Regression and Prediction Week 4

Learning Objectives of the Session

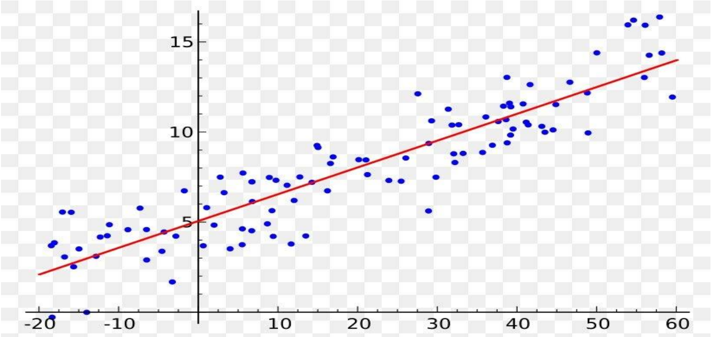
- Basics of Linear Regression
- Evaluation metrics for Regression
- Overfitting and Underfitting
- Bias-Variance trade off
- Regularization
- Cross Validation
- Regression Trees
- Random Forest Regressor

Discussion Questions

1. What is linear regression?
2. How to find best fit line in linear regression
3. What are different evaluation metrics and their interpretation?
4. What is bias variance trade off and problem of overfitting?
5. What is Regularization and how it helps in reduce overfitting?
6. What is cross validation and why need to use it?
7. What are some Non-Linear regressors and why they are used and when?

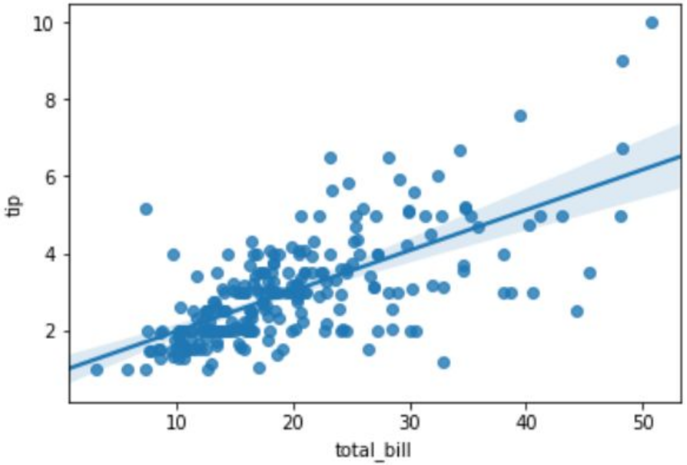
Linear Regression

1. Linear regression is a way to identify a relationship between the independent variable(s) and the dependent variable
2. We can use these relationships to predict values for one variable for given value(s) of other variable(s)
3. It assumes the relationship between variables can be modeled through linear equation or an equation of line.
4. The variable, which is used in prediction is termed as independent/explanatory/regressor where the predicted variable is termed as dependent/target/response variable.
5. In case of linear regression with a single explanatory variable, the linear combination can be expressed as : $\hat{Y} = \beta_0 + \beta_1 X$. The terms β_0& β_1 are coefficients.



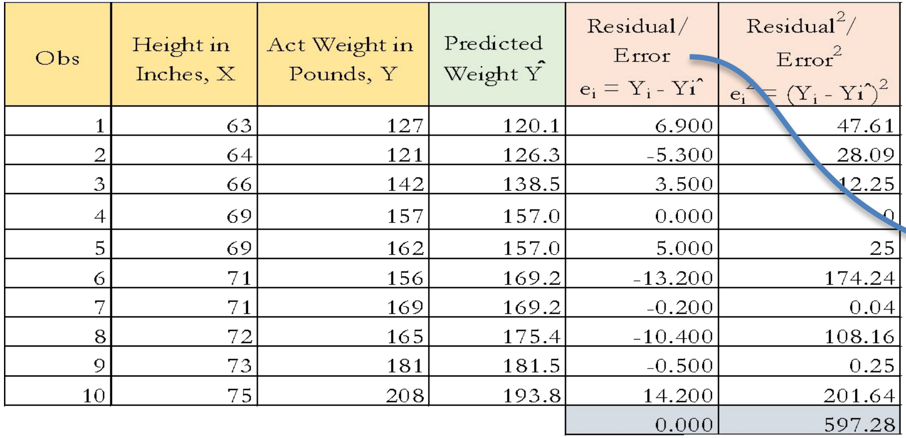
Best fit line or Best linear predictor in the linear regression

- Learning from the data, the model generates a line that fits the data.
- Our aim is to find a regression line that best fits the data
- By best fit, it means that the line will be such that the cumulative distance of all the points from the line is minimized
- Mathematically, the line that minimizes the sum of squared error of residuals is called Regression Line or the Best Fit Line.

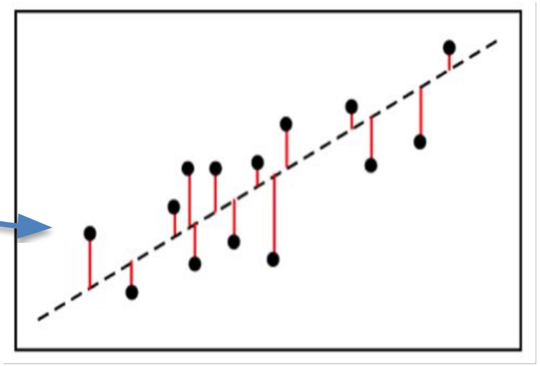


- In the example here, you can see a scatter plot between the *tip* amount and the *total_bill* amount
- We can see that there is positive correlation between these two - as the bill amount increases, the tip increases
- The line in blue that you see is the 'best fit' line - those in red are some examples of all other lines that are not the 'best fit'

Regression Example



Obs	Height in Inches, X	Act Weight in Pounds, Y	Predicted Weight $\hat{Y}$	Residual/ Error $e_i = Y_i - \hat{Yi}$	Residual^2/ Error^2 $e_i^2 = (Y_i - \hat{Yi})^2$
1	63	127	120.1	6.900	47.61
2	64	121	126.3	-5.300	28.09
3	66	142	138.5	3.500	12.25
4	69	157	157.0	0.000	0
5	69	162	157.0	5.000	25
6	71	156	169.2	-13.200	174.24
7	71	169	169.2	-0.200	0.04
8	72	165	175.4	-10.400	108.16
9	73	181	181.5	-0.500	0.25
10	75	208	193.8	14.200	201.64
				0.000	597.28



Sum of Squared Residuals

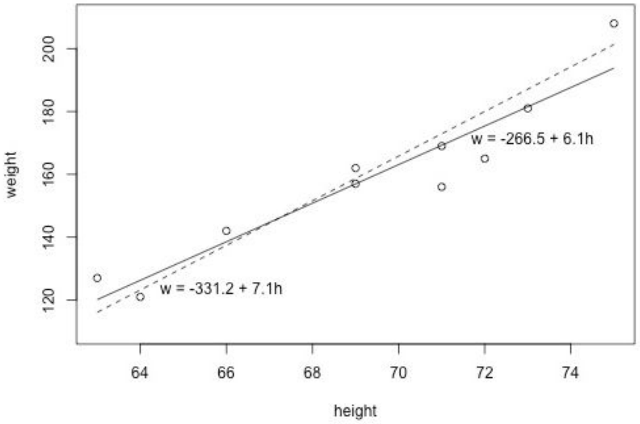
1. Say weight is regressed on height of an individual
2. Linear regression model for the above data: **$\hat{Y}$= -266.53 + 6.1376X**
3. Model is obtained by **minimizing the sum of squares of residuals.**
4. Sum of residuals is always equal to zero.
5. The line will always pass through the centroid **($\bar{X}$, $\bar{Y}$)**

Regression Example – Interpretation of Intercept

- The intercept b_0 is the measure of **y** when **x=0**. Agree/disagree
- **Never extrapolate** the model beyond the range of x values.
- When range of x does not include zero, y @ x=0 is not meaningful.
- Simple Linear Regression helps in prediction of y within the range of x values in the data
- Ex: What would be the weight of an individual having height = 67.5 inches?

$$\hat{Y} = b_0 + b_1 X$$

$$\hat{Y} = -266.53 + 6.1376X$$



Regression - Evaluation Methods

R-squared	Adjusted R-squared	Mean Absolute Error	Root Mean Square Error
● Measure of the % of variance in the target variable explained by the model ● Generally the first metric to look at for linear regression model performance ● Higher the better	● Conceptually, very similar to R-squared but penalizes for addition of too many variables ● Generally used when you have too many variables as adding more variables always increases R^2 but not Adjusted R^2 ● Higher the better	● Simplest metric to check prediction accuracy ● Same unit as dependent variable ● Not sensitive to outliers i.e. errors doesn't increase too much if there are outliers ● Difficult to optimize from mathematical point of view (pure maths logic) ● Lower the better	● Another metric to measure the accuracy of prediction ● Same unit as dependent variable ● Sensitive to outliers - errors will be magnified due to square function ● But has other mathematical advantages that will be covered later ● Lower the better

$$R^2 = 1 - \frac{\frac{1}{n}\sum_{i=1}^{n}(y_i - yhat_i)^2}{\frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

$$Adjusted\ R^2 = 1 - \frac{(1 - R^2)(N-1)}{N-p-1}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - yhat_i|$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - yhat_i\,)^2}$$

Applications of Regression

- Finance & economics
  - Sales forecasting
- Logistics & operations
  - Demand forecasting (number of units)
- Number of flights in an airport
  - Duration or delay of flights (time as Y)
- Sociology
  - Growth of population rate, GDP
- Environment
  - Prediction of rainfall (what is unit of Y?)

Bias-Variance: Underfitting and Overfitting

- **Bias:** Bias is the difference between the prediction of our model and the correct value which we are trying to predict. Model with high bias gives less attention to the training data and overgeneralize the model which leads to high error on training and test data.

- **Variance:** Variance is the value which tells us spread of our data. Model with high variance pays a lot of attention to training data and does not generalize on the test data. Therefore, such models perform very well on training data but has high error on test data

- In supervised learning, **underfitting** happens when a model is not able to capture the underlying pattern of the data. These models usually have high bias and low variance whereas, **overfitting** happens when our model captures the noise along with the underlying pattern in data. These models usually have low bias and high variance.

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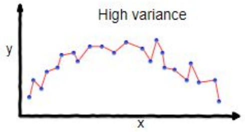
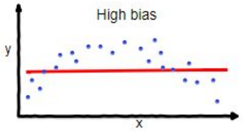
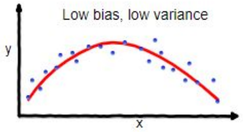


overfitting



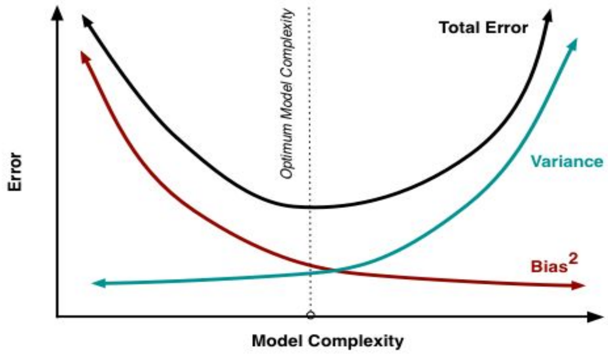
underfitting



Good balance

Bias-Variance Trade off

- If our model is too simple and has very few parameters then it may have high bias and low variance. On the other hand if our model has large number of parameters then it's going to have high variance and low bias. So we need to find the right/good balance without overfitting and underfitting the data.
- An optimal balance of bias and variance would never overfit or underfit the model.



Regularization and its types

Regularization is the process which regularizes or shrinks the coefficients towards zero. In other words, this technique discourages learning a more complex or flexible model, so as to avoid the risk of overfitting.

Regularization, significantly reduces the variance of the model, without substantial increase in its bias.

There are two types of regularization:

Lasso Regression: In this technique we add $\alpha*\sum|\beta|$ as the shrinkage quantity. It only penalizes the high coefficients. It has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning parameter λ is sufficiently large. This technique is also called L1 regularization.

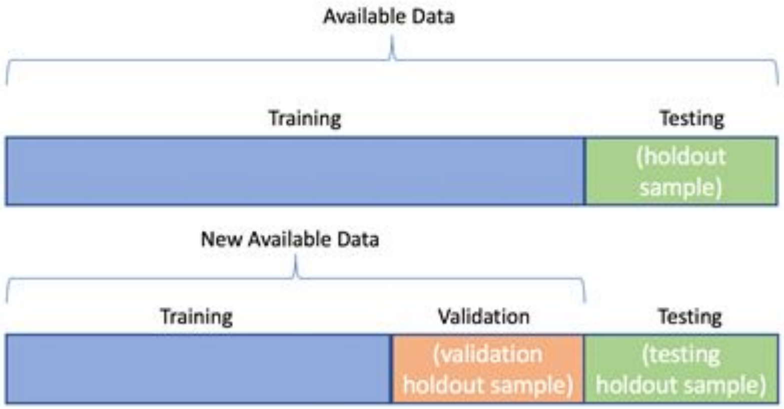
Ridge Regression: In this technique, we modify the residual sum of squares by adding the shrinkage quantity $\alpha*\sum\beta^2$ and use α as the tuning parameter that decides how much we want to penalize the flexibility of our model. This technique is also called L2 regularization.

Cross Validation

Cross-validation is a technique in which we train our model using the subset of the data-set and then evaluate using the complementary subset of the dataset.

It provides some kind of assurance that your model has got most of the pattern from the data set correct and it is not picking up some noise.

On the most used cross validation Method is K-Fold Cross-validation

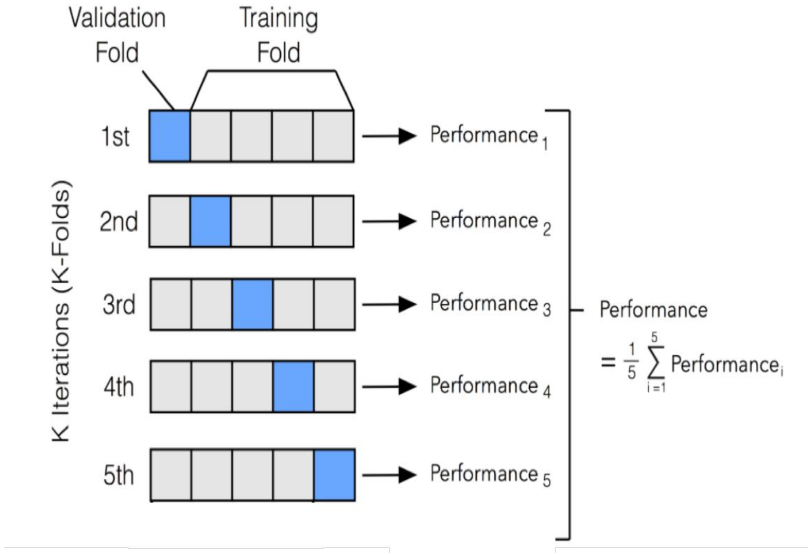


K-Fold Cross Validation

This algorithm has a single parameter called K that refers to the number of groups that a given data sample is to be split into.

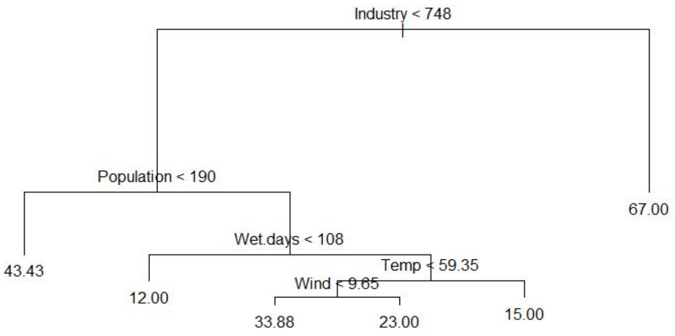
This algorithm has following procedure:

1. Shuffle the dataset randomly.
2. Split the whole dataset into K groups
3. For each unique group, take one as a hold out set and remaining as training set.
4. Repeat the step 3, for all groups
5. Summarize the skill of the model using the sample of model evaluation scores of all groups



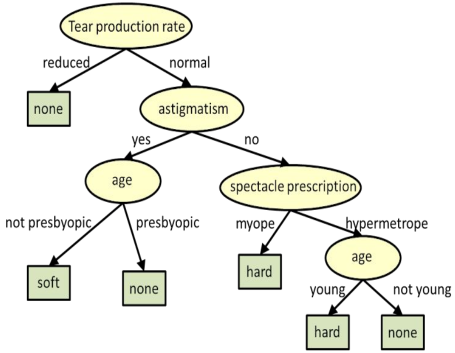
Regression Trees

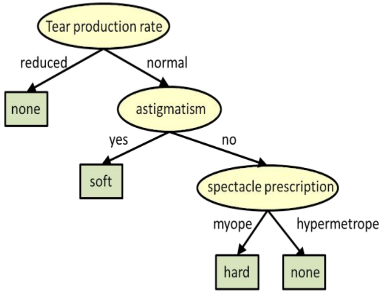
- A decision tree is one of the most popular and effective supervised learning techniques for Regression and classification problems, that works equally well with both categorical and continuous variables.
- It is a graphical representation of all the possible solutions to a decision that is based on a certain condition.
- In this algorithm, the training sample points are split into two or more sets based on the split condition over input variables.



Tree Pruning

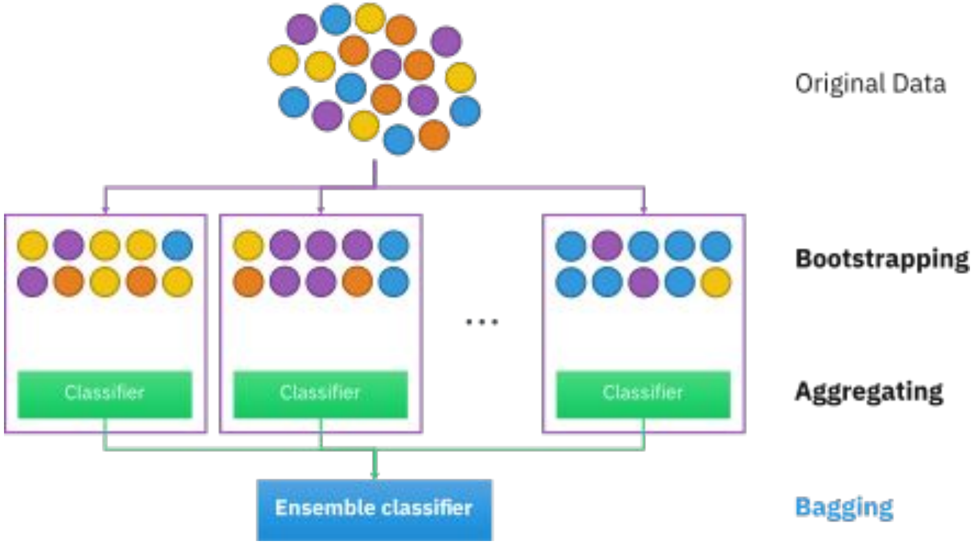
- One of the problems with the decision tree is it gets easily overfit with the training sample and becomes too large and complex.
- A complex and large tree poorly generalizes to new sample data whereas a small tree fails to capture the information of the training sample data.
- Pruning may be defined as shortening the branches of the tree. It is the process of reducing the size of the tree by turning some branch node into a leaf node and removing the leaf node under the original branch.
- By removing branches we can reduce the complexity of tree which helps in reducing the overfitting of the tree.





Bootstrap Aggregation (Bagging)

- Bagging is a technique of merging the outputs of various models to get a final result
- It reduces the chances of overfitting by training each model only with a randomly chosen subset of the training data. Training can be done in parallel.
- It essentially trains a large number of “strong” learners in parallel (each model is an overfit for that subset of the data)
- Then it combines (averaging or voting) these learners together to "smooth out" predictions.



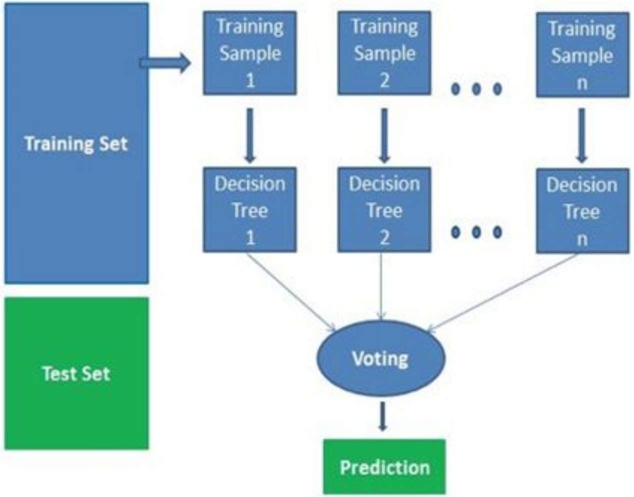
Random Forest

- Random Forest is a supervised machine learning algorithm which can be used for both classification and regression.
- It generates small decision trees using random subsamples of the dataset where the collection of the generated decision tree is defined as forest. Every individual tree is created using an attribute selection indicator such as entropy, information gain, etc.
- In classification, problem voting is done by each tree and the most voted class is considered the final result whereas in case of regression the average method is used to get the final outcome.
- Random Forest is used in various domains such as classification of images, feature selection and recommendation engines.

Steps involved in the Random Forest algorithm

The following steps are involved in this algorithm:

1. Selection of a random subsample of a given dataset.
2. Using attribute selection indicators create a decision tree for each subsample and record the prediction outcome from each model.
3. Applying the voting/averaging method over predicted outcomes of individual models.
4. Considering the final results as the average value or most voted value.



Case Study
Regression

Great Learning

Happy Learning !