

We will be using the nine features to predict the **price**. We can begin by computing the Pearson correlation matrix heatmap for these features in the dataset in Figure 1. Note that a pearson correlation coefficient r is defined as such:

$$r = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2}} \quad (1)$$

We have assigned quantitative values to the qualitative labels **cut,color,clarity** as ascending natural numbers based on ideality.

Feature	Correlation	Feature	Correlation
carat	0.9215914337868304	carat	0.7694571626172851
cut	-0.05349263851362828	cut	0.00542011950342582
color	-0.1725093772499559	color	-0.011980043670033661
clarity	-0.14680175361025616	clarity	0.04512538515850012
depth	-0.010647725608533299	depth	-0.03572374489729493
table	0.12713358133531918	table	0.08458507638109278
x	0.8844357793744166	x	0.7873455524189906
y	0.865421694764742	y	0.7717301198408058
z	0.861250266123968	z	0.7655421629234554

(a) Price
(b) Price per Carat

Table 1: Pearson Correlation Coefficients

The values for correlation for **price** is given in Table 1(a). We see that, unsurprisingly, there is a massive collection of high correlation squares at the bottom right. These indicate high Pearson correlation coefficient between **price** and **x, y, z**. Similarly, there is also a high correlation with **carat**. All of these suggest that the size of the diamond itself is the most significant predictor as to its price.

However, unexpectedly, we had a negative pearson coefficient for the quality of the **cut, color, and clarity**. This was odd, so we similarly calculated the Pearson correlation values for Price per Carat instead, given in Table 1(b). We observed that the coefficient for **cut** and **clarity** became slightly positive, while color became close to zero. These seemed more in line with our expectations, and confirmed that the rarity of high carat and high clarity in a diamond at the same time was making the corresponding values in Table 1(a) negative.

Question 1.2

Feature	Skewness	Feature	Method	Skewness
carat	1.116645920812613	carat	Box Cox	0.020450070764268666
depth	-0.08229402630189467	depth	No Change	-0.08229402630189467
table	0.7968958486695427	table	Logrithm	0.5993289324435086
x	0.3786763426463927	x	No Change	0.3786763426463927
y	2.4341667164885554	z	Square Root	0.0139742634447758
z	1.5224225590685583			

(a) Before Processing
(b) After Processing

Table 2: Skewness of Features

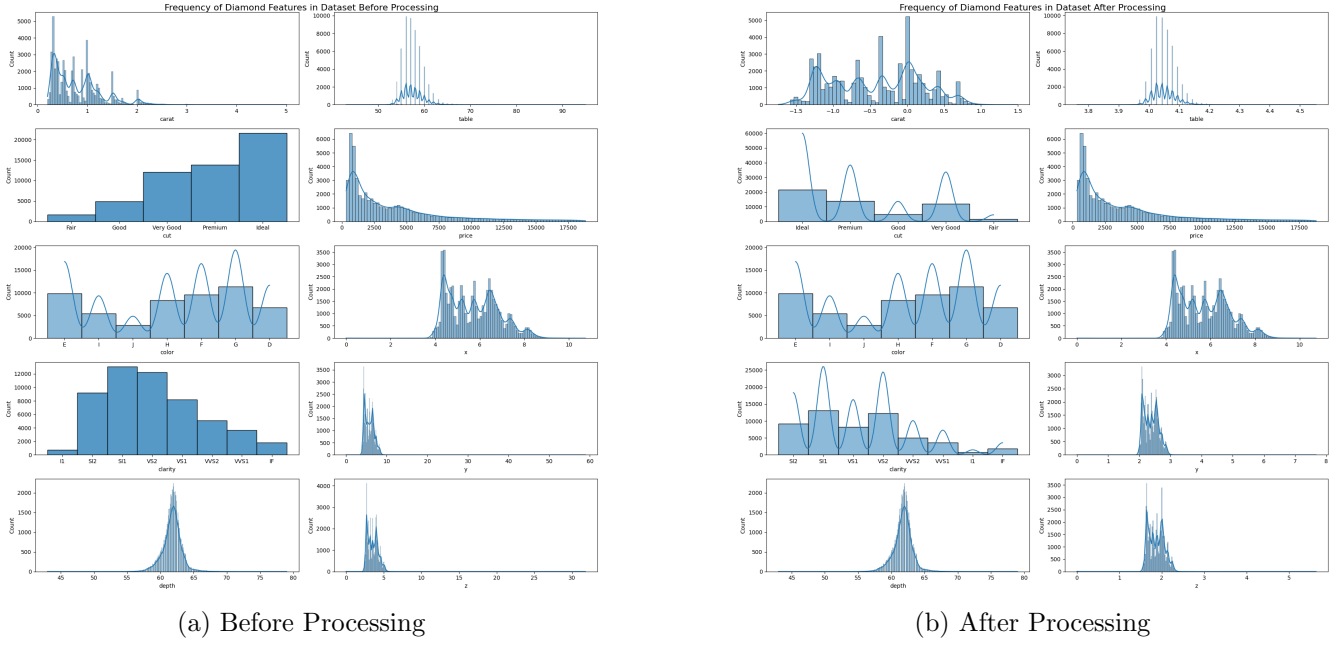


Figure 2: Histogram and KDE for Features

Now, we examine the frequency distributions within each feature. We find that some of our numerical features are somewhat skewed—apparent from Table 2(a) and Figure 2(a). We target a skewness less than 0.5, as this would imply that the distribution is somewhat symmetric. As such, we try three different methods: square-root, logarithm, and box-cox transformation. The first two are somewhat self-explanatory; box-cox uses a non-zero value of λ and conducts the following transformation:

$$y'_\lambda = \frac{y^\lambda - 1}{\lambda \cdot \bar{g}_y^{\lambda-1}} \quad (2)$$

where \bar{g}_y is defined as the geometric mean of y .

We next try all of these methods, along with no transformation, and take the minimum to try to minimize skewness in our data. The results are shown in Table 2(b) and Figure 2(b).

Question 1.3

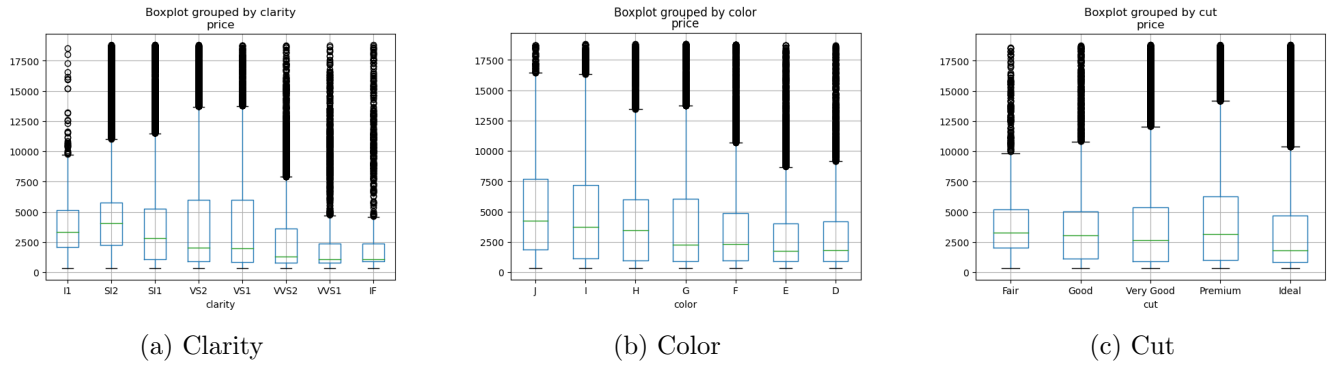


Figure 3: Categorical feature vs price boxplots

Begin by noting that in these boxplots, the features are arranged from left to right in terms of ascending desirability.

Begin by observing the boxplot for `clarity`. Note that the trend for the outlier cutoffs ($1.5 \times \text{IQR}$) seems to mirror the frequency histogram plot in Figure 2(a). This is somewhat interesting, as this implies that we simply find more expensive diamonds of average clarity, which also have a wider range of prices. Meanwhile, the diamonds with the best clarity seem to have a low cutoff, which could be attributed to the small sample size, but also the fact that these diamonds are also likely to be smaller. This is apparent from Figure 1, where we see that there is a negative coefficient in the case comparing `clarity` with `x`, `y`, and `z`. Note that size of the diamond was established as the best predictor for the price of the diamond from earlier. Meanwhile, it is apparent that the diamond with worst clarity have few that breach the 10000 dollar price mark, as we only see a few individual dots on the boxplot indicating these diamonds.

Now, let us analyze the boxplot for `color`. We see that there is a negative trend for the outlier cut-off as the desirability of the color increases. This To analyze the boxplot for `cut`, we need to also look as the histogram of diamond features in Figure 2(a). Note that we also have increasing numbers of diamonds as we move left to right. We see that the data generally follows our expectation, as the outlier cutoff seems to be higher for each one. However, this changes when the `cut` is Ideal. This makes sense, most of the diamonds are cut ideally, and smaller diamonds are also probably easier to cut well; meanwhile, if a diamond isn't cut very well, but there was some attempt to cut it to some reasonable extent, it was probably very large. This explains why Ideal seems to break the observed trend.

Finally, let us observe the boxplot for `cut`. This plot can be explained with similar explanation to that of `clarity`. In fact,

Question 2.1

Now, before we train our regression models, we begin by splitting our data into training and testing sets. As such, we must now standardize the feature columns. The function used to do this, `scaledTrainTest()`, as well as `scaledTrainTestSplit()` can be found in `utils.py`.

Question 2.2

Next, we begin with feature selection. We note that some of the features may not be useful or may cause overfitting in our models as they do not carry useful information about the variable that we are trying to predict. To tell whether this is the case, we use two metrics: Mutual Information (MI) and F score.

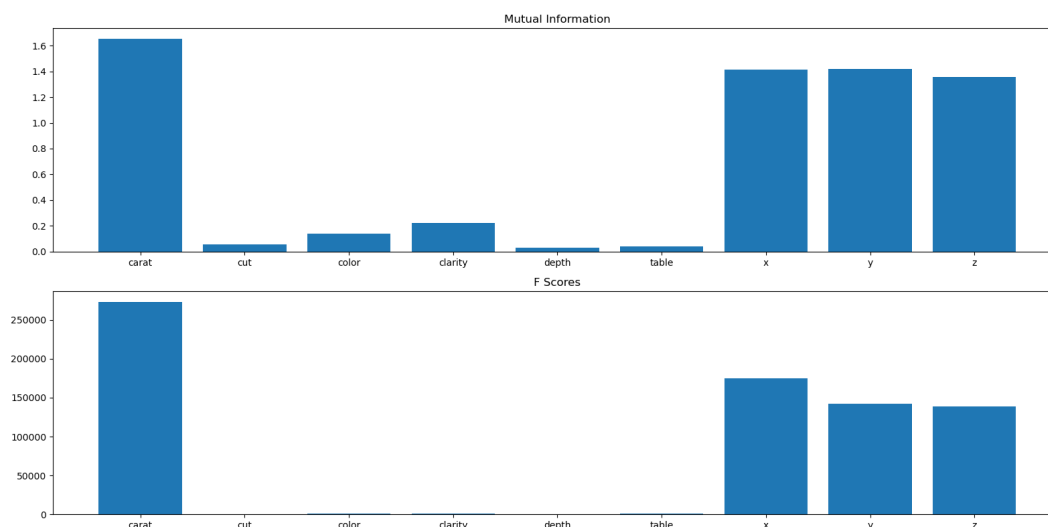


Figure 4: Bar graph of F score and Mutual Information for features

Feature	Mutual Information	F Score
carat	1.64589286853222835	273144
cut	0.058351547792578895	139
color	0.13968295427702282	1465
clarity	0.21672877051000627	1079
depth	0.030486803506200033	5.074
table	0.03818752327438668	802
x	1.4058664238563194	174973
y	1.4172107199595354	142130
z	1.3569258463570115	138947

Table 3: Mutual Information and F Score Values for features

It is clear by observation from Figure 3 and Table 2 that the lowest mutual information is present in **depth** and **table**. It is also important to note that the mutual information in **cut** is also very small. This makes sense as we saw earlier that the Pearson correlation coefficient for **cut** with respect to price per carat was almost zero. Similarly, the Pearson correlation coefficients for **depth** and **table** were very close to zero.

From this point, we will be testing the regression models without these three features, and with these three features and comparing the performance to determine the general performance.

Regression Models

Question 3

For this entire section we perform 10-fold cross validation and then measure the average RSME error for the training and validation sets. For the random forest model we also measure "Out-of-Bag Error" and R^2 score.

To explain OOB error, let us first examine how a Random Forest algorithm with bootstrapping works. If we bootstrap, we sample the training data, and then use this small sample of the training data in order to train a single decision tree model. We can then ensemble many such trees, all trained with different

samples of the original data. OOB error is calculated on the training set, where we calculate the average error of the trees' predictions on data that was not included in its bootstrap sample.

R^2 score is normally used as the coefficient of determination—that is—the proportion of the variation in the labels that can be predicted from the features. For random forests, we compute it as:

$$R^2 = 1 - \frac{\text{MSE}}{\text{Var}(\text{labels})}$$

Note that R^2 for non-linear predictors like random forest can in fact be negative.

Linear Regression

Question 4.1

We begin with a simple regression, least square linear regression. Begin by noting the optimization problem:

$$\underset{\theta}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{Y} - \theta^T \hat{\mathbf{X}}\|^2 \quad (3)$$

Taking the derivative with respect to θ and setting it equal to zero gives us

$$\theta = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \quad (4)$$

Now, we can add regularization terms, beginning with the simple L1 regularization, also known in this case as a Lasso regression. This would make our new optimization problem:

$$\underset{\theta}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{Y} - \theta^T \hat{\mathbf{X}}\|^2 + \alpha \|\theta\| \quad (5)$$

Note that in this case, our learned values for θ would become somewhat sparse as L1 regularization linearly penalizes any non-zero parameters. As such, the gradient for the regularization term does not change until the parameter is zero, which leads to sparsity. However, in this case, as there aren't many terms, we would simple disconsider features that aren't very important.

With L2 regularization, also known as a Ridge regression, we would have:

$$\underset{\theta}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{Y} - \theta^T \hat{\mathbf{X}}\|^2 + \lambda \|\theta\|^2 \quad (6)$$

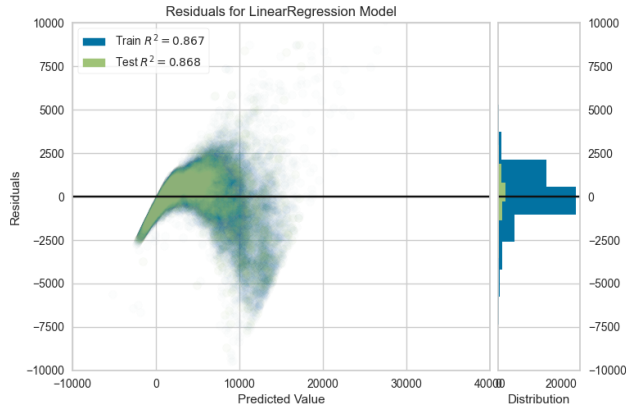
Note in this case, we wouldn't have parameters that are zero; rather, we would have extremely small parameters. This is because the gradient for L2 regularization decreases rapidly as the parameter itself becomes smaller and smaller due to the parabolic nature of the term.

Question 4.2 and 4.3

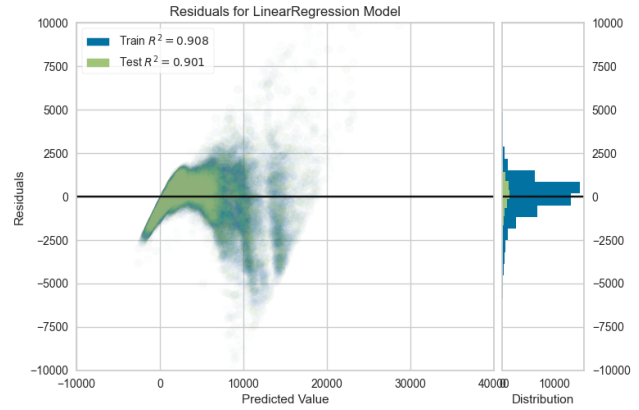
Model	Description	Train RSME	Test RSME
1	Features processed	1434.7215231192772	1443.41152861054185
2	Features unprocessed	1216.495767837737	1217.7987618616985
3	Features processed using $\log(\text{price})$	963.6508209107394	963.0840609301274
4	Features unprocessed using $\log(\text{price})$	1215.167267164955	1292.934288205552

Table 4: Ordinary Least Squares Regression Model

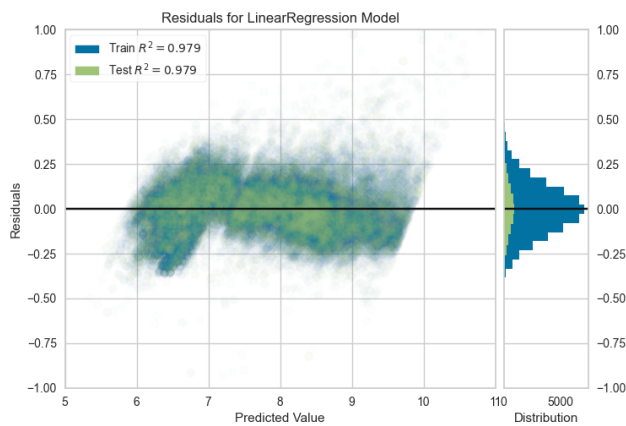
Beginning with ordinary least squares regression, I first varied the number of features available to the model based on mutual information and quickly found that keeping all the features led to the best regression model. This makes sense due to the nature of a linear regression—if a feature isn't very relevant, its associated parameter will be very small—and so for Ridge and Lasso, we also kept all of the features.



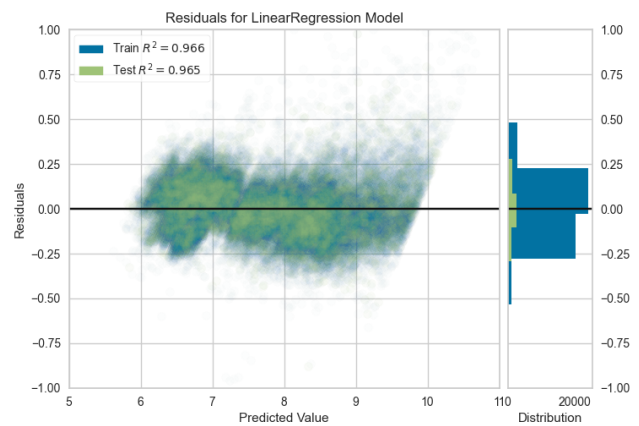
(a) Model 1 Residuals



(b) Model 2 Residuals



(c) Model 3 *log* Residual



(d) Model 4 *log* Residuals

Figure 5: Residual Plots

We then tested the linear regression model with processed data (deskewed as in Question 1.2) and unprocessed data. We noted that the model without processed features seemed to perform much better as shown in Table 4 and visualized in Figure 5. Note that Model 2's residual histogram is distributed far more symmetrically than Model 1, implying that the linear regression fit better in this case. However, we see in both Figures 5(a) and 5(b) that Models 1 and 2 predict many of the prices to be negative.

As such, we decided to test the model by taking the natural logarithm of `price` before fitting the regression. Note in Table 4 that with unprocessed Features, this model performed about the same, but with processed features the RSME decreased very significantly. We also see that our new *log* residual plots seem to follow a linear trend, which makes sense as this implies that the error is increasing as the price of the diamond itself increases. We also note that unlike earlier, Model 3 has normally distributed residuals while Model 4 does not. This is interesting, because this is the opposite of Models 1 and 2; that is, this time, the model with deskewed data has the more normal distribution of residuals.

Next, we test the Lasso Model by iterating through alpha values 10^k such that $k \in \mathbb{Z}$ and $-4 \geq k \leq 1$. We also try both the $\log(\text{price})$ model, and try both with and without deskewing. As seen in Table 5, we see that the best performing model is the same as for ordinary least squares regression, as well as the general trends across the models. The only difference in this case that we see is that leaving the features unprocessed while also taking the $\log(\text{price})$ leads to the error blowing up. We note that this issue persists for all future models referred to in this report as well.

Model	Description	Best Alpha	Best Train RSME	Best Test RSME
1	Features processed	1	1434.8446180295655	1443.270394653097
2	Features unprocessed	1	1216.5716991188874	1217.1322328759766
3	Features processed using $\log(\text{price})$	0.001	953.1890102312589	952.4417958988445
4	Features unprocessed using $\log(\text{price})$	10	4270.277347211739	4270.276711329372

Table 5: Lasso Regression Model

Next we test the Ridge model with all the same parameters are the Lasso model, except we also test whether or not feature standardization is palyng a role in improving the model performance. Note the description column has been left out as it is the same as the previous two models. We see in Table 6 that contrary to our expectations, scaling/standardizing the features did not seem to play a very big roll in improving the model. This was surprising, given how a linear regression is usually sensitive to changes in magnitude (making scaling beneficial).

Model	Standardized	Best Alpha	Best Train RSME	Best Test RSME
1	Yes	10	1434.8513489310335	1442.9008267138393
1	No	10	1435.8556914721148	1442.1066793353307
2	Yes	10	1216.6969576343665	1217.9346926613257
2	No	1	1216.4978665798574	1217.7934651327528
3	Yes	0.001	964.0857752044615	963.5016367407248
3	No	0.0001	963.4272568650325	962.8249050664665
4	Yes	1	1215.16766015031	56321.703744924875
4	No	1	1215.1676667481079	56321.78526878937

Table 6: Ridge Regression Model

Ultimately, we find that our best performing model was Lasso Model 3 with an alpha value of 0.001, as this gave us the lowest RSME of all our linear regression models.

Question 4.4

p -values for different features tell us the chance that a certain parameter is zero—that is, a parameter corresponding to a certain feature is zero. This means that if a p -value for a feature is very small, the feature is also probably not very important to the linear model.

Polynomial Regression

Question 5.1

After creating an array of the polynomial features, we find, unsurprisingly, that `carat` is involved in all of them. However, we never use a higher power of `carat`—rather, we multiply by different powers of

Feature	Mutual Information
<code>carat × clarity</code>	1.8159676557242
<code>carat × clarity²</code>	1.8052014657565039
<code>carat × color²</code>	1.7327044648084868
<code>carat × clarity⁴</code>	1.7102713903040332
<code>carat × color²clarity²</code>	1.6728060460257277

Table 7: Most Salient Polynomial Features

`clarity`, and in one case by `color2`. This is interesting, as earlier it seemed as if all of the categorical features were either not very important, or we made some mistake in assigning ascending natural numbers as values for them. However, we see here that the product is somewhat valuable. This confirms our findings when we analyzed Figure 3 in Question 1.3; we find that keeping `carat` constant, higher values for `clarity` and `color` do in fact increase the price of the diamond. This confirms that the misleading trends were simply due to the rarity of larger diamonds as we have better `clarity` and `color`. Thus, although `carat` is by far the most important singular feature, we find that when used in conjunction, `clarity` and `color` can be interpreted to have some meaning as well.

Interestingly, features like `x`, `y`, and `z` that had high mutual information were not included in the most salient feature terms. I concluded that this was because the information from `x`, `y`, and `z` is encompassed within `carat` and the singular dimension doesn't tell us as much about the diamond as the weight.

Question 5.2

In order to test and find the best polynomial degree, we tested integer values between 2 and 6 inclusive while also testing different alpha values between 10^{-3} and 10^2 for the Ridge regularization. We quickly notice that the higher degree polynomials are almost definitely overfitting, with extremely low training error and extremely high validation error. This makes sense, as higher order polynomials are less generalized in shape, and tend to try to fit the data more "perfectly"—in other words, it's simply a more complicated model. We see that the model is performing much better than the linear regression almost universally, as the best linear model, which involved taking the logarithm of `price` is still worse than the best polynomial model. Note that the best polynomial model was of 5th degree. Similarly note that our alpha constant values are very high, meaning that we've had to add extremely high amounts of regularization to our model because of the overfitting nature of polynomial regression. Note that the non-linear models so far have performed best—including the $\log(\text{price})$ linear regression and now the polynomial regression.

Degree	log vs raw Price	Best Alpha	Training RMSE	Testing RMSE
2	Raw	10	900.3779319488907	932.1444972450224
3	Raw	10	877.2503108198043	973.1487742305775
4	Raw	10	860.7751295043215	1050.162477614935
5	Raw	10	616.7122497398685	904.9899982439823
6	Log	0.001	363.5332636480957	999.3493546367806

Table 8: Polynomial Regression Performance

Neural Network

Question 6.1

We tested three different classes of networks: Wide and Shallow, Wide and Deep, Narrow and Deep. Imperically, from previous experience, Narrow and Deep performs best, but we found that the performance of both deep models were about the same after some tuning of hyperparameters to deal with overfitting in the Wide and Deep Neural Network. Note that we used a batchsize of 200 for all of the models, with learning rate of 0.0001, adam as the optimizer, and RELU as the activation function between layers. We implemented early stopping along with momentum, and for the two deep networks had a inverse scaling learning rate.

Model	Num Layers	Hidden Layer Size	Training Accuracy	Testing Accuracy
Wide and Deep	8	100	567.115903287934	528.0967129827669
Wide and Shallow				
Narrow and Deep				

Table 9: Multilayer Perceptron Performance

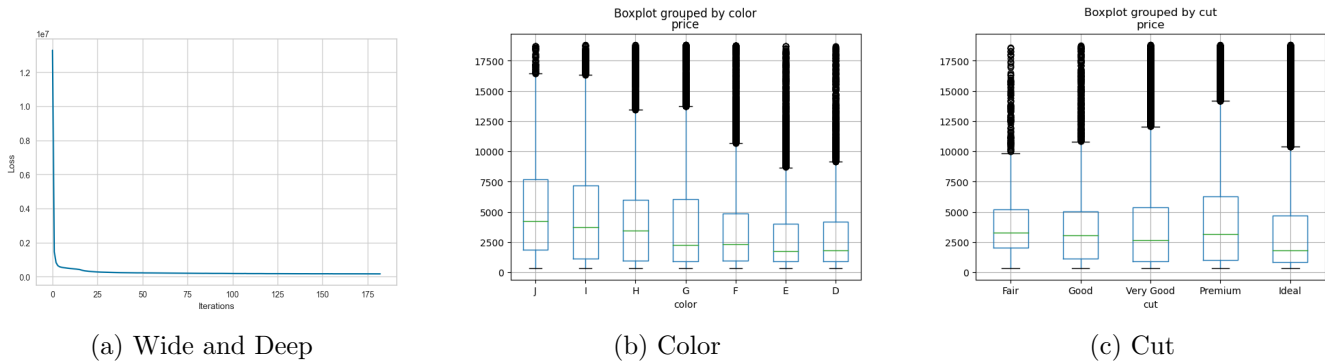


Figure 6: Loss Curves

Question 6.2

The performance is significantly better than the linear regression, although the time to train for even a singular model is almost as long as the entire grid search for linear or Ridge regression. The difference in all of the models used can be found in Table where we have compiled the best models of each type.

Question 6.3

We did not use an activation function for the output from the last fully connected layer. Initially, we were planning on simply taking the output from the fully connected layer as we were just interested in the raw numebrs predicted by the model; however, we realized that it is an obvious assumption that the price must always be positive and as such we decided to try RELU. However, it imperically performed worse, so we simply did not use an activation function.

Question 6.4

If the depth of the network is very high, the obvious risk is of course overfitting. This is simply because we are increasing the number of neurons, so the network becomes more likely to memorize the training data. At this point, the model would not be able to generalize as well. There is also a higher risk of

vanishing or exploding gradients, as they are carried over from one layer onto the next layer. We also face the issue of internal covariate shift, where every hidden layer's input distribution has to change every time a parameter updates in the previous layer leading to extremely slow training that is not possible without good parameter initializations.

Random Forest

We began by noting that increasing the number of trees always increased the overall performance. I did not increase the number of trees beyond 200 because of the time it took to run, but the ensembling nature of having more trees is what leads to better performance. We do not provide justification in ways of a graph for this but rather have our tables at the end of this report to justify this answer. Similarly, we will assume for the following plot that using no function for max features is best.

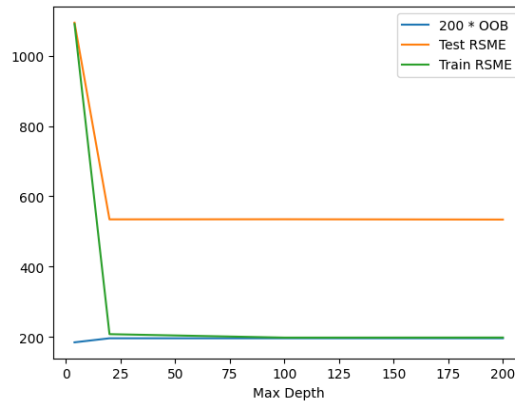


Figure 7: Random Forest Loss vs Max Depth

Max Depth	OOB Error	Test RSME	Train RSME
4	0.9244489827	1093.68057	1090.131115
20	0.9819323954	534.4829574	208.1138089
100	0.9818788398	534.7722537	198.3342015
200	0.9818834686	533.9593106	198.5191772

We thus find that our best model is that of max depth 100, no function for max features, and 200 trees.

Quesiton 7.1

Maximum number of features has a regulariation effect on the model. This is simply because we are considering less features, and disregarding the features that aren't as useful. As such, we have a simpler model and thus setting this maximum number of features for the tree to split on allows for regularization. However, eliminating too many featurers could be harmful to the model as we could simply be eliminating features that are valuable. The number of trees refers to the number of seperate tree models created that are going to be ensembled. The more models we ensemble while also using bootstrapping allows for more regualrization. However, at the same time, we must balance having enough data for the individual trees to actually train on. Lastly, the depth of each tree obviously has a regularization effect on the model, as we are effectively reducing the complexity and "number of neurons" of the model. We can also try to change the depth by adjusting the minimum number of samples needed in order to split into multiple leaves.

Quesiton 7.2

Random forests are essentially combining small piecewise linear decision boundaries at each of its nodes into a larger non-linear structure. Thus, our final decision boundary is somewhat more complex, and can in fact be non-linear. Logically, we see the decision tree itself can overfit any dataset y setting harsher and harsher if-statements, meaning it can perfectly model/overfit any training set.

Question 7.3

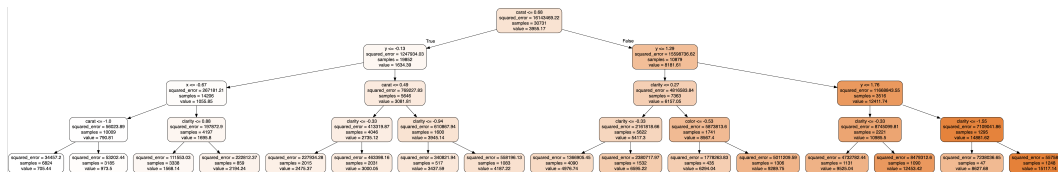


Figure 8: Random 4 depth Tree from Random Forest

We see that the feature selected for branching at the root node is **carat** as expected. We noted earlier that **carat** was the most important feature, as it corresponds to the literal weight and size of the diamond. It also has the highest mutual information with **price** of all the features. It does agree with our earlier findings somewhat. We see that **clarity** and **color** become the most common classifier. This generally makes sense from a human standpoint as it suggests that the model is getting a general ballpark of how much the diamond is worth from its weight and then proceeding to use the finer features to price the diamond. The only exception is the appearance of the **x** node, by note that this too is closely correlated with **carat**. The reason we do not see more is because the information of **x** is mostly encompassed within **carat**, as we simply care about size of the diamond.

Question 7.4

To explain OOB error, let us first examine how a Random Forest algorithm with bootstrapping works. If we bootstrap, we sample the training data, and then use this small sample of the training data in order to train a single decision tree model. We can then ensemble many such trees, all trained with different samples of the original data. OOB error is calculated on the training set, where we calculate the average error of the trees' predictions on data that was not included in its bootstrap sample.

R^2 score is normally used as the coefficient of determination—that is—the proportion of the variation in the labels that can be predicted from the features. For random forests, we compute it as:

$$R^2 = 1 - \frac{\text{MSE}}{\text{Var}(\text{labels})}$$

Note that R^2 for non-linear predictors like random forest can in fact be negative.

LightGBM, CatBoost, and Bayesian Optimization

Question 8.1

The hyperparameters we chose to vary were:

1. `Tree_Learning_Rate` drawn from a uniform distribution between 0.005 and 5
2. `Treee__max_depth` drawn as an integer value between 2 and 32 inclusve

-
3. `tree__min_split_gain` drawn between 0 and 0.3
 4. `tree__n_estimators` drawn as an integer value between 100 and 200 inclusive
 5. `reg_alpha` drawn as an integer value between 0 and 0.1

We of course used `n_jobs` in order to parallelize the task. We used these hyperparameters, as the others did not seem very useful—we included regularization parameters, along with parameters like learning rate and max depth that allow us to make sure the model is actually learning (we don't over regularize).

Question 8.2

Our best model corresponding to the hyperparameters referred to in the previous question used (Note the order will be the same as above):

1. `Tree_Learning_Rate` is 0.356790985277557
2. `Tree__max_depth` is 3
3. `tree__min_split_gain` is 0.11439104645067763
4. `tree__n_estimators` is 200
5. `reg_alpha` is 0.0723842703480234

Note it had RMSE 592.498771288194

Question 8.3

We see that the best performance is provided by

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Max Feature Function	Max Depth	Number of Trees	OOB	Test RSME	Train RSME
Sqrt	4	10	0.888507545	1159.959716	1152.848945
Sqrt		50	0.9171313504	1140.563857	1134.275963
Sqrt		100	0.9191165157	1129.346395	1123.858801
Sqrt		200	0.9188510884	1134.089141	1128.10018
Sqrt	20	10	0.9538068624	574.710234	270.643099
Sqrt		50	0.9801764999	548.0368293	234.7525084
Sqrt		100	0.9810110937	544.337696	229.7962548
Sqrt		200	0.9813714943	541.9969573	227.829509
Sqrt	100	10	0.952074361	584.8709897	251.5979829
Sqrt		50	0.9801804006	548.2237846	209.7595994
Sqrt		100	0.9809620903	543.0336185	204.1539647
Sqrt		200	0.9813119671	540.9774691	201.4067505
Sqrt	200	10	0.9524553607	581.9463059	249.9683452
Sqrt		50	0.9800355171	549.180965	210.5645585
Sqrt		100	0.9808838459	545.553042	204.4457473
log		200	0.9813853014	543.6600276	201.2575916
log	4	10	0.8883054168	1157.457366	1150.956749
log		50	0.917231479	1140.118984	1133.194543
log		100	0.919291226	1129.281357	1122.782338
log		200	0.918920738	1134.014515	1127.519151
log	20	10	0.9527329601	576.6097058	271.1668142
log		50	0.9802277603	545.6922031	234.9126577
log		100	0.9809636018	543.2411822	230.2138979
log		200	0.981371479	541.1313816	227.5167292
log	100	10	0.9508821205	582.2038386	251.3593473
log		50	0.9801277275	547.6444163	209.9927989
log		100	0.9809551574	542.9125848	203.8702072
log		200	0.9813605768	541.0191076	201.3292414
log	200	10	0.9515704197	578.0423422	250.3845501
log		50	0.9801532065	551.3455731	210.0763147
log		100	0.9810080433	544.0830238	203.7966355
log		200	0.9813756034	542.2773565	201.1595134
none	4	10	0.9023035324	1097.538401	1094.664785
none		50	0.9241238739	1093.927796	1090.392225
none		100	0.9244161312	1092.986609	1089.681183
none		200	0.9244489827	1093.68057	1090.131115
none	20	10	0.9564292592	557.9466554	242.4763037
none		50	0.9812088369	537.8696376	214.0872931
none		100	0.9817084472	535.6808118	210.1387262
none		200	0.9819323954	534.4829574	208.1138089
none	100	10	0.9566362724	558.9295058	235.81578
none		50	0.9811235288	537.2029647	204.7660947
none		100	0.9816142316	535.4227102	200.3857282
none		200	0.9818788398	534.7722537	198.3342015
none	200	10	0.956278795	561.0361648	236.9948476
none		50	0.9811670519	540.1592345	205.2858802
none		100	0.9816291442	535.0693099	200.8452532
none		200	0.9818834686	533.9593106	198.5191772