers) and minimizes the small errors. Inevitably meaning a single outlier in our dataset could skew our analysis greatly, due to the fact that we could get the same MSE for a predictor with one large error as a predictor with lots of small errors.

The best way to solve such a problem would be through either identifying outliers in our dataset through visualization or using different error metrics which are more robust against outliers (eg. Median Absolute Deviation).

(f) (3 points) Our next step will be to evaluate the performance of the fitted models using Mean Squared Error (MSE). Report the MSE of the data in regression_part1.csv for your prediction of exam_score. You should report the MSE for the linear model fitted using sklearn and the model resulting from your closed-form solution. Comment on any differences in their performance.

Implementation evaluation using MSE

 $MSE_{sklearn} = 30.985472614541305$

 $MSE_{closed-form} = 30.98547261454129$

Differences in performance:

 $MSE_{\text{sklearn}} = MSE_{\text{closed-form}} + 1.4210854715202004 * 10^{-14}$

Given that both of these models were calculated on the exact same dataset, we can see that the solution of our closed-form implementation was a tiny bit more accurate than that of our sklearn implementation.

Your Answer Here			

(g) (4 points) Assume that the optimal value of w_0 is 20, it is not but let's assume so for now. Create a plot where you vary w_1 from -2 to +2 on the horizontal axis, and report

Question 2: (18 total points) Nonlinear Regression

In this question we will tackle regression using basis functions.

(a) (5 points) Fit four different polynomial regression models to the data by varying the degree of polynomial features used i.e. M=1 to 4. For example, M=3 means that $\phi(x_i)=[1,x_i,x_i^2,x_i^3]$. Plot the resulting models on the same plot and also include the input data.

Hint: You can again use the sklearn implementation of Linear Regression and you can also use PolynomialFeatures to generate the polynomial features. Again, set fit_intercept = False.

Your Answer Here	

ur different polynomial regression models from the previous question.					
Your Answer Here					

(b) (3 points) Create a bar plot where you display the Mean Squared Error of each of the

on these results, which model would you choose?				
Your Answer Here				

(c) (4 points) Comment on the fit and Mean Squared Error values of the M=3 and M=4 polynomial regression models. Do they result in the same or different performance? Based

(d) (6 points) Instead of using polynomial basis functions, in this final part we will use another type of basis function - radial basis functions (RBF). Specifically, we will define $\phi(x_i) = [1, rbf(x_i; c_1, \alpha), rbf(x_i; c_2, \alpha), rbf(x_i; c_3, \alpha), rbf(x_i; c_4, \alpha)]$, where $rbf(x; c, \alpha) = \exp(-0.5(x-c)^2/\alpha^2)$ is an RBF kernel with center c and width α . Note that in this example, we are using the same width α for each RBF, but different centers for each. Let $c_1 = -4.0$, $c_2 = -2.0$, $c_3 = 2.0$, and $c_4 = 4.0$ and plot the resulting nonlinear predictions using the regression_part2.csv dataset for $\alpha \in \{0.2, 100, 1000\}$. You can plot all three results on the same figure. Comment on the impact of larger or smaller values of α .

Your Answer Here	

Question 3: (26 total points) Decision Trees

In this question we will train a classifier to predict if a person is smiling or not.

(a) (4 points) Load the data, taking care to separate the target binary class label we want to predict, smiling, from the input attributes. Summarise the main properties of both the training and test splits.

Your Answer Here		

(b) (4 points) Even though the input attributes are high dimensional, they actually consist of a set of 2D coordinates representing points on the faces of each person in the dataset. Create a scatter plot of the average location for each 2D coordinate. One for (i) smiling and (ii) one not smiling faces. For instance, in the case of smiling faces, you would average each of the rows where smiling = 1. You can plot both on the same figure, but use different colors for each of the two cases. Comment on any difference you notice between the two sets of points.

Hint: Your plot should contain two faces.

Your Answer Here	

neasure compared to entropy?					
Your Answer	Here				

(c) (2 points) There are different measures that can be used in decision trees when evaluating the quality of a split. What measure of purity at a node does the DecisionTreeClassifier in sklearn use for classification by default? What is the advantage, if any, of using this

Give one potential problem for small values and two for large values.					
Your Answer	Here				

(d) (3 points) One of the hyper-parameters of a decision tree classifier is the maximum depth of the tree. What impact does smaller or larger values of this parameter have?

(e) (6 points) Train three different decision tree classifiers with a maximum depth of 2, 8, and 20 respectively. Report the maximum depth, the training accuracy (in %), and the test accuracy (in %) for each of the three trees. Comment on which model is best and why it is best.

Hint: Set random_state = 2001 and use the predict() method of the DecisionTreeClassifier so that you do not need to set a threshold on the output predictions. You can set the maximum depth of the decision tree using the max_depth hyper-parameter.

Your Answer Here		

with the higher Hint: Use the	_			
Your Answe	er Here			

(f) (5 points) Report the names of the top three most important attributes, in order of importance, according to the Gini importance from DecisionTreeClassifier. Does the one

(g) (2 points) Are there any limitat 2D point locations? If so, name one	ions of the current choice of input attributes used i.e.
Your Answer Here	

Question 4: (14 total points) Evaluating Binary Classifiers

In this question we will perform performance evaluation of binary classifiers.

(a) (4 points) Report the classification accuracy (in %) for each of the four different models using the \mathtt{gt} attribute as the ground truth class labels. Use a threshold of >= 0.5 to convert the continuous classifier outputs into binary predictions. Which model is the best according to this metric? What, if any, are the limitations of the above method for computing accuracy and how would you improve it without changing the metric used?

Your Answer Here			

accuracy? If not, why not?

int: You can use the roc_auc_score function from sklearn.					
Your Answe	er Here				

(b) (4 points) Instead of using classification accuracy, report the Area Under the ROC Curve (AUC) for each model. Does the model with the best AUC also have the best

of alg_3 without having to retrain the model?

Your Answer Here			

(c) (6 points) Plot ROC curves for each of the four models on the same plot. Comment on the ROC curve for alg_3? Is there anything that can be done to improve the performance