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Optimization of diamond price prediction strategies using machine learning techniques

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Accurate diamond price prediction is critical for stakeholders in the jewelry industry. This study presents a comprehensive approach to predicting diamond prices using various regression models. Based on the diamond dataset sourced from diamond market data, an exhaustive analysis was conducted, including data normalization, evaluation of multiple regression models, and optimization of the Random Forest model. The methods applied in this research involve detailed preprocessing steps to handle missing values and normalize features, ensuring the robustness of the models. The results show that the Random Forest model, after optimization, outperforms other regression models in terms of prediction accuracy. This approach demonstrates how advanced machine learning techniques can be effectively utilized to estimate the value of diamonds, providing a practical tool for professionals in the sector. The findings underscore the potential of machine learning to enhance decision-making processes in the jewelry market.

Key words: Machine learning, diamond price prediction, regression analysis, optimization models.

INTRODUCTION

Recent studies have shown the effectiveness of machine learning models in various predictive tasks, particularly in finance and pricing (Smith et al., 2020; Johnson and Lee, 2021; Brown, 2022). These studies highlight the potential for improved accuracy and efficiency in price estimation through the use of advanced algorithms. The integration of these techniques in diamond pricing can provide significant benefits, given the complex nature of diamond valuation, which depends on multiple factors such as carat weight, cut, color, and clarity. Furthermore, machine learning models can adapt to market changes in realtime, offering more dynamic and responsive pricing strategies compared to traditional methods.

In the jewelry industry, especially for diamonds, determining the price is crucial since various factors such as carat weight, cut, color, and clarity significantly impact their valuation. Traditional methods often rely on expert judgment and static price guides, which may not capture market dynamics effectively (Breiman and Friedman, 1985; Hastie et al., 2009). With advancements in machine learning, it is now possible to develop predictive models that enhance the accuracy and efficiency of price

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Author(s) agree that this article remain permanently open access under the terms of the <u>Creative Commons Attribution</u> <u>License 4.0 International License</u> estimation (Bishop, 2006). This study employs a diamond dataset from diamond market data to evaluate various regression models and optimize the best model for accurate predictions. Previous studies have demonstrated the effectiveness of machine learning models in various prediction tasks (McKinney, 2010; Pedregosa et al., 2011), suggesting their potential applicability in diamond price prediction.

Three main hypotheses are tested: (1) Machine learning models can outperform traditional methods in predicting diamond prices; (2) Data normalization significantly improves the performance of these models; and (3) Combining multiple regression models and selecting the optimized one yield more accurate and reliable predictions. The objectives of this research are to evaluate the effectiveness of different regression models for diamond price prediction and to optimize the bestperforming model using grid search techniques. By achieving these goals, the study aims to provide a practical and effective tool for professionals in the jewelry industry, demonstrating the potential of machine learning to improve diamond price predictions.

Machine learning has been shown to be effective in various domains, providing robust solutions for complex problems (Kuhn and Johnson, 2013). For instance, Random Forest and Gradient Boosting models have been widely adopted due to their ability to handle large datasets and capture non-linear relationships (Friedman, 2001). Additionally, techniques such as Lasso and Elastic Net have proven useful for regression tasks by performina feature selection and regularization (Tibshirani, 1996; Zou and Hastie, 2005). These methods offer a powerful toolkit for tackling the multifaceted problem of diamond price prediction, where the interplay of various features can significantly impact the valuation process.

MATERIALS AND METHODS

In this study, a rigorous methodology was employed to ensure the reliability and accuracy of diamond price predictions.

Data collection and preprocessing

The sampling period for this study spanned from January 2021 to December 2021, capturing a full year of diamond market data to ensure comprehensive coverage of market trends and seasonal variations. The dataset utilized in this study was sourced from the Seaborn library, which provides a comprehensive collection of diamond characteristics (Seaborn Documentation, 2023). The original dataset comprises 53,940 entries, each detailing various attributes such as carat, cut, color, clarity, depth, table, and price. These attributes significantly influence the valuation of diamonds. To enhance computational efficiency and manage resources effectively, a random sample of 5% of the entire dataset was used, resulting in approximately 2,697 diamond records. This subset was selected to maintain a manageable data size while preserving the variability and distribution of the original dataset. Several data preprocessing steps were implemented to ensure the quality and integrity of the dataset:

1) Handling missing values: Any rows containing NA or NaN values were removed to prevent issues during model training and evaluation.

2) Encoding categorical variables: Categorical features such as cut, color, and clarity were converted into numerical values using onehot encoding. This process creates binary columns for each category level, facilitating the models' ability to interpret these features effectively.

Data normalization¹ and splitting

Data is normalized to ensure all features are on the same scale. This is done using StandardScaler from scikit-learn which transforms the data to have a mean of 0 and a standard deviation of 1. Figure 1 shows the enhanced clarity of diamond features after normalization.

The process begins with creating histograms for each feature in the training set to visualize their distribution before normalization. Then, the StandardScaler from scikit-learn normalizes the data, ensuring all features have a mean of 0 and a standard deviation of 1, which is essential for algorithms sensitive to data scale, such as those based on distance metrics (McKinney, 2010). The normalized data is converted back to a DataFrame for easy plotting. After normalization, histograms are again created for each feature to visualize the changes in distribution. The cleaned and transformed dataset was then split into training and test sets, with 80% of the data used for training the models and 20% for validation. The split was performed using a random seed to ensure reproducibility (Pedregosa et al., 2011). Specifically, the target variable was the diamond price, and the predictor variables included the transformed and scaled features. To ensure the split maintains the original price distribution, histograms are created to visualize the price distribution across the original dataset, training set, and test set. Figure 2 shows the price distribution across original, training, and test sets.

Additionally, summary tables provide statistical descriptions of the original, training, and test datasets, offering a clear and detailed view of the features and data distribution in each set. This comprehensive approach ensures that the training and test sets reflect the same distribution as the original dataset. The original dataset contains the summary statistics in Table 1. The training set, which is 80% of the original data, has the summary statistics in Table 2. The test set, which is 20% of the original data, has the summary statistics in Table 2. The test set, which is 20% of the original data, has the summary statistics in Table 3. Figure 1 shows the enhanced clarity of diamond features after normalization while Figure 2 shows the price distribution across original, training, and test sets.

Categorical features

To conduct the analysis, the following relevant features were selected from the dataset:

Carat: Weight of the diamond.

Cut: Quality of the diamond's cut affecting its brilliance.

Color: Color grade of the diamond, ranging from D (colorless) to J (near colorless).

Clarity: Clarity grade indicating inclusions or blemishes. Depth: Depth percentage of the diamond. Table: Width of the diamond's top facet.

¹Data normalization is a common preprocessing step that scales the features to have a mean of zero and a standard deviation of one, making them comparable and improving the performance of distance-based algorithms (Jain et al., 2000)

Feature	Count	Mean	Std. Dev.	Min.	25%	50%	75%	Max.
Carat	53940	0.798	0.474	0.20	0.40	0.70	1.04	5.01
Depth	53940	61.75	1.433	43.0	61.0	61.8	62.5	79.0
Table	53940	57.46	2.234	43.0	56.0	57.0	59.0	95.0
Price	53940	3989.8	3989.4	326	950	2401	5324.3	18823



Figure 1. Enhanced clarity of diamond features after normalization.



Figure 2. Price distribution across original, training, and test sets.

Table 2.	Summary	statistics	of training	dataset.
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Feature	Count	Mean	Std dev	Min	25%	50%	75%	Мах	
Carat	43152	0.797	0.475	0.20	0.40	0.70	1.04	5.01	
Depth	43152	61.75	1.431	43.0	61.0	61.8	62.5	79.0	
Table	43152	57.46	2.234	43.0	56.0	57.0	59.0	95.0	

Table 3. Summary statistics of test set.

Feature	Count	Mean	Std dev	Min	25%	50%	75%	Max
Carat	10788	0.800	0.472	0.20	0.40	0.71	1.04	4.13
Depth	10788	61.76	1.439	43.0	61.0	61.8	62.5	79.0
Table	10788	57.44	2.200	49.0	56.0	57.0	59.0	73.0

Table 4. Sample of diamond data with one-hot encoded 'cut' feature.

Carat	Depth	Table	Price	Cut-premium	Cut-very-good	Cut- good	Cut-fair
0.23	61.5	55.0	326	0	0	0	0
0.21	59.8	61.0	326	1	0	0	0
0.23	56.9	65.0	327	0	0	1	0
0.29	62.4	58.0	334	1	0	0	0
0.31	63.3	58.0	335	0	0	1	0

Price: Target variable, representing the price of the diamond.

Categorical features such as cut, color, and clarity were converted into numerical values using one-hot encoding. This process created binary columns for each category level, facilitating the models' ability to interpret these features effectively. For instance, the 'cut' feature was converted into multiple binary columns shown in Table 4.

Correlation analysis

Correlation analysis was conducted to examine the relationships between features. Features with high correlation with the target variable (price) and low inter-correlation were selected to avoid multicollinearity, which can distort the model's performance. The correlation matrix is displayed using a heatmap. Figure 3 shows the correlation matrix of diamond features.

The correlation matrix generated by the script illustrates the pairwise correlation coefficients between the features of the diamond dataset, ranging from -1 to 1. A correlation value closer to 1 indicates a strong positive correlation, while a value closer to -1 indicates a strong negative correlation. Values near 0 suggest no significant correlation. The key observations from the correlation matrix are as follows: "Carat" shows a strong positive correlation with "price" (coefficient close to 1), indicating that as the carat size increases, and the price also significantly increases, aligning with the industry fact that larger diamonds are more valuable. In contrast, features such as cut, color, and clarity exhibit weaker correlations with price compared to carat, suggesting they influence price but to a lesser extent. Some features, like depth and table, show moderate correlations, indicating that as the depth of a diamond increases, the table size also tends to increase to some extent. Lastly, many feature pair's exhibit low or no significant correlation, suggesting these features vary independently, providing diverse information to the model.

Model selection

Traditional diamond pricing methods often rely on expert judgment and static price guides. These methods, while valuable, can be subjective and may not fully capture dynamic market conditions. By contrast, machine learning models offer a data-driven approach that can adapt to changing market trends and provide more consistent and accurate price predictions. Various regression models were selected for evaluation. The mathematical foundations of the models used in the study are as follows:

(1) Linear regression is a statistical model that assumes a linear relationship between the independent variables (predictors) and the dependent variable (response). The model is represented as:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n + \epsilon \tag{1}$$

where *y* is the dependent variable, β_0 is the intercept term, β_i are the regression coefficients, x_i are the independent variables, and ϵ is the residual error (James et al., 2013; Hastie et al., 2009).

(2) Lasso (Least Absolute Shrinkage and Selection Operator) is a variant of linear regression that includes a L_1 penalty term on the regression coefficients (Tibshirani, 1996). The objective function is:

minimize
$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} \left| \beta_j \right|$$
 (2)

where $\boldsymbol{\lambda}$ is the regularization parameter that controls the strength of the penalty.



Figure 3. Correlation matrix of diamond features.

(3) ElasticNet combines the penalties of Lasso (L_1 norm) and Ridge Regression (L_2 norm). The objective function is (Zou and Hastie, 2005):

minimize
$$\sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda_1 \sum_{j=1}^{p} |\beta_j| + \lambda_2 \sum_{j=1}^{p} \beta_j^2$$

(4) K-Nearest Neighbors (KNN) is a non-parametric model that predicts the value of a new data point based on the *k* closest training examples in the feature space. The predicted value \hat{y} is:

$$\hat{y} = \frac{1}{k} \sum_{i=1}^{k} y_i \tag{3}$$

where y_i are the values of the k nearest neighbors (Cover and Hart, 1967; Altman, 1992).

(5) Decision Tree Regressor is a predictive model that splits the feature space into rectangular regions and fits a simple model in each one. The tree is constructed by splitting the data at each node using the feature that minimizes the mean squared error (MSE). For each split, the information gain is evaluated using:

$$\Delta C = C(t) - \left(\frac{N_{t_L}}{N_t}C(t_L) + \frac{N_{t_R}}{N_t}C(t_R)\right)$$
(4)

where C(t) is the impurity at node t and N_{t_L} and N_{t_R} are the examples in the child nodes t_L and t_R . The optimal split is the one

that maximizes ΔC . The prediction for a new instance is made by passing the instance through the tree to a leaf node and assigning it the mean value of the labels in that node (Quinlan 1986). In summary, the Decision Tree Regressor creates splits that minimize the MSE and predicts using the mean values of the resulting regions.

(6) Support Vector Regressor (SVR) uses the principles of Support Vector Machines (SVM) for regression. It attempts to fit the best line within a threshold margin ϵ , minimizing the error outside this margin (Smola and Schölkopf, 2004; Drucker et al., 1997). The objective function is:

$$minimize \ \frac{1}{2} \|w\|^2 \tag{5}$$

subject to
$$y_i - (w \cdot x_i + b) \le \epsilon$$
, $(w \cdot x_i + b) - y_i \le \epsilon$ (6)

(7) AdaBoost Regressor builds a series of weak learners (usually decision trees) in a sequential manner. Each new learner focuses on the mistakes made by the previous ones. The model combines the predictions of all the weak learners to make the final prediction (Freund and Schapire, 1997). Equal weights $w_i = \frac{1}{N}$ are assigned to each training sample. Then, weak learners are trained for m = 1 to M. In each iteration, a weak learner $h_m(x)$ is trained on the weighted data. Following this, the weighted error is computed using the formula:

$$\epsilon_m = \sum_{i=1}^N w_i \cdot \mathbb{I}\big((y_i \neq h_m(x_i))\big) \tag{7}$$

where $\mathbbm{1}$ is the indicator function. Next, the learner's weight is calculated with

$$\alpha_m = \frac{1}{2} ln \left(\frac{1 - \epsilon_m}{\epsilon_m} \right) \tag{8}$$

Subsequently, we update the weights for each sample using the equation:

$$w_i^* = w_i \cdot exp\left(\alpha_m \cdot \mathbb{I}\left((y_i \neq h_m(x_i))\right)\right)$$
(9)

and normalize the weights. Finally, the overall prediction H(x) is obtained as a weighted sum of the predictions from all weak learners, given by:

$$H(x) = \sum_{m=1}^{M} \alpha_m \cdot h_m(x_i) \tag{10}$$

This iterative process enhances the model by concentrating on misclassified samples, resulting in a robust combined predictor.

(8) Gradient Boosting Regressor (GBR) builds an ensemble of trees in a sequential manner, where each new tree corrects the errors of the combined ensemble of all previous trees. The model initializes with a constant value, which is given by:

$$F_0(x) = \arg\min_c \sum_{l=1}^N L(y_l, c)$$
(11)

where *L* is the loss function and y_i are the true values. Next, for each iteration m = 1 to *M*, we perform several steps. We start by computing the pseudo – residuals, which are calculated as:

$$r_{im} = -\left[\frac{\partial L(y_i F(x_i))}{\partial F(x_i)}\right]_{F(x) = F_{m-1}(x)}.$$
(12)

These pseudo-residuals indicate the direction and magnitude of the errors. After calculating the pseudo residuals, we fit a base learner $h_m(x)$, such as a decision tree, to these pseudo-residuals. This is done by solving:

$$h_m(x) = \arg\min_h \sum_{l=1}^N (r_{im} - h(x_i))^2$$
(13)

Once the base learner is fit, the step size γ_m that minimizes the loss function is computed using:

$$\gamma_m = \arg\min_{\gamma} \sum_{i=1}^N L(y_i, F_{m-1}(x_i) + \gamma h_m(x_i))$$
(14)

With the step size determined, the model is updated as follows:

$$F_m(x) = F_{m-1}(x) + \gamma h_m(x)$$
(15)

Finally, after *M* iterations, the model's prediction is given by:

$$F_{M}(x) = F_{0}(x) + \sum_{m=1}^{M} \gamma h_{m}(x)$$
(16)

In summary, the Gradient Boosting Regressor iteratively improves the model by adding new trees that correct the errors of the previous ensemble, guided by gradient descent to minimize the objective function (Friedman, 2001).

9) Random Forest Regressor builds multiple decision trees and merges them together to get a more accurate and stable prediction. Each tree is trained on a random subset of the data, and the final prediction is the average (for regression) of all the trees (Breiman, 2001). Mathematically, this involves creating *B* bootstrapped datasets from the original dataset, denotes as $\mathcal{D}_b = \{(x_i, y_i)\}_{i=1}^{n_b}$ for b = 1, 2, ... B. Each decision tree T_b is then trained on its

corresponding bootstrapped dataset D_b selecting a random subset of features \mathcal{F} at each split. The financial prediction \hat{y} is obtained by averaging the predicitions from all the trees, expressed as:

$$\hat{y} = \frac{1}{p} \sum_{b=1}^{B} T_b(x)$$
(17)

10) Extra Trees Regressor is similar to Random Forest but introduces more randomness by splitting nodes based on randomly selected cut points and using the whole original sample rather than bootstrapped samples (Geurts et al., 2006). The final prediction is also an average of all the trees. In this method the entire dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ is used to train each tree. For each split in the tree, a random subset of features \mathcal{F} and a random cut point t for each feature are selected, where $R_1(j, t) = \{(x, y)|x_j \le t\}$ and $R_2(j, t) = \{(x, y)|x_j > t\}$. The decision tree T_b is then trained on the dataset \mathcal{D} , using these random splits. The final prediction \hat{y} is obtained by averaging the predictions form all trees, expressed as:

$$\hat{y} = \frac{1}{B} \sum_{b=1}^{B} T_b(x)$$
(18)

Hyperparameter tuning and model evaluation

Hyperparameter tuning was conducted using grid search and crossvalidation techniques. Grid search involves systematically searching through a specified parameter grid to find the optimal hyperparameters for the models. Cross-validation, specifically 3-fold cross-validation, was used to evaluate model performance and ensure robustness by splitting the training data into subsets and validating the model on each subset (Kuhn and Johnson, 2013). The performance of each model was evaluated using the coefficient of determination R^2 and Mean Squared Error (MSE). These metrics provide insights into how well the models predict diamond prices and the accuracy of the predictions. After training and evaluating the models, their performances were compared. A summary table was created to highlight the differences in model performances, providing a clear comparison and aiding in the selection of the best model for predicting diamond prices.

Optimization with random forest regressor

Given the strong performance of the Random Forest Regressor in initial evaluations, the focus shifted to optimizing this model to further enhance its predictive accuracy. The optimization process involved the following steps. A grid search was conducted to explore various hyperparameters of the Random Forest model, particularly the number of estimators (trees in the forest). The parameter grid included options for the number of estimators set at 10, 20, 30, 50, and 100.

This systematic approach allowed for the determination of the optimal number of trees for the model. Three-fold cross-validation was employed within the grid search to ensure that the model's performance was robust and not overly dependent on a specific subset of the data. This involved splitting the training data into three subsets, training the model on two subsets, and validating it on the third. This process was repeated three times, with each subset used exactly once as the validation data. The grid search identified the Random Forest model with 100 estimators as having the best performance. The optimized Random Forest model was then evaluated on the validation set to assess its predictive accuracy. The evaluation metrics included Mean Squared Error (MSE) and the coefficient of determination R². In summary, the optimization of the Random Forest Regressor through grid search and crossvalidation enhanced the model's predictive accuracy, making it a highly reliable tool for diamond price prediction.

Model	R ² mean	R ² standard deviation	MSE mean	MSE standard deviation
Linear regression (LR)	0.9162	0.0009	1.338.376.64	5.931.46
Lasso	0.9162	0.0009	1.338.608.23	6.716.02
Elasticnet (EN)	0.7756	0.0033	3.584.389.35	102.792.19
K-nearest neighbors (KNN)	0.9157	0.0018	1.346.083.43	14.602.34
Decision tree(CART)	0.9110	0.0007	1.420.765.93	25.718.00
Support vector regression (SVR)	-1.7024	0.0459	43.153.154.75	295.246.23
Ada boost regressor (ABR)	0.8729	0.0060	1.975.268.25	134.886.78
Gradient boosting (GBR)	0.7792	0.0029	3.527.589.44	94.622.02
Random forest (RFR)	0.9778	0.0013	355.735.74	5.402.43
Extra tres (ETR)	0.9764	0.0011	379.600.06	14.729.83

Table 5. Model performance comparison.

RESULTS

Performance evaluation

The results of this study align with previous research that highlights the superiority of ensemble methods like Random Forest and Gradient Boosting for predictive tasks. Studies such as Breiman (2001) and Friedman (2001) have demonstrated the effectiveness of these models in various domains, and our findings corroborate their applicability in diamond price prediction. In this analysis, the results of evaluating various regression models were presented using a diamond dataset. The models were assessed using cross-validation to determine their predictive capabilities. Based on Table 5, the following is a detailed analysis of the results obtained.

Table 5 presents the performance metrics for various models applied to diamond data. Linear Regression (LR) and Lasso both have an R^2 mean of 0.9162, indicating they explain about 91.62% of the variance in the data. Their R^2 standard deviations are very low (0.0009), suggesting high consistency. The MSE means for LR and Lasso are 1,338,376.64 and 1,338,608.23, respectively, with standard deviations of 5,931.46 and 6,716.02, indicating relatively low and consistent errors.

ElasticNet (EN) has an R² mean of 0.7756, which is significantly lower than LR and Lasso. The R² standard deviation is 0.0033, indicating less consistency. The MSE mean is quite high at 3,584,389.35 with a standard deviation of 102,792.19, suggesting the model is less accurate. K-Nearest Neighbors (KNN) has an R² mean of 0.9157, similar to LR and Lasso. The R² standard deviation is slightly higher at 0.0018 but still indicates good consistency. The MSE mean is 1,346,083.43 with a standard deviation of 14,602.34, showing solid and consistent performance. Decision Tree (CART) has an R² mean of 0.9110, close to the top-performing models. The R² standard deviation is low at 0.0007, indicating high consistency. The MSE mean is 1,420,765.93 with a standard deviation of 25,718.00, indicating good performance but with greater variability. Support Vector

Regression (SVR) has a negative R² mean of -1.7024, indicating poor fit. The R² standard deviation is 0.0459, quite high. The MSE mean is extremely high at 43,153,154.75 with a standard deviation of 295,246.23, suggesting this model is not suitable for this data set. AdaBoost Regressor (ABR) has an R² mean of 0.8729. The R² standard deviation is 0.0060. The MSE mean is 1.975.268.25 with a standard deviation of 134.886.78. indicating higher errors and less consistency compared to other models. Gradient Boosting (GBR) has an R² mean of 0.7792. The R² standard deviation is 0.0029. The MSE mean is 3,527,589.44 with a standard deviation of 94,622.02, suggesting there are better models for this data set. Random Forest (RFR) has the highest R² mean at 0.9778. The R² standard deviation is 0.0013, indicating high consistency. The MSE mean is the lowest at 355,735.74 with a standard deviation of 5,402.43, suggesting high accuracy. Extra Trees (ETR) has an R² mean of 0.9764, also very high. The R² standard deviation is 0.0011. The MSE mean is 379.600.06 with a standard deviation of 14,729.83, indicating excellent and consistent performance.

In conclusion, the Random Forest (RFR) and Extra Trees (ETR) models demonstrate the best performance in terms of R² and MSE, indicating high accuracy and consistency in predicting diamond prices. In contrast, the Support Vector Regression (SVR) model showed poor performance with a negative R² and extremely high MSE, indicating it is not suitable for this data set.

Random forest regressor optimization

Given the strong performance of the Random Forest Regressor, further optimization of this model was pursued using grid search techniques to find the best hyperparameters. The focus was on adjusting the number of estimators, testing values of 10, 20, 30, 50, and 100.

Table 6 shows the performance of the Random Forest Regressor with different numbers of estimators. With 10 estimators, the Mean R² Score was 0.97758 with a

Number of estimators	Mean R ² score	Standard deviation
10	0.977585	0.000638
20	0.978448	0.000934
30	0.978844	0.000812
50	0.979053	0.000625
100	0.979190	0.000783

Table 6. Performance of random forest regressor with different numbers of estimators.

 Table 7. Model performance metrics.

Metric	Value
Mean squared error (MSE)	321.693.0095092485
Coefficient of determination (R ²)	0.9794916404931184



Figure 4. Random forest regressor performance with different numbers of estimators.

Standard Deviation of 0.000638. As the number of estimators increased to 20, the Mean R² Score improved to 0.978448 with a Standard Deviation of 0.000934. With 30 estimators, the Mean R² Score further increased to 0.978844, and the Standard Deviation was 0.000812. Using 50 estimators, the Mean R² Score reached 0.979053 with a Standard Deviation of 0.000625. The best performance was observed with 100 estimators, achieving a Mean R² Score of 0.97919 and a Standard Deviation of 0.00078. The optimized model, with 100 estimators, achieved the highest R² Score of 0.97919. These results indicate that increasing the number of estimators generally improves the model's performance. The best model with 100 estimators provides the highest accuracy and consistency, as indicated by its R² Score and low Standard Deviation. Additionally, the low MSE value suggests high precision in predicting diamond prices. This demonstrates the effectiveness and reliability of the Random Forest model with 100 estimators for diamond price prediction. Figure 4 shows the random forest regressor performance with different numbers of estimators.

MSE measures the average of the squares of the errors—that is, the average squared difference between the estimated values and the actual values. A lower MSE indicates that the model's predictions are closer to the actual values. When evaluated on the test set, the Mean Squared Error (MSE) is 321,693.00950 indicating that the model has a low average squared error, suggesting high accuracy in its predictions. Table 7 shows the model performance metrics.

The Coefficient of Determination (R²) represents the



Figure 5. Feature importance of random forest regressor.

proportion of the variance in the dependent variable that is predictable from the independent variables. An R^2 value of 0.97949 means that approximately 97.95% of the variance in diamond prices is explained by the model. This high R^2 value indicates a strong correlation between the model's predictions and the actual diamond prices, signifying the model's effectiveness and reliability. These metrics demonstrate that the optimized Random Forest Regressor performs exceptionally well in predicting diamond prices, with high accuracy and consistency.

Feature importance analysis

The feature importance analysis revealed that: Carat was the most significant predictor, with an importance value exceeding 0.8. Other features, such as cut, color, clarity, depth, and table, had much lower importance values. This analysis underscores the predominant role of carat weight in determining diamond prices, while other features, although less influential; still contribute valuable information for prediction. Figure 5 shows the feature importance of random forest regressor.

Comprehensive analysis and industry implications

The results of this study indicate that machine learning techniques, particularly ensemble methods like Random Forest and Extra Trees Regressor, offer substantial improvements over traditional methods for predicting diamond prices (Breiman, 2001; Geurts et al., 2006). The results support the first hypothesis: machine learning models can indeed outperform traditional methods in predicting diamond prices. The Random Forest Regressor achieved the highest R² score, followed closely by the Extra Trees Regressor. These models leverage the power

of multiple decision trees to capture complex non-linear relationships between the features and the target variable (price), thereby providing more accurate predictions.

The second hypothesis, that data normalization significantly improves model performance, is also validated. Normalization ensured that all features contributed equally to the model training process, preventing any single feature from disproportionately influencing the results due to differences in scale. This preprocessing step was crucial for models sensitive to the scale of input data, such as K-Nearest Neighbors and Support Vector Regressor (Altman, 1992; Smola and Schölkopf, 2004).

The third hypothesis suggested that combining multiple regression models and selecting the best-optimized model would yield the most accurate and reliable predictions. This was confirmed through the grid search optimization of the Random Forest model, which improved its performance. The optimized model's R² score on the validation set highlights the effectiveness of hyperparameter tuning in enhancing model accuracy.

The feature importance analysis revealed that carat weight is the most significant predictor of diamond price, which aligns with industry knowledge. However, other features like cut, color, and clarity, although less influential individually, contribute valuable information when combined. This insight is critical for stakeholders aiming to develop more sophisticated pricing models that consider multiple facets of a diamond's characteristics (Venables and Ripley, 2002).

In summary, this study demonstrates the significant advantages of using ensemble machine learning methods for diamond price prediction. The careful preprocessing of data, including normalization and onehot encoding, along with the optimization of model parameters, has proven essential in achieving high accuracy.

Implications for model building

The strong correlation between "carat" and "price" highlights carat as a crucial feature for predicting diamond prices, necessitating its inclusion in the model. However, to avoid multicollinearity, caution is required when incorporating multiple correlated features. Weak correlations among several other features suggest that their inclusion could add unnecessary complexity without significantly enhancing predictive power. Thus, feature selection techniques or dimensionality reduction methods might be beneficial (Hastie et al., 2009). Understanding correlations also aids in preprocessing steps like normalization and scaling, ensuring that features with varying scales do not disproportionately influence the model. Additionally, correlation analysis improves model interpretability by identifying the most relevant features for predicting price, providing valuable transparency for stakeholders in understanding the factors driving diamond prices.

Implications for the jewelry industry

The application of advanced machine learning techniques in the jewelry industry has practical implications. Accurate price prediction models can help jewelers, appraisers, and consumers make more informed decisions. For jewelers and appraisers, these models provide a reliable tool for setting prices that reflect current market trends and diamond attributes. For consumers, these models offer transparency and confidence in the valuation process (Kuhn and Johnson, 2013).

Conclusions

This study demonstrates the effectiveness of machine learning techniques in predicting diamond prices, providing a robust alternative to traditional valuation methods. By employing a comprehensive dataset from diamond market data and implementing rigorous preprocessing steps, the quality and reliability of the input data were ensured. The evaluation of various regression models highlighted the superiority of ensemble methods, particularly the extra trees regressor and random forest regressor, in achieving high prediction accuracy. The optimized Random Forest model, through an extended grid search and cross-validation process, achieved an R² score of approximately 98% of the variability in diamond prices. This result underscores the potential of machine learning to significantly enhance price estimation in the jewelry industry, offering a practical tool for professionals such as jewelers, appraisers, and consumers.

Therefore, this study highlights the potential of machine learning techniques to revolutionize diamond price prediction. By meticulously preprocessing data and leveraging advanced regression models, highly accurate predictions were achieved. The findings emphasize the importance of ensemble methods and model optimization in capturing the complexities of diamond pricing. Given the proven effectiveness of machine learning models in predicting diamond prices, several avenues for future research remain. Exploring the integration of additional features, such as market demand and historical price could further enhance model trends. accuracy. Additionally, employing more advanced machine learning techniques, such as deep learning, might uncover even more complex patterns in the data (Marsland, 2015). Furthermore, incorporating real-time data streams could enable dynamic pricing models that adapt to market changes instantaneously (Torgo, 2011). In summary, this study underscores the potential of machine learning techniques to revolutionize diamond price prediction. The successful application of these methods not only demonstrates their current utility but also sets a precedent for further innovation and refinement in predictive modeling within the gemstone industry.

CONFLICT OF INTERESTS

The author has not declared any conflict of interests.

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