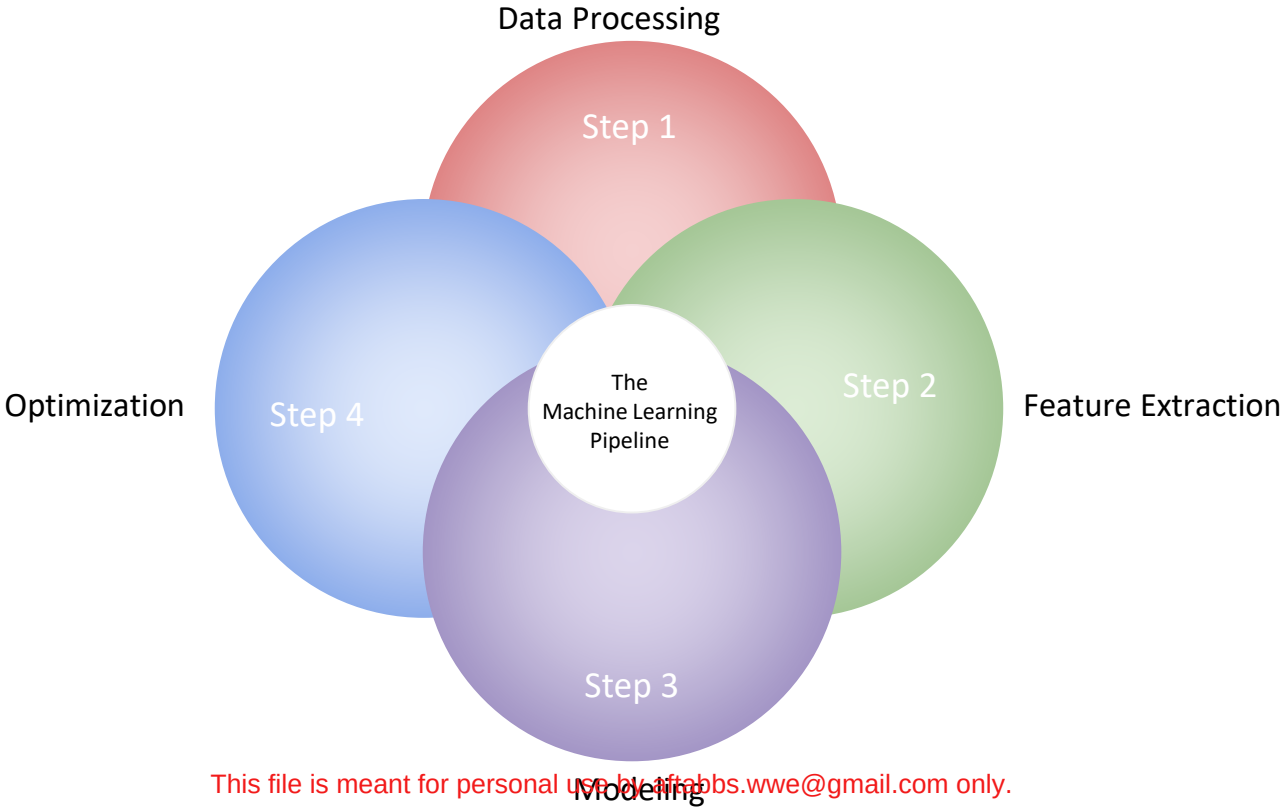
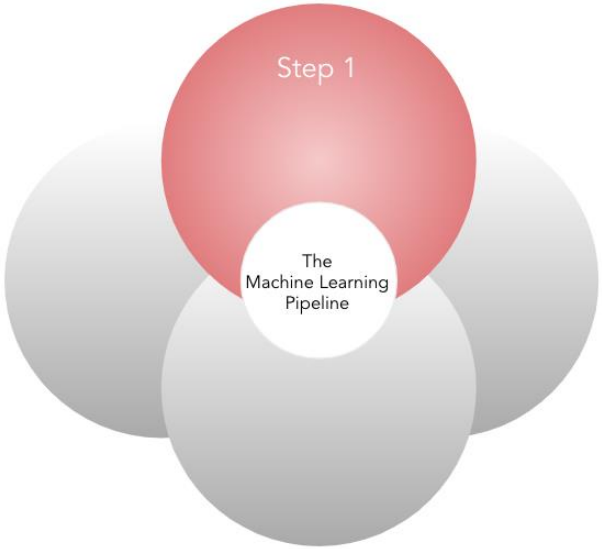
Machine Learning Pipeline

The ML pipeline



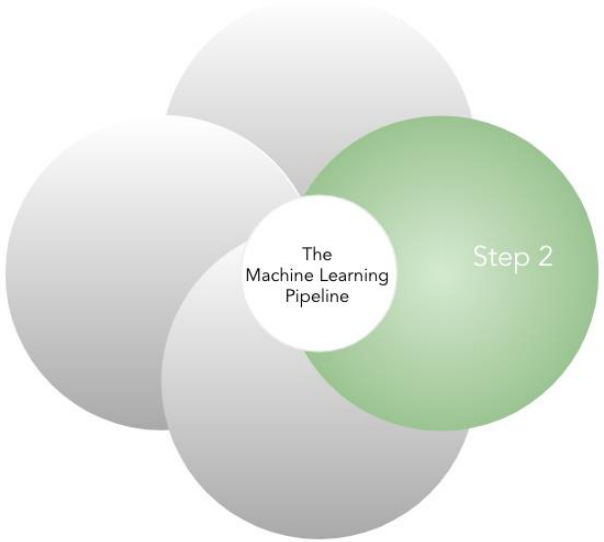
The ML pipeline: Data processing



DATA PROCESSING

- Collection
- Formatting
- Labelling

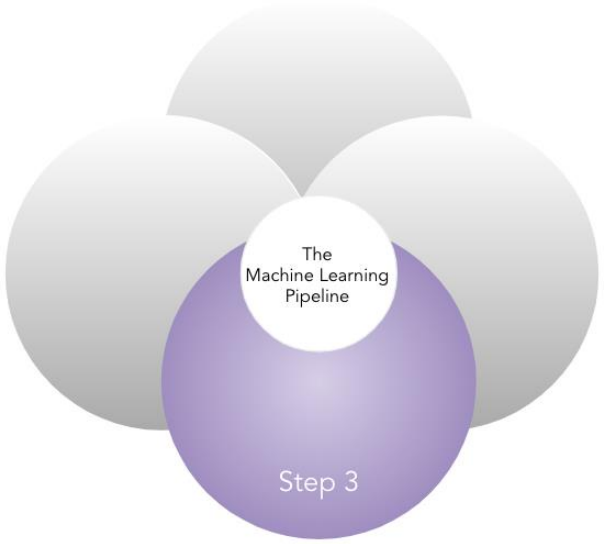
The ML pipeline: Feature extraction



FEATURE EXTRACTION

- Feature Transformation
- Feature Engineering
- Feature Selection

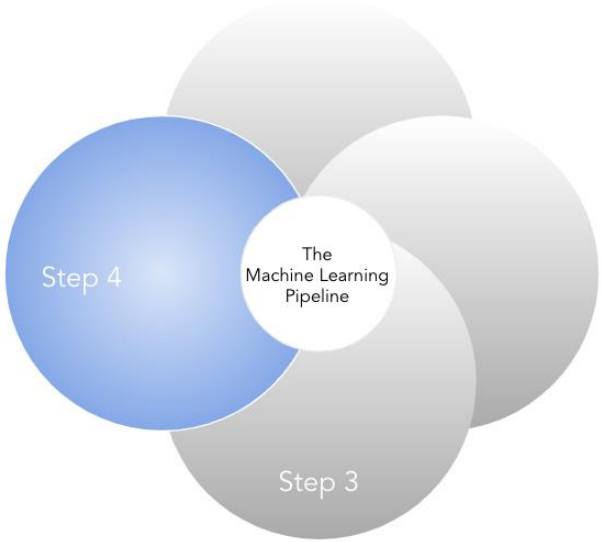
The ML pipeline: Modeling



MODELING

- Model Building
- Model Evaluation

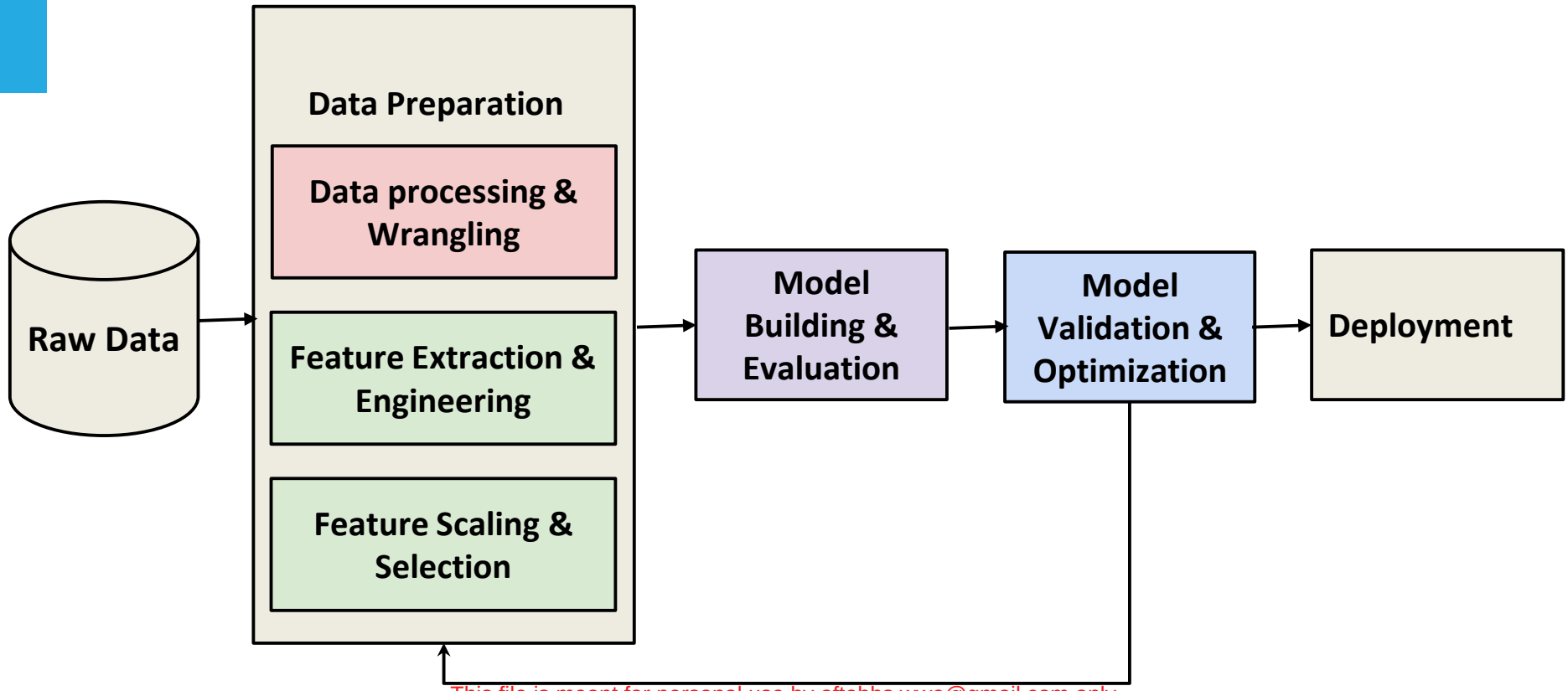
The ML pipeline: Optimization



OPTIMIZATION

- Prediction Evaluation
- Model Validation
- Fine Tuning

The ML pipeline



Data Processing

Data processing

DATA PROCESSING

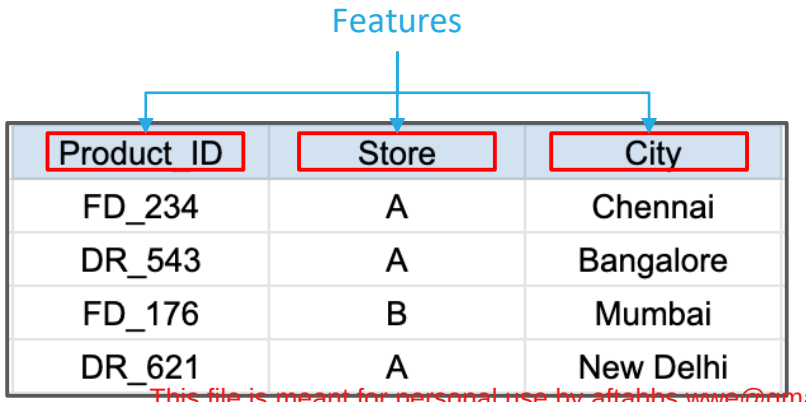
- Collection
- Formatting
- Labelling

- Collection: To extract data from various sources. Generally obtained in the raw form and not immediately suitable for analysis
- Formatting: Organizing the datasets as required for analysis
- Labelling: Manually labelling data

Feature Extraction

Feature

- Feature or attribute is an independent variable that acts as input to our model
- The columns of a dataset are considered as features



Feature Extraction

FEATURE EXTRACTION

- Feature Transformation
- Feature Engineering
- Feature Selection

- Feature Transformation: Replacing the existing features by function of these feature
- Feature Engineering: Creating new features based on empirical relationships
- Feature Selection: Fitting a model of significant features

Feature Transformation

Why do we need feature transformation?

- Incase of skewed (predictor and/or dependent) variable, we transform it to reduce the skewness
- If the assumptions of linear regression are not met, transformation of skewed target variable can be used for making the error terms more compatible to the assumptions
- If the relationship between a predictor and the response variable is non-linear, it can be linearized using transformation

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Assumption of normality

The parametric methods used to compute test statistics or confidence intervals on the predictor variables assume the data to follow a normal distribution

Hence it is favourable that features have approximately normal distribution

Recap: The parametric methods are used when sample statistics adequately represent the population

Rule for transformed variables

Comparison of model performance should be done using the original units for the target variable and not the units after transformation

Transformation methods

- Logarithmic transformation
- Square root transformation
- Reciprocal transformation
- Exponential transformation
- Box-cox transformation

Transformation methods

- Logarithmic transformation
- Square root transformation
- Reciprocal transformation
- Exponential transformation
- Box-cox transformation

Logarithmic transformation

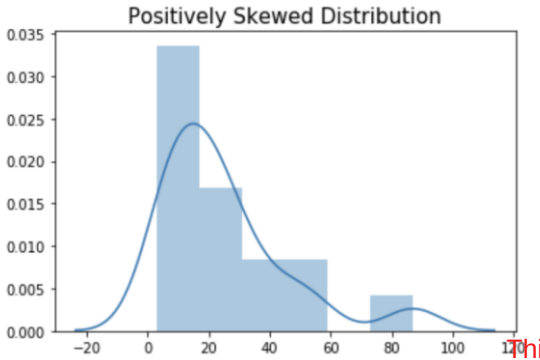
- To linearize, values of a variable are replaced with its natural log
- It cannot be used on a categorical variable after dummy encoding since ln(0) is undefined
- Also if a variable takes zero or negative values, logarithmic transform cannot be used on it

Example of log transformation

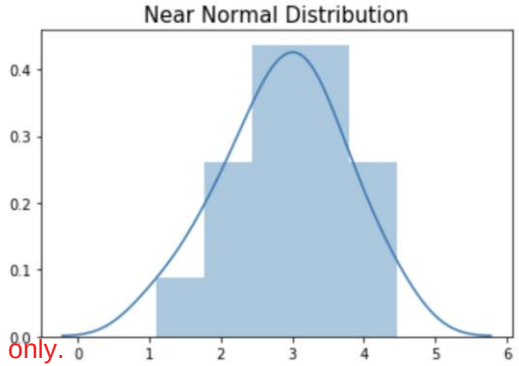
Consider the following data:

Note: Values are rounded to 1 decimals

X	12	9	3	6	24	13	21	6	16	13	54	23	46	32	87	23	34
ln(X)	2.5	2.2	1.1	1.8	3.2	2.6	3.1	1.8	2.7	2.6	3.9	3.1	3.8	3.4	4.5	3.1	3.5



Logarithmic Transformation



Transformation techniques

- Logarithmic transformation
- Square root transformation
- Reciprocal transformation
- Exponential transformation
- Box-cox transformation

Square root transformation

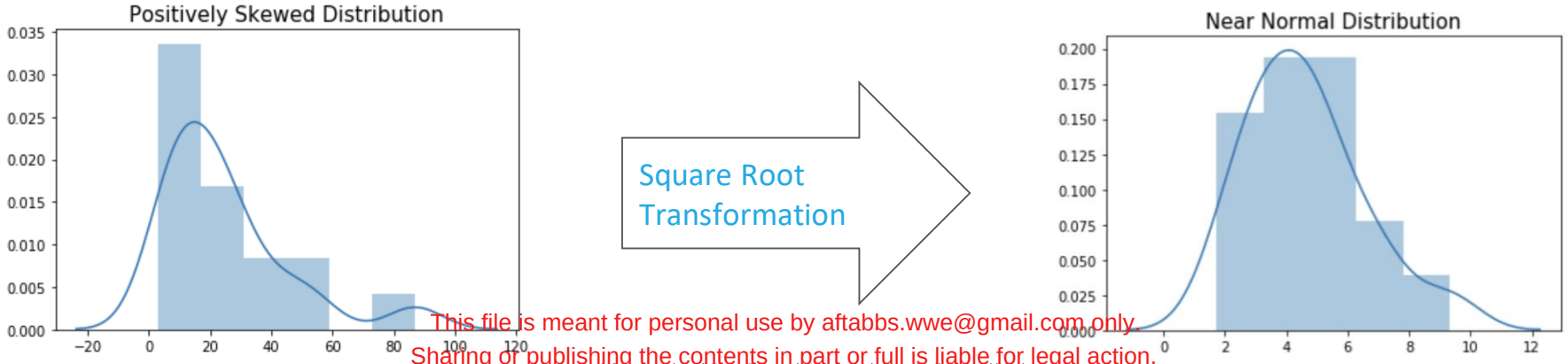
- Values of a variable are replaced with its square root
- To reduce right skewness, we may use square root transformation
- It can be applied even when the variable takes a zero value

Example of square root transformation

Note: Values are rounded to 1 decimals

Consider the following data:

X	12	9	3	6	24	13	21	6	16	13	54	23	46	32	87	23	34
√X	3.5	3	1.7	2.4	4.9	3.6	4.6	2.4	4	3.6	7.4	4.8	6.8	5.7	9.3	4.8	5.8



Transformation techniques

- Logarithmic transformation
- Square root transformation
- Reciprocal transformation
- Exponential transformation
- Box-cox transformation

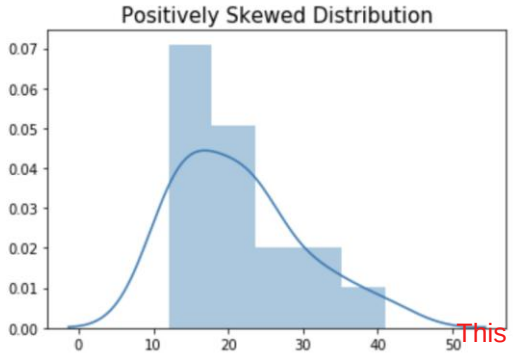
Reciprocal transformation

- Values of a variable are replaced with its reciprocal
- It can not be applied only when the variable takes zero values
- However, can be applied to negative values
- Example: population per area (population density) transforms to area per person

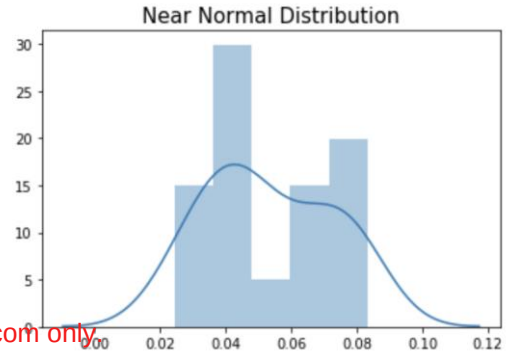
Example of reciprocal

Consider the following data :

X	12	19	23	16	14	13	21	13	16	13	24	23	41	32	27	23	34
1/X	.08	.05	.04	.06	.07	.08	.05	.08	.06	.08	.04	.04	.02	.03	.04	.04	.03



Reciprocal Transformation



Transformation techniques

- Logarithmic transformation
- Square root transformation
- Reciprocal transformation
- Exponential transformation
- Box-cox transformation

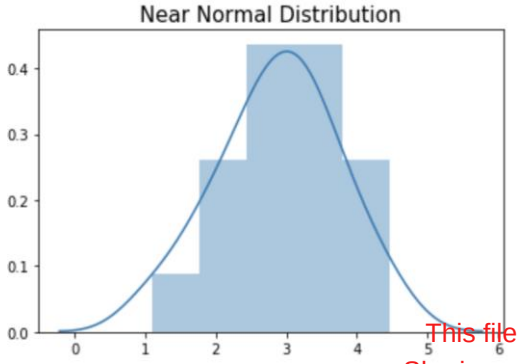
Exponential transformation

- Values of a variable are replaced with its exponential
- It is generally used to transform logarithmic transformed data to get the original data back

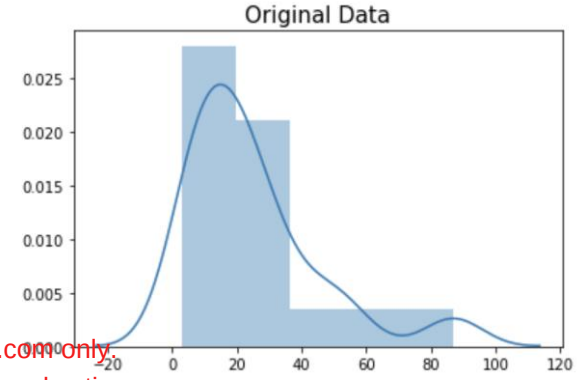
Example of exponential transformation

Consider the data used in logarithmic transformation.

X	12	9	3	6	24	13	21	6	16	13	54	23	46	32	87	23	34
ln(X)	2.5	2.2	1.1	1.8	3.2	2.6	3.1	1.8	2.7	2.6	3.9	3.1	3.8	3.4	4.5	3.1	3.5
exp(X)	12	9	3	6	24	13	21	6	16	13	54	23	46	32	87	23	34



Exponential Transformation



Transformation techniques

- Logarithmic transformation
- Square root transformation
- Reciprocal transformation
- Exponential transformation
- Box-cox transformation

Box cox transformation

- It is defined as

$$X^{\lambda} = \begin{cases} \frac{X^{\lambda}-1}{\lambda} & \text{if} \lambda > 0 \\ \ln(X) & \text{if} \lambda = 0 \end{cases}$$

Here, X is the variable and λ is the transformation parameter and can be tuned according to the data.

- The Box-Cox transformation can only be used on positive variables
- Generalized form of logarithmic transformation

Feature Scaling

Feature scaling

- It is a technique used to transform the data into a common scale
- Since the features have various ranges, it becomes a necessary step in data preprocessing while using machine learning algorithms
- Since most machine learning algorithms use distance calculations, features taking higher values will weigh in more in the distance compared to features taking values of low magnitude

Example

- In a dataset which has variables age and income. The age of a person is measured in years which can takes values between 18 to 65 (retirement age) and income of a person is in thousands
  So it is necessary to bring the two features in the same scale to assign appropriate weights

- In some parts of the world height is measured using metric system (centimetres), while in some other parts the imperial system is used (feet/inches).
  So the results would be different if the height value is 152 cm or 5 feet, when if converted they refer to the exact same height value.

Feature scaling methods

- Normalization
- Standardization

Normalization

Normalization is the process of rescaling features in the range 0 to 1

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)}$$

Standardization

- Standardization rescales the feature such that it has mean 0 and unit variance
- The procedure involves subtracting the mean from observation and then dividing by the standard deviation

$$x' = \frac{x - \bar{x}}{\sigma}$$

When to use Normalization? When to use Standardization?

Normalization is a good technique to use when you do not know the distribution of your data or when you know the distribution is not Gaussian (a bell curve).

Standardization assumes that your data has a Gaussian (bell curve) distribution. This does not strictly have to be true, but the technique is more effective if your attribute distribution is Gaussian.

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Normalization or Min-Max normalization tries to get the values closer to mean, but when there are outliers in the data which are important and we don't want to lose their impact, we go with Standardization or Z score normalization

Min- Max tries to get the values closer to mean. But when there are outliers in the data which are important and we don’t want to lose their impact, we go with Z score. In this case, we rescale an original variable to have a mean of zero and a standard deviation of one. It does not have any units: hence is useful for comparing variables expressed in different units. Standardization makes no difference to the shape of a distribution.

Feature Selection

Feature selection

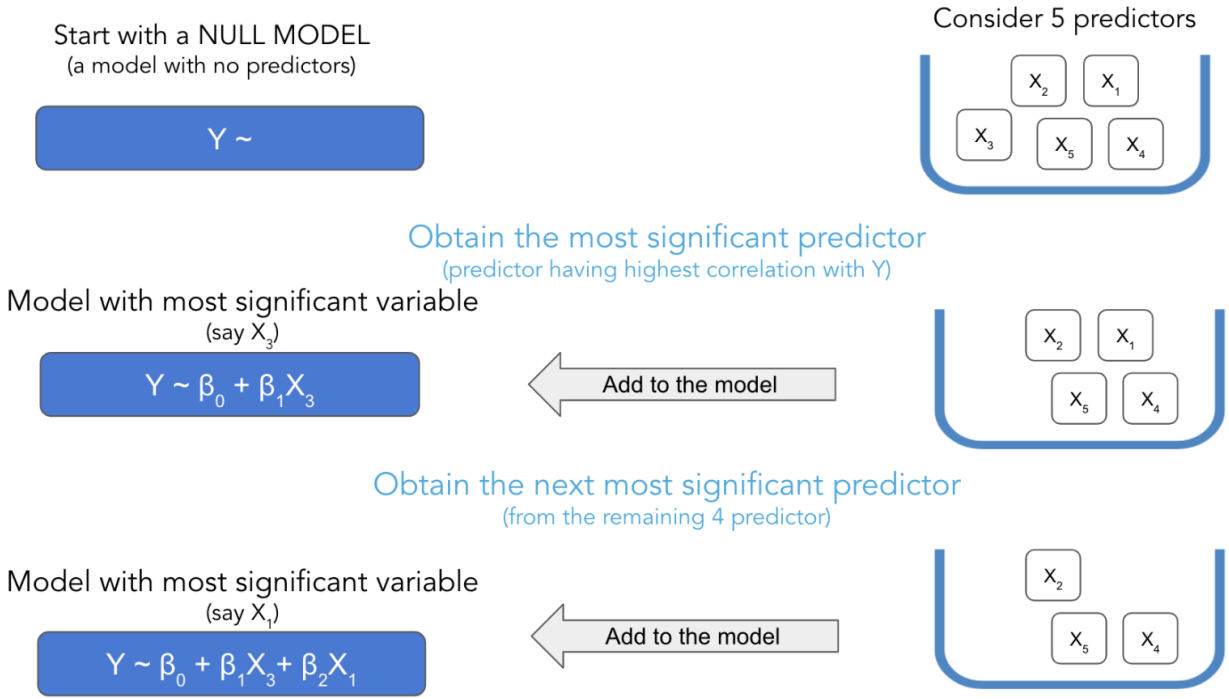
- Feature selection is the process of including the significant features in the model
- This can be achieved by:
  - Forward selection method
  - Backward elimination method
  - Stepwise method
- To understand the above methods let X_1, X_2, ... , X_k be k predictor variables and Y be the response variable

Forward selection method

Procedure

1. Start with a null model (with no predictors)
2. Obtain the correlation between Y and each variable. The variable with highest correlation gets added to the model (say X_m). Build a model $Y \sim X_m$
3. Obtain the correlation between Y and remaining (k-1) variables. The next variable (say X_p) is included, which has the highest correlation with Y after removing X_m
4. Build a model $Y \sim X_m + X_p$. If X_p is significant include it in the model else discard
5. Repeat steps (3) and (4) until reaching the stopping rule or running out of variables

Forward selection method



Backward elimination method

Procedure

1. Start with a full model (model with all k predictors)
2. Remove the variable which is least significant (variable with largest p-value)
3. Fit a new model with remaining (k-1) regressors
4. The next variable (say X_p) is removed if it is least significant
5. Repeat steps (3) and (4) until reaching the stopping rule or all variables are significant

Backward elimination method

Start with a FULL MODEL
(a model with all the 5 predictors)

$$Y \sim \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4 + \beta_5 X_5$$

Obtain the least significant predictor
(predictor having highest p-value)

Model after removing the least significant variable
(say X_3 the least significant)

$$Y \sim \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_4 + \beta_4 X_5$$

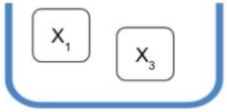
Remove X_3

Obtain the next least significant predictor
(predictor having highest p-value after removing X_3)

Model after removing the least significant variable
(say X_1 is least significant)

$$Y \sim \beta_0 + \beta_1 X_2 + \beta_2 X_4 + \beta_3 X_5$$

Remove X_1

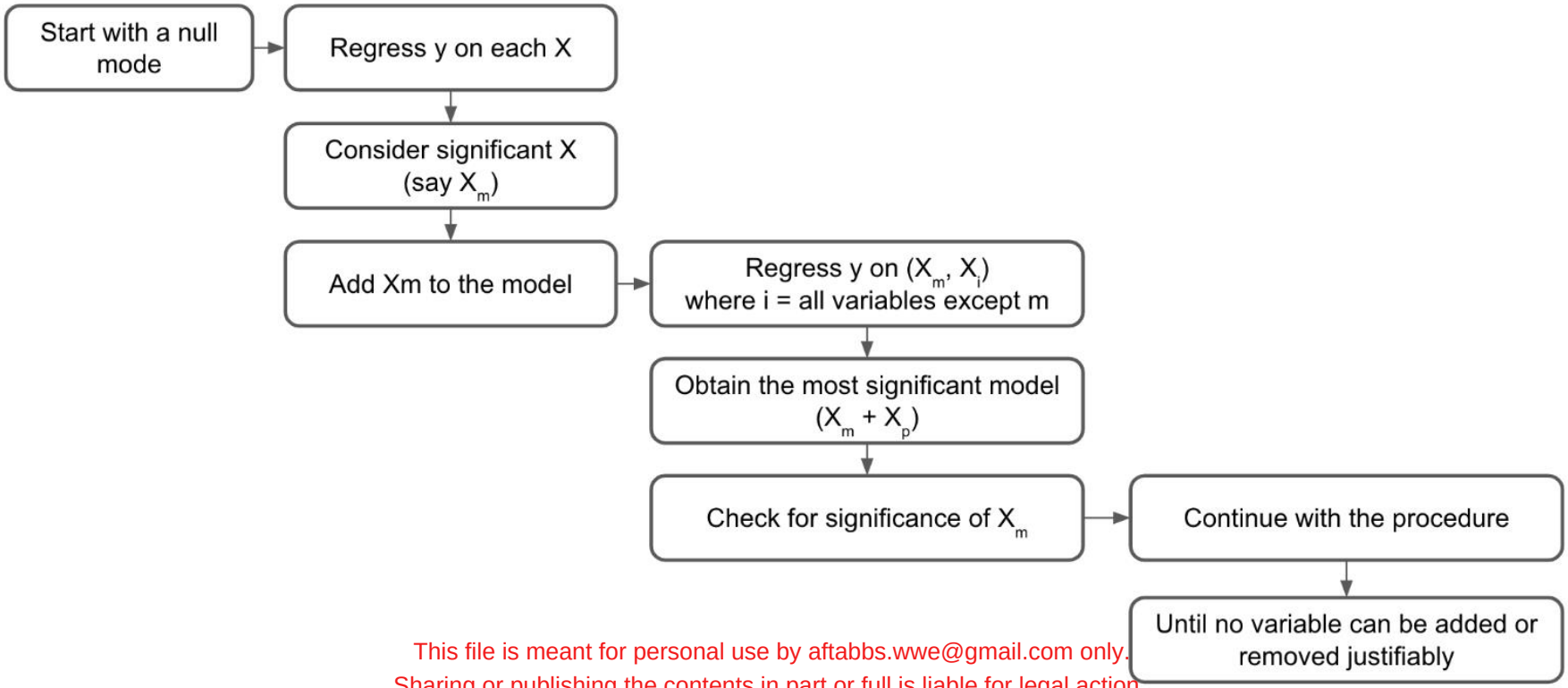


Continue until reaching the stopping rule or running out of variables

Stepwise regression

- It is a combination of forward selection and backward elimination method
- Procedure:
  - Start with a null model (with no predictors)
  - At each step add or remove variable based on its corresponding p-value
  - Stop when no variable can be added or removed justifiably

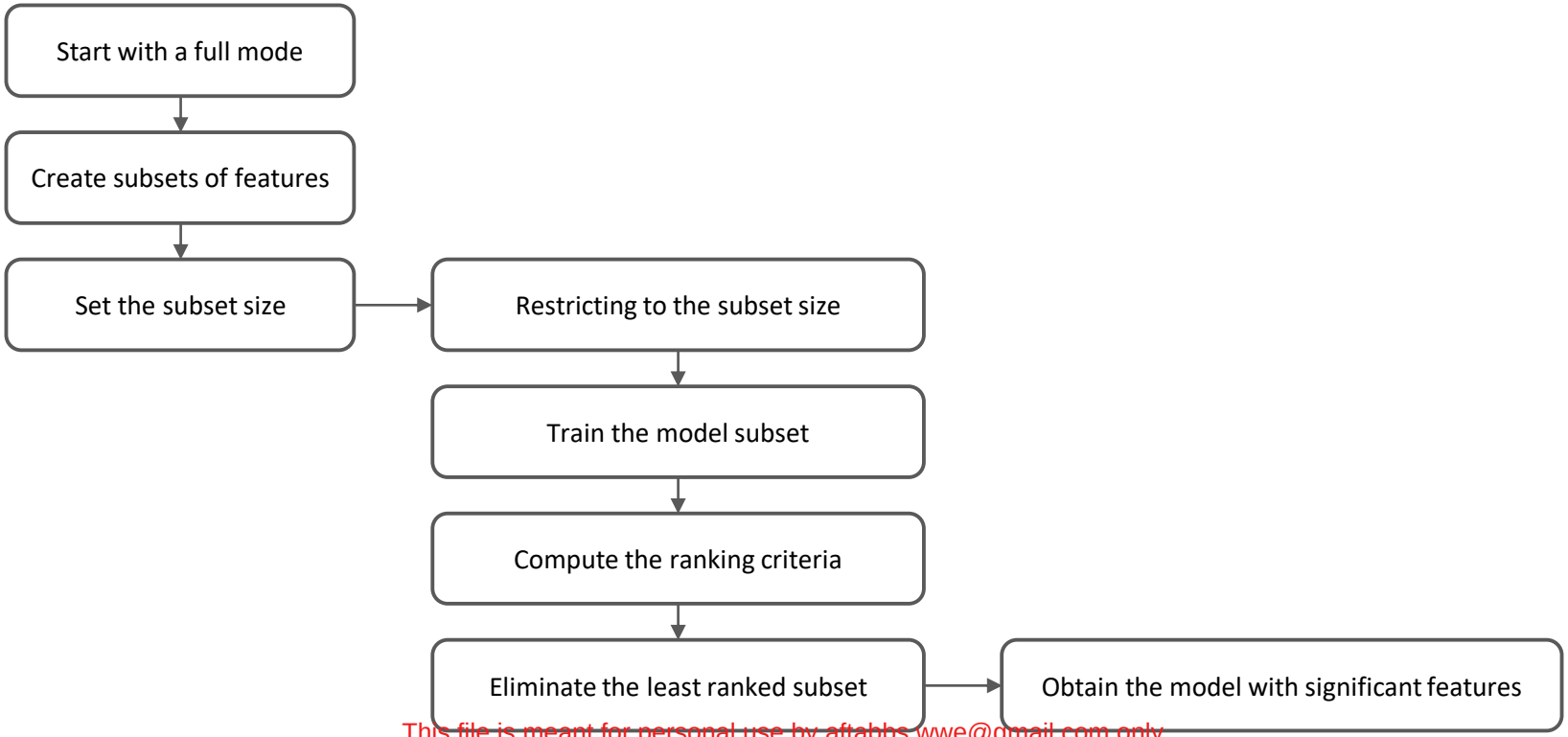
Stepwise regression



Recursive feature elimination (RFE)

- It is an instance of backward feature elimination
- Procedure:
  - Train a full model
  - Create subsets for features
  - Set the subset size
  - Compute the ranking criteria for each feature subset
  - Remove the feature subset that has the least ranking

Recursive feature elimination (RFE)



Optimization

Optimization

OPTIMIZATION

- Prediction Evaluation
- Model Validation
- Fine Tuning

- Prediction Evaluation: Process of evaluating how effectively the constructed model performs predictions
- Model Validation:Using test data to validate the model built using train data
- Fine Tuning: Maximizing the performance of a constructed model

Prediction Evaluation

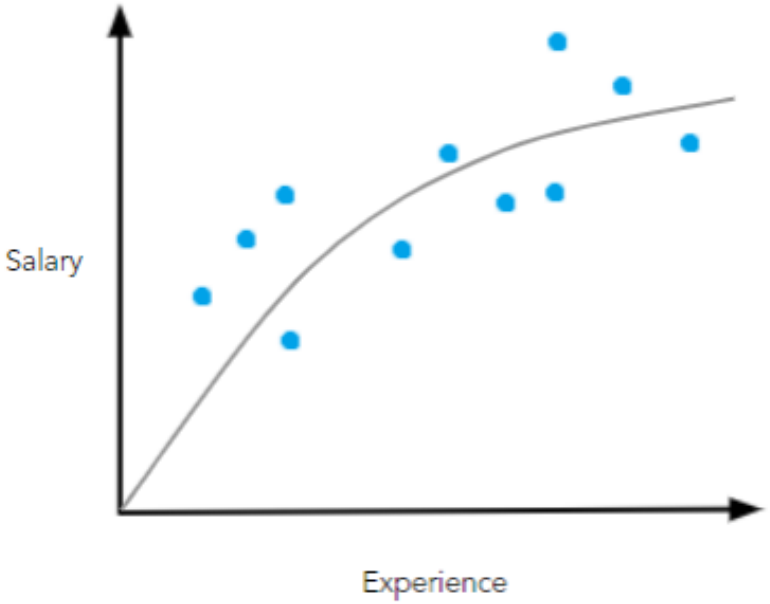
Prediction Evaluation

To construct a model with high prediction efficacy it is important to consider the prediction errors:

- Bias
- Variance

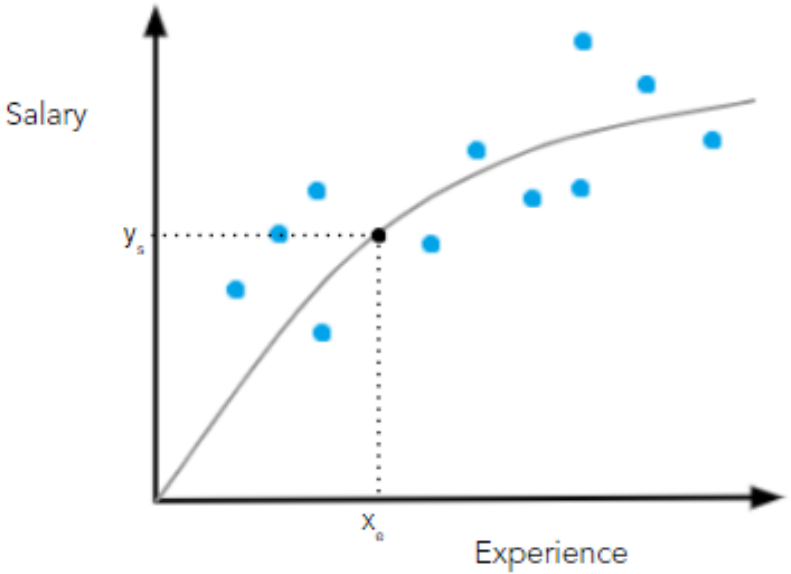
Bias and Variance

Bias and variance



- Consider the example of influence of years of experience on salary
- The plot represents a relationship between salary and experience
- Let us assume a grey curve that captures the true trend for the points in the plot

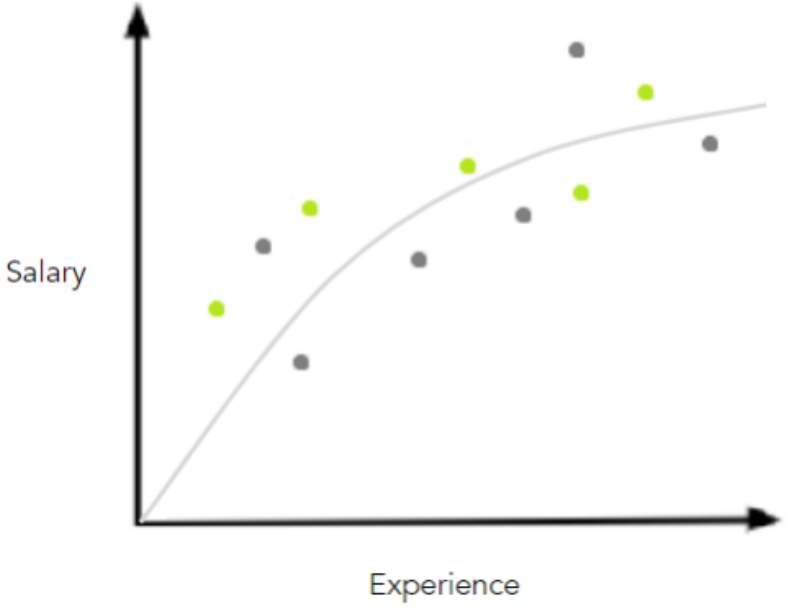
Bias and variance



Given the years of experience information (x_e), we can determine the salary (y_s) using the grey curve

But we do not actually know the grey curve for this plot

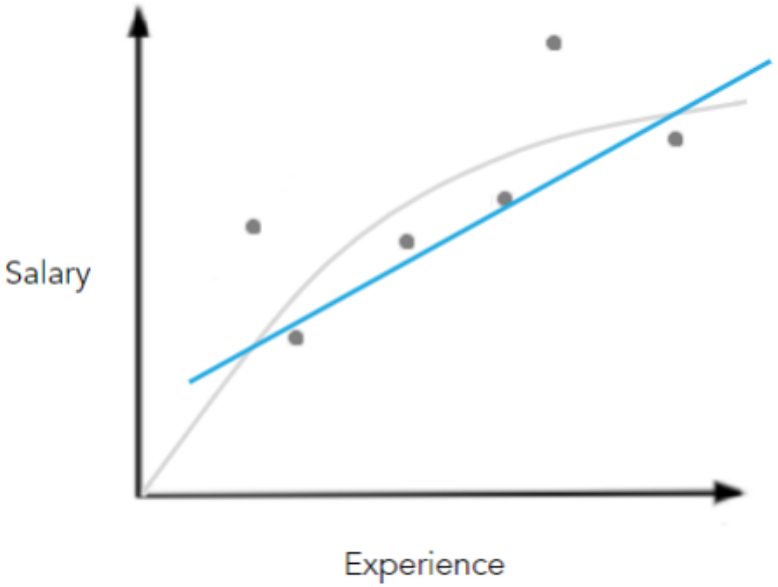
Bias and variance



To find the curve that captures the true trend we divide the data into :

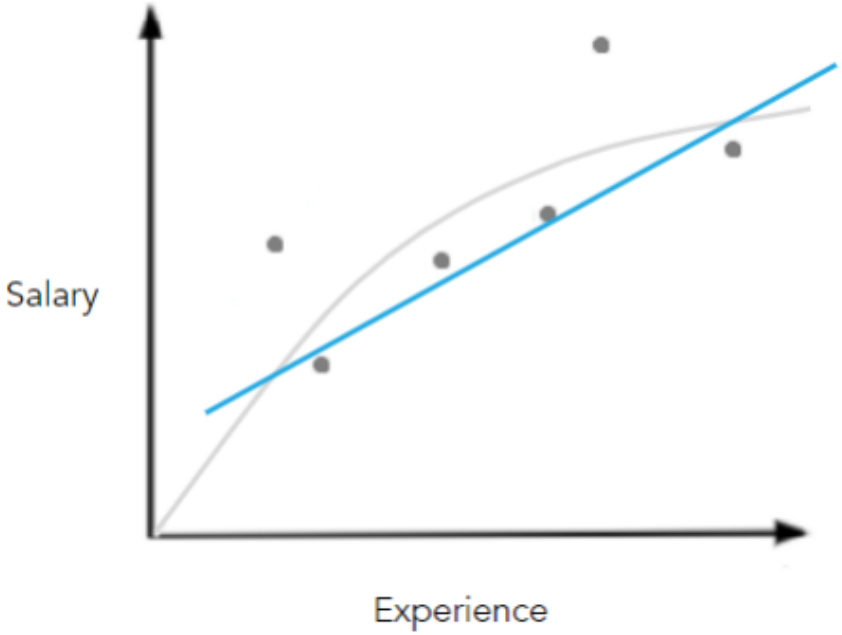
- Train data
- Test data

Bias and variance



- We first estimate a regression line to capture the trend in the train data
- But compared to the line, the grey curve seems to better capture the relationship between experience and salary

Bias

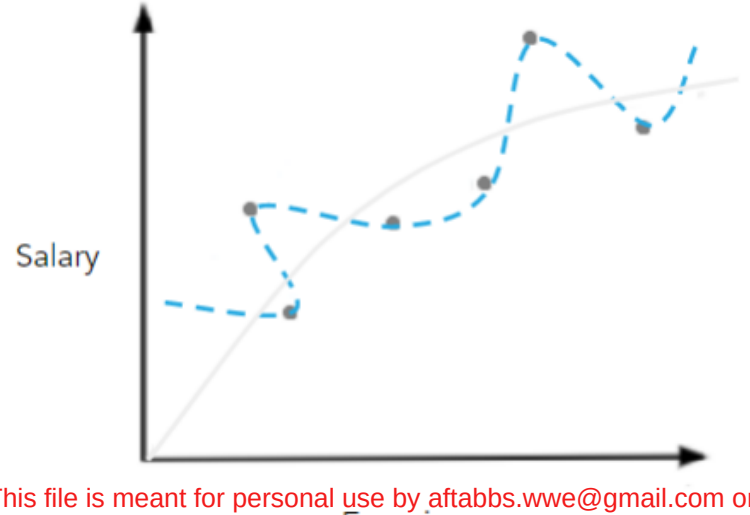


- The linear regression line will never bend and hence will never capture the “true” relationship

- This inability to capture the “true” relationship is called bias

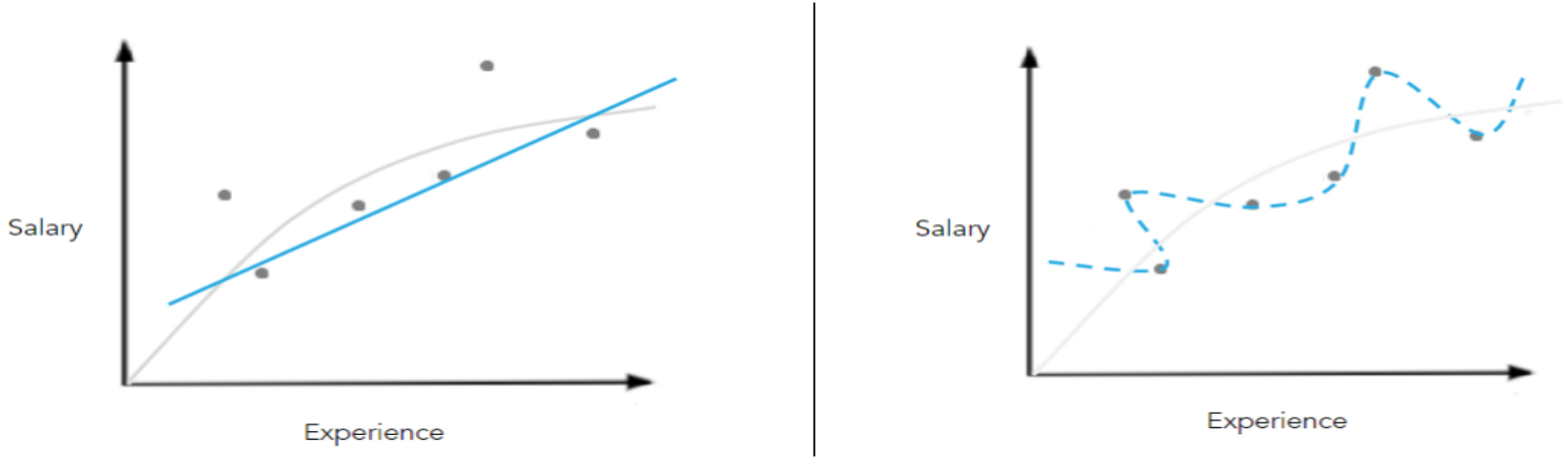
Bias and variance

We then estimate a blue curve that captures the trend in train data perfectly, even better than the grey curve



Error calculation

Error is measured by adding the squares of difference between the actual and the fitted values.



The curve fits the data points so perfectly, the difference between the actual and fitted values is actually zero.

Bias and variance

We use the same blue line and blue curve to estimate trends in test data

Bias and variance

Even though the blue curve fits the train data with zero error, it does not predict well on test data

Variance

This difference in fits is called variance

Bias and variance

- Bias is the difference between a model's predicted values and the observed values

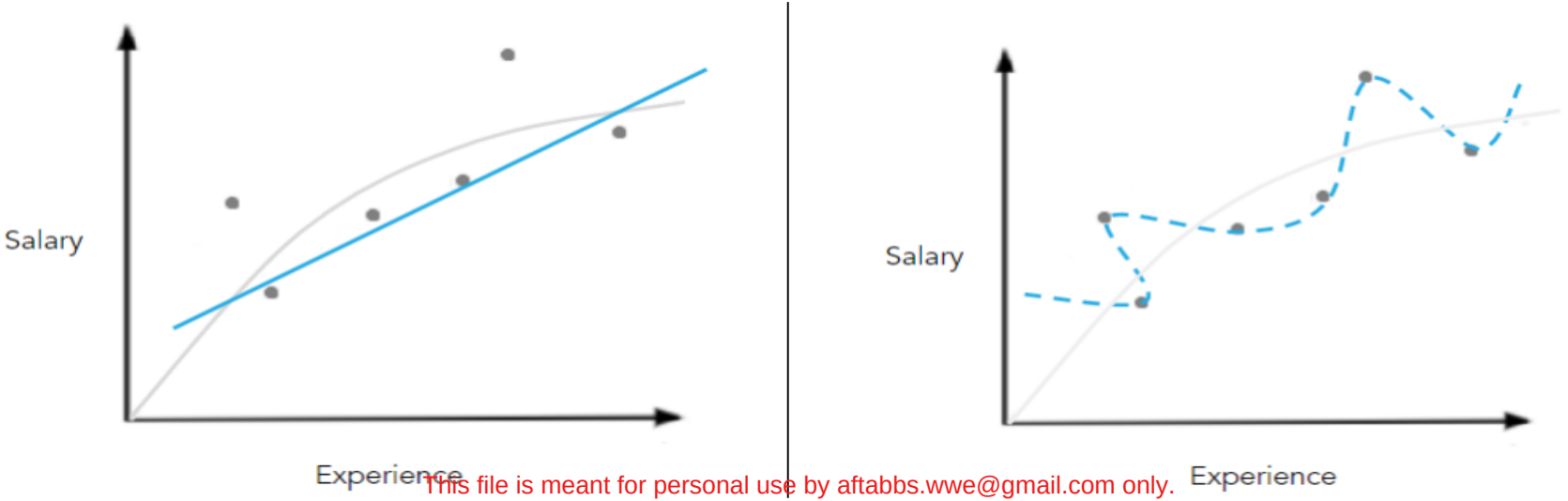
- Variance of a model is the difference between predictions if the model is fit to different datasets

Bias-Variance for a simple model

- If the model is too simple it will have a high bias and low variance
- Such a model will give not perfectly accurate predictions, but the predictions will be consistent
- The model will not be flexible enough to learn from majority of given data, this is termed as underfitting

Example for bias

As we can see compared to the blue line, the blue curve captured the trend in train data perfectly. Hence we can say that the blue line has a high bias.



Bias-Variance for a complex model

- If the model is too complex it will have a low bias and high variance
- Such a model will give accurate predictions but inconsistently
- The high variance indicates it will have a much better fit on the train data compared to the test data, this is termed as overfitting

Model Validation

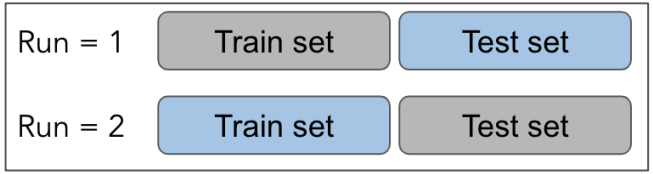
Model validation

- The model validation methods use test data to validate the model built using train data

- The model validation:
  - k - fold cross validation
  - Leave one out cross validation (LOOCV)

Cross validation

- Procedure:
  - Consider a data having ‘2n’ observations
  - Partition the dataset into two subsets: train and test sets of the equal size (n)
  - Measure the model performance
  - Swap the train and test sets
  - Total error is obtained by summing up the errors for both runs



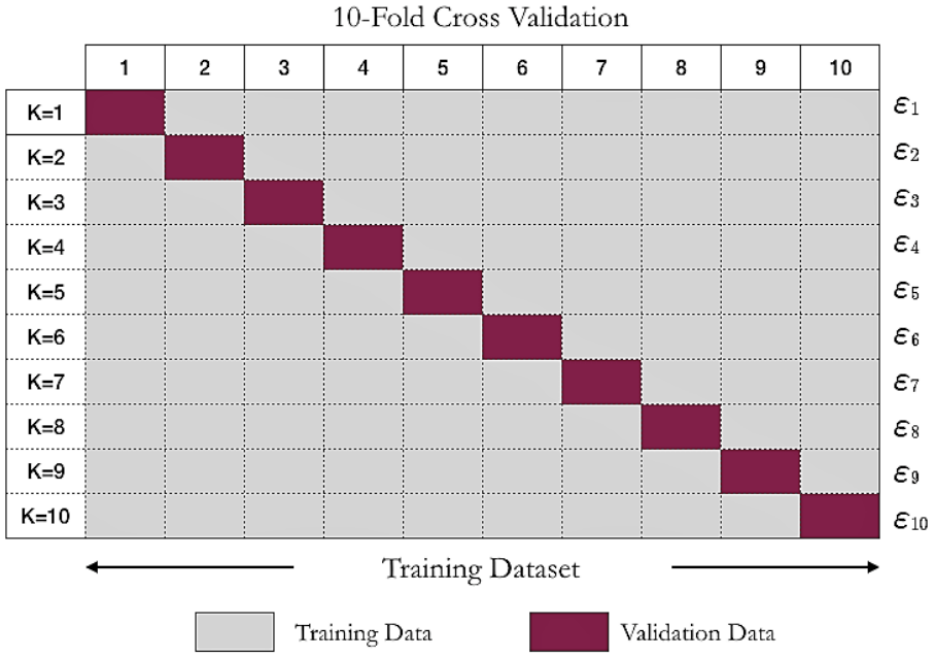
- This method is known as two fold cross validation
- Here, each observation is used exactly once for training and once for testing

The k - fold cross validation

- Procedure:
  - Partition the dataset into ‘k’ subsets
  - Consider one subset as the test set and remaining subsets as train set
  - Measure the model performance
  - Repeat this until all k subsets are considered as test set
  - Total error is obtained by summing up the errors for all the k runs
- This method is known as the k - fold cross validation
- Here, each observation is used exactly k times for training and exactly once for testing

10 - Fold cross validation

The split of training and test for each run.



And the total error is given by:

$$\epsilon = \frac{1}{10} \sum_{i=1}^{n=10} \epsilon_i$$

LOOCV

- It is a special case of k - fold cross validation method. Instead of subsetting the data, at every run one observation is considered as the test set
- For n observations, there are n runs
- The total error is the sum of errors for n runs
- In LOOCV, the estimates from each fold are highly correlated and their average can have a high level of variance

Thank You