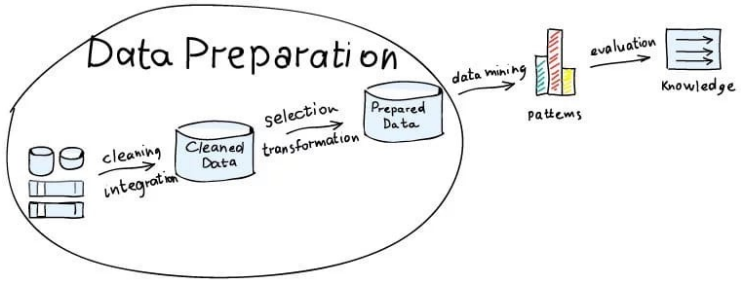
CHULA ENGINEERING
Foundation toward Innovation

COMPUTER



Data Preparation with Python

2110531: Data Science and Data Engineering Tools

Peerapon Vateekul, Ph.D.
Department of Computer Engineering,
Faculty of Engineering, Chulalongkorn University
Peerapon.v@chula.ac.th

+

Recap of "Introduction to Data Science"

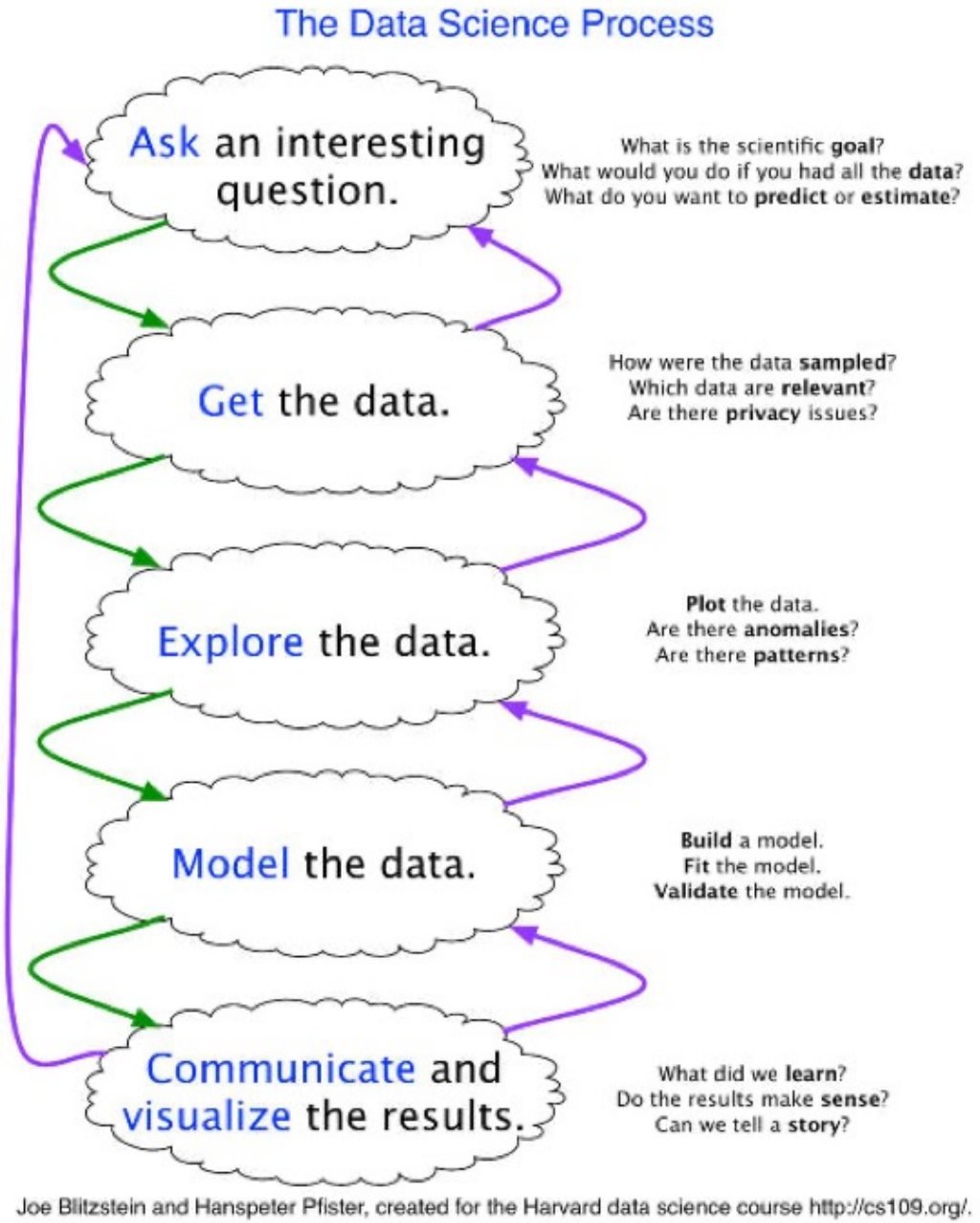
Data Science Process

Dr.Virote

1. Transform data into valuable insights
2. Transform data into data products
3. Transform data into interesting stories

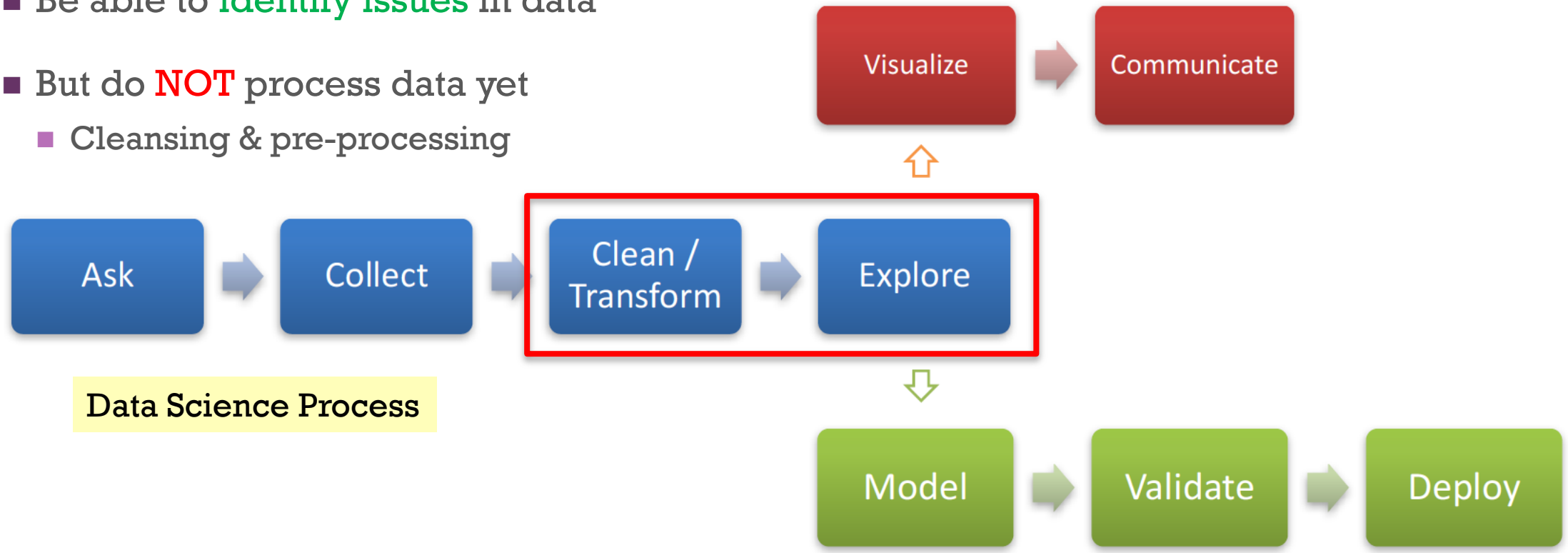
Aj.Natawut

1. Measurement
2. Insights
3. Data Products



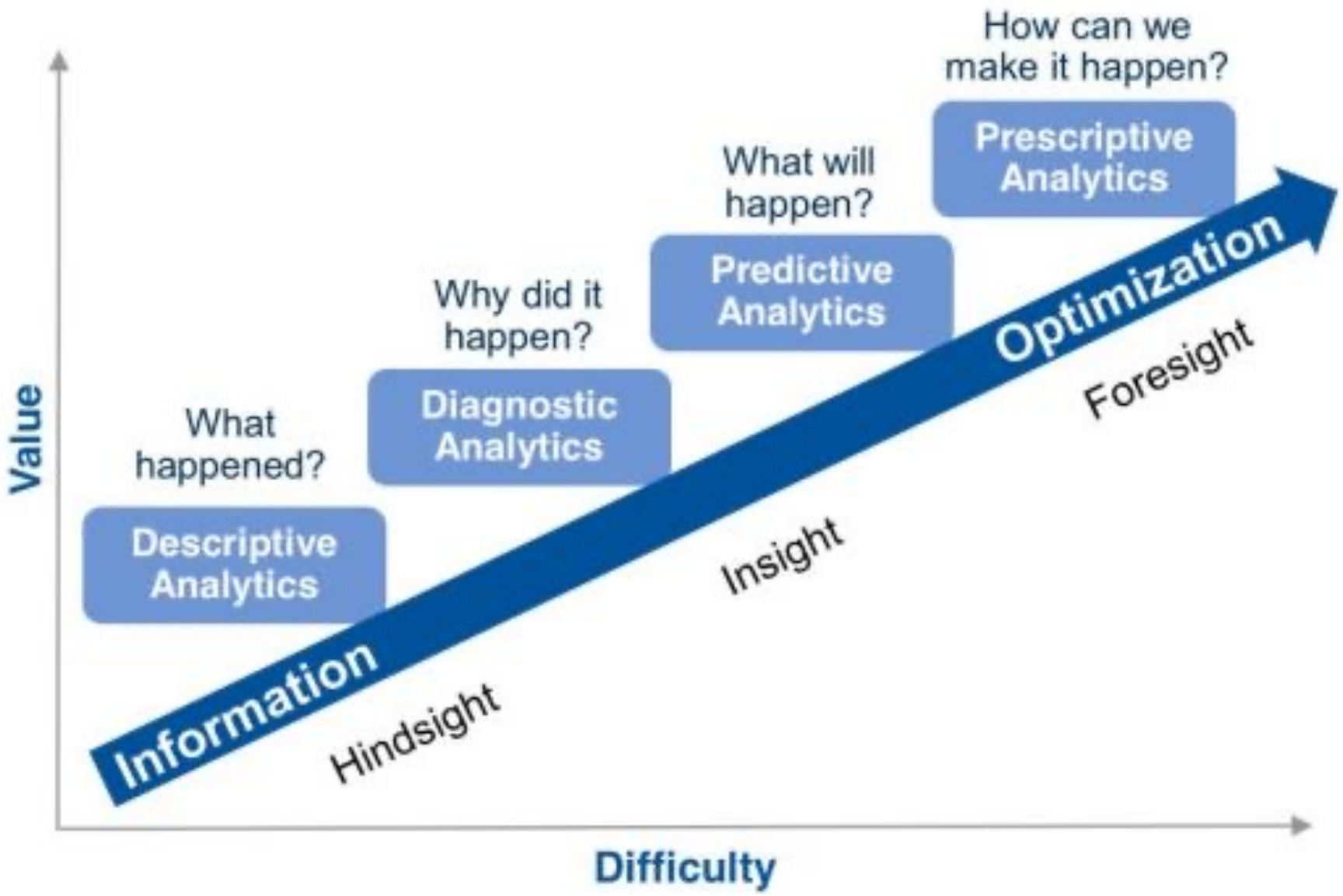
Data Science Process

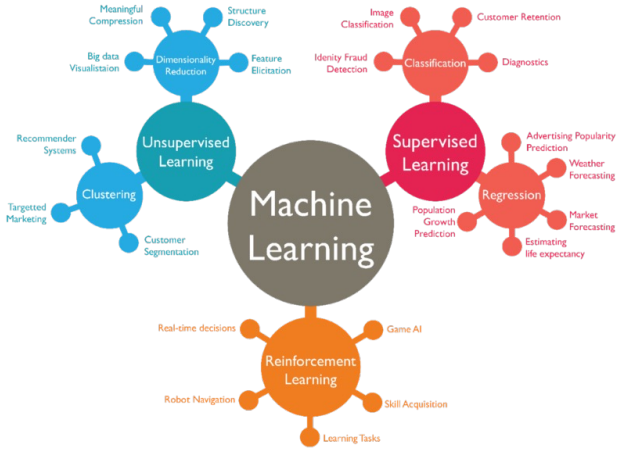
- Be able to explore data
- Be able to identify issues in data
- But do NOT process data yet
  - Cleansing & pre-processing

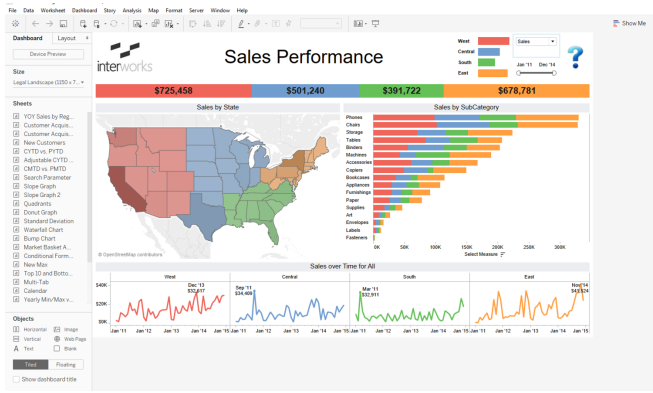


Data Science Process

Data Analytics







Data Preparation

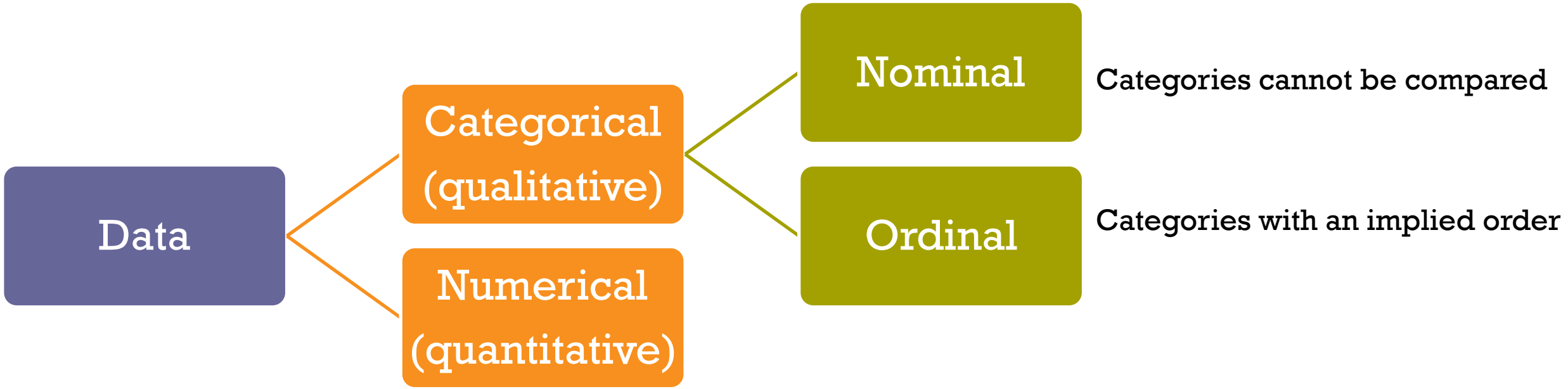
Terminology: Data table

inputs | target

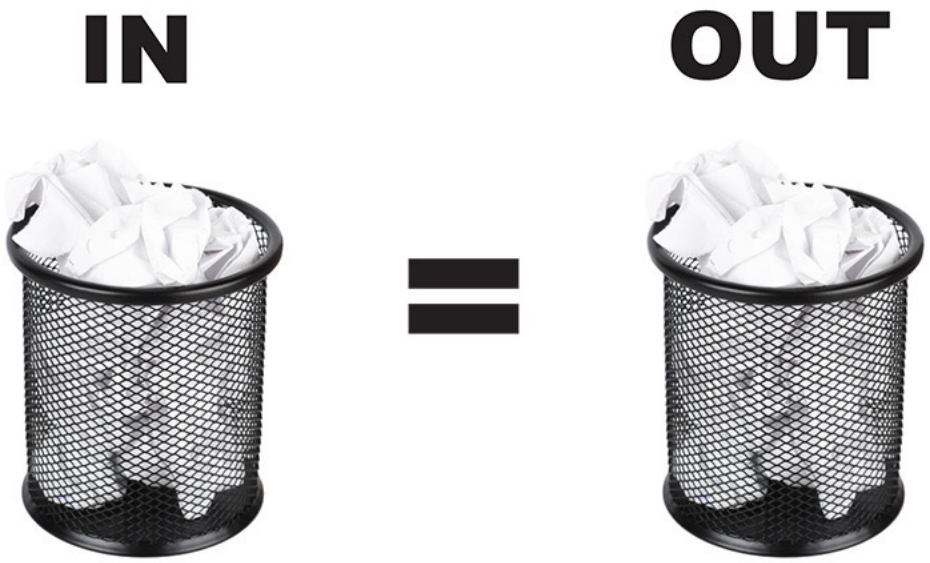
Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes
35	50,000	Female	Nontaburi	Yes
32	35,000	Male	Bangkok	No

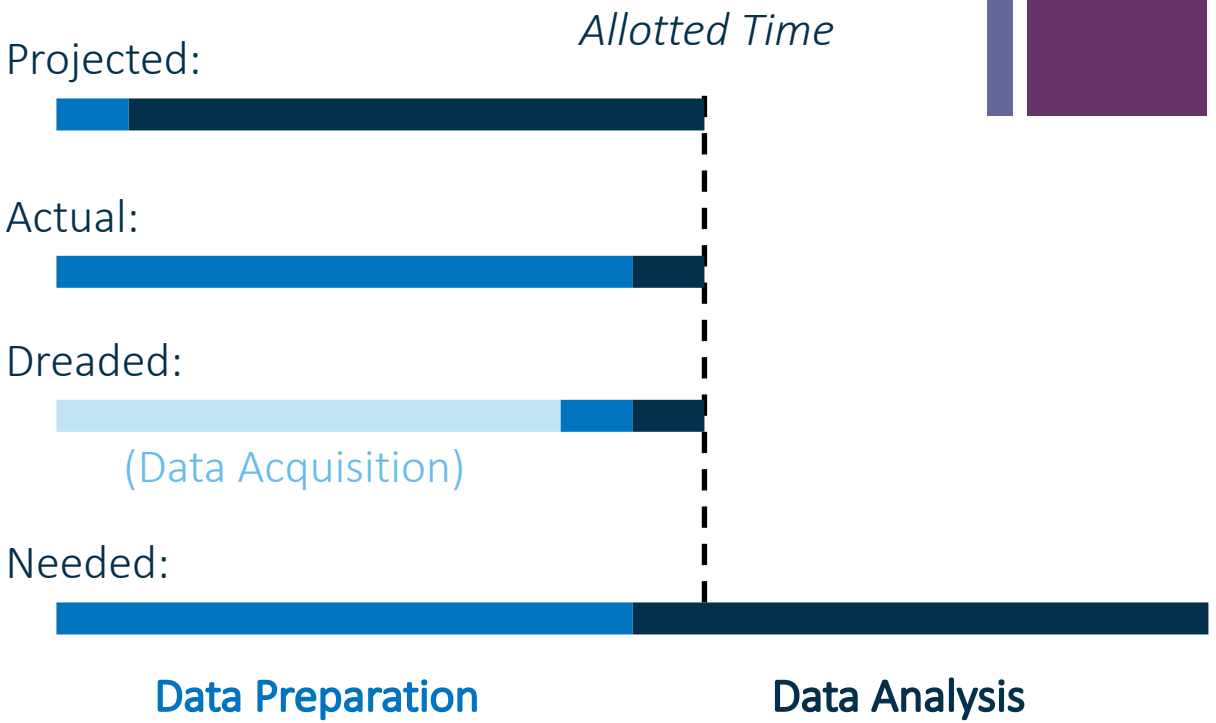
- Row
  - Example, instance, case, observation, subject
- Column
  - Feature, variable, attribute
- Input
  - Predictor, independent, explanatory variable
- Target
  - Output, outcome, response, dependent variable

Terminology: Kinds of data

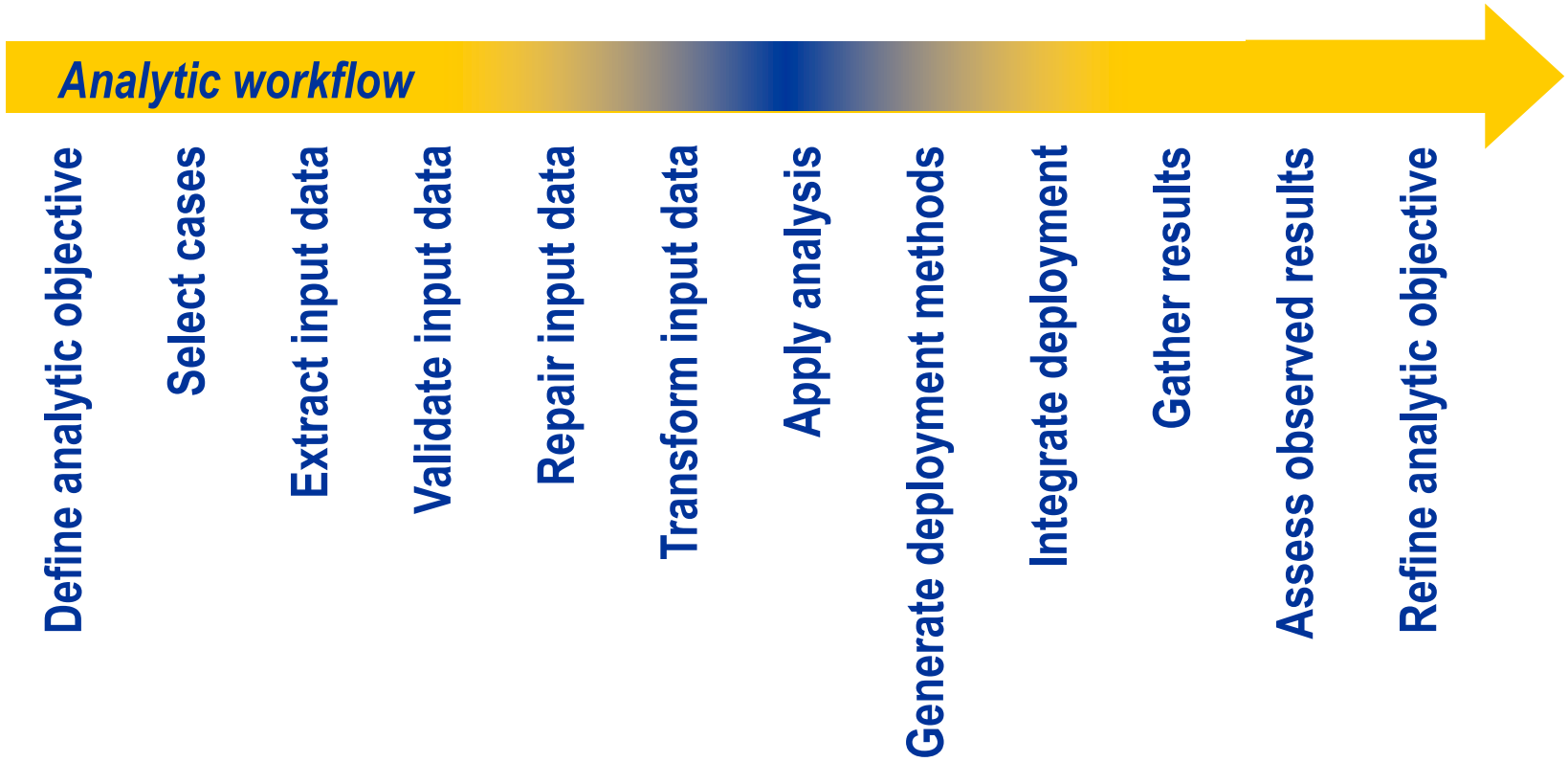


Data preparation is very important!





Analytics workflow



Data preparation challenges

- Massive data sets

- Temporal infidelity

- Transaction and event data

$$\hat{y} = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2$$

- Non-numeric data

$$Spend = 500 + 2 \times Age + 3 \times Province$$

- Exceptional, extreme, and missing values

- Stationarity


Practice is everything.
Periander
quotefancy

28 DECEMBER 2016 / DATA CLEANING

Preparing and Cleaning Data for Machine Learning

- 1) Examining the Data Set
- 2) Narrowing down columns manually
  - Remove Id's
  - Irrelevant variables
  - Remove zipcode & date
  - Temporal infidelity (data from future)
  - Calculated variables
  - Decide target
    - Select studied cases
    - Distribution of target variables
  - Remove flat values
- 3) Preparing features for ML
  - Preview data
  - Handling missing values
    - Drop unqualified features
  - Investigate categorical features
    - Drop too many unique values (treat as Id)
    - Convert ordinal to numeric
    - Convert categorical to numeric
  - Check all numeric variables
- 4) Other preprocessing steps:
  - Train/Test/Validate

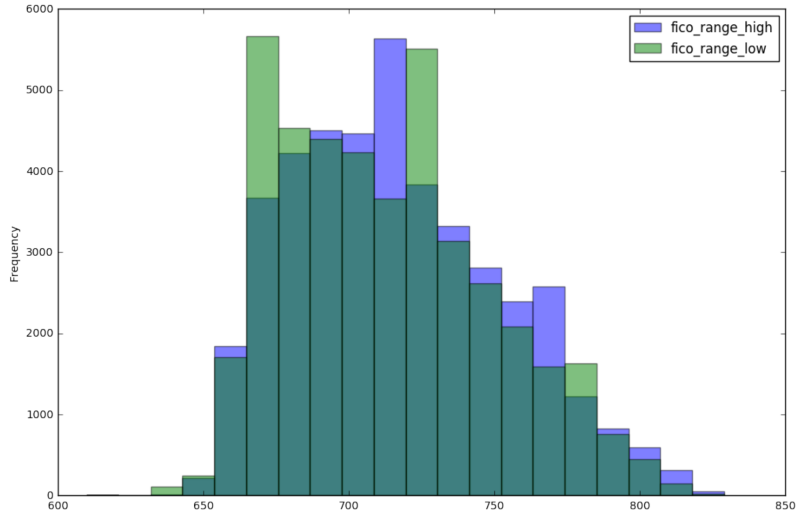
https://www.dataquest.io/blog/machine-learning-preparing-data/

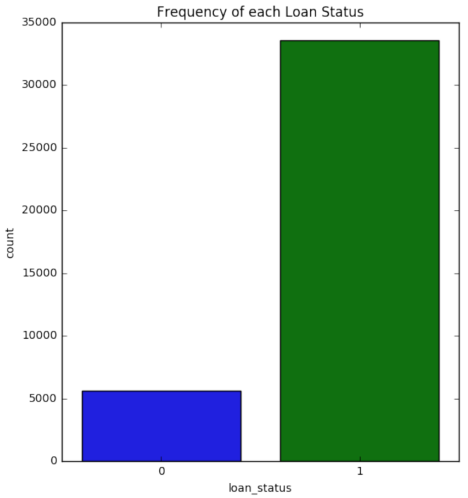
1) Examining the Data Set

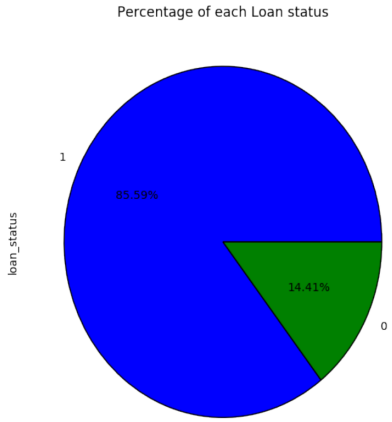
- Numerical variables
  - Out of ranges
  - Distribution: histogram

- Categorical variables
  - Miscodes
  - Distribution: frequency table, bar chart

- Target variable
  - Understand class distribution (proportion of each class): bar chart, pie chart







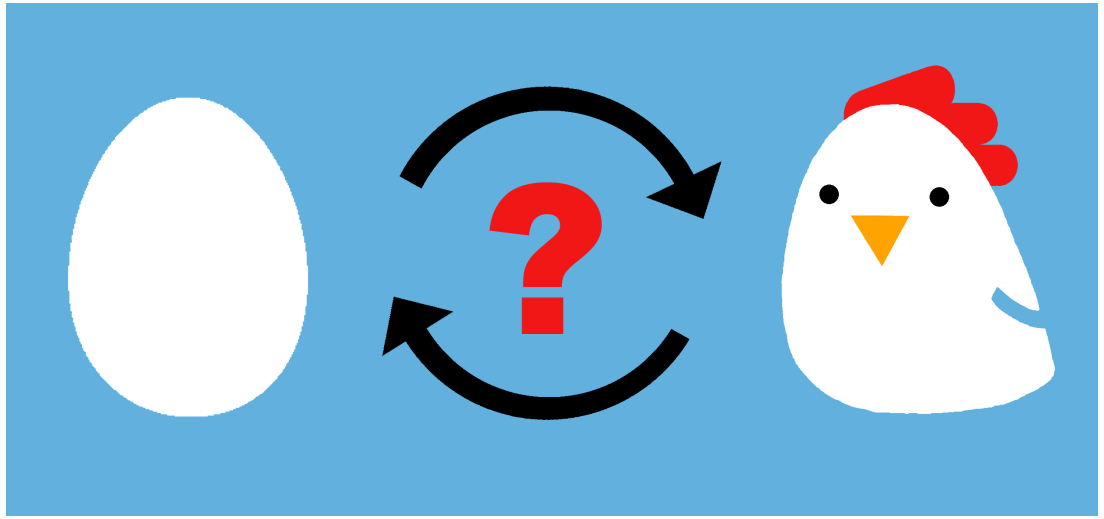
2) Narrowing down columns: Feature understanding is extremely important!

Remove irrelevant features manually

Domain expert

Inputs

Target



2) Narrowing down columns (cont.): Remove unqualified features

- Remove unqualified features
- ID's (lack of generalization; overfit)
- Variables with missing values > 50%
- Categorical variables
  - Too many unique values (treat as ID's)
  - Flat values (underfit)

- Special ways to treat these data
- High cardinalities of categorical inputs
  - Recode, consolidation (grouping)
- Zip code
  - Distance to closet branch
- Date/time
  - Recency
  - Month, day of week, year
  - Hours, period of days

2) Narrowing down columns (cont.): Remove temporal Infidelity features

- Occurs when the input variables contain information that will be unavailable at the time that the prediction model is deployed.
- Assume that the model will be deployed in July-2017
  - Should we include a variable called "FICO2017", which is calculated at the end of the year?

2) Narrowing down columns (cont.): Remove leaking-target features

Target variables quantify account responses during the current campaign season.

Name	Label	Description
B_TGT	Tgt Binary New Product	A binary target variable. Accounts coded with a 1 contracted for at least one product in the previous campaign season. Accounts coded with a zero did not contract for a product in the previous campaign season.
INT_TGT	Tgt Interval New Sales	The amount of the financial services products (sum of sales) per account in the previous campaign season, denominated in US dollars.
CNT_TGT	Tgt Count Number New Products	The number of the financial services products (count) per account in the previous campaign season.

3) Preparing features for ML (cont.): 3.1 Impute missing values

? != 0

$$\hat{y} = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2$$

$$Spend = 500 + 10 \times IncomeK - 20 \times Age$$

- For missing in target, those examples must be removed.
- For missing in inputs, either remove those examples or impute missing values

- 1) Statistical approach
- Numerical variables:
  - Mean
  - Median
- Categorical variables:
  - Mode (most-frequent)
- Stats by group can improve the performance, e.g., income by age group.
- 2) Model-based approach
  - x1 ~ (x2, x3, x4, …)
  - Income ~ Age
  - Tree-based imputation

$$Spend = 500 + 10 \times IncomeK - 20 \times Age + 3 \times Province$$

3) Preparing features for ML (cont.): 3.2 Categorical to numeric variables

- Ordinal variable
  - Enumerate

Grade	GradeNum
A	4.00
B+	3.50
B	3.00
C+	2.50
C	2.00
D+	1.50
D	1.00
F	0.00

Size	SizeNum
XL	5
L	4
M	3
S	2
XS	1

- Nominal variable
  - (1) One-hot vector (dummy codes)
  - (2) Target Averaging (prob)
  - (3) Weight of Evidence (WoE)
  - (4) Smoothed weight of evidence (SWoE)

(1) One-hot vector (dummy codes)

- Dummy coding = (n-1) dummy codes

Branch	BranchNum	D_BKK	B_Patum	D_Non	D_BKK	B_Patum	
BKK	1	1	0	0	1	0	
Patumtani	2	0	1	0	0	1	
Nontaburi	3	0	0	1	0	0	reference

(1) One-hot vector (dummy codes) – Example2

Level	D_A	D_B	D_C	D_D	D_E	D_F	D_G	D_H	D_I
A	1	0	0	0	0	0	0	0	0
B	0	1	0	0	0	0	0	0	0
C	0	0	1	0	0	0	0	0	0
D	0	0	0	1	0	0	0	0	0
E	0	0	0	0	1	0	0	0	0
F	0	0	0	0	0	1	0	0	0
G	0	0	0	0	0	0	1	0	0
H	0	0	0	0	0	0	0	1	0
I	0	0	0	0	0	0	0	0	1

(1) One-hot vector (dummy codes) – Example2

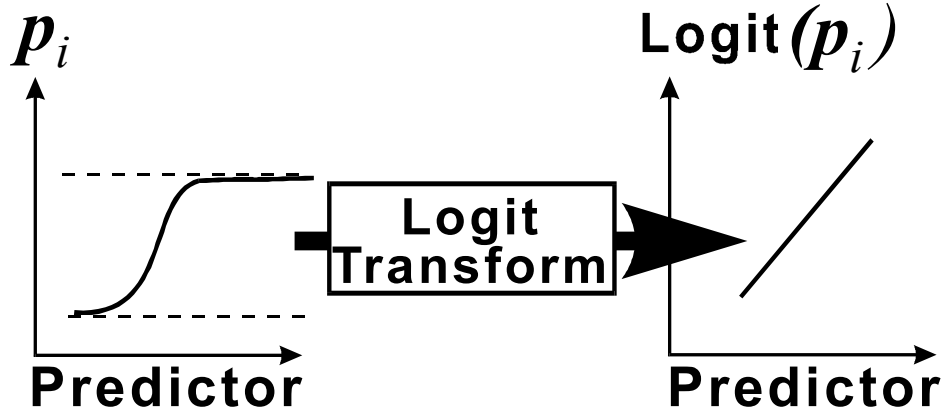
Level	D_A	D_B	D_C	D_D	D_E	D_F	D_G	D_H	D_I
A	1	0	0	0	0	0	0	0	0
B	0	1	0	0	0	0	0	0	0
C	0	0	1	0	0	0	0	0	0
D	0	0	0	1	0	0	0	0	0
E	0	0	0	0	1	0	0	0	0
F	0	0	0	0	0	1	0	0	0
G	0	0	0	0	0	0	1	0	0
H	0	0	0	0	0	0	0	1	0
I	0	0	0	0	0	0	0	0	1

(2) Target Averaging

Level	N_i	ΣY_i	p_i
J	5	5	1.00
I	12	6	0.50
B	970	432	0.45
F	50	20	0.40
G	23	8	0.35
D	111	36	0.32
H	17	5	0.29
A	1562	430	0.28
E	85	23	0.27
C	223	45	0.20

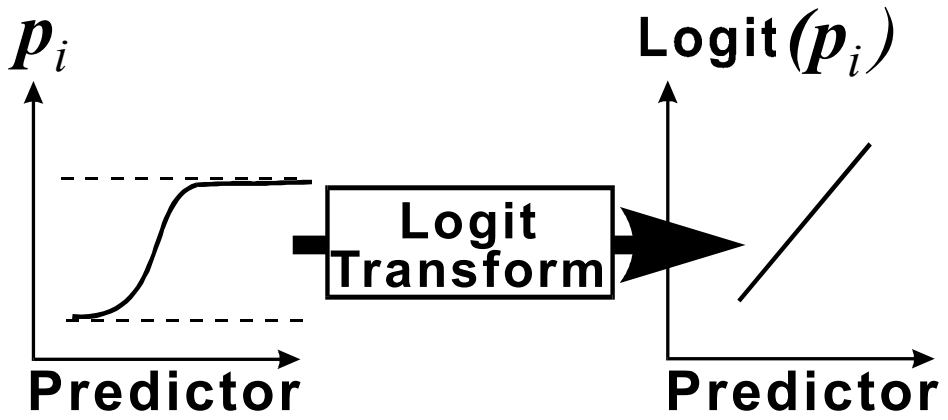
(3) Weight of Evidence (WoE)

Level	N_i	ΣY_i	p_i	$\log(p_i/1-p_i)$
J	5	5	1.00	.
I	12	6	0.50	0.00
B	970	432	0.45	-0.10
F	50	20	0.40	-0.18
G	23	8	0.35	-0.27
D	111	36	0.32	-0.32
H	17	5	0.29	-0.38
A	1562	430	0.28	-0.42
E	85	23	0.27	-0.43
C	223	45	0.20	-0.60

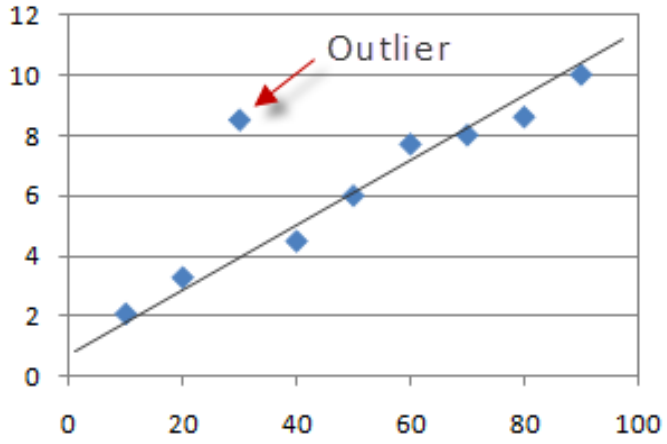


(4) Smoothed Weight of Evidence (SWoE)

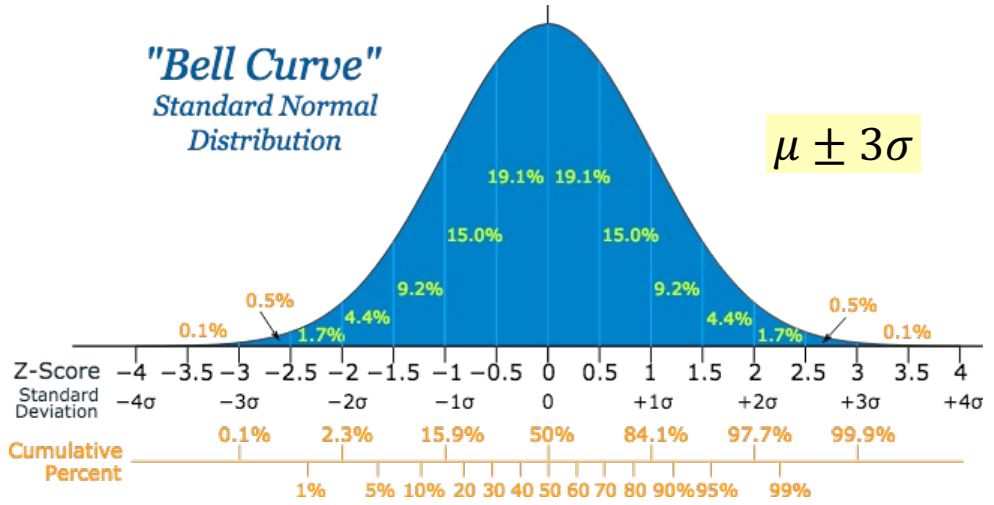
Level	N_i		ΣY_i		p_i	$\log(p_i/1-p_i)$
J	5	+24	5	+8	0.45	-0.09
I	12	+24	6	+8	0.39	-0.19
B	970	+24	432	+8	0.44	-0.10
F	50	+24	20	+8	0.38	-0.22
G	23	+24	8	+8	0.34	-0.29
D	111	+24	36	+8	0.33	-0.32
H	17	+24	5	+8	0.32	-0.33
A	1562	+24	430	+8	0.28	-0.42
E	85	+24	23	+8	0.28	-0.40
C	223	+24	45	+8	0.21	-0.56

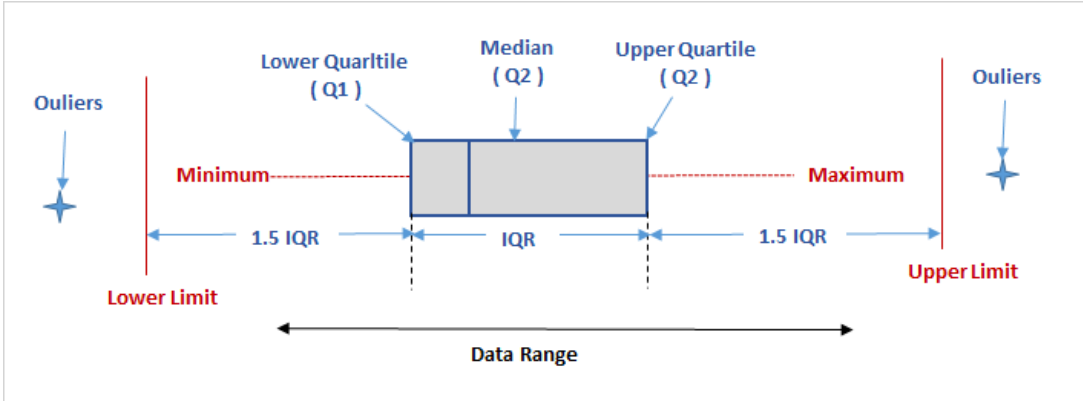


3) Preparing features for ML (cont.): 3.3 Truncate outliers



- Outlier, leverage points, extreme values

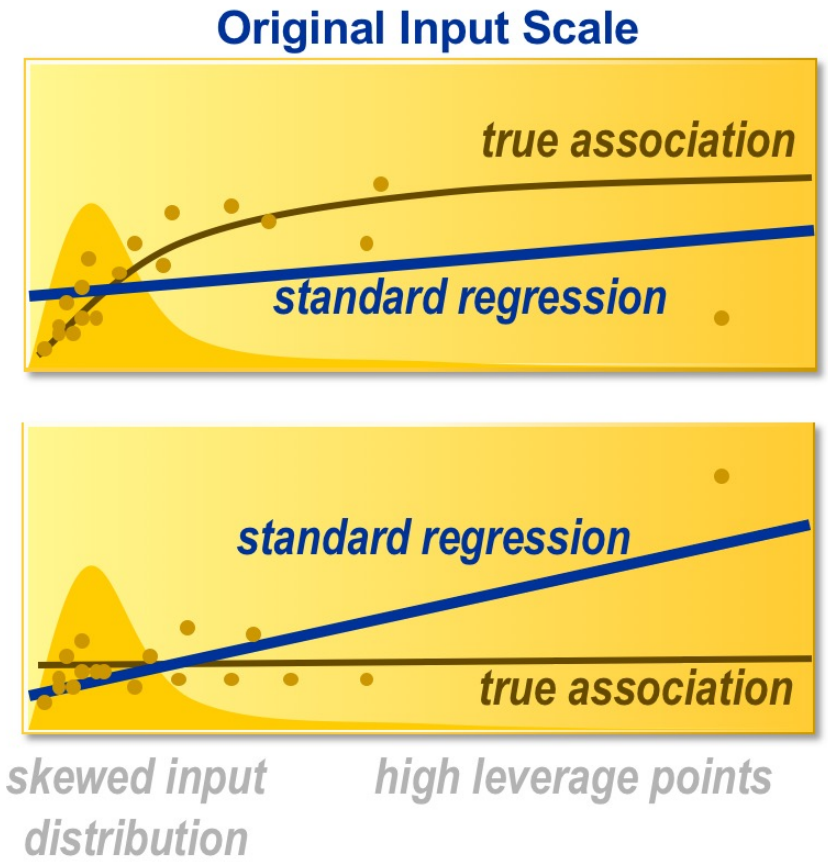




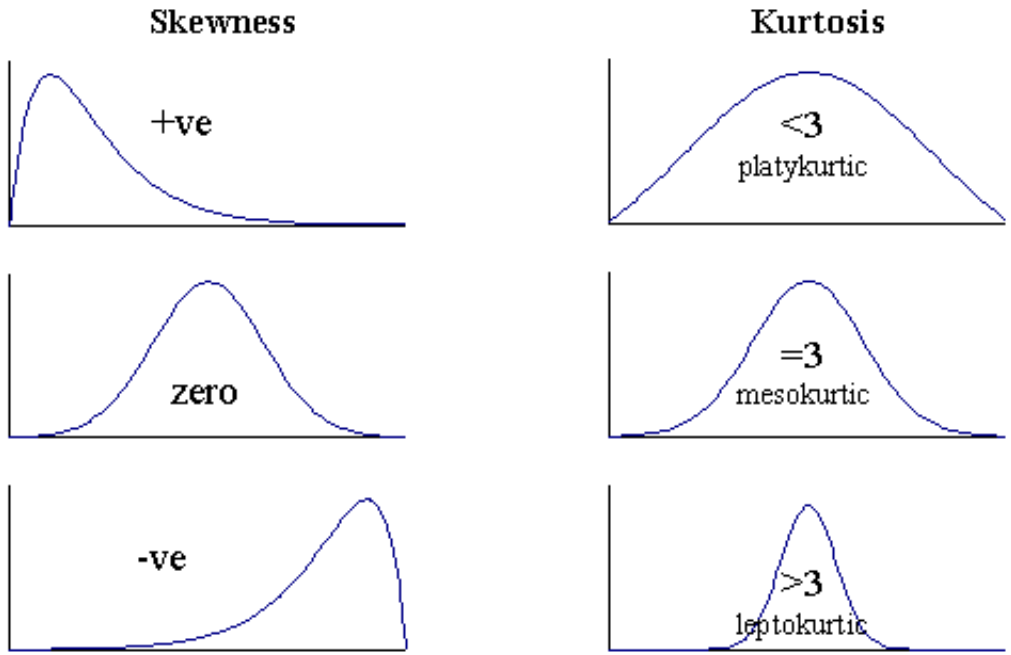
Percentile
1st
2.5th
5th
10th
25th
50th
75th
90th
95th
97.5th
99th

$$\hat{y} = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2$$

3) Preparing features for ML (cont.): 3.4 Feature transformation



- Skewness
- Example: Salary, Balance in bank account
- **Solutions: Log, Binning**



3) Preparing features for ML (cont.): 3.4 Feature transformation - Log

	Spending	Spending with outliers	LOG10(Spending)	LOG10(Spending with outliers)
	2,500.00	2,500.00	3.40	3.40
	2,900.00	2,900.00	3.46	3.46
	3,200.00	3,200.00	3.51	3.51
	4,000.00	4,000.00	3.60	3.60
	4,500.00	4,500.00	3.65	3.65
	6,200.00	6,200.00	3.79	3.79
		10,000,000.00		7.00
mean	**3,883.33**	**1,431,900.00**	**3.57**	**4.06**

3) Preparing features for ML (cont.): 3.4 Feature transformation - Binning

	Spending	Spending with outliers	LOG10(Spending)	LOG10(Spending with outliers)	Binning (Spending)	LOG10(Spending with outliers)
	2,500.00	2,500.00	3.40	3.40	1	1
	2,900.00	2,900.00	3.46	3.46	1	1
	3,200.00	3,200.00	3.51	3.51	2	2
	4,000.00	4,000.00	3.60	3.60	2	2
	4,500.00	4,500.00	3.65	3.65	2	2
	6,200.00	6,200.00	3.79	3.79	3	3
		10,000,000.00		7.00		3
mean	**3,883.33**	**1,431,900.00**	**3.57**	**4.06**	**1.83**	**2.00**

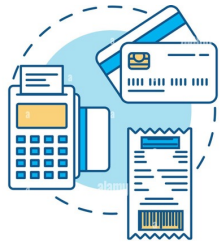
3) Preparing features for ML (cont.): 3.5 Feature engineering

- Feature engineering
  - Calculated variables
  - Behavior from transactional data (RFM/RFA)

Recency	Frequency	Monetary Value
The time when they last placed an order	How many orders they have placed in the given period	How much money have they spent since their first purchase (CLV/LTV)

3) Preparing features for ML (cont.): 3.5 Feature engineering (cont.)

- Feature engineering
  - Calculated variables
  - Behavior from transactional data (RFM/RFA)

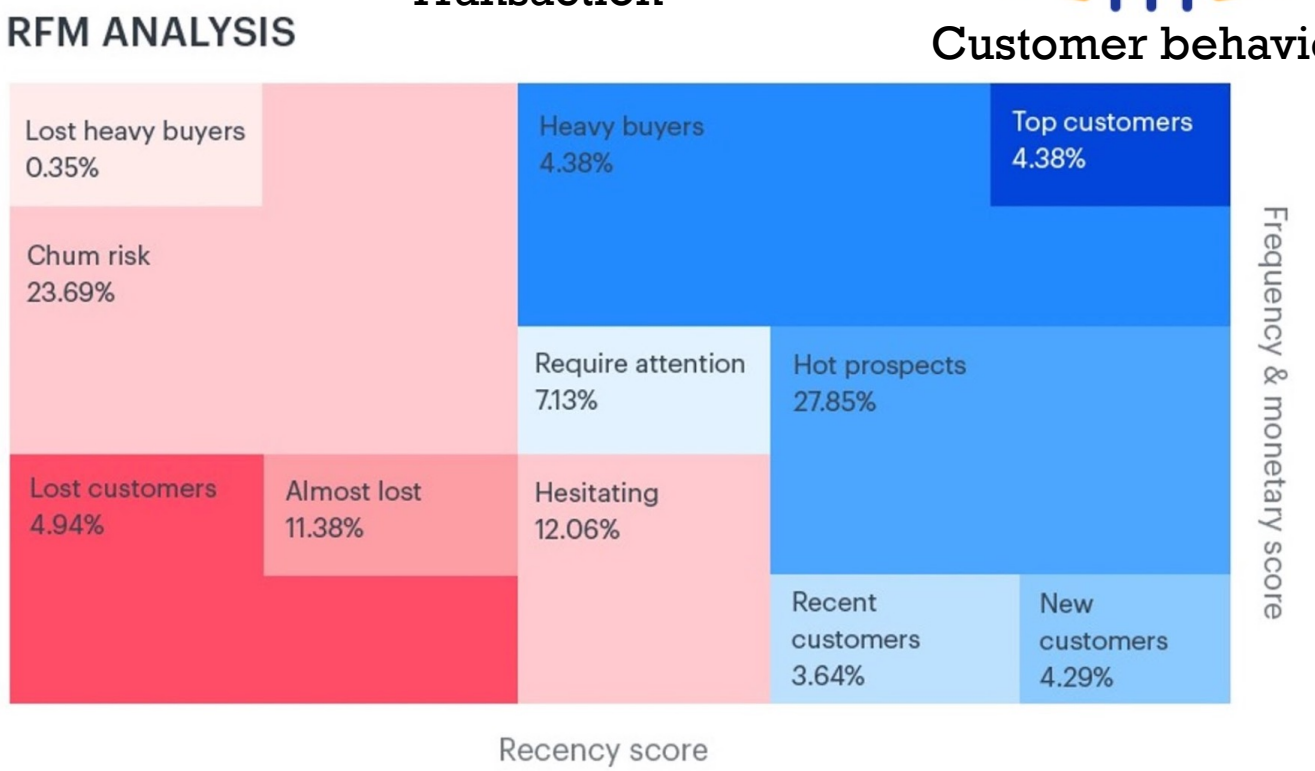


POS terminal

Transaction

Customer behavior

Recency	Frequency	Monetary Value
The time when they last placed an order	How many orders they have placed in the given period	How much money have they spent since their first purchase (CLV/LTV)



4) Other preprocessing steps: Train/Test/Validate – Overfitting issue on train

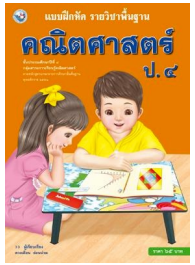
Training Data

inputs

target

Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes
35	50,000	Female	Nontaburi	Yes
32	35,000	Male	Bangkok	No

Validation Data



Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes
35	50,000	Female	Nontaburi	Yes

Testing Data

Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	?

Which method is the winner?

Training Data

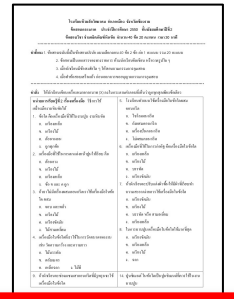
inputs

Age	Income	Gender	Province
25	25,000	Female	Bangkok
35	50,000	Female	Nontaburi
32	35,000	Male	Bangkok

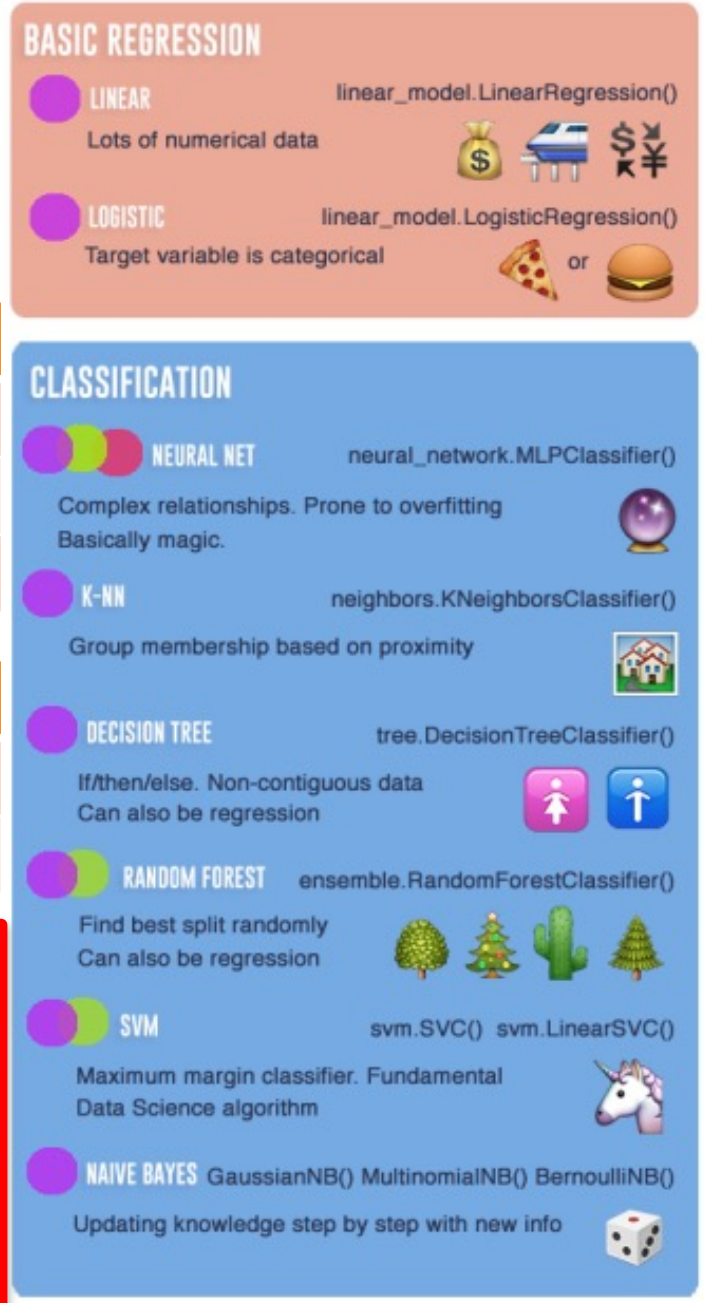
Validation Data

Age	Income	Gender	Province
25	25,000	Female	Bangkok
35	50,000	Female	Nontaburi

Testing Data



Age	Income	Gender	Province
25	25,000	Female	Bangkok



What is the best setting for decision tree?

Training Data

inputs

target

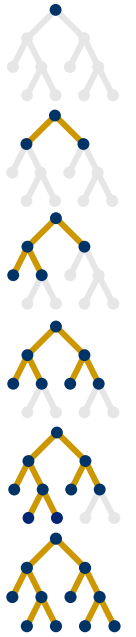
Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes
35	50,000	Female	Nontaburi	Yes
32	35,000	Male	Bangkok	No

Validation Data

Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes
35	50,000	Female	Nontaburi	Yes

Testing Data

Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	?

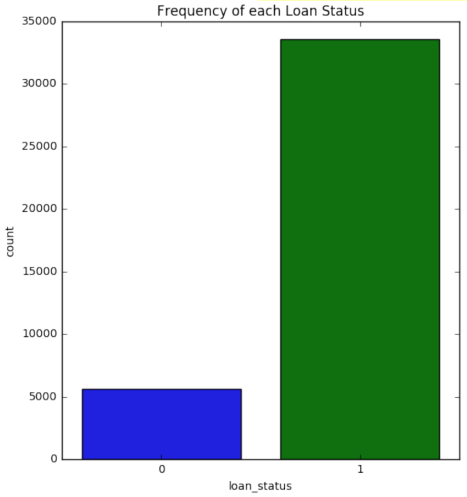


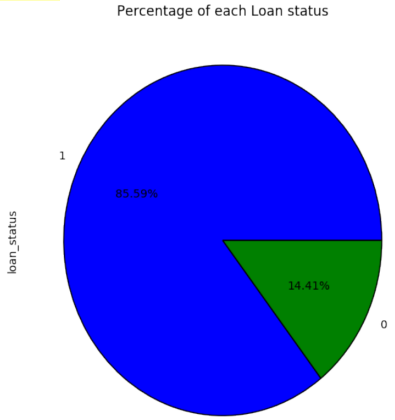
Model Complexity

4) Other preprocessing steps: Train/Test/Validate (cont.)

Simple random sample

Stratification

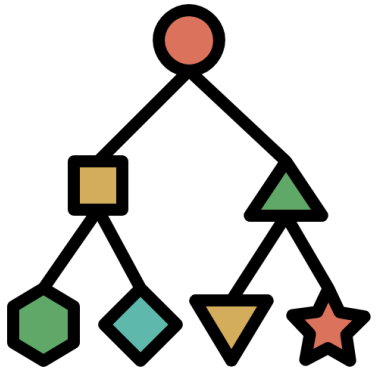




K-Fold Cross Validation

How to fix overfitting issue on test

Iteration 1	Test	Train	Train	Train	Train	75%
Iteration 2	Train	Test	Train	Train	Train	80%
Iteration 3	Train	Train	Test	Train	Train	90%
Iteration 4	Train	Train	Train	Test	Train	75%
Iteration 5	Train	Train	Train	Train	Test	84%



- Which model to be used?
- 1) The model on the best fold
- 2) Use "all data" to create a new model

Overall performance = mean(folds) = 80.8%

https://towardsdatascience.com/cross-validation-explained-evaluating-estimator-performance-e51e5430ff85

Data leaking from testing data in training data

- Split by subjects/videos rather than individual images
- For time series data, split by period of time

Remark: Random Seed

- The experiment must be able to reconstruct (replicate).
- All randoms must be assigned a radom seed.
  - random.seed(12345)
  - random_state option

Other data preparation processes

- Impute missing values
- Outlier detections
- Feature transformation
  - Skewness
- Split train/test
  - Simple random sampling
  - Stratification
- Feature clustering
- Feature selection
  - Statistical approach
  - Model-based approach

1.13.2. Univariate feature selection ¶

Univariate feature selection works by selecting the best features based on univariate statistical tests. It can be seen as a preprocessing step to an estimator. Scikit-learn exposes feature selection routines as objects that implement the `transform` method:

- **SelectKBest** removes all but the k highest scoring features
- **SelectPercentile** removes all but a user-specified highest scoring percentage of features
- using common univariate statistical tests for each feature: false positive rate **SelectFpr**, false discovery rate **SelectFdr**, or family wise error **SelectFwe**.
- **GenericUnivariateSelect** allows to perform univariate feature selection with a configurable strategy. This allows to select the best univariate selection strategy with hyper-parameter search estimator.

For instance, we can perform a χ^2 test to the samples to retrieve only the two best features as follows:

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.feature_selection import SelectKBest
>>> from sklearn.feature_selection import chi2
>>> X, y = load_iris(return_X_y=True)
>>> X.shape
(150, 4)
>>> X_new = SelectKBest(chi2, k=2).fit_transform(X, y)
>>> X_new.shape
(150, 2)
```

https://scikit-learn.org/stable/modules/feature_selection.html

These objects take as input a scoring function that returns univariate scores and p-values (or only scores for **SelectKBest** and **SelectPercentile**):

- For regression: **f_regression**, **mutual_info_regression**
- For classification: **chi2**, **f_classif**, **mutual_info_classif**

1.13.4. Feature selection using SelectFromModel

`SelectFromModel` is a meta-transformer that can be used alongside any estimator that assigns importance to each feature through a specific attribute (such as `coef_`, `feature_importances_`) or via an `importance_getter` callable after fitting. The features are considered unimportant and removed if the corresponding importance of the feature values are below the provided `threshold` parameter. Apart from specifying the threshold numerically, there are built-in heuristics for finding a threshold using a string argument. Available heuristics are “mean”, “median” and float multiples of these like “0.1*mean”. In combination with the `threshold` criteria, one can use the `max_features` parameter to set a limit on the number of features to select.

For examples on how it is to be used refer to the sections below.

Examples

- Model-based and sequential feature selection

1.13.4.1. L1-based feature selection

Linear models penalized with the L1 norm have sparse solutions: many of their estimated coefficients are zero. When the goal is to reduce the dimensionality of the data to use with another classifier, they can be used along with `SelectFromModel` to select the non-zero coefficients. In particular, sparse estimators useful for this purpose are the `Lasso` for regression, and of `LogisticRegression` and `LinearSVC` for classification:

```
>>> from sklearn.svm import LinearSVC
>>> from sklearn.datasets import load_iris
>>> from sklearn.feature_selection import SelectFromModel
>>> X, y = load_iris(return_X_y=True)
>>> X.shape
(150, 4)
>>> lsvc = LinearSVC(C=0.01, penalty="l1", dual=False).fit(X, y)
>>> model = SelectFromModel(lsvc, prefit=True)
>>> X_new = model.transform(X)
>>> X_new.shape
(150, 3)
```

Statistical approach

- Chi-squared
- Correlation, F-test

Type of Response \ Type of Predictors	Categorical	Continuous	Continuous and Categorical
Continuous	Analysis of Variance (ANOVA)	Ordinary Least Squares (OLS) Regression	Analysis of Covariance (ANCOVA)
Categorical	Contingency Table Analysis or Logistic Regression	Logistic Regression	Logistic Regression

Chi-Square Test (categorical variables)

Type of Response \ Type of Predictors	Categorical	Continuous	Continuous and Categorical
Continuous	Analysis of Variance (ANOVA)	Ordinary Least Squares (OLS) Regression	Analysis of Covariance (ANCOVA)
Categorical	Contingency Table Analysis or Logistic Regression	Logistic Regression	Logistic Regression

Categorical Variables Association

- An **association** exists between **two categorical variables** if the distribution of one variable changes when the value of the other variable changes.
- If there is **no association**, the distribution of the first variable is the same regardless of the level of the other variable.

Categorical Variables Association (cont.)

Confusion Matrix, Contingency Table

	
70%	30%
70%	30%

There seems to be **no association** between your mood and the weather because the row percentages are the **same** in each column.

Categorical Variables Association (cont.)

Confusion Matrix, Contingency Table

	
90%	**10%**
30%	**70%**

There seems to be **an association** because the row percentages are the **different** in each column.

Chi-Square Test (cont.)

	Outcome		Total
	Yes	No	
Group A	60	20	80
Group B	90	10	100
Total	150	30	180

- Under the **null hypothesis** that there is **no association between the Row and Column variables**.
  - **The expected percentage** in any R*C cell will be equal to the percent in that cell's row (R/T) times the percent in the cell's column (C/T) = (R/T)*(C/T).
  - **The expected count** is then only that expected percentage times the total sample size = (R/T)*(C/T)*T = (R*C)/T.

$$Exp_{ij} = \frac{T_i \; x \; T_j}{N}$$

- Chi-square tests and the corresponding p-values
  - determine whether an association exists
  - do not measure the strength of an association
  - depend on and reflect the sample size.

$$\chi^2 = \sum_{i=1}^{R} \sum_{j=1}^{C} \frac{(Obs_{ij} - Exp_{ij})^2}{Exp_{ij}}$$

Chi-Square Test

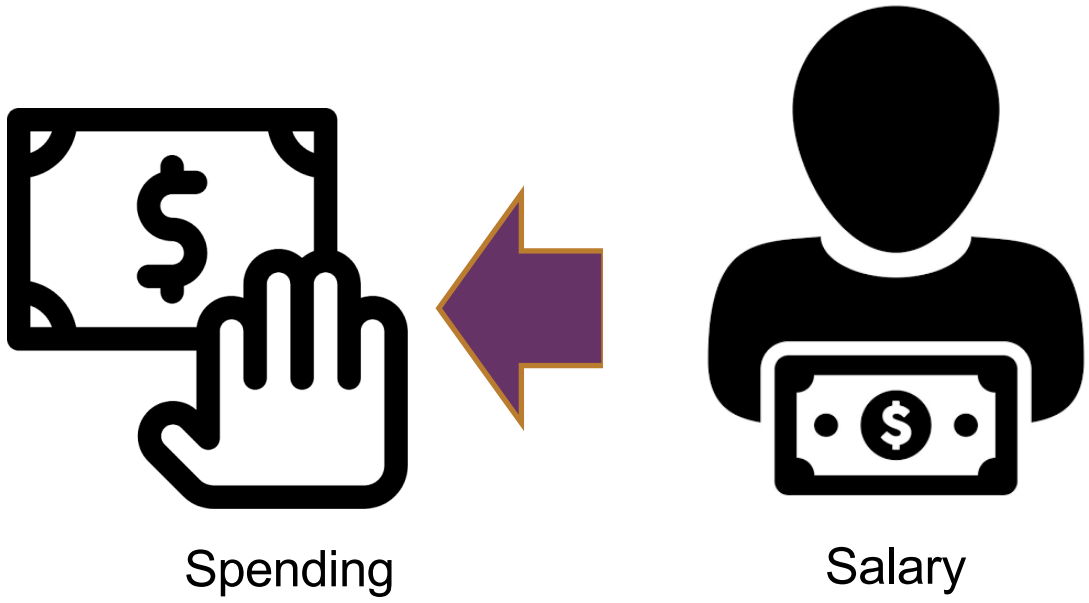
- A commonly used test to check whether there is an association between two categorical variables

- The chi-square test **measures** the difference between the **observed frequencies** and the **expected frequencies**
  - **H0: Observed freq. = expected freq.** → **No Association**
  - **H1: Observed freq. ≠ expected freq.** → **Association**

- If you have a significant chi-square statistic, there is strong evidence that there is **an association** between your variables.

Continuous ~ Continuous (Correlation, Regression)

One-to-One



Type of Response \ Type of Predictors	Categorical	Continuous	Continuous and Categorical
Continuous	Analysis of Variance (ANOVA)	Ordinary Least Squares (OLS) Regression	Analysis of Covariance (ANCOVA)
Categorical	Contingency Table Analysis or Logistic Regression	Logistic Regression	Logistic Regression

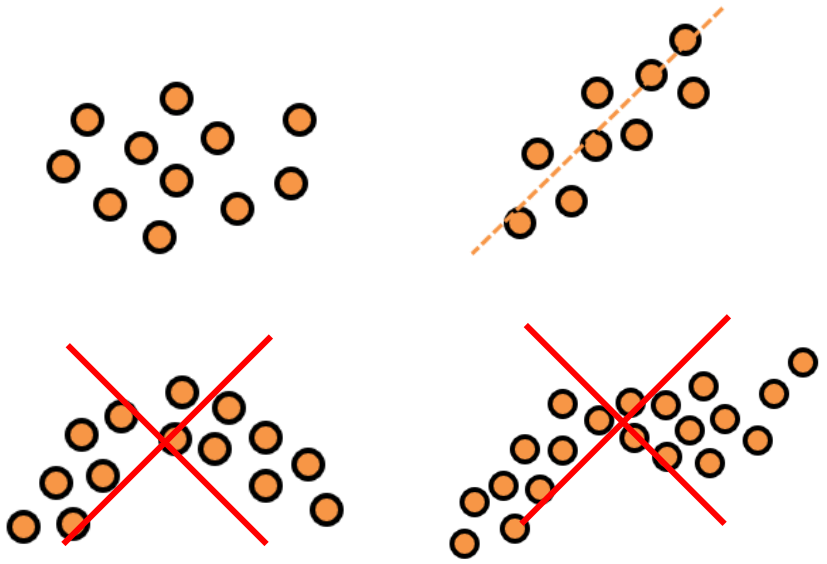
Correlation

- Correlation is a measure that describes the **strength and direction of a relationship** between two variables. It is commonly used in statistics, economics and social sciences for budgets, business plans and etc.
- The method used to understand how closely each variable is related is called **correlation analysis**.

Pearson Correlation

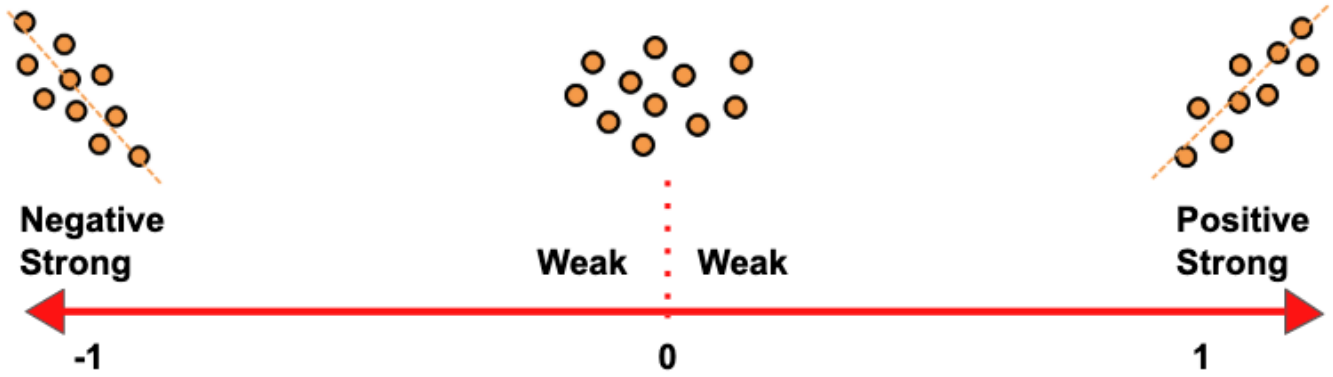
- Pearson Correlation, which is the Pearson Product Moment Correlation (PPMC), is used to evaluate **linear relationships** between two **continuous variable**
- Here's the most commonly used formula to find the Pearson correlation coefficient, which can be called Pearson's R:

$$r = \frac{\sum(x_i - x_{\text{average}})\,(y_i - y_{\text{average}})}{\sqrt{\sum(x_i - x_{\text{average}})^2 * \sum\left(y_i - y_{\text{average}}\right)^2}}$$



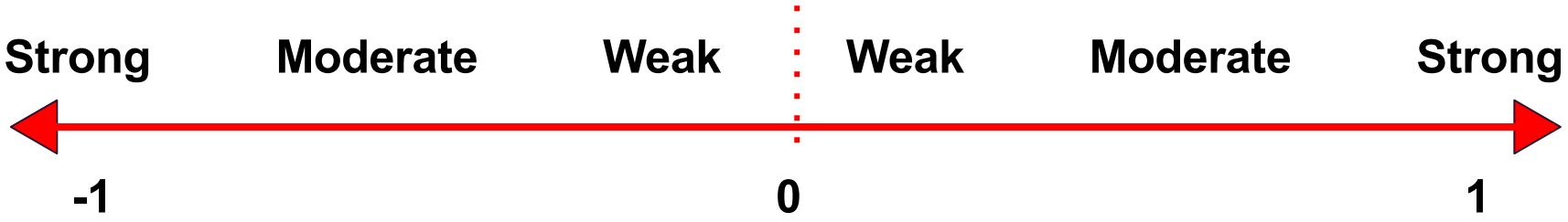
Correlation Coefficient

- The numerical measure of the degree of association between two continuous variables is called the **correlation coefficient (r)**.
- The coefficient value is always between -1 and 1 and it measures both the **strength** and **direction** of the linear relationship between the variables.



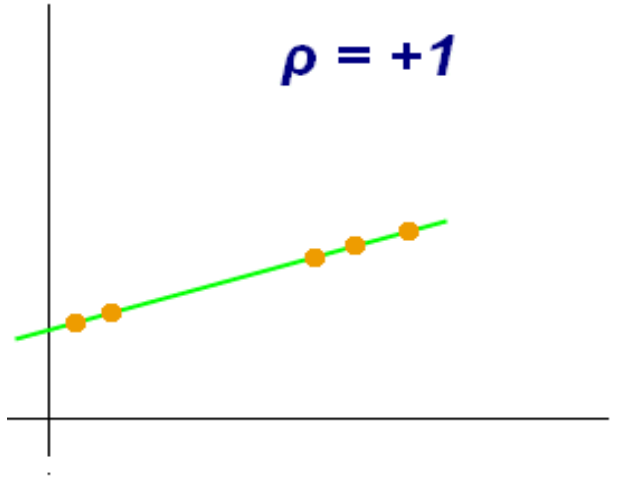
Correlation Coefficient (cont.): Strength

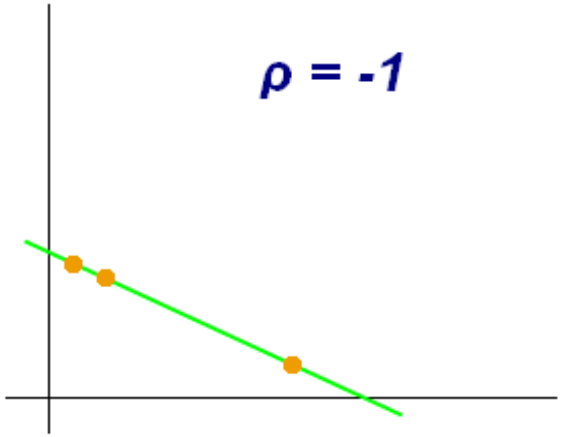
- **Strength**
  - The values of **-1 and 1** indicate a perfect **linear relationship** when all the data points fall on a line. Normally, either positive or negative, is **rarely** found.
  - A coefficient of **0** indicates no linear relationship between the variables. This is what you are likely to get with two sets of random numbers.
  - Values **between 0 and +1/-1** represent a scale of weak, moderate and strong relationships. As the coefficient gets closer to either -1 or 1, the strength of the relationship increases.



Correlation Coefficient (cont.): Direction

- **Direction**
  - **Positive coefficients** represent **direct** linear association (upward-sloping)
  - **Negative coefficients** represent **inverse** linear association (downward-sloping)



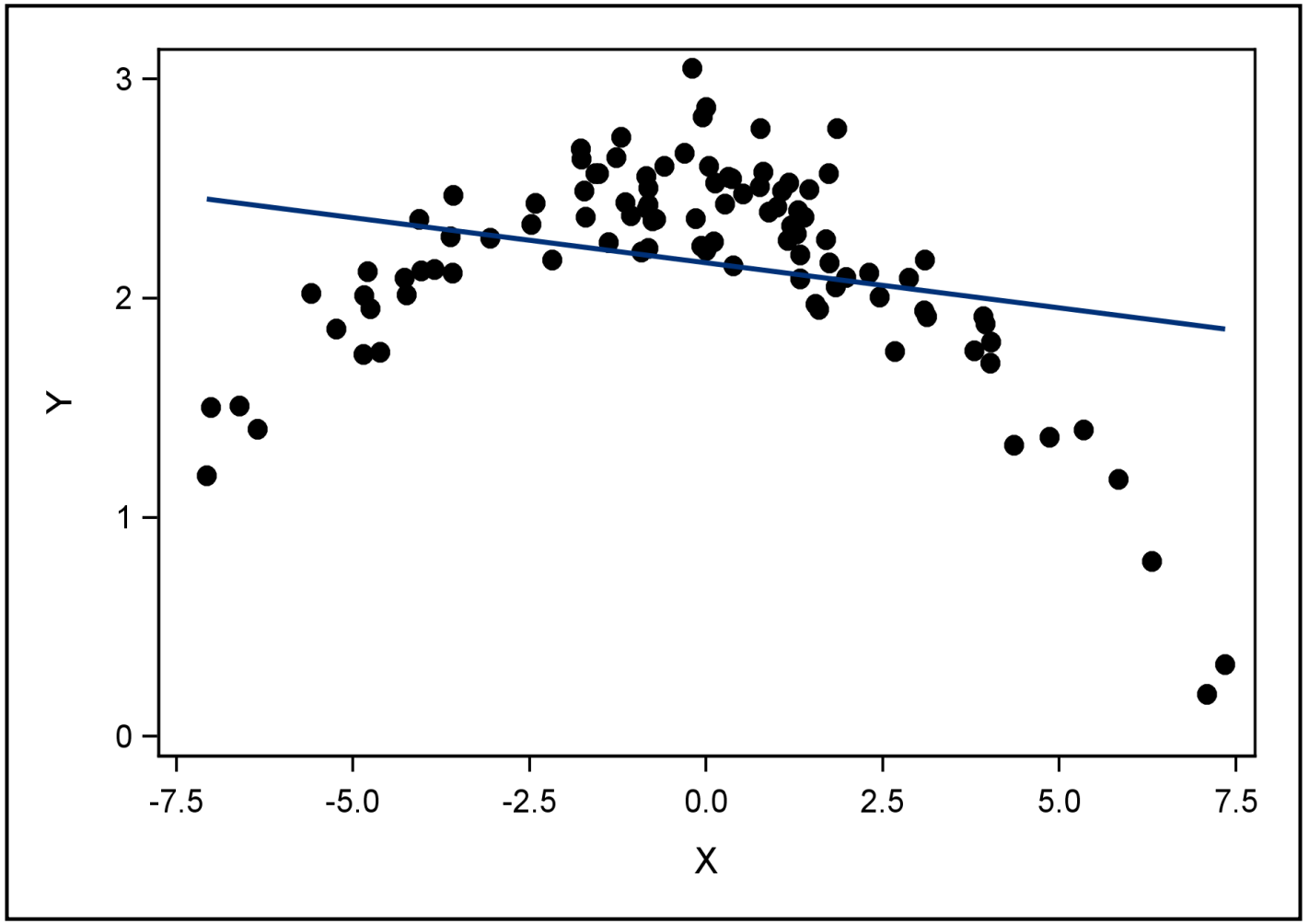


Hypothesis Test for a Correlation

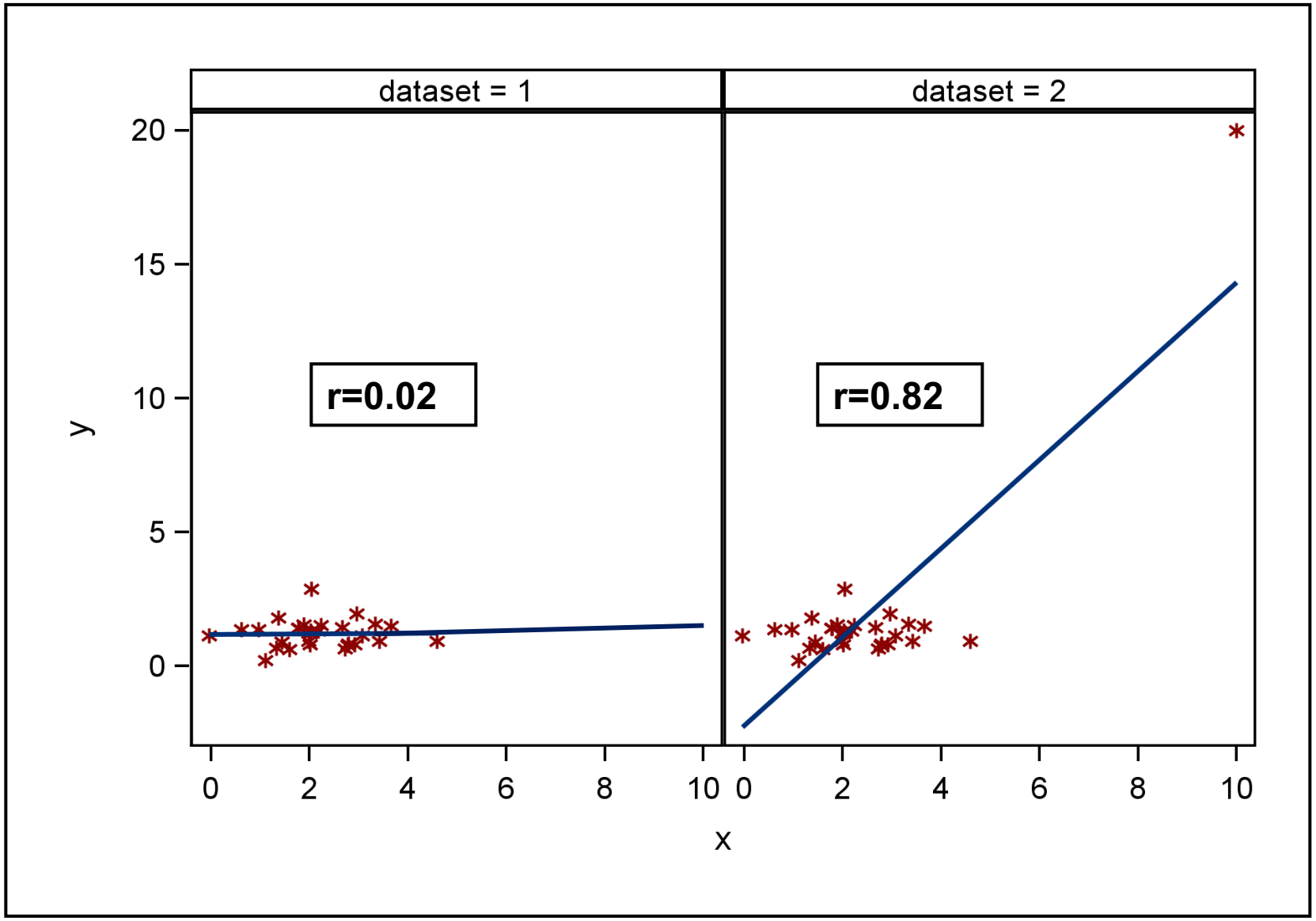
- The parameter representing correlation is ρ.
- ρ is estimated by the sample statistic *r*.

- H_0: $\rho=0$
- Rejecting H0 indicates only great confidence that ρ is not exactly zero.
- A *p*-value does not measure the magnitude of the association.
- Sample size affects the *p*-value.

Remark1: Missing Another Type of Relationship



Remark2: Extreme Data Values



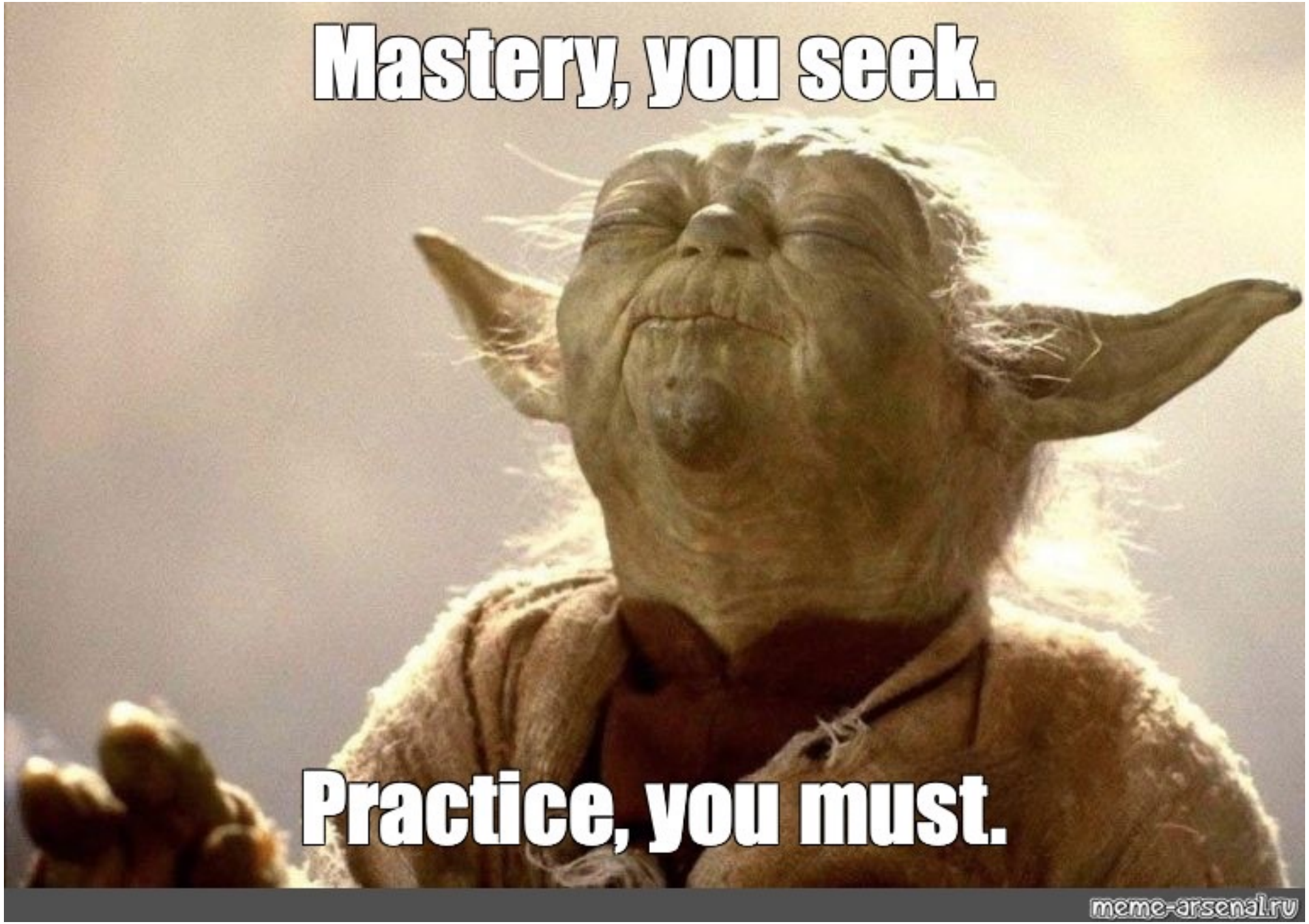
Conclusion

28 DECEMBER 2016 / DATA CLEANING

Preparing and Cleaning Data for Machine Learning

- 1) Examining the Data Set
- 2) Narrowing down columns manually
  - Remove Id's
  - Irrelevant variables
  - Remove zipcode & date
  - Temporal infidelity (data from future)
  - Calculated variables
  - Decide target
    - Select studied cases
    - Distribution of target variables
  - Remove flat values
- 3) Preparing features for ML
  - Preview data
  - Handling missing values
    - Drop unqualified features
  - Investigate categorical features
    - Drop too many unique values (treat as Id)
    - Convert ordinal to numeric
    - Convert categorical to numeric
  - Check all numeric variables
- 4) Other preprocessing steps:
  - Train/Test/Validate

https://www.dataquest.io/blog/machine-learning-preparing-data/


Mastery, you seek.
Practice, you must.
meme-arsenal.ru