



IDARE®

AI Success Metrics

Module 10 ML Success and Performance Assessment

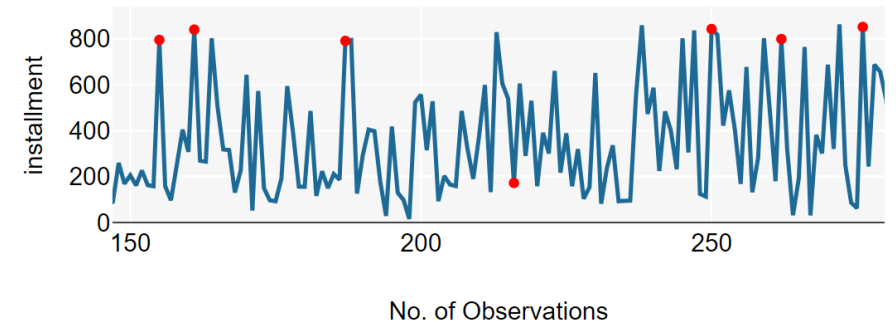
ML Success Tactics

Minimizing Data Uncertainty

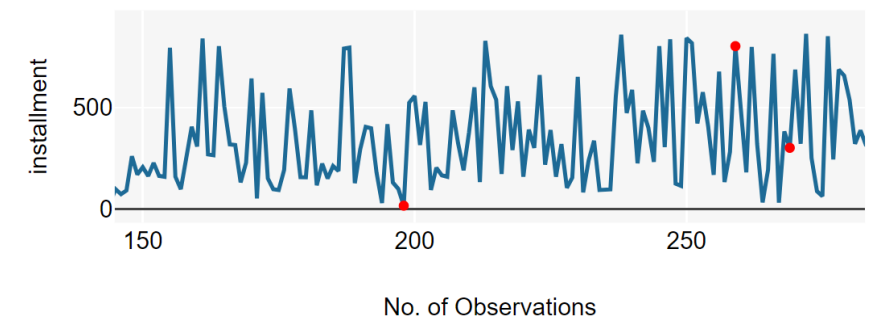
Data Quality

Types of Trouble you may face in Data

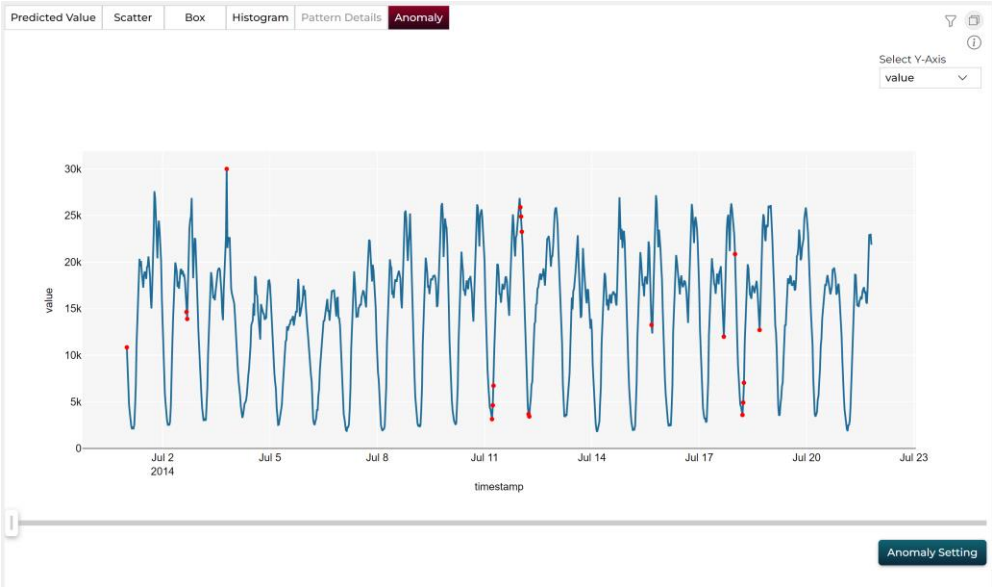
- **Missing Value**, Null Value, Blank Value, inf value, NA value
 - Removing is the easy option, however in many cases those values means major cause of the target.
 - Replace with either 0 or avg or other statistical parameters will be wise
- **Anomalous Data or Outlier**
 - Sudden picks and valleys in the data
 - Use anomaly detector to detect or isolate
 - Talk to domain expert or use your knowledge to understand
 - That anomaly is the part of a process or means something. Twik the anomaly detector to isolate right anomalies
 - Or simply data error
 - If those anomalies mean something, categories them based on their recognized category, if not remove them
 - Removing anomalies for a variable will lead to removing other variables from that point so be careful



Twiking Anomaly parameter shows lesser anomalies



Anomaly Detection Example



Anomaly Setting

Anomaly Detect

Period

Enter Period

Detect

Anomaly Delete

Columns

value

×

|

×

▼

Detect

ML Success Tactics

Variable Selection (Feature Engineering)

**Right use of Correlation & Causation
in variable selection in training**

Variable Selection Defines success of an AI Solution

Most Important Process in Solution Creation
is to determine the right predictor variables
or features

- Variable that doesn't have any affect on the target
 - Start your analysis unselecting these variables
- that cause the target
 - Try keeping these variables under any circumstances unless there are compelling reasons
- The relationship between the selected variables i.e. correlation coefficient
 - If p-value < 0.05 try keep the variable
- Check Feature Importance after each analysis
 - If Pearson correlations coefficient
 - high w.r.t target try keeping these variables
 - high w.r.t other predictor variable, try not to use one of the two
- Create science driven variables
- Perform extensive parametric study
- Try to stick to One Algorithm during Variable selection

Recommended Practice for being successful in variable selection process

Key practices

- Brainstorm to understand the problem and study the target
- Utilize your Domain expertise
- Gather domain knowledge
 - Do extensive literature survey
 - Talk to domain experts
- Use critical and analytical skills to determine

Correlation and Causation

**Right use of Correlation & Causation
in variable selection in training**

Correlation & Causation for Variable Selection

- Causation:**

- Variable that directly comes from domain expertized are used or not
- Variables that are low p-values considered or not
- High P-values are avoided or not unless domain experts recommends that
- IF p-values are 0 check t-value, high t-value suggest high significance with the target

- Correlation:**

- If variables are highly correlated or high coefficient with respect to TARGET should be used
- If variables within themselves are highly correlated should be avoided unless domain knowledge suggested or parametric study suggested

Variable Statistics		Validation Result		Variable Importance		Compare KPI
Variables	Data Type	Missing Values Count	p value	t value	Pearson Correlation	
Lever_Pos	float	0	0.4	0.84	0	
Ship_Speed	int	0	0	11.33	0	
GT_Shft_torq	float	0	0	106.99	0	
GT_RPM	float	0	0	61.11	0	
Gas_Genrtr_RPM	float	0	0	100.25	0.01	
Strbrd_Proplr_Trq	float	0	0	-139.25	0	
Port_Proplr_Trq	float	0	0	-139.25	0	
HP_Trbin_exit_temp	float	0	0	-96.02	-0.04	
GT_Comprsr_inlet_air_Temp	int	0	0.04	2.11		
GT_Comprsr_outlet_air_Temp	float	0	0	16.55	-0.02	
HP_Trbin_exit_press	float	0	0	24.18	0	
GT_Comprsr_inlet_air_Press	float	0	0.04	2.11		
GT_Comprsr_outlet_air_Press	float	0	0	-177.8	-0.02	
HP_Trbin_exahst_gas_press	float	0	0	12.86	0.01	
Trbin_Injecton_Cntrl	float	0	0	-36.89	-0.02	
Fuel_flow	float	0	0	82.69	-0.02	
GT_Trbin_decay_coeff	float	0			1	

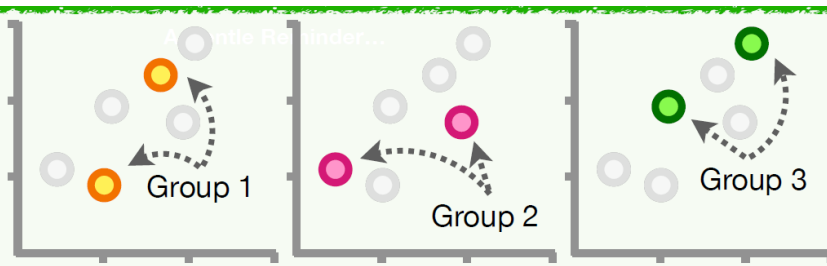
Cross Validation for Variable Selection

Right use of cross validation in training

Cross Validation: Details Part 3

8 Because we have **3** groups of data points, we'll do **3** iterations, which ensures that each group is used for **Testing**. The number of iterations are also called **Folds**, so this is called **3-Fold Cross Validation**.

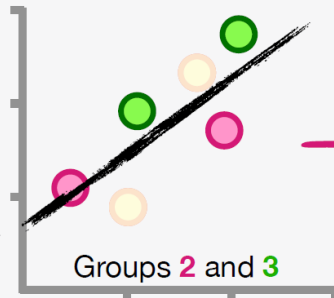
Gentle Reminder:
These are the original **3** groups.



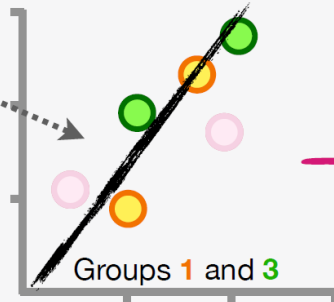
9 So, these are the **3** iterations of **Training**...

NOTE: Because each iteration uses a different combination of data for **Training**, each iteration results in a slightly different fitted line.

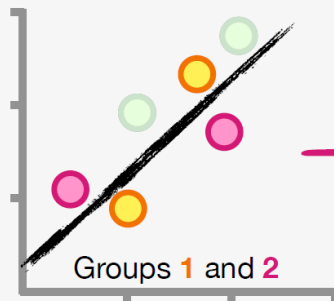
Iteration #1



Iteration #2



Iteration #3



10 ...and these are the **3** iterations of **Testing**.

A different fitted line combined with using different data for **Testing** results in each iteration giving us different prediction errors.

We can average these errors to get a general sense of how well this model will perform with future data...

...or we can compare these errors to errors made by another method.

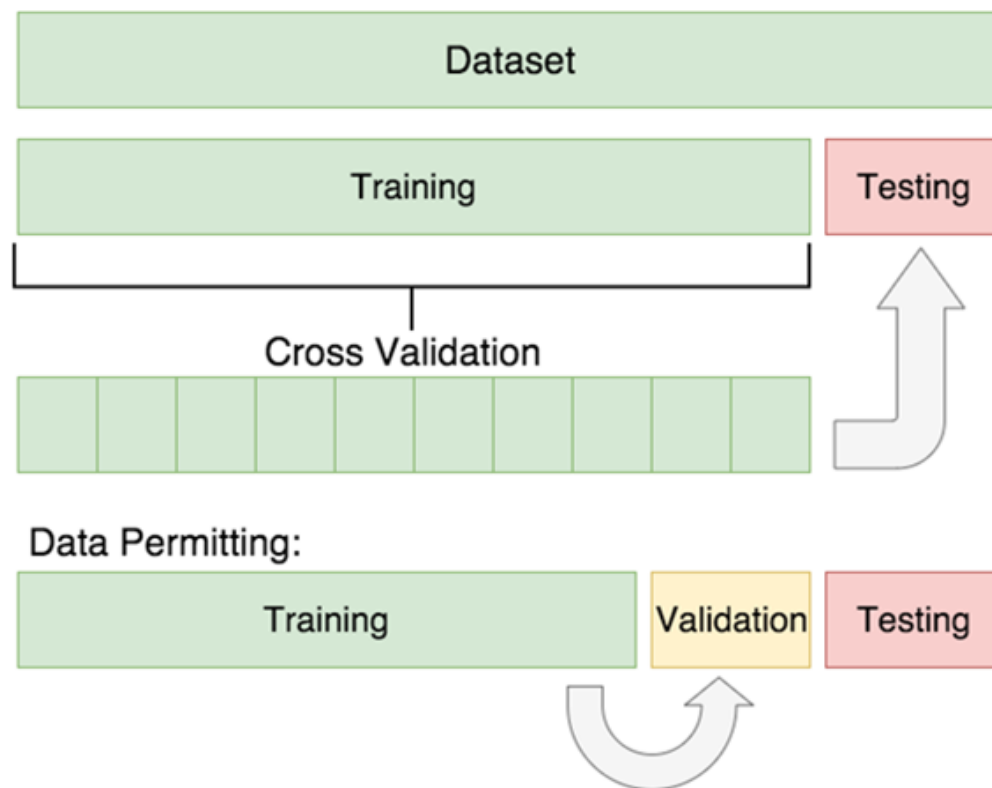
Cross Validation with Data Split

Train Data: Data Sample ML will Learn From

Test Data: Unseen data or Out of Sample data

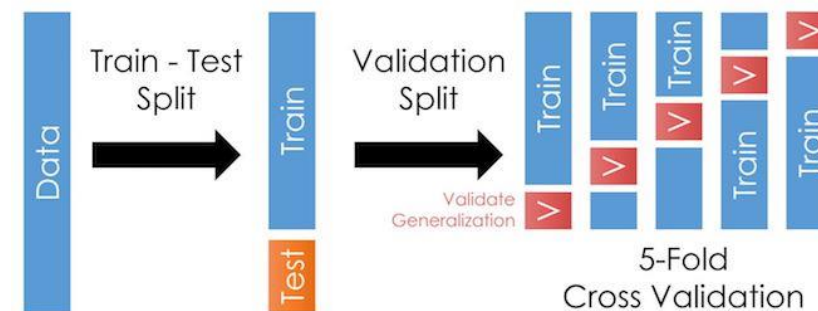
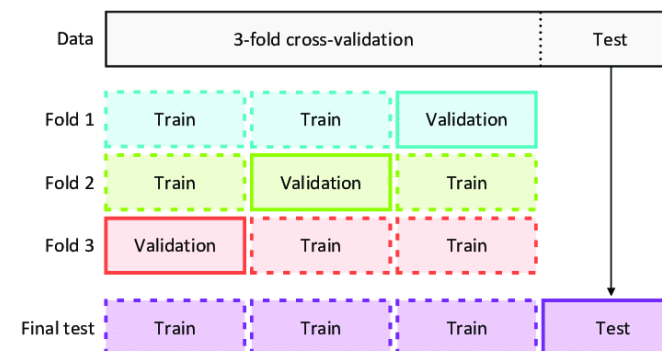
potentially you will see when in production

Validation Data: Part of Train data kept unseen for cross validation



Kinds

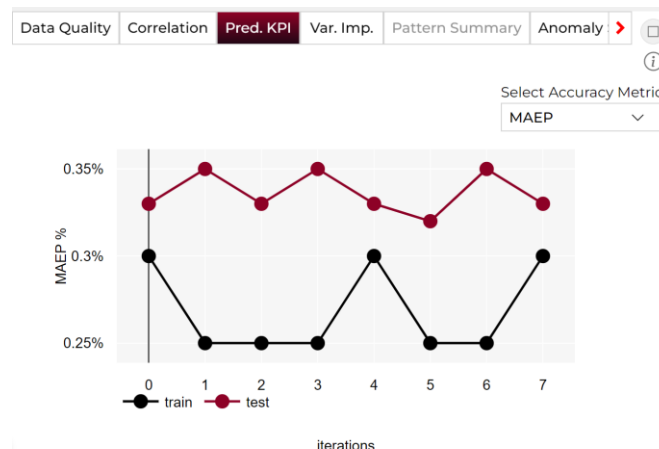
- 3-fold
- 5-fold
- 10-fold



Error Check with Cross-Validation

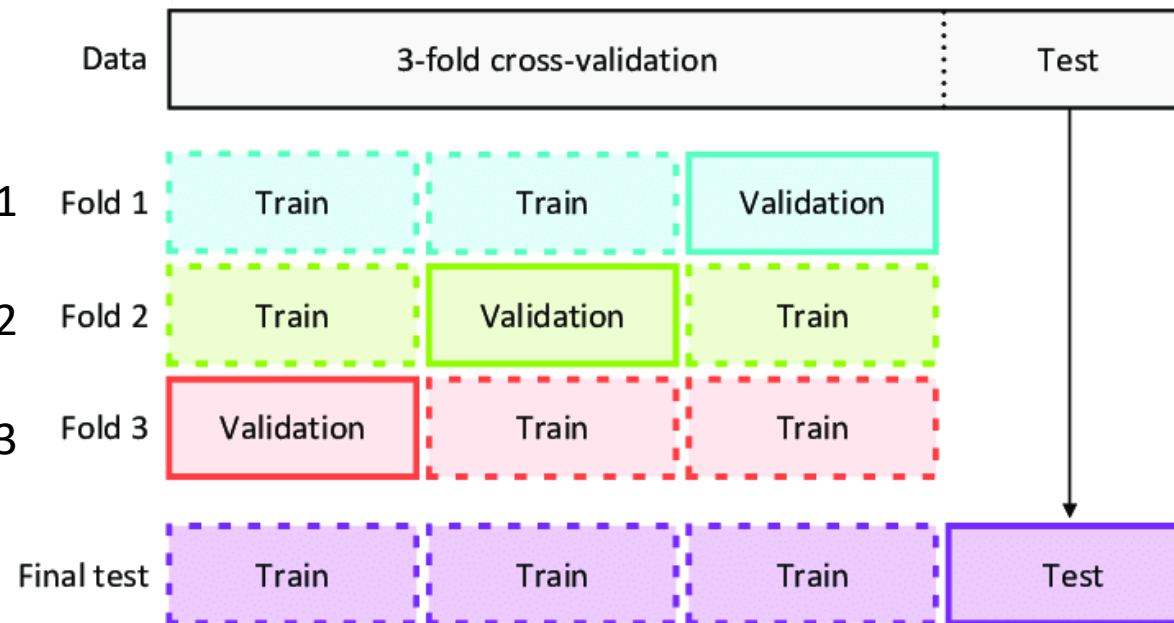
Error to Look at

- Train Error (Bias)
- Cross Validation Error
- Test Error (Variance)
- Variation of Error between folds



Variable Statistics		Validation Result	Variable Importance			Compare KPI
ML Algorithm	Mean CV MAEP	Test MAEP	Split_1 CV MAEP	Split_2 CV MAEP	Split_3 CV MAEP	Stand Dev of CV MAEP
Random Forest	0.2	0.32	0.28	0.08	0.24	-0.09
XGB	0.23	0.35	0.28	0.11	0.28	-0.08
Linear regression	0.21	0.33	0.22	0.16	0.26	-0.04

- Cross Validation
- Avg. Error
- Standard Deviation



AI Success Metrics

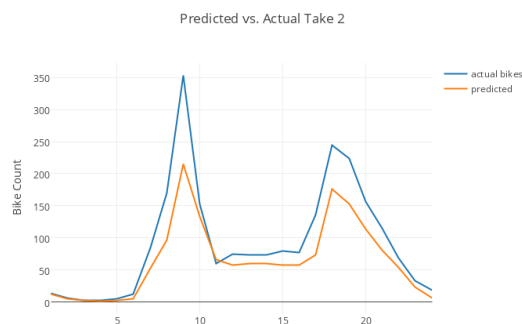
Module 10 ML Success and Performance Assessment
Performance Assessment



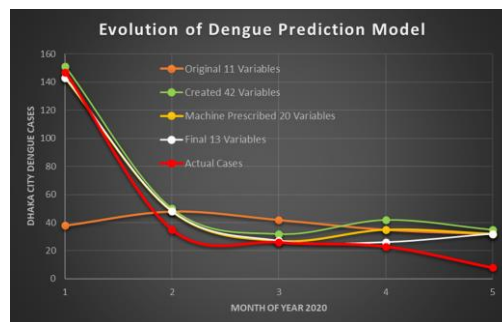
Fundamentals

Performance Check: Regression

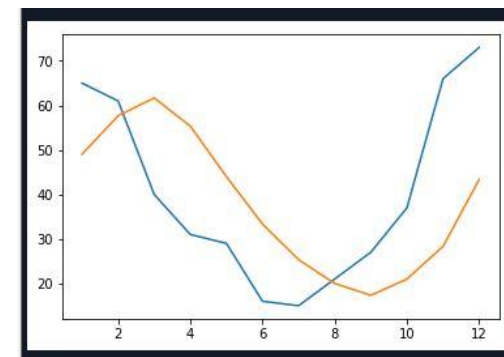
- The zeroth law: Compare actual versus predicted line chart for Test data
- Check whether predicted line captures the pattern of the actual or not
- If pattern doesn't match, major work will be needed in variable selection



Captures the pattern
But error will be high.
BIAS is ok though
variances are high



All prediction captures
the pattern except one

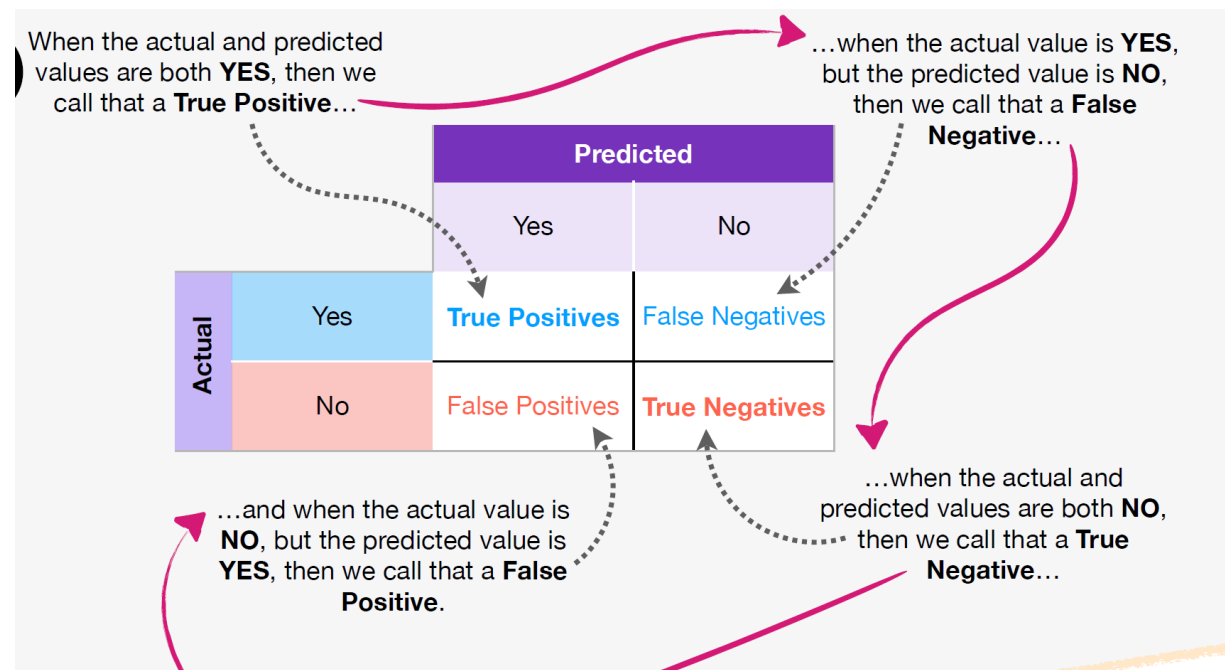


Captures the pattern,
the pattern shifted

Performance Check Classification

- The zeroth law: check confusion matrix
- check true positive, false positive, true negative and false negative
- Reduce false positive or false negative based on the problem

		Predicted	
		Has Heart Disease	Does Not Have Heart Disease
Actual	Has Heart Disease	142	22
	Does Not Have Heart Disease	29	110



Understanding Model Stability or Prediction Consistency

Model Stability or Consistence

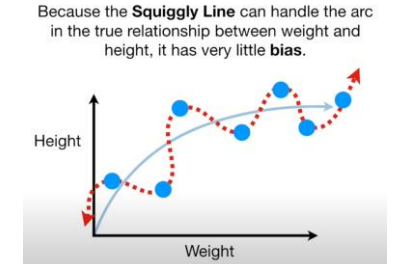
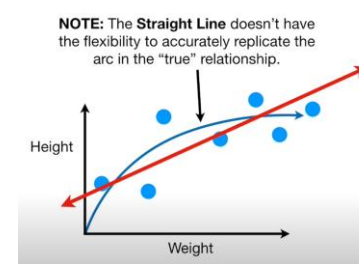
Remember Bias and Variance?

4. Bias: How well the algorithm learns the true behavior or how complicated your model is

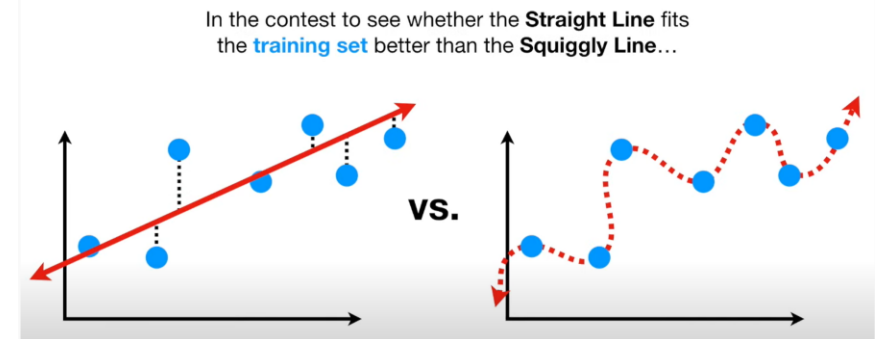
- *Low bias: over complicated model or too many variable used*
- *High bias: over simplified model or too less variable used*
- Sum of Squared Error for each predicted points with training data set

5. Variance: Measures the differences between actual and predictions.

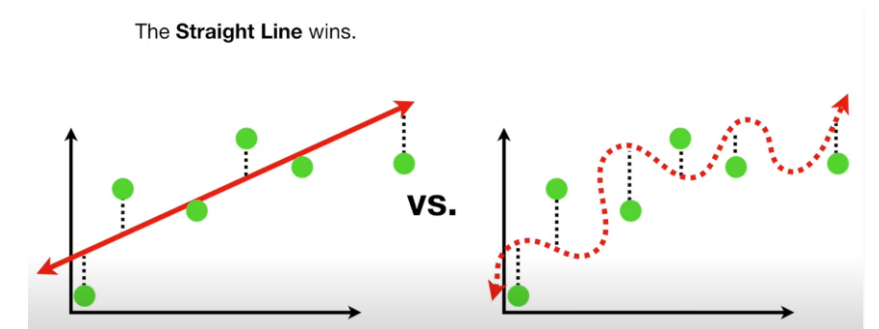
- Sum of Squared Error for each predicted points with test data set



Training data set trains with 2 algorithm

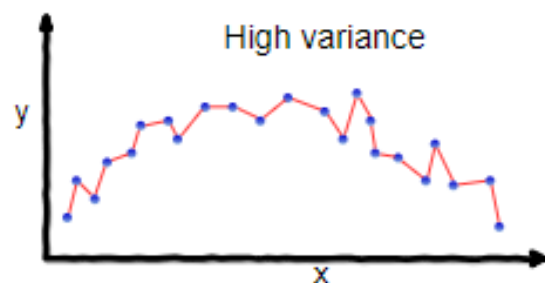


Error for Training Data sets

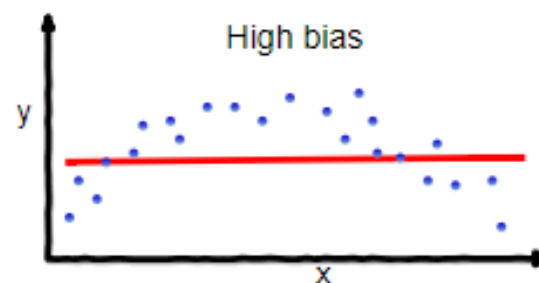


Error for Test Data sets

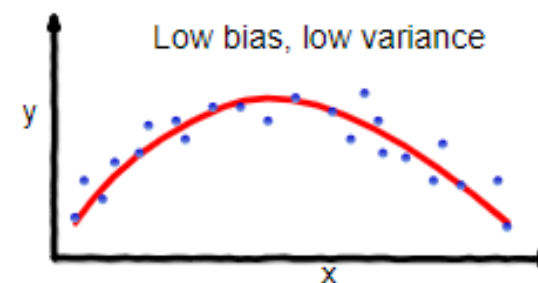
Overfitting Underfitting



overfitting



underfitting



Good balance

Overfitting: Training error low ,testing error high → Model Low Bias high variance

- Extra unrelated variables cause reduce bias and cause more error later, leads to instable and inconsistent result

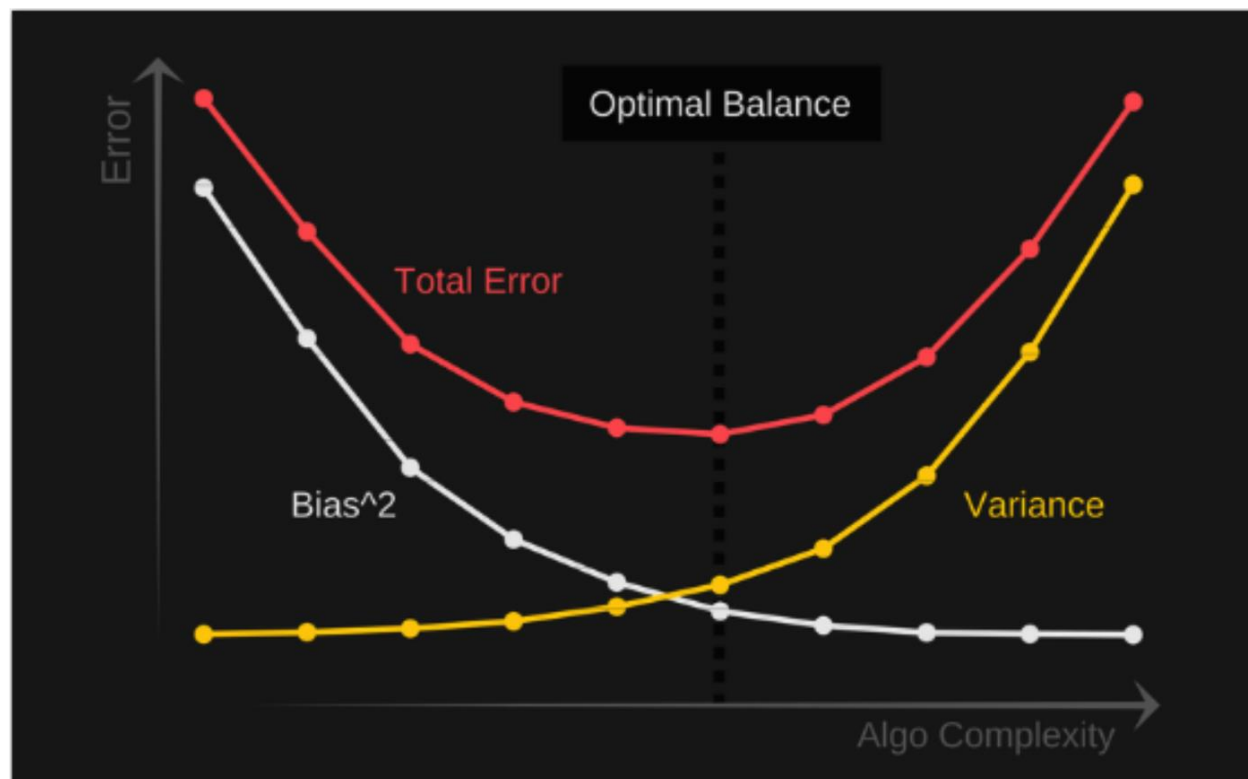
Underfitting: Training error high, testing error high → Model high Bias, high variance

- Missing important variable increase bias and also cause more error later leads to highly instable and inconsistent prediction

Good Balance: Training error low, testing error low → Optimal Bias, low variance

- Good variable selection and science driven AI reduces chances of overfitting or underfitting

$$\text{Total Error} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$



Total Error Scale on the order of Bias squared, which in most cases is substantially big, downplays testing error. Best way to understand a stable model is to do a eye check.

- Minimum difference between training and testing error
- Both error are low
- Standard deviations of cross validation data sets are low

Error Metrics

Error metrics for Regression

Residual = Observed - Predicted

SSR = Sum of Squared Residuals

$$\text{SSR} = \sum_{i=1}^n (\text{Observed}_i - \text{Predicted}_i)^2$$

$$\text{Mean Squared Error (MSE)} = \frac{\text{SSR}}{n}$$

...where **n** is the sample size

$$R^2 = \frac{\text{SSR}(\text{mean}) - \text{SSR}(\text{fitted line})}{\text{SSR}(\text{mean})}$$

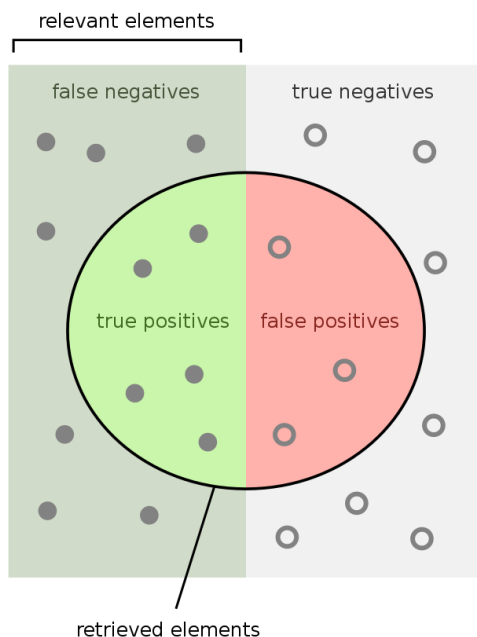
$$RMSE = \sqrt{MSE}$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |\hat{y}_i - y_i|$$

$$MAPE = \frac{100\%}{n} \sum_{i=1}^n \left| \frac{\hat{y}_i - y_i}{y_i} \right|$$

MAEP = Sum of absolute Error / Sum of Actuals

Error metrics for Classification



How many retrieved items are relevant?

$$\text{Precision} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$

How many relevant items are retrieved?

$$\text{Recall} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$

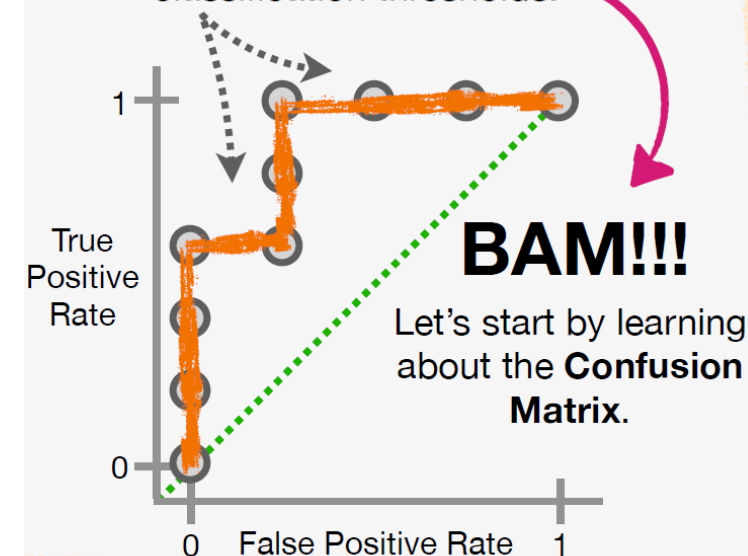
$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

$$F = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

...to **Receiver Operator Curves (ROCs)**, which give us an easy way to evaluate how each model performs with different classification thresholds.



AI Success Metrics

Module 10 ML Success and Performance Assessment

ML Parameter on Performance (Hyper Parameter Tuning)

Hyper Parameter (HP) Tuning for ML Algorithm

Hyper parameters are variables specific to machine learning algorithms that helps the ML learning process.

Hyper parameters has no influence on the performance of the model but affect the speed and quality of the learning process.

The HP tuning process is little expensive, costs computation time as it runs many time to find best models

Following are some key parameters applicable for many ML algorithm

- **No. of Iteration:** how many times the algorithm search for best results
- **No. of Trees or Layers:** no. of Paths and combinations of path to reach the outcome
- **Depth:** How many elements or parameters of a tree or paths to consider
- **Learning Rate:** How small the step of the learning
- **Bootstrap:** Way of data sampling, combinations of rows or variables etc
- **Solver:** Algorithm to tune the hyperparameter

Hyperparameters for different Algorithm

Random Forest (RF)

- **Criterion:** Criterion is a loss function to measure the quality of a split inside a tree.
 - Mean Squared Error and Mean Absolute Error
- **The maximum number of features:** The number of features to consider when looking for the best split. Decreasing the maximum number of features helps control overfitting.
 - All, Square Root, Logarithm: Use the logarithm (base 2) of the total number of features
- **Maximum depth of each tree:** The deeper the tree, the more branches it has and it captures more information about the data.
- **Bootstrap:** It's a sampling technique
- **The number of trees in the forest:** The default value for this parameter is 100, which means that 100 different decision trees will be constructed in the random forest. A higher number of trees give you better performance but makes the training slower.

XG Boost

- **Maximum depth of each tree:** Same as RF
- **The number of trees in the forest:** Same as RF
- **Learning Rate:** Lower learning rate means the model is more robust to overfitting but makes the training slower.

Neural Network

1. **Hidden Layers and Neurons:** Hidden Layers Similar like Trees
2. **Activation Function:** decides whether a neuron's input to the network is important or not in the process of prediction
3. **Solver:** Solver is an algorithm to optimize the weights of the neural network.
Stochastic Gradient Descent & Adam:
4. **Initial Learning Rate:** How small the step of the learning
5. **The number of epochs:** no. of iterations.

Hyperparameter Examples

Random Forest Regressor



Hyperparameters	Values
Criterion [?]	<input checked="" type="checkbox"/> Mean Squared Error [?] Loss of Accuracy <input type="checkbox"/> Mean Absolute Error [?]
Maximum number of features [?]	<input checked="" type="checkbox"/> All [?] Solver <input type="checkbox"/> Square Root [?] <input type="checkbox"/> Logarithm [?]
Bootstrap [?]	<input checked="" type="radio"/> True <input type="radio"/> False Data Sampling
The number of trees in the forest [?]	<input checked="" type="radio"/> List [?] <input type="radio"/> Range [?] 100 No. of Iteration
Maximum depth of each tree [?]	<input checked="" type="radio"/> List [?] <input type="radio"/> Range [?] None Depth

XGBoost Regressor



Hyperparameters	Values
The number of trees [?]	<input checked="" type="radio"/> List [?] <input type="radio"/> Range [?] 100 No. of Paths
Maximum depth of each tree [?]	<input checked="" type="radio"/> List [?] <input type="radio"/> Range [?] 6 Depth
Learning Rate [?]	<input checked="" type="radio"/> List [?] <input type="radio"/> Range [?] 0.3 Learning Rate

Neural Network Regressor



Hyperparameters	Values
Hidden Layers and Neurons [?]	100 Depth
Activation Function [?]	<input checked="" type="checkbox"/> Rectified Linear Unit [?] Loss of Accuracy <input type="checkbox"/> Hyperbolic tan Function [?]
Solver [?]	<input type="checkbox"/> Stochastic Gradient Descent [?] Solver <input checked="" type="checkbox"/> Adam [?]
Initial Learning Rate [?]	<input checked="" type="radio"/> List [?] <input type="radio"/> Range [?] 0.001 Learning Rate
The number of epochs [?]	<input checked="" type="radio"/> List [?] <input type="radio"/> Range [?] 200 No. of Iteration

Final Selection of Model and Variables

Decide the best ML models and Variables based on

- Check which ML model's Variable Importance most consistent with the physical understanding of the target
- Select your model by setting 1 error metric.
- The changes of errors based on ML models and different selected variables are very similar for between the error metrics
- Consider minimum difference between training and testing error
- Consider when Both error are the lowest
- Consider when all the cross-validation errors are similar or Standard deviations of cross validation data sets are the lowest
- Use your judgement

