





# The Methods in Data Mining

Information Systems Undergraduate Program School of Industrial Engineering



#### PLO & CLO to be achieved:

**PLO01 –** Able to analyze complex INFOKOM issues, defining and modeling requirements in the context of enterprises or society by applying knowledge in the fields of computing, information and communication technology, and other relevant disciplines

**CLO07 –** Students are able to apply fundamental statistical knowledge in the scope of information systems science .



#### **Outline:**

- 1. Clustering
- 2. Regression
- 3. Classification

#### Reference:

- 1. <u>James, Gareth et al. 2023. An Introduction Statistical Machine Learning With Applications in Python. Springer</u>
- 2. Walpole, Ronald E., Myers, Raymond H., Myers, Sharon L. 2013. Probability & Statistics for Engineers & Scientists. 9th ed.. Pearson Education. United States of America
- 3. <u>Han, Jiawei, Jian Pei, and Hanghang Tong. 2023. Data Mining Concepts and Techniques. 4th ed. ed. Beth LoGiudice. Cambridge: Katey Birtcher.</u>
- 4. Moreira, J. M., Carvalho, A. C. P. L. F., & Horváth, T. (2018). A General Introduction to Data Analytics. In A General Introduction to Data Analytics. https://doi.org/10.1002/9781119296294

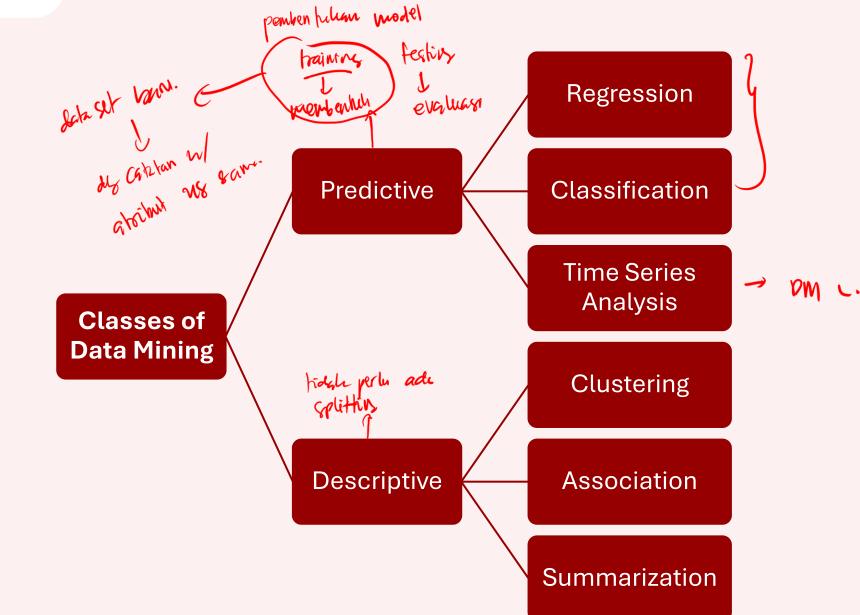




# Introduction to the Methods in Data Mining

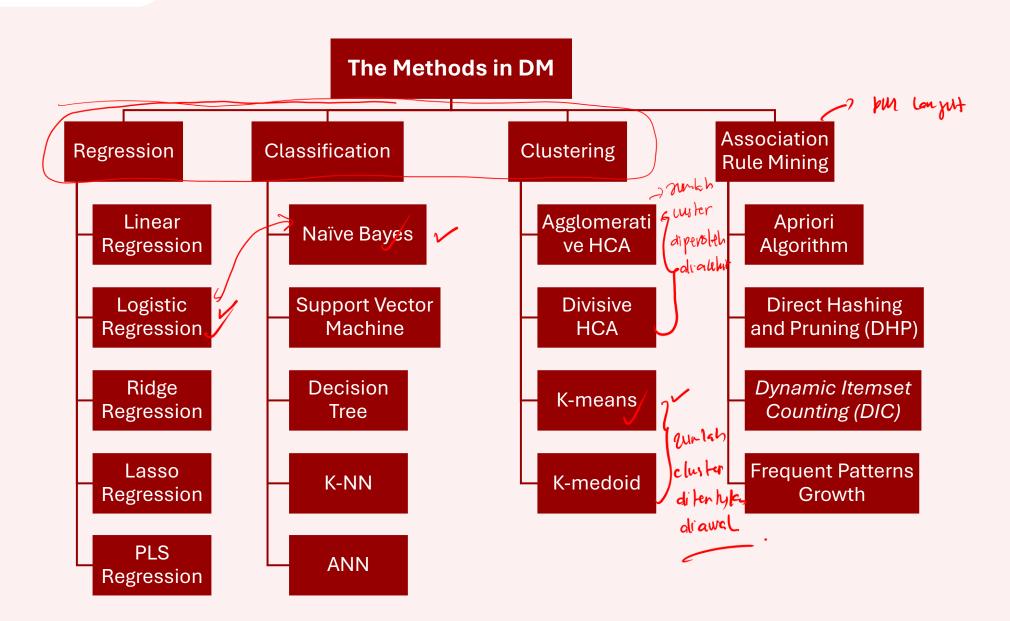
















## Clustering





Clustering Felompole 1

Kelompoli 2

Kelompole 3

- Unsupervised learning is a type of machine learning where the algorithm is given data without any explicit instructions or labeled examples.
- Its goal is to identify patterns, structures, or relationships in the data independently.
- Unsupervised learning deals with unlabeled data, meaning the algorithm must work without prior guidance.
- Clustering is one of algorithms/ methods in unsupervised learning
- Clustering is the process of dividing a set of data objects into subsets called clusters, where objects in the same cluster are similar and different from those in other clusters.
- The goal of clustering is to organize data into meaningful subgroups so that data points within the same cluster are more similar than those in other clusters.
- Clustering is also called data segmentation in some applications because clustering partitions large data sets into groups according to their similarity.



#### Requirement in Clustering

#### Scalability

Many clustering algorithms excel with small datasets but struggle with large databases containing millions or billions of objects, as seen in web search. Sampling from these extensive datasets can lead to biased results, highlighting the need for scalable clustering algorithms.

#### Ability to deal with different types of attributes

Many algorithms are designed for clustering numeric data, but there is a growing need for techniques that can manage mixed data types, such as binary, nominal, ordinal, and numerical data, along with various object types like text, graphs, sequences, images, and videos.

#### Discovery of clusters with arbitrary shape

Many clustering algorithms use Euclidean or Manhattan distance measures, which typically identify spherical clusters of similar size and density. However, clusters can take on various shapes.



#### Requirement in Clustering

- Requirements for domain knowledge to determine input parameters
   Many clustering algorithms need users to specify parameters, such as the number of clusters, based on domain knowledge. This makes results sensitive to these parameters.
  - clusters, based on domain knowledge. This makes results sensitive to these parameters, which are difficult to define, especially in high-dimensional datasets. This requirement increases user burden and makes it harder to ensure clustering quality.
- Ability to deal with noisy data
  - Most real-world datasets have outliers and may contain missing, unknown, or erroneous data. Clustering algorithms often struggle with this noise, resulting in poor-quality clusters, highlighting the need for robust methods that can effectively handle noise.
- Incremental clustering and insensitivity to input order
  In many applications, incremental updates can occur at any time, but some clustering
  algorithms cannot incorporate these updates and must recompute clusters from scratch.
  Moreover, the order of input data can significantly impact results, resulting in different
  clustering based on the presentation order.



#### Requirement in Clustering

#### Capability of clustering high-dimensionality data

Datasets can have numerous dimensions or attributes. In document clustering, each keyword is a dimension, often resulting in thousands of dimensions. Most clustering algorithms handle low-dimensional data well, but finding clusters in high-dimensional spaces is challenging due to data sparsity and skewness.

#### Constraint-based clustering

Real-world clustering often involves constraints. The challenge is to find data groups that exhibit good clustering behavior while meeting these constraints.

#### Interpretability and usability

Clustering results should be interpretable, comprehensible, and usable, often requiring alignment with specific semantic interpretations and applications.





Method	General Characteristics
Partitioning	<ul> <li>Find mutually exclusive clusters of spherical shape</li> </ul>
methods	- Distance-based
	<ul> <li>May use mean or medoid (etc.) to represent cluster center</li> </ul>
	Effective for small- to medium-size data sets
Hierarchical	- Clustering is a hierarchical decomposition (i.e., multiple levels)
methods	<ul> <li>Cannot correct erroneous merges or splits</li> </ul>
	<ul> <li>May incorporate other techniques like microclustering or</li> </ul>
	consider object "linkages"
Density-based	— Can find arbitrarily shaped clusters
methods	<ul> <li>Clusters are dense regions of objects in space that are</li> </ul>
	separated by low-density regions
	<ul> <li>Cluster density: Each point must have a minimum number of</li> </ul>
	points within its "neighborhood"
	- May filter out outliers
Grid-based	Use a multiresolution grid data structure
methods	<ul> <li>Fast processing time (typically independent of the number of</li> </ul>
	data objects, yet dependent on grid size)

#### **Clustering Methods**

This section just described the partitioning method, especially k-means clustering

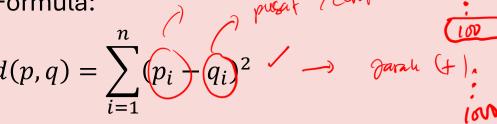




#### The Distance in Clustering

#### 1. Euclidean Distance

Formula:



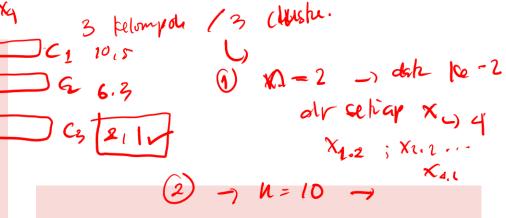
Use Cases: Suitable for continuous numerical data and is the default distance metric for K-means.

#### 2. Manhattan Distance

Formula:

$$d(p,q) = \sum_{i=1}^{n} |p_i - q_i| \rightarrow (\uparrow)$$

Use Cases: Useful for high-dimensional spaces and when you want to measure distance in a grid-like path.



#### Where:

 $p_i$  is point one of the observation  $q_i$  is point two of the observation n is the number of the observation



#### **Application of Clustering**

#### Market Segmentation

Businesses use clustering to segment customers based on purchasing behavior, demographics, or preferences.

#### Image Segmentation

Clustering techniques are applied in image processing to segment images into distinct regions based on color or texture, aiding in object recognition and classification.

#### Anomaly Detection

Clustering helps identify outliers in data, which is useful in fraud detection, network security, and monitoring for unusual patterns in various fields.

#### Social Network Analysis

Clustering identifies communities or groups within social networks based on user interactions, providing insights into social dynamics and user behavior.

#### Telecommunications

Clustering analyzes call data records to identify patterns of usage or detect fraudulent activities.





## **K-Means Clustering**







- K-means clustering is a simple and elegant approach for partitioning n observation of a dataset into k distinct, non-overlapping clusters, where  $k \le n$ .
- K-means clustering is an effective and widely used algorithm for grouping similar data points into clusters.
- The algorithm groups data points based on their similarity, aiming to minimize the variance within each cluster while maximizing the variance between clusters.







#### The Characteristics

#### Centroid-Based Clustering

Each cluster is represented by a centroid, which is the mean of all data points assigned to that cluster.

#### Sensitivity to Initialization

Results can vary based on the initial placement of centroids, potentially leading to different clustering outcomes.

#### Sensitivity to Outliers

K-means is sensitive to outliers, which can skew the position of centroids and affect the quality of the clusters.

#### Iterative Process

K-means follows an iterative process consisting of two main steps: assignment and update.



#### 1. Initialization



• Randomly initialize k centroids from the dataset. These centroids will act as the starting points for each cluster.

How K-Means Works

#### 2. Assignment Step

- For each data point, calculate its distance to each centroid (typically using Euclidean distance).
- Assign each data point to the cluster of the nearest centroid. This initial grouping creates preliminary clusters.  $n_1 + kd C_2$   $n_1 + kd C_2$

#### 3. Update Step

• For each cluster, update the centroid by calculating the mean (average) position of all the data points within that cluster.

9-1 (9-5)2+ (5-8)2+ (7-5)2 =

• This updated centroid represents the new "center" of the cluster.

#### 4. Iterative Process

• Repeat assignment and update step until convergence. The convergence criteria is centroids no longer move significantly between iterations, meaning that data points stay in the same clusters.



#### The Advantages and Disadvantages

#### **Advantages:**

- 1. Efficiency and Speed: K-means is computationally efficient and has a linear time complexity, making it suitable for large datasets.
- **2. Simplicity:** The algorithm is straightforward and easy to implement, widely understood, and accessible.
- **3. Scalability:** K-means performs well with high-dimensional data and can easily scale to large datasets.

#### **Disadvantages:**

- **1. Sensitivity to Initialization:** Poor initialization of centroids can lead to suboptimal clustering results.
- **2. Sensitivity to Outliers:** Outliers and noise can distort the cluster centroids, affecting accuracy.
- **3. Limited to Numeric Data**: It's best suited for numerical data and requires adaptations for categorical data.





## Regression

- General Linear Model (GLM) is a statistical model that used to describe the relationship between a dependent variable and one or more independent variables.
- The basic form of the GLM is:

$$Y = X\beta + \varepsilon$$

- Like the GLM, regression describes the relationship between a response/ dependent and predictor/ independent variables
- So, we can say that regression is a part of the GLM.





## **Logistic Regression**

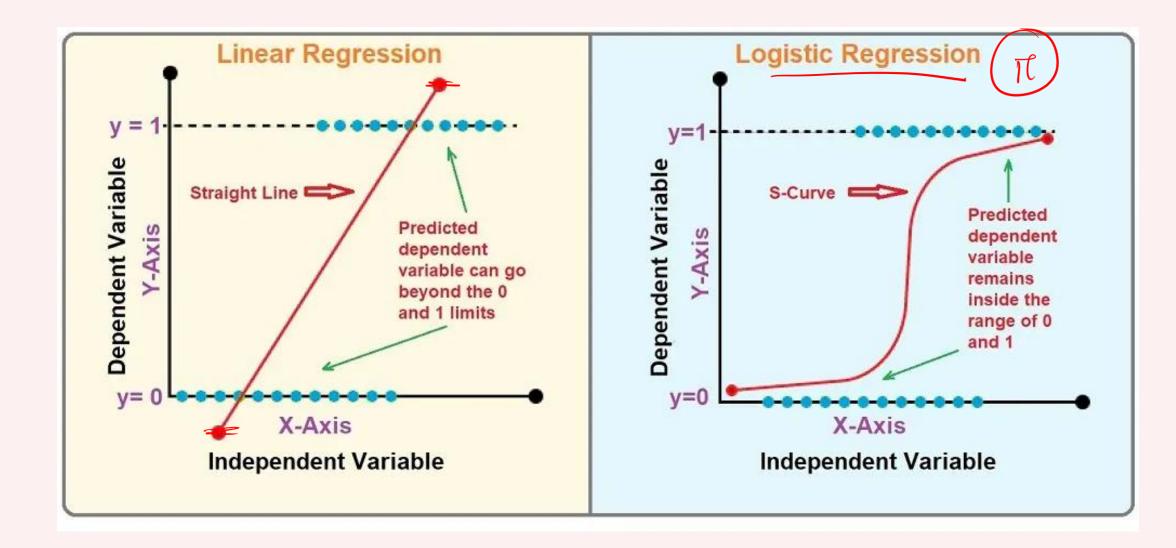


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- Logistic regression is a statistical method used for binary classification problems,
   where the outcome or dependent variable is categorical and typically represents two classes.
- It predicts the probability that a given input point belongs to a certain class, using a logistic function (also called the sigmoid function) to map any real-valued number into the interval between 0 and 1.
- Probabilistic Output: It outputs the probability of the input belonging to a class, which can be thresholded to make a decision (if the probability  $\geq$  0.5, then classify as 1).

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#### Form of logistic regression (using sigmoid model)

Simple logistic regression (single predictor)

$$p(X) = P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X)}} = \frac{e^{(\beta_0 + \beta_1 X)}}{1 + e^{(\beta_0 + \beta_1 X)}}$$

Multiple logistic regression (two or more predictors)

$$p(X) = P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p)}} = \frac{e^{(\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p)}}{1 + e^{(\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p)}}$$



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- 1. Model Fit (Goodness of fit model) 🗸
  - Hosmer-Lemeshow Test -> A p-value greater than 0.05 suggests that there is no significant difference between observed and predicted values, indicating a good fit.
  - Pseudo R-Squared
    - McFadden's R<sup>2</sup>: This is the most common pseudo R-squared for logistic regression. It ranges between 0 and 1, with higher values indicating a better fit, although values between 0.2 and 0.4 are considered reasonable.
    - Cox & Snell R<sup>2</sup>: It is another pseudo R-squared that compares the likelihood of the model to the null model. It can be difficult to interpret directly as it does not reach a maximum value of 1.
    - Magelkerke R<sup>2</sup>: This is an adjusted version of Cox & Snell R<sup>2</sup>, which adjusts the scale to allow it to reach a maximum value of 1.
  - Confusion matrix (accuracy, precision, recall, f1-score)

2. The relationship between the response and predictors -> using hypothesis testing

$$H_0: \beta_1 = \beta_2 = \dots = \beta_p = 0$$

(there is no relationship between the response and predictors)

 $H_1$ : at least one  $\beta_i$  is non – zero

(At least one predictor that relates to the response)

Statistics test: *likelihood ratio test* (*G test*)

 $G test = -2 \times (log likelihood of restricted model - log likelihood of the full model)$ 

Rejected 
$$H_0$$
 if  $G$  test  $> \chi^2_{table}$ 

#### Deciding on Important Variables (partial testing) -> backward, forward method

$$H_0$$
:  $\beta_i = 0$ 

(There is no relationship between X and Y)

$$H_1$$
:  $\beta_i$  is non – zero

(There is a relationship between X and Y)

Statistics test: Wald test (W)

$$W = \frac{\hat{\beta}_{j}}{SE(\hat{\beta}_{j})} \text{ or } W^{2} = \left(\frac{\hat{\beta}_{j}}{SE(\hat{\beta}_{j})}\right)^{2}$$
 Rejected  $H_{0}$  if  $W > Z_{table}$  or  $W^{2} > \chi_{table}^{2}$  
$$P\text{-value } C \text{ of } S \text{ if } W$$



#### **Assumption in Logistic Regression:**

- 1) Independence: Observations must be independent of each other.
- 2. Linearity of the logit: The relationship between independent variables and the log odds of the dependent variable should be linear.
- No Multicollinearity: Independent variables should not be highly correlated.

  Multicollinearity can be checked using Variance Inflation Factor (VIF) or correlation matrices



#### How to modelling:

- 1. Split the dataset into training set and testing set
- 2. Model Training (Fitting) -> using training set
- 3. Model evaluation -> check the goodness of fit model using Pseudo R-Squared, Hosmer-Lemeshow test, or confusion matrix
- 4. Model interpretation -> check the significant variables using G test and W ald test
- 5. Model testing -> using testing set -> apply the model to the testing dataset (or unseen data) to evaluate its performance and generalizability; use the same evaluation metrics to determine how well the model performs on the test data compared to the training data.





### Classification



#### **Classification:**

- Predict the class of item
- Creating a model based on training dataset

#### **Application:**

- Credit approval
- Diagnosis of disease
- Fraud detection
- Churn detection



- Proses untuk menyatakan suatu objek ke salah satu kategori yg sudah didefinisikan sebelumnya.
- Proses pembelajaran fungsi target (model klasifikasi) yg memetakan setiap sekumpulan atribut x (input) ke salah satu class/label y yang didefinisikan sebelumnya.
  - Input : sekumpulan record (training set)
  - Setiap record terdiri atas sekumpulan atribut, salah satu atribut adalah class.
  - Mencari model utk atribut class sebagai fungsi dari nilai2 utk atribut yg lain.
- Tujuannya: record yang belum diketahui kelasnya akan diberi label seakurat mungkin.



## Classification algorithms principles

- Distance-based algorithms: K-Nearest Neighbor
- Probability-based algorithms: Naïve Bayes, Logistic Regression
- Search-based algorithms: Decision Tree H condition
- Optimization-based algorithms: Artificial Neural Network,
  Support Vector Machines

## Bayesian Classification

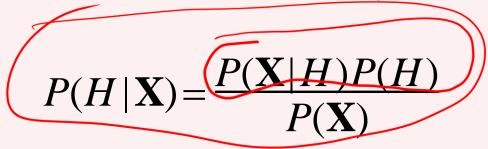
P(AIR) = P(AOR)
P(R)

- P(H|X) Kemungkinan H benar jika X. X adalah kumpulah atribut.
- P(H) Kemungkinan H di data, independen terhadap X
- P ("Single" | "muka sayu", "baju berantakan",
   ←"jalan sendiri") # nilainya besar
  - P ("Non Single" | "muka ceria", "baju rapi", "jalan selalu berdua") # nilainya besar
  - P ("Single") = jumlah single / jumlah mahasiwa



## **Bayesian Classification**

- P(H|X) \*posterior
- P (X | H) probabilitas X, jika kita ketahui bahwa H benar #data training
- Kegiatan klasifikasi: kegiatan mencari P (H | X) yang paling maksimal
- Teorema Bayes:



P(B|A) P(A)



## Klasifikasi

```
X = ("muka cerah", "jalan sendiri", "baju rapi")
Kelasnya Single atau Non Single?
Cari P(H|X) yang paling besar:
("Single" | "muka cerah", "jalan sendiri", "baju
  rapi")
Atau
("Non Single" | "muka cerah", "jalan sendiri",
  "baju rapi")
```



Harus memaksimalkan (C<sub>i</sub>: kelas ke i)

$$P(C_i|\mathbf{X}) = \frac{P(\mathbf{X}|C_i)P(C_i)}{P(\mathbf{X})}$$

Karena P(X) konstan untuk setiap C*i* maka bisa ditulis, pencarian max untuk:

$$P(C_i|\mathbf{X}) = P(\mathbf{X}|C_i)P(C_i)$$

## Naïve Bayes Classifier

 Penyederhanaan masalah: Tidak ada kaitan antar atribut "jalan sendiri" tidak terkait dengan "muka sayu"

$$P(\mathbf{X} \mid C_i) \prod_{k=0}^{n} P(x_k \mid C_i) = P(x_k \mid C_i) \times \left| \begin{array}{ccc} |C_i| \times ... \times & |C_i| \\ |C_i| \times ... \times & |C_i| \end{array} \right|$$

$$= \sum_{k=0}^{n} P(x_k \mid C_i) = P(x_k \mid C_i) \times \left| \begin{array}{ccc} |C_i| \times ... \times & |C_i| \\ |C_i| \times ... \times & |C_i| \end{array} \right|$$

X<sub>1</sub>: atribut ke-1 ("jalan sendiri")

X<sub>n</sub>: atribut ke-n



## Naïve Bayes Classifier

- Jika bentuknya kategori ,
   P(x<sub>k</sub>|C<sub>i</sub>) = jumlah kelas C<sub>i</sub> yang memiliki x<sub>k</sub>
   dibagi | C<sub>i</sub> | (jumlah anggota kelas C<sub>i</sub> di data contoh)
- Jika bentuknya continous dapat menggunakan distribusi gaussian

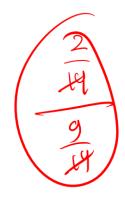
Contoh Naïve Bayes

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	<b>\</b> \\	N <sub>2</sub>		• 0
age	income	student	redit_rating	_com
<=30 ~	high	no	fair	no)
<=30 -	high	no	excellent	no)
3140	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no)
3140	low	yes	excellent	yes
<=30	medium	no	fair	noj
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no)

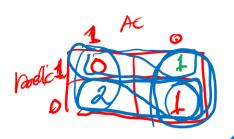
target output

## Contoh Naïve Bayes

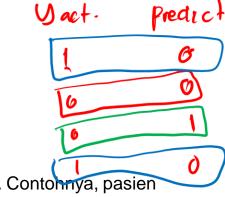
```
P(Ci):
                                                     yes beli konfuter.
P(buys_computer = "yes") = 9/14 = 0.643
P(buys_computer = "no") = 5/14 = 0.357
Training: Hitung P(X|Ci) untuk setiap kelas
   P(age = "<=30" | buys\_computer = "yes") = 2/9 = 0.222
   P(age = "<= 30" | buys_computer = "no") = 3/5 = 0.6
   P(income = "medium" | buys_computer = "yes" > = 4/9 = 0.444
   P(income = "medium" | buys_computer = "no") = 2/5 = 0.4 -
   P(student = "yes" | buys_computer = "yes) = 6/9 = 0.667
   P(student = "yes" | buys_computer = "no") = 1/5 = 0.2
   P(credit_rating = "fair" | buys_computer = "yes") = 6/9 = 0.667
   P(credit_rating = "fair" | buys_computer = "no") = 2/5 = 0.4
Klasifikasi: X = (age <= 30 , income = medium, student = yes, credit_rating
= fair) 🗸
P(X|Ci): P(X|buys_computer = "yes") = 0.222 \times 0.444 \times 0.667 \times 0.667 = 0.044
         P(X|buys\_computer = "no") = 0.6 \times 0.4 \times 0.2 \times 0.4 = 0.019
P(X|Ci)*P(Ci) :
P(X|buys_computer = "yes") * P(buys_computer = "yes") = 0.028 ← ✓
P(X|buys_computer = "no") * P(buys_computer = "no") = 0.007
```

## Pro, Cons Naïve Bayes

- Keuntungan
  - Mudah untuk dibuat
  - Hasil bagus
- Kerugian
  - Asumsi independence antar atribut membuat akurasi berkurang (karena biasanya ada keterkaitan)



## Metriks Evaluasi



Atrurasi: 1	م العبد	Actual Values		
/ Mikasi	25%=	1 (Postive)	0 (Negative)	
presisi: $\frac{0}{1} = 0$	d Values 1 (Postive)	<b>TP</b> (True Positive)	FP (False Positive) Type I Error	
Recall: $\frac{0}{2} = 0$	Predicte 0 (Negative)	FN (False Negative) Type II Error	<b>TN</b> (True Negative)	

#### True Positive (TP)

Merupakan data positif yang diprediksi benar. Contohnya, pasien menderita kanker (*class* 1) dan dari model yang dibuat memprediksi pasien tersebut menderita kanker (*class* 1).

#### • True Negative (TN)

Merupakan data negatif yang diprediksi benar. Contohnya, pasien tidak menderita kanker (*class* 2) dan dari model yang dibuat memprediksi pasien tersebut tidak menderita kanker (*class* 2).

#### False Postive (FP) — Type I Error

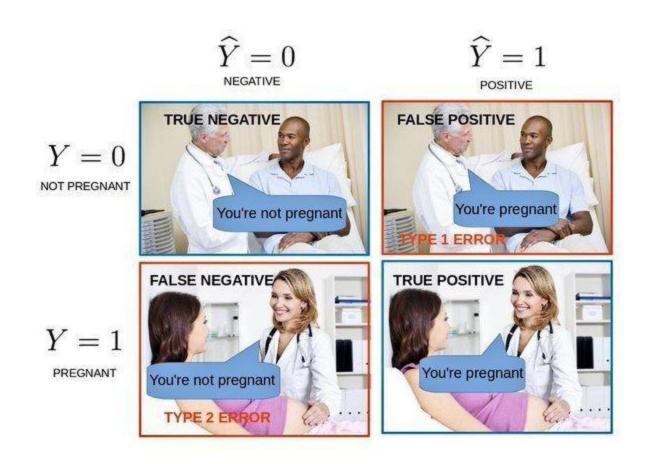
Merupakan data negatif namun diprediksi sebagai data positif. Contohnya, pasien tidak menderita kanker (*class* 2) tetapi dari model yang telah memprediksi pasien tersebut menderita kanker (*class* 1).

#### • False Negative (FN) — Type II Error

Merupakan data positif namun diprediksi sebagai data negatif. Contohnya, pasien menderita kanker (*class* 1) tetapi dari model yang dibuat memprediksi pasien tersebut tidak menderita kanker (*class* 2).

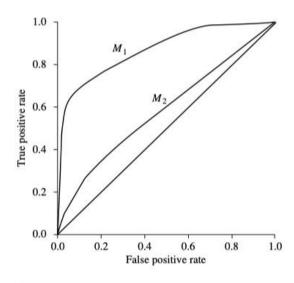
F1 score = 
$$\frac{2(\text{Recall} + \text{Presisi})}{(\text{recall} + \text{Presisi})}$$
 = 0 =  $\frac{2(0.5 \times 0.33)}{(0.5 \times 0.33)}$ 

## **Confusion Matrix**



## Receiver Operating Characteristic Curves (ROC curve)

Receiver operating characteristic curves are a useful visual tool for comparing two classification models.



**Figure 8.20** ROC curves of two classification models,  $M_1$  and  $M_2$ . The diagonal shows where, for every true positive, we are equally likely to encounter a false positive. The closer an ROC curve is to the diagonal line, the less accurate the model is. Thus,  $M_1$  is more accurate here.







# The Methods in Data Mining (Regression)

Thankyou