

## Machine Learning Assignment-5

**Ans1** - R-squared ( $R^2$ ) is a statistical measure that represents the proportion of variance in the dependent variable that is explained by the independent variables in the model. It ranges between 0 and 1, with higher values indicating a better fit. An  $R^2$  value closer to 1 implies that a larger proportion of the variance in the dependent variable is explained by the independent variables, suggesting a better fit of the model.

On the other hand, Residual Sum of Squares (RSS) is the sum of the squared differences between the observed values and the predicted values by the regression model. It quantifies the total amount of unexplained variance or errors in the model. Lower values of RSS indicate a better fit, as they represent smaller differences between the observed and predicted values.

Comparing the two:

**Interpretation:** R-squared provides an overall measure of how well the independent variables explain the variance in the dependent variable, while RSS quantifies the magnitude of errors or residuals in the model.

**Relative Assessment:** R-squared is more useful for comparing different models as it standardizes the measure of goodness of fit, enabling a comparison of how much variance is explained across different models. RSS, however, doesn't allow direct comparisons between models unless they have the same number of observations.

**Contextual Understanding:** R-squared might overstate the goodness of fit when more independent variables are added to the model, even if they don't significantly improve the model's predictive power. In contrast, RSS directly measures the model's error, making it more straightforward for understanding the magnitude of errors but doesn't necessarily convey how much variance is explained.

Ultimately, the choice between R-squared and RSS depends on the context and the purpose of the analysis. R-squared is commonly used for model comparison and to understand the proportion of variance explained, while RSS is helpful for understanding the absolute magnitude of errors in the model. It's often recommended to consider both metrics along with other evaluation techniques to comprehensively assess a regression model's performance.

**Ans2-** In regression analysis, TSS (Total Sum of Squares), ESS (Explained Sum of Squares), and RSS (Residual Sum of Squares) are metrics used to quantify the variance and goodness of fit of a regression model. Here's a brief explanation of each metric and the equation relating them:

1. TSS (Total Sum of Squares): TSS represents the total variability or dispersion in the dependent variable (the variable being predicted) around its mean. It measures the total

deviation of each data point from the mean of the dependent variable. TSS can be calculated as the sum of the squared differences between each data point and the mean of the dependent variable.

2. ESS (Explained Sum of Squares): ESS represents the variability or dispersion in the dependent variable explained by the regression model. It measures the deviation of each predicted value from the mean of the dependent variable. ESS can be calculated as the sum of the squared differences between each predicted value and the mean of the dependent variable.
3. RSS (Residual Sum of Squares): RSS represents the remaining variability or dispersion in the dependent variable that is not explained by the regression model. It measures the deviation of each observed value from its corresponding predicted value. RSS can be calculated as the sum of the squared differences between each observed value and its corresponding predicted value.

The equation relating these three metrics is :

This equation highlights that the total sum of squares (TSS) can be decomposed into the sum of the explained sum of squares (ESS), which represents the variability explained by the model, and the residual sum of squares (RSS), which represents the unexplained or residual variability. In other words, TSS measures the total variability in the dependent variable, which can be partitioned into the variability explained by the model (ESS) and the remaining unexplained variability (RSS).

**Ans 3** - Regularization in machine learning is a technique used to prevent overfitting and improve the generalization ability of a model. Overfitting occurs when a machine learning model captures noise from the training data and performs well on the training set but fails to generalize to new, unseen data.

The key need for regularization arises due to the following reasons:

1- Preventing Overfitting: When a model is excessively complex or has too many parameters relative to the amount of training data available, it can start memorizing the noise or specific patterns in the training data that may not be relevant for making predictions on new data. Regularization techniques help to control the model complexity and reduce overfitting by penalizing overly complex models.

2- Improving Generalization: Regularization techniques encourage the model to learn simpler patterns in the data by imposing constraints on the model parameters. This helps the model generalize better to unseen data by focusing on the more important underlying patterns rather than fitting the noise in the training data.

3- Handling Multicollinearity: In regression problems with highly correlated features, regularization methods like Lasso (L1 regularization) or Ridge (L2 regularization) can help in

handling multicollinearity by shrinking the coefficients of less important features or eliminating some features entirely.

4- Controlling Model Complexity: Regularization acts as a way to control the complexity of the model, preventing it from becoming too flexible and ensuring that it doesn't capture noise, outliers, or irrelevant details in the training data.

Common regularization techniques in machine learning include:

- a) L1 Regularization (Lasso): It adds a penalty term proportional to the absolute value of the coefficients, encouraging sparsity and feature selection by driving some coefficients to exactly zero.
- b) L2 Regularization (Ridge): It adds a penalty term proportional to the squared magnitude of the coefficients, preventing large coefficient values and reducing the impact of less influential features.
- c) Elastic Net: Combines L1 and L2 regularization to leverage the benefits of both techniques.
- d) Dropout(for Neural Networks): In neural networks, dropout regularization randomly drops neurons during training to prevent over-reliance on specific neurons or features.

Regularization helps to strike a balance between bias and variance, leading to more robust and generalized models that perform better on unseen data, which is crucial for real-world applications in machine learning.

**Ans4-** Gini-Impurity is a measurement used to build Decision Trees to determine how the features of a dataset should split nodes to form the tree. More precisely, the Gini impurity of a dataset is a number between 0-0.5, which indicates the likelihood of new, random data being misclassified if it were given a random class label according to the class distribution in the dataset.

**Ans5-** Decision trees have a tendency to overfit to the training set because they can keep growing deeper and more complex until they perfectly classify the training data. This can lead to the tree capturing noise in the data, rather than the underlying relationships, and thus performing poorly on new, unseen data. Regularization techniques such as pruning, setting a minimum number of samples required to split a node, or limiting the maximum depth of the tree can help mitigate overfitting in decision trees. Regularization techniques aim to simplify the tree and prevent it from becoming overly complex, thus improving its ability to generalize to new data.

Yes, unregularized decision trees can be prone to overfitting. The primary reason is that decision trees have the capacity to grow deep and complex, allowing them to perfectly fit the training data. Without any form of regularization, the tree can keep splitting nodes until each

training sample is assigned to its own leaf node, resulting in a highly specialized model that captures noise and inconsistencies in the data.

Decision trees make splits based on the available features and try to minimize impurity or maximize information gain at each step. If the tree is allowed to grow without any constraints, it may start to memorize the training data, including its noise and outliers, rather than learning the underlying general patterns.

This overfitting phenomenon occurs because the decision tree becomes too specific to the training set and fails to generalize well to new, unseen data. As a result, when the model encounters new samples during testing or deployment, it may struggle to make accurate predictions.

To address this issue, various regularization techniques are employed, such as pruning, setting minimum sample requirements for node splitting, or limiting the maximum depth of the tree. These techniques aim to simplify the tree structure, prevent it from becoming overly complex, and promote better generalization to unseen data.

**Ans6-** Ensemble techniques in machine learning involve combining multiple individual models to create a more robust and accurate predictive model. The idea behind ensembling is to leverage the collective wisdom and diverse perspectives of multiple models to improve overall performance.

There are two main types of ensemble techniques:

1. **Bagging:** Bagging stands for bootstrap Aggregating. It involves training multiple models independently on different subsets of the training data, obtained through random sampling with replacement. Each model in the ensemble is trained on a different subset of the data, and their predictions are combined through averaging or voting. Random Forest is a popular ensemble technique that uses bagging with decision trees.
2. **Boosting:** Boosting is an iterative ensemble technique where models are trained sequentially, with each subsequent model focusing on the samples that were misclassified or given higher weights in previous iterations. After each iteration, the weights of misclassified samples are increased, allowing subsequent models to pay more attention to these samples. The final prediction is typically made through a weighted combination of the prediction of all models.

Examples of boosting algorithms include AdaBoost, Gradient Boosting Machines (GBM) and XGBoost.

Ensemble techniques offer several benefits. They can improve the generalization ability of models by reducing overfitting and increasing their robustness to noise and outliers. They can also capture complex relationships and patterns in the data that may be missed by individual

models. Ensemble models tend to exhibit better performance and stability compared to single models, and they are often considered a powerful approach in machine learning.

**Ans7-** Bagging and boosting are both ensemble techniques in machine learning, but they differ in their approach to building the ensemble models and combining their predictions. Here are the key differences between bagging and boosting:

1. Training Approach:

- Bagging: Bagging involves training multiple models independently on different subsets of the training data, obtained through random sampling with replacement. Each model is trained on a different subset of the data, and their predictions are combined through averaging or voting. Each model in the ensemble has an equal say in the final prediction.
- Boosting: Boosting is an iterative technique where models are trained sequentially. Each subsequent model focuses on the samples that were misclassified or given higher weights in previous iterations. After each iteration, the weights of misclassified samples are increased, allowing subsequent models to pay more attention to these samples. The final prediction is typically made through a weighted combination of the predictions of all models, where models with higher accuracy or lower error are assigned higher weights.

2. Model Independence:

- Bagging: In bagging, each model in the ensemble is trained independently of the others. The models are typically of the same type and have no knowledge of each other's predictions. They are trained on different subsets of the data and provide diverse perspectives, which helps reduce variance and improve stability.
- Boosting: In boosting, models are trained sequentially, and each subsequent model tries to correct the mistakes or deficiencies of the previous models. The models are dependent on each other, and their training process is influenced by the performance of earlier models. Boosting focuses on reducing bias and improving accuracy by iteratively adjusting the model's focus on difficult samples.

3. Weighting of Models:

- Bagging: In bagging, each model's prediction is given equal weight in the ensemble. The final prediction is typically obtained by averaging the predictions of all models or using majority voting.
- Boosting: In boosting, each model's prediction is weighted based on its performance and importance. Models with higher accuracy or lower error are assigned higher weights, and their predictions contribute more to the final prediction. The weights are typically determined through optimization algorithms that minimize the overall error.

4. Handling of Errors:

- Bagging: Bagging tends to focus on reducing variance. By training models independently on different subsets of data, bagging reduces the impact of individual model's errors or biases. The ensemble combines the predictions of multiple models to improve overall

performance, especially in situations where individual model may overfit or be sensitive to noise.

- **Boosting:** Boosting focuses on reducing bias. It iteratively corrects the mistakes made by earlier models by assigning higher weights to misclassified samples. Boosting aims to improve accuracy by learning from the errors and giving more attention to challenging samples.

Bagging emphasizes reducing variance and improving stability through an ensemble of independently trained models, while boosting focuses on reducing bias and improving accuracy by iteratively adjusting the model's focuses on challenging samples.

**Ans8-** In Random Forest, the out-of-bag(OOB) error is a metric used to estimate the performance of the model without the need for a separate validation set. It is a way to assess the accuracy of the Random Forest model during training.

When building a Random Forest, each individual tree is trained on a bootstrap sample, which is created by randomly selecting samples from the original dataset with replacement. As a result, some samples are left out or not included in the bootstrap sample for each tree. These left-out samples are referred to as "out-of-bag" samples.

The OOB error is calculated by evaluating the prediction of each individual tree in the Random Forest on their corresponding out-of-bag samples. Since these sample were not used in training the tree, they effectively act as a validation set for that computed as the average error across all trees, typically using a suitable performance metric such as classification accuracy or mean squared error.

The OOB error serves as an estimate of the model's performance on unseen data. It provides a measure of how well the Random Forest models, tuning hyperparameters, or assessing the need for additional model refinement.

The OOB error can also be used for feature importance estimation in Random Forest. By comparing the prediction performance on out-of-bag samples before and after permuting the values of a particular feature, one can determine the impact of that feature on the model's accuracy.

The OOB error in Random Forest provides a convenient and efficient way to estimate the model's performance during training without requiring a separate validation set.

**Ans9-** K-fold cross-validation is a technique used to assess the performance and generalization ability of a machine learning model. It involves splitting the available data into K equally sized subsets or folds. The model is then trained and evaluated K times, each time using a different fold as the validation set and the remaining folds as the training set.

**Ans10-** Hyperparameter tuning, also known as hyperparameter optimization, refers to the process of finding the optimal values for the hyperparameter of a machine learning model. Hyperparameters are parameters that are set before the learning process begins and are not learned from the data like model parameters. They control the behavior of the learning algorithm and impact the performance and generalization ability of the model.

Hyperparameter tuning is done for several reasons:

1. **Optimizing Model Performance:**  
Hyperparameters significantly influence the performance of a model. By tuning hyperparameters, you can find the combination that maximizes the model's performance metric, such as accuracy, F1 score, or mean squared error. Selecting appropriate hyperparameter values can improve the model's ability to capture patterns and make accurate predictions.
2. **Addressing Overfitting and Underfitting:**  
Hyperparameters play a crucial role in controlling the complexity of a model. Overfitting occurs when a model becomes too complex and learns the training data too well, resulting in poor generalization to unseen data. Underfitting, on the other hand, occurs when a model is too simple and fails to capture important patterns in the data. By tuning hyperparameters, you can find the right balance between model complexity and generalization performance.
3. **Improving Efficiency:**  
Hyperparameters can affect the computational efficiency and resource requirements of a model. Adjusting hyperparameters can help in improving the training speed and reducing memory usage, making the model more practical and scalable.
4. **Adapting to Specific Datasets:**  
Different datasets may require different hyperparameter settings. By tuning hyperparameter settings. By tuning hyperparameters, you can adapt the model to the specific characteristics and complexities of the dataset at hand, enhancing its performance on that particular data.

Hyperparameter tuning is performed to find the optimal values for the hyperparameters of a machine learning model. It helps improve model performance, address overfitting/underfitting, enhance efficiency, and adapt the model to specific datasets, leading to better predictive accuracy and generalization ability.

**Ans11-** If a large learning rate is used in gradient descent, it can lead to several issues, including:

1. **Divergence:** With a large learning rate, the updates to the model parameters can become too large, causing them to overshoot the optimal values. This can result in the loss function increasing instead of decreasing, leading to the model diverging and failing to converge to a good solution.
2. **Overshooting the Minimum:** When the learning rate is too large, the algorithm may overshoot the minimum of the loss function and keep oscillating around it. This can slow down the convergence process and prevent the algorithm from reaching the optimal solution.
3. **Instability:** Large learning rates can make the optimization process unstable. The model parameters may fluctuate dramatically from one iteration to the next, making it difficult to obtain consistent and reliable results. The instability can be particularly problematic when dealing with noisy or ill-conditioned data.
4. **Slow Convergence:** Although it may seem counterintuitive, using a very large learning rate can slow down the convergence of the optimization algorithm. The algorithm may end up taking very small steps in the parameter space, zigzagging around the minimum, and requiring more iterations to reach convergence.
5. **Difficulty in Escaping Local Minima:** Gradient descent can sometimes get stuck in local minima, especially in non-convex optimization problems. A large learning rate can make it challenging for the algorithm to escape from these local minima as it may skip over potential improvements in the loss function landscape.

It is important to choose an appropriate learning rate for gradient descent.

**Ans12-** Non-linear problems can't be solved with logistic regression because it has a linear decision surface.

If we suspect that the decision boundary is nonlinear we may get better results by attempting some nonlinear functional forms for the logit function. Logistic Regression is a classification technique used in machine learning. It uses a logistic function to model the dependent variable.

**Ans13-** \* Adaboost is computed with a specific loss function and becomes more rigid when comes to a few iterations.

But in gradient boosting, it assists in finding the proper solution to additional iteration modeling problem as it is built with some generic features.

\* In gradient boosting the trees with weak learners are constructed using a greedy algorithm based on split points and purity scores. The trees are grown deeper with eight to thirty-two



terminal nodes. The weak learners should stay a week in terms of nodes, layers, leaf nodes, and splits.

But in Adaboost the trees are called decision stumps.

\* In gradient boosting the classifiers are weighted precisely and their prediction capacity is constrained to learning rate and increasing accuracy

But in Adaboost every classifier has different weight assumptions to its final prediction that depend on the performance.

**Ans14-** Bias-variance trade off describe the relationship between a model's complexity, the accuracy of its predictions, and how well it can make prediction on previously unseen data that were not used to train the model.

It is important to understand prediction errors when it comes to accuracy in any machine-learning algorithm. There is a tradeoff between a model's ability to minimize bias and variance which is referred to as the best solution for selecting a value of Regularization constant.

**Ans15-** Linear Kernel : A linear kernel in SVM assumes that the data can be separated by a straight line or hyperplane in the input feature space. It computes the dot product between two data points in the original feature space, effectively measuring their similarity.

RBF Kernel: In machine learning, the radial basis function kernel, is a popular kernel function used in various kernelized learning algorithms. It is commonly used in support vector machine classification.

Polynomial Kernels: The polynomial kernel is a kernel function commonly used with support vector machines and other kernelized models, that represents the similarity of vectors in a features space over polynomials of the original variables, allowing learning of non-linear models.

