

# **Demystifying Artificial Intelligence Sorcery**

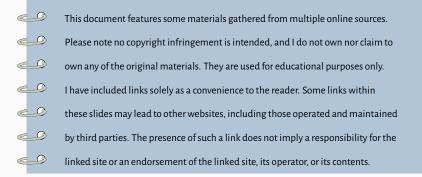
(Part 2: Machine Learning)<sup>a</sup>

Abdelbacet Mhamdi abdelbacet.mhamdi@bizerte.r-iset.tn

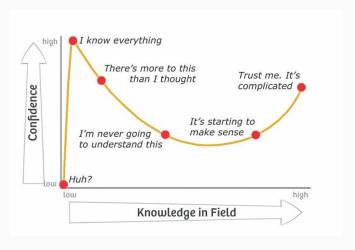
Dr.-Ing. in Electrical Engineering Senior Lecturer at ISET Bizerte

<sup>&</sup>quot;Available @ https://github.com/a-mhamdi/jlai/





#### **DUNNING-KRUGER EFFECT**

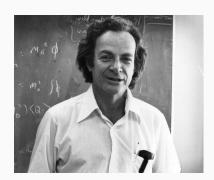


Kruger, J. and Dunning, D. (1999) Unskilled and unaware of it: How difficulties in recognizing one's own incompetence lead to inflated self-assessments. **J Pers Soc Psychol.** 77(6) pp. 1121–1134.

doi:10.1037/0022-3514.77.6.1121

"Knowledge isn't free. You have to pay attention."

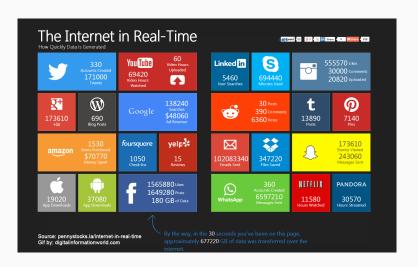
Richard P. Feynman



#### **ROADMAP**

- 1. An overview
- 2. Supervised Learning
- 3. Unsupervised Learning
- 4. Complementary Lab. Project
- 5. ML Landscape through Quizzes

An overview



Update on the internet in real time is available here.

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# LITERATURE REVIEW (1/3)

"The field of machine learning is concerned with the question of how to construct computer programs that automatically improve with experience."

Mitchell, T. (1997) Machine Learning. McGraw-Hill International Editions. McGraw-Hill.

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# LITERATURE REVIEW (2/3)

"Machine learning (ML) is a scientific discipline that concerns developing learning capabilities in computer systems. Machine learning is one of central areas of Artificial Intelligence (AI). It is an interdisciplinary area that combines results from statistics, logic, robotics, computer science, computational intelligence, pattern recognition, data mining, cognitive science, and more."

Wojtusiak, J. (2012) Machine learning. In Encyclopedia of the Sciences of Learning, pages 2082-2083. Springer US.

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# **LITERATURE REVIEW (3/3)**

"Machine learning is an evolving branch of computational algorithms that are designed to emulate human intelligence by learning from the surrounding environment. They are considered the working horse in the new era of the so-called big data. Techniques based on machine learning have been applied successfully in diverse fields ranging from pattern recognition, computer vision, spacecraft engineering, finance, entertainment, and computational biology to biomedical and medical applications. [...] The ability of machine learning algorithms to learn from current context and generalize into unseen tasks would allow improvements in both the safety and efficacy of radiotherapy practice leading to better outcomes."

El Naga, I. and Murphy, M. J. (2015) What Is Machine Learning?, pages 3-11. Springer International Publishing.

#### DEBRIFE

#### Arthur Samuel (1959)

Machine Learning: Field of study that gives computers the ability to learn without being explicitly programmed.

#### Tom Mitchell (1998)

Well-posed Learning Problem: A computer is said to learn from experience  $\mathcal E$  with respect to some task  $\mathcal T$  and some performance measure  $\mathcal P$ , if its performance on  $\mathcal T$ , as measured by  $\mathcal{P}$ , improves with experience  $\mathcal{E}$ .

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#### Task #1

Suppose your email program watches which emails you do or do not mark as spam, and based on that learns how to better filter spam. What is the task  $\mathcal{T}$  in this setting?

- 1. Classifying emails as spam or not spam;
- 2. Watching you label emails as spam or not spam:
- 3. The number (or fraction) of emails correctly classified as spam/not spam;
- 4. None of the above-this not a machine learning problem.

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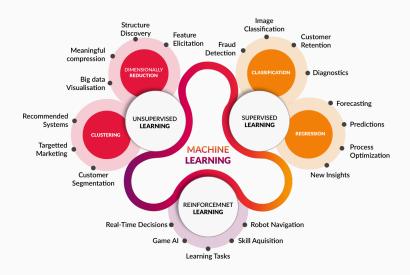
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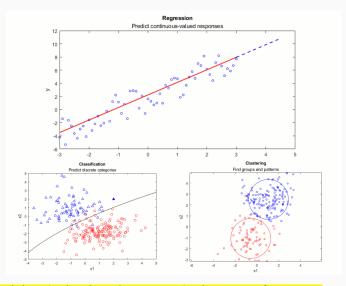


https://www.cognub.com/index.php/cognitive-platform/



https://vitalflux.com/great-mind-maps-for-learning-machine-learning/

# REGRESSION | CLASSIFICATION | CLUSTERING



https://github.com/MathWorks-Teaching-Resources/Machine-Learning-for-Regression



#### **PROGRAMMING LANGUAGE**

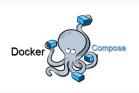




#### **DEVELOPMENT ENVIRONMENTS**







- ▲ \$ docker compose up
- ▼ \$ docker compose down







#### **JULIA IN A NUTSHELL**

- ▲ **Fast:** native code for multiple platforms via LLVM;
- **Dynamic:** good support for interactive use (like a a scripting language);
- **Reproducible:** environment recreation across platforms, with pre-built binaries;
- **Composable:** multiple dispatch as a paradigm (oop & functional programming);
- General: asynchronous I/O, metaprogramming, debugging, logging; profiling, pkg, ...
- Open Source: GitHub repository at <a href="https://github.com/JuliaLang/julia">https://github.com/JuliaLang/julia</a>.



# **JULIA MICRO-BENCHMARKS (1/2)**



https://julialang.org/benchmarks



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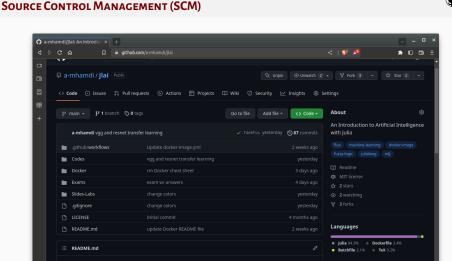
# **JULIA MICRO-BENCHMARKS (2/2)**

### Geometric Means<sup>1</sup> of Micro-Benchmarks by Language

1	С	1.0	
2	Julia	1.17006	
3	LuaJIT	1.02931	
4	Rust	1.0999	
5	Go	1.49917	
6	Fortran	1.67022	
7	Java	3.46773	
8	JavaScript	4.79602	
9	Matlab	9.57235	
10	Mathematica	14.6387	
11	Python	16.9262	
12	R	48.5796	
13	Octave	338.704	



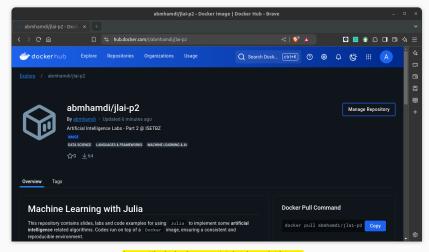




https://github.com/a-mhamdi/jlai

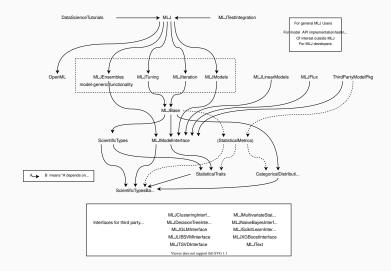
Fuzzy Logic, Machine Learning and Deep Learning with Julia

#### **DOCKER IMAGE**



https://hub.docker.com/r/abmhamdi/jlai-p2

# A MACHINE LEARNING FRAMEWORK FOR JULIA



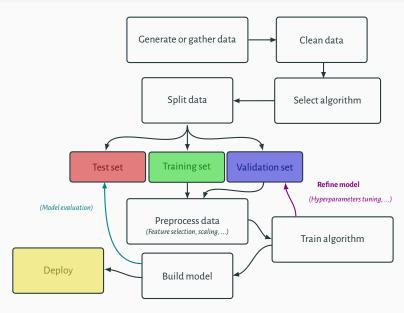
#### https://docs.juliahub.com/MLJ/

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Supervised Learning

### WORKFLOW IN MACHINE LEARNING



#### **DATA PREPROCESSING**

How?

Cleaning Identifying and correcting or removing inaccuracies and inconsistencies in the data

**Transformation** Converting data from one format or structure to another.

**Normalization** Scaling the data so that it fits within a specific range. This is often done to make the data more amenable to certain operations or algorithms.

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- Raw data is often messy and may need to be cleaned and formatted before it can be used for machine learning.
  - (This may involve removing missing or invalid data, handling outliers, and encoding categorical variables.)
- Normalizing the data can help to scale the features so that they are on the same scale. (This can be important for algorithms that use distance measures, as features on different scales can dominate the distance measure.)
- Preprocessing techniques such as feature selection and feature extraction can help to reduce the dimensionality of the data.
  - (This may improve the performance of the model and reduce the risk of overfitting.)
- Preprocessing techniques such as feature selection can help to identify the most important features in the data
  - (This can make the model more interpretable and easier to understand.)

### **DATA PREPROCESSING**

**FEATURE SCALING** 

#### Normalization

# $\frac{X - \min(X)}{\max(X) - \min(X)}$

▲ No assumption on data distribution

#### **Standardization** (Standardizer)

$$\langle \triangleq \frac{X - \mu}{\sigma}$$

▲ More recommended when following normal distribution



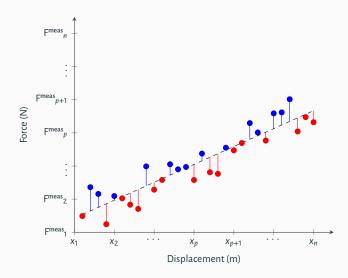
The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  ml-workflows.il

 $\rightarrow$  Jupyter  $\rightarrow$  ml-workflows.ipynb

Pluto.jl 🛢





Consider the example of a spring. Our main goal is to determine the stiffness *k* of this spring, given some experimental data. The mathematical model (*Hooke's law*):

$$F = kx (1)$$

Restoring force is proportional to displacement.

**Table 1:** Measurements of couple  $(x_i, F^{\text{meas}}_i)$ 

Xi	<i>x</i> <sub>1</sub>	 Хp	 Xn
F <sup>meas</sup> i	F <sup>meas</sup> <sub>1</sub>	 F <sup>meas</sup> <sub>p</sub>	 F <sup>meas</sup> n

$$F^{\text{meas}}_{i} = F_{i} + \varepsilon_{i}$$
$$= kx_{i} + \varepsilon_{i}, \qquad (2)$$

where  $F_i$  denotes the unknown real value of the force applied to the spring. In order to estimate the stiffness value k, we can consider the quadratic criterion:

$$\mathcal{J} = \sum_{i=1}^{n} \varepsilon_i^2$$
$$= \sum_{i=1}^{n} (F^{\text{meas}}_i - kx_i)^2$$

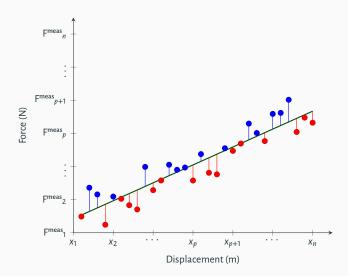
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$$\frac{\partial \mathcal{J}}{\partial k} = 0 \tag{3}$$

$$2\sum_{i=1}^{n} (F^{\text{meas}}_{i} - kx_{i}) \sum_{i=1}^{n} \frac{\partial (F^{\text{meas}}_{i} - kx_{i})}{\partial k} = 0$$

$$\sum_{i=1}^{n} (F^{\text{meas}}_{i} - kx_{i}) \sum_{i=1}^{n} x_{i} = 0$$

$$\sum_{i=1}^{n} \mathsf{F}^{\mathsf{meas}_{i}} x_{i} = k \sum_{i=1}^{n} x_{i}^{2} \iff \hat{k} = \frac{\sum_{i=1}^{n} \mathsf{F}^{\mathsf{meas}_{i}} x_{i}}{\sum_{i=1}^{n} x_{i}^{2}}$$





The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  simple-regression.jl

 $\rightarrow$  Jupyter  $\rightarrow$  simple-regression.ipynb

Pluto.jl 🛢



$$y = y_0 + v_0 t \tag{4}$$

Table 2: Measurements of position y

$t_k$	$t_1$	 $t_p$	 t <sub>n</sub>
y <sup>meas</sup> k	y <sup>meas</sup>	 y <sup>meas</sup> <sub>v</sub>	 y <sup>meas</sup> <sub>n</sub>

$$y^{\text{meas}}_{k} = y_{k} + \varepsilon_{k}$$
$$= y_{0} + v_{0}t_{k} + \varepsilon_{k}, \tag{5}$$

where  $y_k$  denotes the unknown real value of the position y at time point  $t_k$ .

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$$\mathcal{J} = \sum_{k=1}^{n} \varepsilon_k^2$$
$$= \varepsilon^{\mathsf{T}} \times \varepsilon$$

The vector  $\boldsymbol{\varepsilon}$  is set by  $\boldsymbol{\varepsilon}_k, \ \forall k \geq 1$ :

$$\varepsilon = \begin{bmatrix} \varepsilon_1 & \cdots & \varepsilon_n \end{bmatrix}^T$$

$$\frac{\partial \mathcal{J}}{\partial \left[\begin{array}{c} y_0 \\ \end{array}\right]} = 0 \tag{6}$$



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 $\rightarrow$  Pluto  $\rightarrow$  multivariable-regression.jl

 $\rightarrow$  Jupyter  $\rightarrow$  multivariable-regression.ipynb

Pluto.jl 🖁



Consider the following multivariable equation:

$$y = \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_m x_m \tag{7}$$

For a particular single measurement, eq. (7) can be updated as

$$y_k = \theta_1 x_{(1,k)} + \theta_2 x_{(2,k)} + \cdots + \theta_m x_{(m,k)} + \varepsilon_k$$

We denote hereafter by  $\boldsymbol{\theta}$  the vector  $\begin{bmatrix} \boldsymbol{\theta}_1 \\ \boldsymbol{\theta}_2 \\ \vdots \\ \boldsymbol{\theta}_m \end{bmatrix}$ . The function  $y_k$  becomes:

$$y_k = \underbrace{\left[x_{(1,k)}, x_{(2,k)}, \cdots, x_{(m,k)}\right]}_{\mathbf{x}_{l_k}^T} \boldsymbol{\theta} + \varepsilon_k$$

We assume that we have n measurements for y. Then we can transform the previous equation into

$$y = X\theta + \varepsilon$$

where 
$$\mathbf{y}^{\mathsf{T}} = [y_1, y_2, \cdots, y_n], \mathbf{X} = \begin{bmatrix} \mathbf{x}_1^{\mathsf{T}} \\ \mathbf{x}_2^{\mathsf{T}} \\ \vdots \\ \mathbf{y}^{\mathsf{T}} \end{bmatrix}$$
, and  $\boldsymbol{\varepsilon}^{\mathsf{T}} = [\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_n]$ .

We can consider the mean squared error or quadratic criterion in order to compute the approximated value of  $\theta$ :

$$\mathcal{J} = \sum_{k=1}^{n} \varepsilon_k^2$$
$$= \varepsilon^{\mathsf{T}} \varepsilon$$

The best well estimated value of  $\hat{\theta}$  corresponds to the absolute minimum of  $\mathcal{J}$ . This leads to calculate the gradient of  $\mathcal{J}$  with respect to  $\theta$ :

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}} = \frac{\partial (\boldsymbol{\varepsilon}^{\mathsf{T}} \boldsymbol{\varepsilon})}{\partial \boldsymbol{\theta}}$$

$$\frac{\partial (\boldsymbol{\varepsilon}^{\mathsf{T}} \boldsymbol{\varepsilon})}{\partial \boldsymbol{\theta}} = 2 \left( \frac{\partial \boldsymbol{\varepsilon}}{\partial \boldsymbol{\theta}} \right)^{\mathsf{T}} \boldsymbol{\varepsilon}$$

Recall that  $\varepsilon = y - X\theta$ , the term  $\frac{\partial \varepsilon}{\partial \theta}$  hence becomes:

$$\frac{\partial \varepsilon}{\partial \theta} = -X$$

$$\frac{\partial J}{\partial \boldsymbol{\theta}} = 2(-\mathbf{X})^{\mathsf{T}} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$$
$$= 0$$

The vector  $\hat{\boldsymbol{\theta}}$  is given by

$$\hat{\boldsymbol{\theta}} = \left( \mathbf{X}^{\mathsf{T}} \mathbf{X} \right)^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{y}$$



 $X^TX$  is not invertible (singular/degenerate)

▼ Redundant Features

Some features are linearly dependent, i.e,  $\exists$  some  $x_p \propto \text{some } x_l$ , e.g.,  $x_p$  in feet and  $x_l$  in m.

▼ Too many features

Fewer observations compared to the number of features, i.e,  $m \ge n$ .

- ▲ Delete some features
- ▲ Add extra observations

Use regularization: 
$$\underbrace{\lambda \sum_{i=2}^{m} |\theta_i|}_{\text{LASSO}} \underbrace{\frac{1}{2} \lambda \sum_{i=2}^{m} \theta_i^2}_{\text{RIDGE}} \underbrace{r \lambda \sum_{i=2}^{m} |\theta_i| + \frac{(1-r)}{2} \lambda \sum_{i=2}^{m} \theta_i^2}_{\text{ELASTICNET}}$$

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ \vdots & 1 & \ddots & \vdots \\ \vdots & \ddots & 1 & \ddots & \vdots \\ \vdots & \ddots & 1 & 0 \\ 0 & \cdots & \cdots & 0 & 1 \end{bmatrix}^{-1}$$

$$\boldsymbol{\chi}^{\mathsf{T}} \mathbf{y}^{\mathsf{T}} \mathbf{y}^{\mathsf$$

### PRACTICAL IMPLEMENTATION





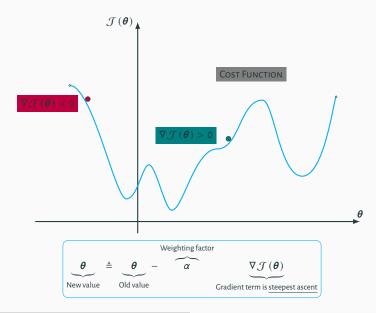
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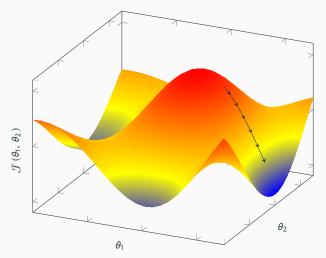
 $\rightarrow$  Pluto  $\rightarrow$  polynomial-regression.jl

 $\rightarrow$  Jupyter  $\rightarrow$  polynomial-regression.ipynb

Pluto.jl 🛢







- ① Start with some random values of  $\theta_1$  and  $\theta_2$
- ② Keep changing  $\theta_1$  and  $\theta_2$  to reduce  $\mathcal{J}(\theta_1, \theta_2)$  until we hopefully end up at minimum

$$\theta_i \triangleq \theta_i - \underbrace{\alpha}_{\text{Learning Rate}} \frac{\partial \mathcal{J}}{\partial \theta_i}$$

Recall that

$$\mathcal{J} = \frac{1}{2n} \sum_{k=1}^{n} (y_k - h_{\theta}(\mathbf{x}_k))^2 \quad \Longrightarrow \quad \frac{\partial \mathcal{J}}{\partial \theta_i} = -\frac{1}{n} \sum_{k=1}^{n} (y_k - h_{\theta}(\mathbf{x}_k)) x_{(i,k)}$$

$$\underbrace{\left(\theta_{1} \triangleq \theta_{1} + \alpha \frac{1}{n} \sum_{k=1}^{n} \left(y_{k} - h_{\theta}\left(\mathbf{x}_{k}\right)\right) \mathbf{x}_{\left(1,k\right)}\right)}_{:}$$

$$\vdots$$

$$\theta_{m} \triangleq \theta_{m} + \alpha \frac{1}{n} \sum_{k=1}^{n} (y_{k} - h_{\theta}(\mathbf{x}_{k})) x_{(m,k)}$$

$$\theta_i \triangleq \theta_i - \underbrace{\alpha}_{\text{Learning Rate}} \frac{\partial \mathcal{J}}{\partial \theta_i}$$

Recall that with L2 regularization term

$$\mathcal{J} = \frac{1}{2n} \sum_{k=1}^{n} (y_k - h_{\theta}(\mathbf{x}_k))^2 + \frac{\lambda}{2n} \sum_{i=2}^{m} \theta_i^2 \quad \Longrightarrow \quad \frac{\partial \mathcal{J}}{\partial \theta_i} = -\frac{1}{n} \sum_{k=1}^{n} (y_k - h_{\theta}(\mathbf{x}_k)) x_{(i,k)} + \frac{\lambda}{n} \theta_i \text{ iff } i \neq 1$$

$$\theta_{1} \triangleq \left(1 - \alpha \frac{1}{n}\right) \theta_{1} + \alpha \frac{1}{n} \sum_{k=1}^{n} \left(y_{k} - h_{\theta}\left(\mathbf{x}_{k}\right)\right) x_{(1,k)}$$

$$\theta_{2} \triangleq \left(1 - \alpha \frac{\lambda}{n}\right) \theta_{2} + \alpha \frac{1}{n} \sum_{k=1}^{n} \left(y_{k} - h_{\theta}\left(\mathbf{x}_{k}\right)\right) x_{(2,k)}$$

$$\theta_{m} \triangleq \left(1 - \alpha \frac{\lambda}{n}\right) \theta_{m} + \alpha \frac{1}{n} \sum_{k=1}^{n} \left(y_{k} - h_{\theta}\left(\mathbf{x}_{k}\right)\right) x_{(m,k)}$$

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# HANDS-ON EXAMPLE (1/3)

#### Task#2

The yield y of a chemical process is a random variable whose value is considered to be a linear function of the temperature x. The following data of corresponding values of x and y is found:

Temperature in °C ( $x$ )	0	25	50	75	100
Yield in grams (y)	14	38	54	76	95

The linear regression model  $y = \theta_1 + \theta_2 x$  is used. Determine the values of  $\theta_0$ ,  $\theta_1$ .

- 1. Using normal equation,
- 2. Using gradient descent for 5 iterations, given the following initial settings:

$$\alpha = 0.01$$
 and  $\boldsymbol{\theta} = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix}$ 

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# HANDS-ON EXAMPLE (2/3)

### **1** Normal Equation

$$\mathbf{y} = \begin{bmatrix} 14 \\ 38 \\ 54 \\ 76 \\ 95 \end{bmatrix} \text{ and } \mathbf{X} = \begin{bmatrix} 1 & 0 \\ 1 & 25 \\ 1 & 50 \\ 1 & 75 \\ 1 & 100 \end{bmatrix} \implies \hat{\boldsymbol{\theta}} = \begin{bmatrix} \hat{\theta}_1 \\ \\ \hat{\theta}_2 \end{bmatrix} = \begin{bmatrix} 15.4 \\ 0.8 \end{bmatrix}$$

#### ② Stochastic Gradient Descent

k	1 2		3	4	5	
у	14	38	54	76	95	
$h_{\boldsymbol{\theta}}(\mathbf{x}_k)$	1	13.63	330.999	-9894.410	734688.376	
$\hat{\boldsymbol{\theta}} = \begin{bmatrix} \hat{\theta}_1 \\ \hat{\theta}_2 \end{bmatrix}$	0.5	6.592	-1.396       -131.907	98.308 7345.901	-7247.626       -727247.475	

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# HANDS-ON EXAMPLE (3/3)

```
X = [1 \ 0: 1 \ 25: 1 \ 50: 1 \ 75: 1 \ 100] # Features
      y = [14, 38, 54, 76, 95] # Target
 3
      \alpha, n, \theta = 0.01, 5, [1; .5]
 4
 5
      J = \Gamma I
 6
      for k in 1:5
         h_{th} = X[k, :]' * \theta
         println("h_th = $(h_th)")
 9
         cost = (y[k] - h_th)^2
10
         push!(J, cost);
11
         \theta += \alpha * (y[k] - h_th) * X[k, :]
12
         println("\theta = $(\theta)\n")
13
      end
14
```



https://github.com/a-mhamdi/journey-into-ML/blob/main/Julia/gradient-descent.jl

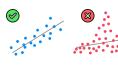
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# **Assumptions of Linear Regression**



1. Linearity

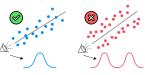
(Linear relationship between Y and each X)



2. Homoscedasticity



3. Multivariate Normality (Normality of error distribution)



4. Independence

(of observations. Includes "no autocorrelation")



5. Lack of Multicollinearity
(Predictors are not correlated with each other)



6. The Outlier Check
(This is not an assumption, but an "extra")



© SuperDataScience



▶ Source

# **EVALUATION METRICS (1/2)**

Mean Absolute Error (MAE) measures the average difference of absolute values between predicted and actual targets.

$$\mathbf{MAE} \ = \ \frac{1}{n} \sum_{k=1}^{n} |y_k - \hat{y}_k|$$

Root Mean Squared Error (RMSE) measures the root of the average squared difference between predicted and actual values.

**RMSE** = 
$$\sqrt{\frac{1}{n} \sum_{k=1}^{n} (y_k - \hat{y}_k)^2}$$

Mean Absolute Percentage Error (MAPE) is a measure of the prediction quality. It is equivalent to doing weighted MAE.

**MAPE** = 
$$\frac{1}{n} \sum_{k=1}^{n} \left| \frac{y_k - \hat{y}_k}{y_k} \right| \times 100\%$$

A lower error indicates a better fit of the model to the data.

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# **EVALUATION METRICS (2/2)**

**R-squared** is a statistical measure that quantifies the proportion of the variance in the dependent variable that is explained by the independent variables in the model.

$$\mathcal{R}^{2} = 1 - \frac{SS_{\text{residuals}}}{SS_{\text{total}}} = 1 - \frac{\sum_{k=1}^{n} (y_{k} - \hat{y}_{k})^{2}}{\sum_{k=1}^{n} (y_{k} - \bar{y})^{2}}$$

1 indicates that the model explains ALL the variance in the dependent variable

• O indicates that the model explains **NONE** of the variance in the dependent variable

Adjusted R-squared is a modified version of R-squared that accounts for the number of independent variables in the model.

Adjusted 
$$\mathcal{R}^2 = 1 - (1 - \mathcal{R}^2) \frac{n-1}{n-m-1}$$

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# HANDS-ON EXAMPLE (1/3)

Task#3

We consider a univariate regression problem with only two predictors m = 2. Compute the error metrics for the given data.

у	1	1	-2	5	-3.5	1
ŷ	0.9	0.85	-2.2	4.8	-3.3	1.2

# HANDS-ON EXAMPLE (2/3)

MAE: 
$$\frac{1}{6} \sum_{k=1}^{6} |y_k - \hat{y}_k| \approx 0.175$$

RMSE:  $\sqrt{\frac{1}{6} \sum_{k=1}^{6} (y_k - \hat{y}_k)^2} \approx 0.179$ 

MAPE:  $\frac{1}{6} \sum_{k=1}^{6} \left| \frac{y_k - \hat{y}_k}{y_k} \right| \times 100\% \approx 10.786$ 
 $\mathcal{R}^2$ :  $1 - \frac{\sum_{k=1}^{6} (y_k - \hat{y}_k)^2}{\sum_{k=1}^{6} (y_k - \bar{y})^2} \approx 0.996$ 

Adjusted  $\mathcal{R}^2$ :  $1 - (1 - \mathcal{R}^2) \frac{6 - 1}{6 - 2 - 1} \approx 0.992$ 

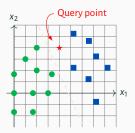
# HANDS-ON EXAMPLE (3/3)

```
v = [1 \ 1 \ -2 \ 5 \ -3.5 \ 1]
 2
    \hat{\mathbf{v}} = [-9.85 - 2.24.8 - 3.31.2]
 3
     mae = 1/6 * sum( abs.(y .- \hat{y}) ) # 0.17500000000000007
4
     rmse = \sqrt{(1/6 \times \text{sum}((y.-\hat{y}).^2))} # 0.1791182105017057
 5
     mape = 1/6 * sum( abs.((v.-\hat{v})./v)) * 100 # 10.785714285714288
 6
     v = 1/6 * sum(v): # 0.416666666666666663 (u\bar = ...)
 8
     # using Statistics: y = mean(y) (y bar = mean(y))
9
     r2 = 1 - sum((y.-\hat{y}).^2)/sum((y.-y).^2) # 0.9955448408871745
10
     adi r2 = 1 - (1-r2) * (6-1)/(6-2-1) # 0.9925747348119576
11
```



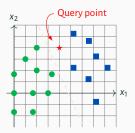
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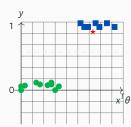
Classification is a type of supervised machine learning algorithm. A model is trained on a set of *labeled data*, where each data point is associated with a known <u>class</u> or <u>category</u>. The goal of the algorithm is to learn the relationship between the *input features x* and the corresponding *output classes y*, so that it can accurately predict the class of new, unseen query points.



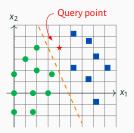


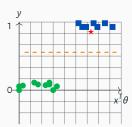
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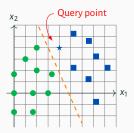


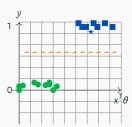
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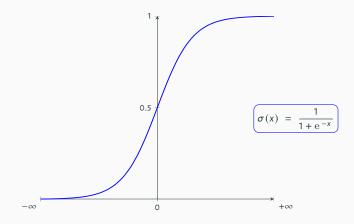


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### Logistic or S-shaped function $\sigma$



- $\sigma$  squashes range of distance from  $]-\infty, +\infty[$  to [0, 1]
- $\sigma$  is differentiable and easy to compute:  $(\dot{\sigma} = \sigma \times (1 \sigma))$

#### **DECISION BOUNDARY**

$$y = \sigma (\theta_1 x_1 + \theta_2 x_2 + \dots + \theta_m x_m)$$
$$y = \frac{1}{1 + e^{-\mathbf{x}^T} \theta}$$

## Hypothesis

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = P(y = 1 | \mathbf{x}; \boldsymbol{\theta}) = \frac{1}{1 + e^{-\mathbf{x}^T \boldsymbol{\theta}}}$$

For some given  $x_k$ 

$$h_{\boldsymbol{\theta}}(\mathbf{x}_k) = P(y=1|\mathbf{x}_k; \boldsymbol{\theta}) = \frac{1}{1 + e^{-\mathbf{x}_k^T \boldsymbol{\theta}}}$$

### **Cost function**

$$\mathcal{J} = \begin{cases} -\ln(h_{\theta}(\mathbf{x})) & \text{if} \quad y = 1 \\ -\ln(1 - h_{\theta}(\mathbf{x})) & \text{if} \quad y = 0 \end{cases}$$

$$\mathcal{J} = -y \ln \left( h_{\theta}(\mathbf{x}) \right) - (1 - y) \ln \left( 1 - h_{\theta}(\mathbf{x}) \right)$$

$$\theta_i \triangleq \theta_i - \underbrace{\alpha}_{\text{Learning Rate}} \frac{\partial \mathcal{J}}{\partial \theta_i}$$

Generalizing  $\mathcal{J}$  yields:

$$\mathcal{J} = -\frac{1}{n} \sum_{k=1}^{n} (y_k \ln (h_{\theta}(\mathbf{x}_k)) + (1 - y_k) \ln (1 - h_{\theta}(\mathbf{x}_k)))$$

$$\implies \frac{\partial \mathcal{J}}{\partial \theta_i} = -\frac{1}{n} \sum_{k=1}^{n} (y_k - h_{\theta}(\mathbf{x}_k)) x_{(i,k)}$$

$$\theta_1 \triangleq \theta_1 + \alpha \frac{1}{n} \sum_{k=1}^n (y_k - h_{\theta}(\mathbf{x}_k)) \mathbf{x}_{(1,k)}$$

$$\theta_2 \triangleq \theta_2 + \alpha \frac{1}{n} \sum_{k=1}^n (y_k - h_{\theta}(\mathbf{x}_k)) \mathbf{x}_{(2,k)}$$

$$\theta_2 \triangleq \theta_2 + \alpha \frac{1}{n} \sum_{k=1}^{n} (y_k - h_{\boldsymbol{\theta}}(\mathbf{x}_k)) x_{(2,k)}$$

$$\theta_{m} \triangleq \theta_{m} + \alpha \frac{1}{n} \sum_{k=1}^{n} (y_{k} - h_{\theta}(\mathbf{x}_{k})) x_{(m,k)}$$

$$\theta_i \triangleq \theta_i - \underbrace{\alpha}_{\text{LEARNING RATE}} \frac{\partial \mathcal{J}}{\partial \theta_i}$$

Generalizing  $\mathcal{J}$  with  $\mathbf{L}_2$  regularization term yields:

$$\mathcal{J} = -\frac{1}{n} \sum_{k=1}^{n} (y_k \ln (h_{\theta}(\mathbf{x}_k)) + (1 - y_k) \ln (1 - h_{\theta}(\mathbf{x}_k))) + \frac{\lambda}{2n} \sum_{i=2}^{m} \theta_i^2$$

$$\implies \frac{\partial \mathcal{J}}{\partial \theta_i} = -\frac{1}{n} \sum_{k=1}^{n} (y_k - h_{\theta}(\mathbf{x}_k)) x_{(i,k)} + \frac{\lambda}{n} \theta_i \text{ iff } i \neq 1$$

$$\theta_{1} \triangleq \left(1 - \alpha \frac{x}{n}\right) \theta_{1} + \alpha \frac{1}{n} \sum_{k=1}^{n} \left(y_{k} - h_{\theta}\left(\mathbf{x}_{k}\right)\right) x_{(1,k)}$$

$$\theta_2 \triangleq \left(1 - \alpha \frac{\lambda}{n}\right) \theta_2 + \alpha \frac{1}{n} \sum_{k=1}^n \left(y_k - h_{\theta}(\mathbf{x}_k)\right) x_{(2,k)}$$

:

$$\theta_{m} \triangleq \left(1 - \alpha \frac{\lambda}{n}\right) \theta_{m} + \alpha \frac{1}{n} \sum_{k=1}^{n} \left(y_{k} - h_{\theta}\left(\mathbf{x}_{k}\right)\right) \times_{(m,k)}$$



The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

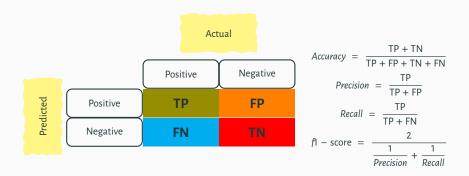
 $\rightarrow$  Pluto  $\rightarrow$  logistic-regression.jl

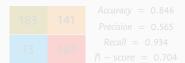
 $\rightarrow$  Jupyter  $\rightarrow$  logistic-regression.ipynb

Pluto.jl 🍍



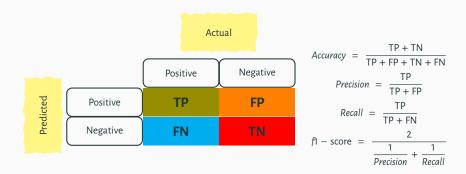
### **CONFUSION MATRIX**

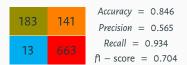




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#### **CONFUSION MATRIX**





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## **EVALUATION METRICS**









Accuracy denotes the ratio of how many we got right over all cases:

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

Precision designates how many positives do we get right over all positive predictions:

$$Precision = \frac{TP}{TP + FP}$$

Recall is the ratio of how many positives we got right over all actual positive cases:

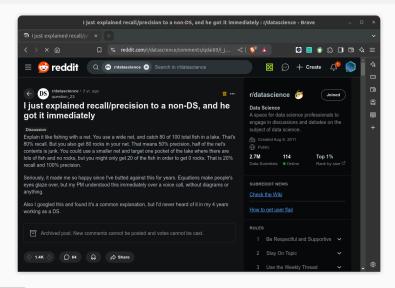
$$Recall = \frac{TP}{TP + FN}$$

f1 - score denotes the Harmonic Mean of Precision & Recall:

$$f1 - score = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}}$$

## **EVALUATION METRICS**

#### AN ANALOGY



### **EVALUATION METRICS**

**FOLLOW UP** 



$$f_{\beta} - \text{score} = \frac{1 + \beta}{\frac{1}{Precision} + \frac{\beta^2}{Recall}}$$

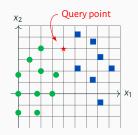
**Case #1:** Prioritize Precision over Recall, e.g.,  $\beta = 0.5$ 

- ► Mail spam detection
- Predicting appropriate day to launch a satellite

**Case #2:** Prioritize Recall over Precision, e.g.,  $\beta = 2$ 

- ► Detection of life threatening diseases like cancer
- ► Fraud detection

# k-Nearest Neighbors (1/2)



$$d(x; y) = \left(\sum_{i=1}^{n} |y_i - x_i|^p\right)^{1/p}$$

$$d(x; y) = \sum_{i=1}^{n} |y_i - x_i|$$

$$d(x; y) = \sum_{i=1}^{n} |y_i - x_i|$$

$$d(x; y) = \sqrt{\sum_{i=1}^{n} (y_i - x_i)^2}$$

## k-NEAREST NEIGHBORS (2/2)

► Evelyn Fix and Joseph Hodges, 1951 ► Thomas Cover, 1966

# Algorithm 1 Summary Construction

1: **procedure** How does *k*-NN work? (Finding Nearest Neighbors)

Input: A query point;

Output: Assign a class label to that point.

- 2: Define how many neighbors will be checked to classify the specific query point;
- 3: Compute the distance d(x; y) of the query point to other data points;
- 4: Count the number of the data points in each category;
- 5: Assign the query point to the class with most frequent neighbors.
- 6: end procedure

# HANDS-ON EXAMPLE (1/2)

#### Task #4

Let be the following coordinate points:

$$A(1, 6)$$
;  $B(2, 6)$ ;  $C(3, 1)$ ;  $D(4, 2)$ ;  $E(6, 0)$ ;  $F(7, 5)$ ;  $G(7, 3)$ ;  $H(10, 3)$ ;  $I(-4, -1)$ 

Using the Euclidean distance, what are the two closest neighbors of point P(5, 5)?

$$d(A; P) = \sqrt{17} \approx 4.12$$
  $d(B; P) = \sqrt{10} \approx 3.16$   $d(C; P) = \sqrt{20} \approx 4.47$ 

$$d(B; P) = \sqrt{10} \approx 3.16$$

$$d(C; P) = \sqrt{20} \approx 4.47$$

$$d(D; P) = \sqrt{10} \approx 3.16$$
  $d(E; P) = \sqrt{26} \approx 5.1$   $d(F; P) = \sqrt{4} = 2$ 

$$d(E; P) = \sqrt{26} \approx 5.1$$

$$d(F; P) = \sqrt{4} = 2$$

$$d(G; P) = \sqrt{8} \approx 2$$

$$d(G; P) = \sqrt{8} \approx 2.83$$
  $d(H; P) = \sqrt{29} \approx 5.38$   $d(I; P) = \sqrt{117} \approx 10.82$ 

$$d(I; P) = \sqrt{117} \approx 10.82$$

## HANDS-ON EXAMPLE (2/2)

```
function dds(a, b) # 'a' and 'b' are coordinates of some point
        d_{squared} = (a-5)^2+(b-5)^2
        (d_squared, sqrt(d_squared))
3
   end
5
   dds(1, 6) # Point 'A'
   dds(2, 6) # Point 'B'
```



# HANDS-ON EXAMPLE (1/3)

Task #5

We try to predict the color of a fruit according to its width (w) and height (h). The following training data is available:

Fruit	F <sub>1</sub>	$F_2$	$F_3$	$F_4$	$F_5$	$F_6$	F <sub>7</sub>	F <sub>8</sub>
w	2	5	2	6	1	4	2	6
h	6	6	5	5	2	2	1	1
Color	Red	Yellow	Orange	Purple	Red	Blue	Violet	Green

The goal here is to study the influence of neighbors on the color property of a fruit. Let U be the new fruit of width w = 1 and height h = 4

- 1. What is its color if we consider 1 neighbor?
- 2. What is its color if we consider 3 neighbors?
- 3. Rather than majority voting, we would like to consider the vote of neighbors weighted by the distance. Each neighbor votes according to a weight inversely proportional to the square of its distance:  $\frac{1}{42}$ . We take 3 neighbors, what is the color of *U*? Compare your results to those in question 2.

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# HANDS-ON EXAMPLE (2/3)

$$d(U; F_1) = \sqrt{5} \approx 2.24$$
  $d(U; F_2) = \sqrt{20} \approx 4.47$   $d(U; F_3) = \sqrt{2} \approx 1.41$ 

$$d(U; F_4) = \sqrt{26} \approx 5.1$$
  $d(U; F_5) = \sqrt{4} = 2$   $d(U; F_6) = \sqrt{13} \approx 3.6$ 

$$d(U; F_7) = \sqrt{10} \approx 3.16$$
  $d(U; F_8) = \sqrt{34} \approx 5.83$ 

- 1. Color of U is Orange because  $d(U; F_3)$  is the smallest.
- 2. Color of U is Red:  $F_1$  and  $F_5$  (+2 to Red class),  $F_3$  (+1 to Orange class)
- 3. Color of U is Orange

$$S(\text{Red}) = \frac{1}{d^2(U; F_1)} + \frac{1}{d^2(U; F_5)} = 0.45 S(\text{Orange}) = \frac{1}{d^2(U; F_3)} = 0.5$$

# HANDS-ON EXAMPLE (3/3)

```
function dds(w, h) # 'w' and 'h' are width and height of some fruit
        d_{squared} = (w-1)^2+(h-4)^2
        (d_squared, sqrt(d_squared))
3
   end
5
   dds(2, 6) # Fruit `F_1`
   dds(5, 6) # Fruit `F_2`
```





The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  knn.jl

 $\rightarrow$  Jupyter  $\rightarrow$  knn.ipynb

Pluto.jl 🍍



### RULE OF THUMB TO CHOOSE k

k is even if the number of classes is odd

k is odd if the number of classes is even

k is an important hyperparameter that can affect the performance of the model.

- 1. Larger values of k will result in a smoother decision boundary, which can lead to a more generalized model.
- 2. Smaller values of k will result in a more complex decision boundary, which can lead to a model that is more prone to overfitting.
- 3. The optimal value of k may depend on the specific dataset and the characteristics of the data.

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# SUPPORT VECTOR MACHINES (SVMs)

Support Vector Machines (SVMs) are supervised learning algorithms for classification and regression. They identify the optimal hyperplane to separate data into distinct classes.

**Hyperplane** A decision boundary separating classes in feature space.

**Support Vectors** Closest data points to the hyperplane, determining its position and orientation.

Margin Distance between the hyperplane and the nearest data points. SVM maximizes this margin.

For a dataset  $\{(\mathbf{x}_k, y_k)\}_{k=1}^n$ , where  $\mathbf{x}_k \in \mathbb{R}^d$  and  $y_k \in \{-1, +1\}$ :

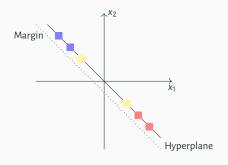
- Find a hyperplane  $\mathbf{x}^T \mathbf{w} + b = 0$  that maximizes the margin.
- Constrained optimization:

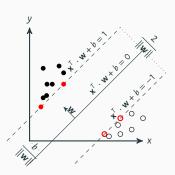
$$\min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2 \quad \text{s.t.} \quad y_k(\mathbf{x}_k^\mathsf{T} \mathbf{w} + b) \ge 1 \quad \forall k$$

### Types of SVMs

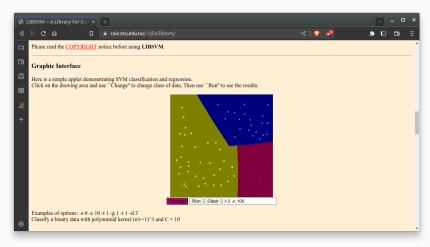
- ► Linear SVM: For linearly separable data.
- ► **Kernel SVM:** Maps data to higher dimensions for non-linear separation.

# **VISUALIZATION OF SVM (1/2)**





## VISUALIZATION OF SVM (2/2)



https://www.csie.ntu.edu.tw/~cjlin/libsvm/

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#### SVM: Loss Function

Hinge Loss Function: The hinge loss is used in SVMs to penalize misclassifications and maximize the margin:

$$L(y, h(\mathbf{x})) = \max(0, 1 - yh(\mathbf{x})),$$

where:

- ▶  $y \in \{-1, +1\}$  is the true label,
- $h(x) = \mathbf{x}^T \mathbf{w} + b$  is the predicted score.

The loss is zero if  $yh(x) \ge 1$  (correct classification with margin), and increases linearly otherwise.

## Why SVMs are powerful

- ▶ **Robustness:** Focuses on support vectors, making it less sensitive to outliers.
- ► **High-Dimensional Data:** Performs well even with a large number of features.
- ▶ **Kernel Trick:** Enables non-linear classification by mapping data to higher dimensions.

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# SOLVING THE LAGRANGIAN PROBLEM IN SVM (1/3)

### Primal Problem (Hard-Margin SVM)

The objective is to maximize the margin between two classes. The primal optimization problem is:

$$\min_{\mathbf{w},b} \frac{1}{2} \|\mathbf{w}\|^2$$
 subject to  $y_k \left(\mathbf{x}_k^\mathsf{T} \mathbf{w} + b\right) \ge 1$ ,  $\forall k$ 

#### Construct the Lagrangian

Introduce Lagrange multipliers  $\alpha_k \geq 0$  for each constraint and form the Lagrangian:

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{k=1}^{n} \alpha_k \left( y_k \left( \mathbf{x}_k^\mathsf{T} \mathbf{w} + b \right) - 1 \right)$$

#### Take Derivatives and Set to Zero

Minimize  $\mathcal{L}$  with respect to **w** and *b*:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{w} - \sum_{k=1}^{n} \alpha_k y_k \mathbf{x}_k = 0 \implies \mathbf{w} = \sum_{k=1}^{n} \alpha_k y_k \mathbf{x}_k$$

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# SOLVING THE LAGRANGIAN PROBLEM IN SVM (2/3)

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{k=1}^{n} \alpha_k y_k = 0 \implies \sum_{k=1}^{n} \alpha_k y_k = 0$$

### Substitute Back into the Lagrangian

Plugging w and the constraint into  $\mathcal{L}$ , we obtain the dual problem:

$$\mathcal{L}_{D}(\boldsymbol{\alpha}) = \sum_{k=1}^{n} \alpha_{k} - \frac{1}{2} \sum_{k,l=1}^{n} \alpha_{k} \alpha_{l} y_{k} y_{l} \mathbf{x}_{k}^{T} \mathbf{x}_{l}$$

#### Solve the Dual Problem

Maximize  $\mathcal{L}_D(\boldsymbol{\alpha})$  subject to:

$$\alpha_k \ge 0$$
 and  $\sum_{k=1}^n \alpha_k y_k = 0$ 

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# SOLVING THE LAGRANGIAN PROBLEM IN SVM (3/3)

#### Obtain the Solution

▶ The optimal  $\mathbf{w}^*$  is a linear combination of support vectors:

$$\mathbf{w}^{\star} = \sum_{k \in SV} \alpha_k y_k \mathbf{x}_k$$

▶ The bias  $b^*$  is computed using any support vector  $\mathbf{x}_{b}$ :

$$b^* = y_k - \mathbf{w}^{*\mathsf{T}} \mathbf{x}_k$$

#### Final Decision Function

For a new input x, the prediction is:

$$f(\mathbf{x}) = \operatorname{sign}\left(\mathbf{w}^{\star \mathsf{T}}\mathbf{x} + b^{\star}\right)$$

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# HANDS-ON EXAMPLE (1/9)

#### Task#6

You are given a dataset with two classes: Class A (y = +1) and Class B (y = -1). The features  $(x_1, x_2)$  and corresponding labels are:

Data Point	1	2	3	4	5	6
<i>x</i> <sub>1</sub>	2	3	1	6	7	8
X2	2	4	1	2	3	2
у	+1	+1	+1	-1	-1	-1

- 1. Plot the data points on a 2D plane.
- 2. Identify the support vectors.
- 3. Determine the optimal hyperplane separating the two classes using SVM.
- 4. Calculate the margin width if the weight vector is  $\mathbf{w} = \begin{bmatrix} -1/2, 1/4 \end{bmatrix}^T$ .

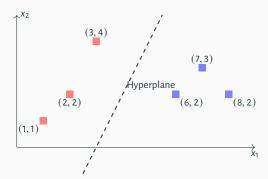
#### Hint!

Support vectors are the data points closest to the hyperplane. The margin width is given by:

$$Margin Width = \frac{2}{\|\mathbf{w}\|}$$

## Q. #1: Plot the Data Points

The data points are visualized on the plane  $(x_1, x_2)$ :



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# HANDS-ON EXAMPLE (3/9)

#### Q. #2: Support Vectors

The support vectors are the points closest to the hyperplane:

$$(2,2)$$
 from Class A,  $(3,4)$  from Class A,  $(6,2)$  from Class B.

### Q. #3: Optimal Hyperplane

$$\mathcal{L}_{D}(\boldsymbol{\alpha}) = \sum_{k=1}^{6} \alpha_{k} - \frac{1}{2} \sum_{k,l=1}^{6} \alpha_{k} \alpha_{l} y_{k} y_{l} \mathbf{x}_{k}^{\mathsf{T}} \mathbf{x}_{l}$$

$$= \alpha_{1} + \alpha_{2} + \alpha_{4}$$

$$- \frac{1}{2} (\alpha_{1} [8\alpha_{1} + 14\alpha_{2} - 16\alpha_{4}] + \alpha_{2} [14\alpha_{1} + 25\alpha_{2} - 26\alpha_{4}] - \alpha_{4} [16\alpha_{1} + 26\alpha_{2} - 40\alpha_{4}])$$

Given

$$\sum_{k=1}^{6} \alpha_k y_k = 0 \therefore \alpha_1 + \alpha_2 - \alpha_4 = 0$$

$$\mathcal{L}_D(\boldsymbol{\alpha}) = 2\alpha_1 + 2\alpha_2 - \frac{1}{2} (16\alpha_1^2 + 13\alpha_2^2 + 24\alpha_1\alpha_2)$$

# HANDS-ON EXAMPLE (4/9)

$$\frac{\partial \mathcal{L}_{D}(\boldsymbol{\alpha})}{\partial \alpha_{1}} = 0 \quad \therefore \quad 16\alpha_{1} + 12\alpha_{2} = 2$$

$$\frac{\partial \mathcal{L}_{D}(\boldsymbol{\alpha})}{\partial \alpha_{1}} = 0 \quad \therefore \quad 12\alpha_{1} + 13\alpha_{2} = 2$$

The resulting linear system is:

$$\begin{bmatrix} 16 & 12 \\ 12 & 13 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

lpha is:

$$\alpha^{T} = \begin{bmatrix} 1/32 & 1/8 & 0 & 5/32 & 0 & 0 \end{bmatrix}$$

► The optimal **w**<sup>\*</sup> is a linear combination of support vectors:

$$\mathbf{w}^{*} = \frac{1}{32} \begin{bmatrix} 2 \\ 2 \end{bmatrix} + \frac{1}{8} \begin{bmatrix} 3 \\ 4 \end{bmatrix} - \frac{5}{32} \begin{bmatrix} 6 \\ 2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} \\ \frac{1}{4} \end{bmatrix}$$

# HANDS-ON EXAMPLE (5/9)

▶ The bias  $b^*$  is computed using any support vector  $\mathbf{x}_{b}$ :

$$b^{\star} = y_k - \mathbf{x}_k^{\mathsf{T}} \mathbf{w}^{\star} = 3/2$$

The separating hyperplane is given by:

$$x_1 w_1 + x_2 w_2 + b = 0$$
 where  $\mathbf{w} = \begin{bmatrix} -1/2 \\ 1/4 \end{bmatrix}^T$ ,  $b = 3/2$ 

Thus, the equation becomes:

$$-2x_1 + x_2 + 6 = 0$$

#### Q. #4: Margin Width

The margin width is calculated as:

Margin Width = 
$$\frac{2}{\|\mathbf{w}\|} = \frac{2}{\sqrt{(1/2)^2 + (1/4)^2}} = \frac{8}{\sqrt{5}}$$

# HANDS-ON EXAMPLE (6/9)

```
using DataFrames, MLJ
     using Plots
 2
 3
     df = DataFrame(
 4
         x1 = [2, 3, 1, 6, 7, 8],
 5
        x2 = [2, 4, 1, 2, 3, 2],
        y = [1, 1, 1, -1, -1, -1]
9
     scatter(df.x1, df.x2, group=df.y)
10
11
     schema(df)
12
     #=
13
14
       names
               scitypes |
                          types
15
16
       x1
               Count
                          Int64
17
       x2
               Count
                          Int64
18
19
               Count
                          Int64
20
```

# HANDS-ON EXAMPLE (7/9)

```
=#
21
22
     coerce!(df, :x1 => Continuous, :x2 => Continuous, :y => OrderedFactor)
23
     scitype(df.y) <: AbstractVector{<:OrderedFactor} # true</pre>
24
     schema(df)
25
     #=
26
27
       names
                scitypes
                                    types
28
29
       x1
                Continuous
                                    Float64
30
               Continuous
                                   Float64
31
       x2
                OrderedFactor{2} | CategoricalValue{Int64. UInt32}
32
33
     =#
34
35
     X = select(df, \Gamma:x1, :x21)
36
     y = df.y
37
38
39
     "[LIBSVM](https://www.csie.ntu.edu.tw/~cjlin/libsvm/)"
     LinearSVC = @load LinearSVC pkg=LIBSVM
40
```

# HANDS-ON EXAMPLE (8/9)

```
# doc("LinearSVC", pka="LIBSVM")
41
42
     svc = LinearSVC()
43
     #=
44
     LinearSVC(
45
       solver = LIBSVM.Linearsolver.L2R L2LOSS SVC DUAL.
46
      tolerance = Inf.
47
      cost = 1.0.
48
       bias = -1.0
49
50
     =#
51
     mach svc = machine(svc. X. v) |> fit!
52
     fitted_params(mach_svc)
53
     #=
54
     (libsvm_model = LIBLINEAR.LinearModel{UInt32}(1, 2, 2, [-0.486189670915792, 0.
55
      →8956996119492998], Int32[1, 2], UInt32[0x00000002, 0x000000001], -1.0, 0.0),
      encoding = Dict{UInt32, CategoricalArrays.CategoricalValue{String, UInt32}}
56
      \hookrightarrow (0x00000002 => "1", 0x00000001 => "-1"),)
57
     =#
```

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# HANDS-ON EXAMPLE (9/9)

using LIBSVM

65 =#

59

```
Data = Matrix(X)'
mdl = svmtrain(D, y, kernel=Kernel.Linear)
mdl.SVs

#=
LIBSVM.SupportVectors{CategoricalArrays.CategoricalVector{Int64, UInt32, Int64, CategoricalArrays.CategoricalValue{Int64, UInt32}, Union{}}, Matrix{Float64}}(3, Int32[2, 1], CategoricalArrays.CategoricalValue{Int64, UInt32}[1, 1, -1], [2.0 3.
→0 6.0; 2.0 4.0 2.0], Int32[1, 2, 4], LIBSVM.SVMNode[LIBSVM.SVMNode(1, 2.0), LIBSVM.SVMNode(1, 3.0), LIBSVM.SVMNode(1, 6.0)])
```





The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

$$\rightarrow$$
 Pluto  $\rightarrow$  svc.jl

$$\rightarrow$$
 Jupyter  $\rightarrow$  svc.ipynb

# Pluto.jl 🛢



## NAIVE BAYES **COVID-19 TESTING**

#### Task #7

Imagine we have the following information:

- ▶ 1% of the population has COVID-19 (prior probability)
- ► A COVID test has 95% sensitivity (true positive rate) if you have COVID, there's a 95% chance the test will be positive
- ► The test has 90% specificity (true negative rate) if you don't have COVID, there's a 90% chance the test will be negative

Now, if someone receives a positive test result, what's the probability they actually have COVID-19?

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### NAIVE BAVES

#### **COVID-19 TESTING**

#### Task #7

Imagine we have the following information:

- ▶ 1% of the population has COVID-19 (prior probability)
- A COVID test has 95% sensitivity (true positive rate) if you have COVID, there's a 95% chance the test will be positive
- ► The test has 90% specificity (true negative rate) if you don't have COVID, there's a 90% chance the test will be negative

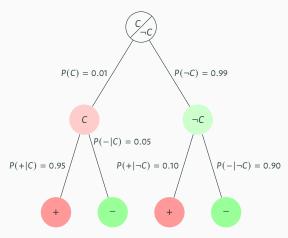
Now, if someone receives a positive test result, what's the probability they actually have COVID-19?

$$P(+) = P(C \cap +) + P(\neg C \cap +) = 0.0095 + 0.099 = 0.1085$$

$$P(C|+) = \frac{P(C \cap +)}{P(+)} = \frac{0.0095}{0.1085} \approx 0.088$$
 (8.8%)

 $\therefore$  Despite a positive test, there's only an 8.8% chance the person actually has COVID-19.

## **NAIVE BAYES COVID-19 TESTING**



$$P(C \cap +) = 0.01 \times 0.95 = 0.0095$$
  
 $P(C \cap -) = 0.01 \times 0.05 = 0.0005$ 

$$P(\neg C \cap +) = 0.99 \times 0.10 = 0.099$$
  
 $P(\neg C \cap -) = 0.99 \times 0.90 = 0.891$ 

## NAIVE BAYES (1/2)

#### DEFINITION AND KEY CONCEPT

Naive Bayes is a probabilistic machine learning algorithm based on Bayes' Theorem. It is commonly used for classification tasks, such as spam detection and text classification.

#### Bayes' Theorem:

$$P(y|X) = \frac{P(X|y) \cdot P(y)}{P(X)}$$

#### where:

- $\triangleright$  P(y|X): Posterior probability of class y given features X.
- $\triangleright$  P(X|y): Likelihood of features X given class y.
- ► P(y): Prior probability of class y.
- $\triangleright$  P(X): Marginal probability of features X.

$$\hat{y} = \arg\max_{y \in Y} P(y|X) = \arg\max_{y \in Y} P(X|y) \cdot P(y)$$

# NAIVE BAYES (2/2)

#### DEFINITION AND KEY CONCEPT



Features: Words in an email (e.g., "free", "offer", "money").

**Classes:** "Spam" (S) or "Not Spam" ( $\neg S$ ).

#### Steps:

- ① Calculate P(S) and  $P(\neg S)$  from the training data.
- ② Calculate P(Word|S) and  $P(Word|\neg S)$  for each word.
- ③ Use Bayes' Theorem to predict the class of a new email.

## HANDS-ON EXAMPLE (1/7)

#### Task #8

You are given a dataset of emails with the following word frequencies and labels:

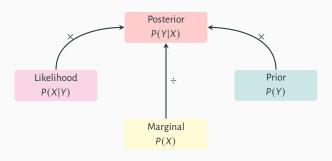
Email	"free"	"money"	Label
1	1	0	S
2	0	1	S
3	0	0	¬S
4	0	1	¬S

- 1. Calculate the prior probabilities P(S) and  $P(\neg S)$ .
- 2. Calculate the likelihoods P("free"|S), P("money"|S),  $P(\text{"free"}|\neg S)$ , and  $P(\text{"money"}|\neg S).$
- 3. Use Naive Bayes to classify a new email with the words "free" and "money".

### Hint!

▶ Use Laplace smoothing (add +1 smoothing) to handle zero probabilities.

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### **Step 1: Calculate Prior Probabilities**

► 
$$P(S) = \frac{\text{Number of Spam Emails}}{\text{Total Emails}} = \frac{2}{4} = 0.5$$

► 
$$P(\neg S) = \frac{\text{Number of Not Spam Emails}}{\text{Total Emails}} = \frac{2}{4} = 0.5$$

# HANDS-ON EXAMPLE (3/7)

### Step 2: Calculate Likelihoods with Laplace Smoothing

$$P("free"|S) = \frac{\text{Count of "free" in Spam} + 1}{\text{Count of Words in Spam} + |\text{Vocabulary}|} = \frac{1+1}{2+2} = \frac{2}{4} = 0.5$$

► 
$$P(\text{"money"}|S) = \frac{\text{Count of "money" in Spam} + 1}{\text{Count of Words in Spam} + |\text{Vocabulary}|} = \frac{1+1}{2+2} = \frac{2}{4} = 0.5$$

► 
$$P(\text{"free"}|\neg S) = \frac{\text{Count of "free" in Not Spam} + 1}{\text{Count of Words in } \neg \text{Spam} + |\text{Vocabulary}|} = \frac{0+1}{1+2} = \frac{1}{3} \approx 0.333$$

$$P(\text{``money''}|\neg S) = \frac{\text{Count of ``money'' in Not Spam} + 1}{\text{Count of Words in } \neg \text{ Spam} + |\text{Vocabulary}|} = \frac{1+1}{1+2} = \frac{2}{3} \approx 0.666$$

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## HANDS-ON EXAMPLE (4/7)

### Step 3: Classify a New Email

► For the email with words "free" and "money":

$$P(S|$$
 "free" and "money")  $\propto P($  "free" $|S) \cdot P($ "money" $|S) \cdot P(S)$ 

$$= 1/2 \cdot 1/2 \cdot 1/2 = 1/6$$

$$P(\neg S|$$
 "free" and "money")  $\propto P($  "free" $|\neg S) \cdot P($  "money" $|\neg S) \cdot P(\neg S)$ 

 $= 1/3 \cdot 2/3 \cdot 1/2 = 1/9$ 

► Since 1/6 > 1/9, the email is classified as **Spam**.

# HANDS-ON EXAMPLE (5/7)

```
using DataFrames, MLJ
 2
     df = DataFrame(
 3
         free = [1, 0, 0, 0],
         money = [0, 1, 0, 1],
 5
         label = ["S", "S", "NS", "NS"]
     schema(df)
 8
     #=
9
10
       names
               scitypes
                           tupes
11
12
      free
                Count
                           Int64
13
                           Int64
       moneu
               Count
14
       label | Textual
                           String
15
16
     =#
17
18
     coerce!(df, :label => OrderedFactor)
19
     scitype(df.label) <: AbstractVector{<:OrderedFactor} # true</pre>
20
```

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# HANDS-ON EXAMPLE (6/7)

```
schema(df)
21
     #=
22
23
               scitypes
       names
                                    types
24
25
                Count
                                    Int64
       free
26
               Count
                                    Int64
27
       money
       label |
               OrderedFactor{2} | CategoricalValue{String, UInt32}
28
29
     =#
30
31
     X = select(df, [:free, :money])
32
     y = df.label
33
34
     MultinomialNBClassifier = @load MultinomialNBClassifier pkg=NaiveBayes
35
     mnb = MultinomialNBClassifier()
36
     #=
37
     MultinomialNBClassifier(
38
39
       alpha = 1)
     =#
40
```

# HANDS-ON EXAMPLE (7/7)

```
mach_nb = machine(mnb, X, y) |> fit!
42
     predict(mach_nb, DataFrame(free = 1, money = 1))
43
     #=
44
     1-element CategoricalDistributions.UnivariateFiniteVector{Multiclass{2}, String,
45
     UInt32, Float64}:
      UnivariateFinite{Multiclass{2}}(NS=>0.471, S=>0.529)
46
47
     =#
```



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## **NAIVE BAYES: KEY ASSUMPTIONS AND TYPES**

## **Key Assumptions**

**Independence:** Features are assumed to be conditionally independent given the class.

**Equal Importance:** All features contribute equally to the prediction.

### **Types**

Gaussian Naive Bayes: Assumes features follow a normal distribution.

Multinomial Naive Bayes: Used for discrete data (e.g., word counts).

Bernoulli Naive Bayes: Used for binary features.

- Simple and fast to train.
- ▲ Works well with high-dimensional data (e.g., text).
- Requires less training data compared to other algorithms.

- Assumes feature independence, which is rarely true in real-world data.
- Struggles with zero probabilities (requires smoothing techniques).
- ▼ Less accurate for complex relationships hetween features



The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  naive-bayes.jl

 $\rightarrow$  Jupyter  $\rightarrow$  naive-bayes.ipynb

Pluto.jl 🛢



#### **DECISION TREE: DEFINITION AND KEY CONCEPTS**

A decision tree is a supervised learning algorithm used for classification and regression. It partitions the feature space into regions by applying a series of decision rules.

## Components

**Root Node:** Represents the entire dataset.

**Decision Nodes:** Split the dataset based on a feature and a threshold.

**Leaf Nodes:** Represent the final output (class label or regression value).

#### **Key Concepts**

Splitting Criteria: Choose the feature and threshold that maximize information gain or minimize

impurity.

**Pruning:** Remove unnecessary branches to prevent overfitting.

Feature Importance: Rank features based on their contribution to the model.

## **GINI INDEX VS ENTROPY**

## Gini Index

- Measures the impurity of a node.
- Lower values indicate purer nodes.

$$G=1-\sum_{i=1}^k p_i^2$$

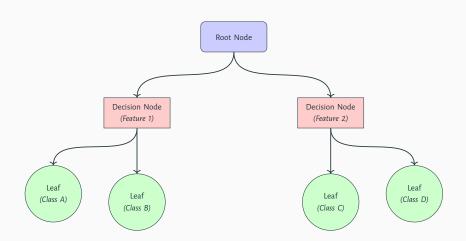
## Entropy

- ► Measures the uncertainty of a node.
- Lower values indicate more certainty.

$$H = -\sum_{i=1}^{k} p_i \log(p_i)$$

#### Comparison

- Both are used for splitting criteria in decision trees.
- ► Gini Index is faster to compute; Entropy provides more precise splits in some cases.



# HANDS-ON EXAMPLE (1/13)

Task#9 Considering the following restaurant wait time dataset, we need to predict if a reservation will be honored (Yes/No). Construct a **decision tree** using Gini Index:

Party Size	Day of Week	Special Occasion?	Reservation Honored?
2	Weekday	No	Yes
4	Weekend	Yes	No
6	Weekend	Yes	No
2	Weekend	No	Yes
4	Weekday	No	Yes
8	Weekend	Yes	No
2	Weekday	Yes	Yes
4	Weekend	No	No
6	Weekday	No	Yes
2	Weekend	Yes	No

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# HANDS-ON EXAMPLE (2/13)

### Step 1: Root Node Gini Impurity

$$G_{\text{Root}} = 1 - \left( \left( \frac{5}{10} \right)^2 + \left( \frac{5}{10} \right)^2 \right) = 1 - (0.25 + 0.25) = 0.5$$

### Step 2: Feature Split Analysis

Split 1: "Party Size"

$$G_{ps=2} = 1 - \left(\left(\frac{3}{4}\right)^2 + \left(\frac{1}{4}\right)^2\right) = 0.375$$

$$G_{ps=4} = 1 - \left(\left(\frac{1}{3}\right)^2 + \left(\frac{2}{3}\right)^2\right) = 0.444$$

$$G_{ps=6} = 1 - \left(\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2\right) = 0.5$$

$$G_{ps=8} = 1 - \left(\left(\frac{0}{1}\right)^2 + \left(\frac{1}{1}\right)^2\right) = 0$$

$$G_{split} = \frac{4}{10} \times 0.375 + \frac{3}{10} \times 0.444 + \frac{2}{10} \times 0.5 + \frac{1}{10} \times 0 = 0.383$$

# HANDS-ON EXAMPLE (3/13)

Split 2: "Weekend?""

$$G_{\text{weekday}} = 1 - \left( \left( \frac{4}{4} \right)^2 + \left( \frac{0}{4} \right)^2 \right) = 0$$

$$G_{\text{weekend}} = 1 - \left( \left( \frac{1}{6} \right)^2 + \left( \frac{5}{6} \right)^2 \right) = 0.278$$

$$G_{\text{split}} = \frac{4}{10} \times 0 + \frac{6}{10} \times 0.278 = 0.167$$

Split 3: "Special Occasion?"

$$G_{\text{special}} = 1 - \left( \left(\frac{1}{5}\right)^2 + \left(\frac{4}{5}\right)^2 \right) = 0.32$$

$$G_{\text{no special}} = 1 - \left( \left(\frac{4}{5}\right)^2 + \left(\frac{1}{5}\right)^2 \right) \approx 0.32$$

$$G_{\text{split}} = \frac{5}{10} \times 0.32 + \frac{5}{10} \times 0.32 \approx 0.32$$

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### HANDS-ON EXAMPLE (4/13)

## Step 3: Optimal Split Selection

- Weekend? has the lowest Gini impurity (G = 0.167)
- ▶ Party Size? (G = 0.383) and Special Occasion? ( $G \approx 0.32$ ) are less optimal

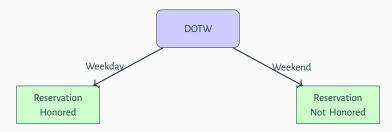
#### **RESULTING DECISION TREE**

1st split: "Weekend?"

**Weekday:** Predict "Reservation Honored" (4/4 samples) (pure leaf node)

Weekend: Predict "Reservation Not Honored" (5/6 samples)

Subsequent splits: Refine with "Party Size" or "Special Occasion?"



# HANDS-ON EXAMPLE (5/13)

Party Size	SO?	RH?
2	No	Yes
4	No	Yes
2	Yes	Yes
6	No	Yes

## Weekday Node Gini Impurity

$$G_{\text{Weekday}} = 1 - \left( \left( \frac{4}{4} \right)^2 + \left( \frac{0}{4} \right)^2 \right) = 0$$

Party Size	SO?	RH?
4	Yes	No
6	Yes	No
2	No	Yes
8	Yes	No
4	No	No
2	Yes	No

## Weekend Node Gini Impurity

$$G_{\text{Weekend}} = 1 - \left( \left( \frac{1}{6} \right)^2 + \left( \frac{5}{6} \right)^2 \right) = 0.278$$

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# HANDS-ON EXAMPLE (6/13)

"Party Size?" Split

$$G_{ps=2} = 1 - \left( \left( \frac{1}{2} \right)^2 + \left( \frac{1}{2} \right)^2 \right) = 0.5$$

$$G_{ps=4} = 1 - \left( \left( \frac{0}{2} \right)^2 + \left( \frac{1}{2} \right)^2 \right) = 0$$

$$G_{ps=6} = 1 - \left( \left( \frac{0}{1} \right)^2 + \left( \frac{1}{1} \right)^2 \right) = 0$$

$$G_{ps=8} = 1 - \left( \left( \frac{0}{1} \right)^2 + \left( \frac{1}{1} \right)^2 \right) = 0$$

$$G_{split} = \frac{2}{6} \times 0.5 + \frac{2}{6} \times 0 + \frac{1}{6} \times 0 + \frac{1}{6} \times 0 = 0.165$$

# HANDS-ON EXAMPLE (7/13)

"Special Occasion?" Split

$$G_{\text{special}}$$
 = 1 -  $\left(\left(\frac{0}{4}\right)^2 + \left(\frac{4}{4}\right)^2\right)$  = 0  
 $G_{\text{no special}}$  = 1 -  $\left(\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2\right)$   $\approx$  0.5  
 $G_{\text{split}}$  =  $\frac{4}{6} \times 0 + \frac{2}{6} \times 0.5$   $\approx$  0.167

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## HANDS-ON EXAMPLE (8/13)

## Optimal Split Selection

Both "Party Size" and "Special Occasion?" have the same Gini Index (0.1667) for the "Weekend" branch.

In this case, we can choose either one. Let's use "Special Occasion?" as our second split.

#### **RESULTING DECISION TREE**

2<sup>nd</sup> split: Special Occasion?

Yes: Predict "Reservation Not Honored" (4 samples)

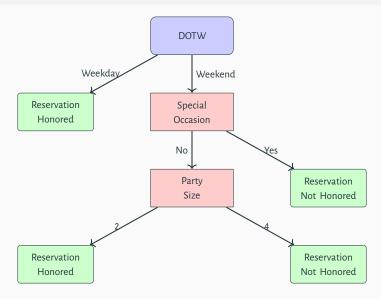
No: Refine with "Party Size" (2 samples)

3<sup>rd</sup> split: Party Size (pure leaf)

2: Predict "Reservation Honored" (1/2 sample)

4: Predict "Reservation Not Honored" (1/2 sample)

# HANDS-ON EXAMPLE (9/13)



# HANDS-ON EXAMPLE (10/13)

19

```
using DataFrames, MLJ
 1
 2
     df = DataFrame(
 3
         PS = [2, 4, 6, 2, 4, 8, 2, 4, 6, 2].
 4
         DOTW = ["Weekday", "Weekend", "Weekend", "Weekday", "Weekday", "Weekend",
 5
      →"Weekday", "Weekend", "Weekday", "Weekend"],
         SO = ["No", "Yes", "Yes", "No", "No", "Yes", "Yes", "No", "No", "Yes"],
 6
         RH = ["Yes", "No", "No", "Yes", "Yes", "No", "Yes", "No", "Yes", "No"]
 8
9
     schema(df)
     #=
10
11
       names | scitupes | tupes
12
13
       PS
               Count
                          Int64
14
       DOTW
               Textual
                         | Strina
15
       SO
               Textual
                        | String |
16
       RH
               Textual
                        | Strina |
17
18
     =#
```

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# HANDS-ON EXAMPLE (11/13)

```
20
     coerce!(df,
21
         :PS => Continuous,
22
         :DOTW => OrderedFactor,
23
         :SO => OrderedFactor,
24
         :RH => OrderedFactor
25
26
     schema(df)
27
     #=
28
29
       names
               scitupes
30
                                    types
31
                Continuous
       PS
                                    Float64
32
       DOTW
                OrderedFactor{2} |
                                    CategoricalValue{String, UInt32}
33
       SO
               OrderedFactor{2} | CategoricalValue{String, UInt32} |
34
                OrderedFactor{2} | CategoricalValue{String, UInt32} |
       RH
35
36
     =#
37
38
     X = select(df, Not(:RH))
39
```

# HANDS-ON EXAMPLE (12/13)

```
v = df.RH
40
41
     ohe = OneHotEncoder(drop_last=true)
42
     mach_ohe = machine(ohe, X) |> fit!
43
     W = MLJ.transform(mach_ohe, X)
44
     first(W, 2)
45
     #=
46
     2×3 DataFrame
47
48
     Row | PS
                    DOTW__Weekday SO__No
           Float64 Float64 Float64
49
50
       1 |
               2.0
                               1.0
                                       1.0
51
       2
               4.0
                              0.0
                                       0.0
52
     =#
53
54
     DecisionTreeClassifier = @load DecisionTreeClassifier pkg=DecisionTree
55
     dt = DecisionTreeClassifier() # an instance of `DecisionTreeClassifier'
56
57
58
     mach_tree = machine(dt, W, y)
     fit!(mach_tree, verbosity=2)
59
```

# HANDS-ON EXAMPLE (13/13)

```
#=
61
    Feature 2: "DOTW__Weekday" < 0.5 ?
62
    ├ Feature 3: "SO__No" < 0.5 ?
63
64
     ⊢ 1 : 4/4
        └ Feature 1: "PS" < 3.0 ?
65
         ⊢ 2 : 1/1
66

    □ 1 : 1/1

67
    □ 2 : 4/4
68
    =#
```

mach\_tree.report[:fit].print\_tree(mach\_tree.fitresult[1])



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60

69



The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  decision-tree-\*.jl

 $\rightarrow$  Jupyter  $\rightarrow$  decision-tree-\*.ipynb

Pluto.jl 🛢



## **ENSEMBLE APPROACH: RANDOM FOREST (1/2)**

A random forest is an ensemble method that combines multiple decision trees to improve classification accuracy. It uses bagging (bootstrap aggregation) and random feature selection.

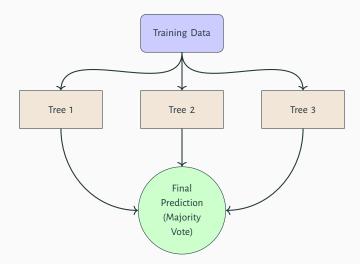
### **Key Features**

- ▶ **Diversity:** Trees are trained on different subsets of data and features.
- ▶ **Voting Mechanism:** For classification, the final output is the mode of the tree predictions.

#### **Loss Function**

► Combines the loss functions of individual trees, e.g., Gini Index or Entropy, during splits.

# **ENSEMBLE APPROACH: RANDOM FOREST (2/2)**





The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  random-forest-\*.jl

 $\rightarrow$  Jupyter  $\rightarrow$  random-forest-\*.ipynb

Pluto.jl 🛢



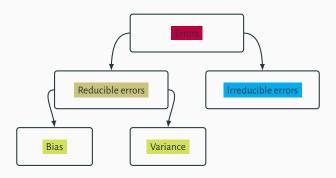
### **SUMMARY**

Method	Pros	Cons
Logistic Regression	▲ Probabilistic	<ul> <li>Almost linearly separable data</li> </ul>
k-NN	Fast and efficient	▼ # of neighbors k
K-ININ	Fast and emicient	<ul> <li>Detecting outliers<sup>2</sup></li> </ul>
	▲ Memory efficient	▼ Kernel's choice
SVM	▲ Versatile	<ul><li>Large datasets</li></ul>
37/71	Noise and outliers	<ul><li>Overlapping classes</li></ul>
	High dimension	<ul><li>Interpretability</li></ul>
Naive Bayes	▲ Simplicity and efficiency	<ul> <li>Independence between features</li> </ul>
Ivaive bayes	High dimension	▼ ∃ of irrelevant features
	▲ Interpretability	▼ Overfitting
Decision Tree	<ul> <li>Numerical and categorical data</li> </ul>	a ▼ Unstable
Decision tree	Robust to outliers	<ul><li>Continuous variables</li></ul>
	▲ High accuracy	▼ # of input features
Random Forest	▲ Less prone to overfitting	▼ Computation
Kunuum Foresi	<ul><li>High dimension</li></ul>	<ul><li>Interpretability</li></ul>

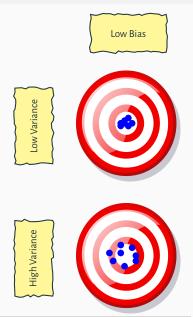
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<sup>&</sup>lt;sup>2</sup>Points that differ significantly from the rest of the data points.

## **ERRORS IN ML**



### **BIAS-VARIANCE TRADEOFF**



High Bias





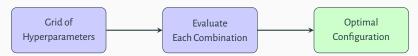
### **GRID SEARCH: OPTIMIZING HYPERPARAMETERS**

Grid Search is a systematic approach to finding the best hyperparameter combination for a machine learning model by evaluating all possible configurations.

### **Key Concepts**

- ► Defines a **grid** of hyperparameter values.
- Evaluates all combinations using a performance metric (e.g., accuracy, precision).
- ▶ Identifies the **optimal configuration** for the model.

#### **Process**



### Challenges

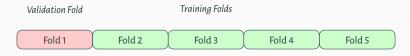
**Computationally expensive:** Large grids require significant resources.

Alternative: Randomized Search samples combinations to reduce computation.

## CROSS-VALIDATION: ENSURING ROBUSTNESS

Cross-validation is a resampling technique used to evaluate model performance by dividing the dataset into multiple subsets (folds) and validating the model on each subset.

- 1. Split the dataset into *k* subsets (folds).
- 2. Train the model on k-1 folds and validate on the remaining fold.
- 3. Repeat *k* times, using a different fold for validation each time.
- 4. Compute the average performance metric across all folds.



EXAMPLE: 5-FOLD CROSS-VALIDATION

#### **Benefits**

- Reduces overfitting by validating on multiple subsets.
- Provides a reliable estimate of model performance.



The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  hp.jl

 $\rightarrow$  Jupyter  $\rightarrow$  hp.ipynb

Pluto.jl 🛢



### PIPELINE MECHANISM: AUTOMATING WORKFLOW

A pipeline automates the sequential application of preprocessing steps and model training, ensuring a consistent and efficient workflow.

### Steps in a Pipeline

- 1. Preprocess data (e.g., scaling, normalization).
- 2. Apply dimensionality reduction or feature selection.
- 3. Train a machine learning model.



#### **Advantages**

- Ensures consistency across training and testing data.
- Simplifies hyperparameter optimization.

### INTEGRATING PIPELINES, GRID SEARCH, AND CROSS-VALIDATION

## Overview

Pipeline: Automates preprocessing and training.

**Grid Search:** Finds the best hyperparameters.

Cross-Validation: Ensures robust performance evaluation.



#### End-to-End Workflow

- 1. Define preprocessing steps in a pipeline.
- 2. Use Grid Search to optimize hyperparameters.
- 3. Validate results using K-Folds Cross-Validation.

# **OVERALL METHODOLOGY (1/2)**

#### 1 Problem Definition

- · Understand the business or research objective.
- Define success metrics (e.g., accuracy, F1-score, ROI).

#### 2 Data Collection

- Gather raw data from databases, APIs, or files.
- Ensure data quality, relevance, and representativeness.

#### 3. Data Preprocessing & Exploratory Analysis (EDA)

- Handle missing values, duplicates, and outliers.
- Perform statistical and visual analysis.

#### 4. Feature Engineering & Selection

- Transform/create meaningful features (e.g., scaling, encoding).
- Select optimal features (e.g., using PCA, feature importance).

#### 5. Model Selection & Training

- Split data into training, validation, and test sets.
- Train multiple algorithms (e.g., regression, neural networks).
- Apply cross-validation techniques.

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#### 6. Model Evaluation

- Test on unseen data (validation/test sets).
- Compare performance metrics (e.g., precision, RMSE, AUC-ROC).

#### 7. Hyperparameter Tuning & Optimization

• Fine-tune models using GridSearch, RandomSearch, or Bayesian methods.

### 8. Deployment & Monitoring

- Deploy the model (e.g., as an API, cloud service, or embedded system).
- · Continuously monitor performance and data drift.

#### 9. Communication & Maintenance

- Document methodology, results, and limitations.
- · Schedule retraining and updates as needed.

Unsupervised Learning

# K-MEANS CLUSTERING (1/3)

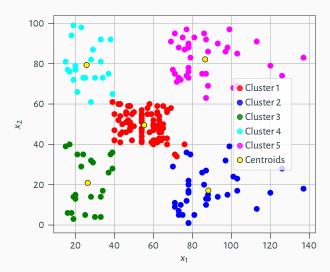
The algorithm *K***-Means** allows to display regularities or patterns in unlabeled data.

- ► The term 'means' refers to averaging the data when computing each centroid;
- A centroid is the arithmetic mean of all the data points belonging to a particular cluster.

This technique identifies a certain number of centroids within a data set. The algorithm then allocates every data point to the nearest cluster as it attempts to keep the clusters as small as possible. At the same time, K-Means attempts to keep the other clusters as different as possible.

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# K-MEANS CLUSTERING (2/3)



## K-Means Clustering (3/3)

## Algorithm 2 Summary Construction

1: **procedure** How does K-Means work? (Discovering similarities)

Input: Unlabeled data sets;

Output: Grouping into clusters.

- 2: Define how many clusters will be used to group the data sets;
- Initialize all the coordinates of the k cluster centers
- 4: repeat
- 5: Assign each point to its nearest cluster;
- 6: Update the centroids coordinates;
- 7: **until** No changes to the centers of the clusters
- 8: Assign new cases to one of the clusters
- 9: end procedure

Of the following examples, which would you address using an <u>unsupervised learning</u> algorithms? (Check all that apply.)

- 1. Given email labeled as spam/not spam, learn a spam filter
- 2. Given a set of news articles found on the web, group them into set of articles about the same story
- Given a database of customer data, automatically discover market segments and group customers into different market segments
- 4. Given a dataset of patients diagnosed as either having diabetes or not, learn to classify new patients as having diabetes or not.

<sup>&</sup>lt;sup>3</sup>From 'Machine Learning' course on 'Coursera'

Of the following examples, which would you address using an <u>unsupervised learning</u> algorithms? (Check all that apply.)

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- Given a database of customer data, automatically discover market segments and group customers into different market segments
- 4. Given a dataset of patients diagnosed as either having diabetes or not, learn to classify new patients as having diabetes or not.

<sup>&</sup>lt;sup>3</sup>From 'Machine Learning' course on 'Coursera'

Use K-Means algorithm to cluster the following eight points intro three clusters:

$$A(2, 10)$$
;  $B(2, 5)$ ;  $C(8, 4)$ ;  $D(5, 8)$ ;  $E(7, 5)$ ;  $F(6, 4)$ ;  $G(1, 2)$  and  $H(4, 9)$ .

- Initial cluster centers are:  $\alpha(2, 10)$ ;  $\beta(5, 8)$  and  $\gamma(1, 2)$
- The distance between two points:  $M(x_m, y_m)$  and  $N(x_n, y_n)$  is defined as

$$d(M; N) = |x_m - x_n| + |y_m - y_n|$$

<sup>4</sup>Credit: Shokoufeh Mirzaei. PhD

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$$d(M; N) = |x_m - x_n| + |y_m - y_n| \quad y$$

$$A \wedge A$$

$$B \wedge B$$

$$F \wedge C$$

<sup>&</sup>lt;sup>4</sup>Credit: Shokoufeh Mirzaei. PhD

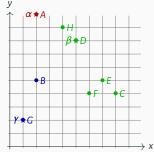
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$$d(M; N) = |x_m - x_n| + |y_m - y_n|$$

Point	$\alpha(2, 10)$	$\beta$ (5, 8)	γ(1, 2)	#
A(2, 10)	0	5	9	1
B(2, 5)	5	6	4	3
C(8, 4)	12	7	9	2
D(5, 8)	5	0	10	2
E(7, 5)	10	5	9	2
F(6, 4)	10	5	7	2
G(1, 2)	9	10	0	3
H(4, 9)	3	2	10	2



<sup>4</sup>Credit: Shokoufeh Mirzaei. PhD

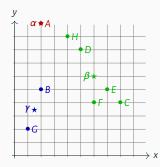
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E(7, 5)	10	5	9	2
F(6, 4)	10	5	7	2
G(1, 2)	9	10	0	3
H(4, 9)	3	2	10	2
α(2,	(10)	$\beta(6, 6)$	γ(1.5, 3.5	5))



<sup>&</sup>lt;sup>4</sup>Credit: Shokoufeh Mirzaei, PhD

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$$d(M; N) = |x_m - x_n| + |y_m - y_n|$$

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A(2, 10)	0	8	7	1
B(2, 5)	5	5	2	3
C(8, 4)	12	4	7	2
D(5, 8)	5	3	8	2
E(7, 5)	10	2	7	2
F(6, 4)	10	2	5	2
G(1, 2)	9	9	2	3
H(4, 9)	3	5	8	1



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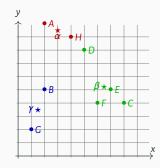
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F(6, 4)	10	2	5	2
G(1, 2)	9	9	2	3
H(4, 9)	3	5	8	1
(x(3 9	S) (B(6	5 5 25)	v(15 35)	<u> </u>



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<sup>&</sup>lt;sup>4</sup>Credit: Shokoufeh Mirzaei. PhD

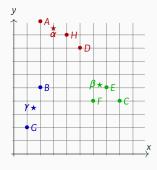
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- The distance between two points:  $M(x_m, y_m)$  and  $N(x_n, y_n)$  is defined as

$$d(M; N) = |x_m - x_n| + |y_m - y_n|$$

Point	$\alpha(3, 9.5)$	β(6.5, 5.25)	γ(1.5, 3.5)	#
A(2, 10)	1.5	9.25	7	1
B(2, 5)	5.5	4.75	2	3
C(8, 4)	10.5	2.75	7	2
D(5, 8)	3.5	4.25	8	1
E(7, 5)	8.5	0.75	7	2
F(6, 4)	8.5	1.75	5	2
G(1, 2)	9.5	8.75	2	3
H(4, 9)	1.5	6.25	8	1



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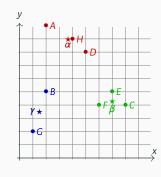
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Point	$\alpha(3, 9.5)$	$\beta$ (6.5, 5.25)	$\gamma(1.5, 3.5)$	#
A(2, 10)	1.5	9.25	7	1
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E(7, 5)	8.5	0.75	7	2
F(6, 4)	8.5	1.75	5	2
G(1, 2)	9.5	8.75	2	3
H(4, 9)	1.5	6.25	8	1
α(3	67. 9)	B(7, 4.3)	γ(1.5, 3.5)	



<sup>4</sup>Credit: Shokoufeh Mirzaei. PhD

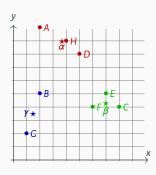
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 $d(M; N) = |x_m - x_n| + |y_m - y_n|$ 

- Initial cluster centers are:  $\alpha(2, 10)$ ;  $\beta(5, 8)$  and  $\gamma(1, 2)$
- The distance between two points:  $M(x_m, y_m)$  and  $N(x_n, y_n)$  is defined as

Point	$\alpha(3.67, 9)$	$\beta$ (7, 4.3)	γ(1.5, 3.5)	#	
A(2, 10)	2.67	10.7	7	1	
B(2, 5)	5.67	5.7	2	3	
C(8, 4)	9.33	1.3	7	2	
D(5, 8)	2.33	5.7	8	1	
E(7, 5)	7.33	0.7	7	2	
F(6, 4)	7.33	1.3	5	2	
G(1, 2)	9.67	8.3	2	3	
H(4, 9)	0.33	7.7	8	1	



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Point	$\alpha(3.67, 9)$	$\beta(7, 4.3)$	$\gamma(1.5, 3.5)$	#
A(2, 10)	2.67	10.7	7	1
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G(1, 2)	9.67	8.3	2	3
H(4, 9)	0.33	7.7	8	1
α(3	67 9)	3(7 4 3)	v(1.5, 3.5)	



<sup>&</sup>lt;sup>4</sup>Credit: Shokoufeh Mirzaei. PhD

## **PRACTICAL IMPLEMENTATION**





The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  kmeans.il

 $\rightarrow$  Jupyter  $\rightarrow$  kmeans.ipynb

Pluto.jl 🍍



### **DBSCAN: OVERVIEW**

DBSCAN (Density-Based Spatial Clustering of Applications with Noise) is a density-based clustering algorithm that groups together points closely packed in space while marking points in sparse regions as outliers.

**Epsilon** ( $\epsilon$ ): Maximum distance between two points to consider them as neighbors.

MinPts: Minimum number of points required to form a dense region.

**Core Point:** A point with at least MinPts neighbors within  $\epsilon$ -distance.

**Border Point:** A point within  $\epsilon$ -distance of a core point but with fewer than MinPts neighbors.

Noise Point: A point that is neither a core point nor a border point.

### Steps of DBSCAN

- 1. Select an unvisited point and check its  $\epsilon$ -neighborhood.
- 2. Mark it as a core, border, or noise point based on MinPts.
- 3. Expand clusters iteratively by connecting core points.
- 4. Continue until all points are visited.

### **DBSCAN: VISUAL REPRESENTATION**



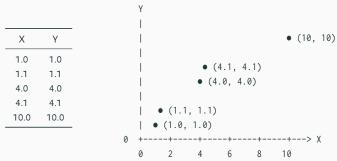


- ▲ Detects clusters of arbitrary shapes.
- Robust to noise and outliers.

- ▼ Sensitive to the choice of  $\epsilon$  and MinPts.
- Struggles with clusters of varying densities.
- Performance degrades with high-dimensional data.

## HANDS-ON EXAMPLE (1/3)

Task #12 Consider the following synthetic 2D dataset with 5 points:



Apply DBSCAN with  $\epsilon=1.5$  and MinPts = 2.

# HANDS-ON EXAMPLE (2/3)

### Compute Pairwise Distances

	(1, 1)	(1.1, 1.1)	(4, 4)	(4.1, 4.1)	(10, 10)
(1, 1)	0.00	0.141	4.243	4.384	12.738
(1.1, 1.1)	0.141	0.00	4.101	4.243	12.586
(4, 4)	4.243	4.101	0.00	0.141	8.485
(4.1, 4.1)	4.384	4.243	0.141	0.00	8.344
(10, 10)	12.738	12.586	8.485	8.344	0.00

### **Identify Core Points**

A point is a **core point** if  $\geq$  MinPts neighbors exist within  $\epsilon$ :

- ▶ (1.0, 1.0): Neighbors =  $\{(1.1, 1.1)\} \rightarrow 1 (<2) \rightarrow Border$
- ► (1.1, 1.1): Neighbors =  $\{(1.0, 1.0)\} \rightarrow 1 (<2) \rightarrow Border$
- ▶ **(4.0, 4.0)**: Neighbors =  $\{(4.1, 4.1)\} \rightarrow 1 (<2) \rightarrow Border$
- ► **(4.1, 4.1)**: Neighbors =  $\{(4.0, 4.0)\} \rightarrow 1 (<2) \rightarrow Border$
- ▶ (10.0,10.0): No neighbors within  $\epsilon \rightarrow Noise$

# HANDS-ON EXAMPLE (3/3)

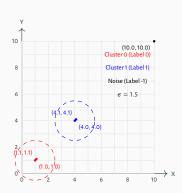
## Cluster Assignment

**Cluster 1**: {(1.0,1.0), (1.1,1.1)} (mutually reachable via *ϵ*)

► Cluster 2: {(4.0,4.0), (4.1,4.1)} (mutually reachable via  $\epsilon$ )

► **Noise**: (10.0,10.0) (no nearby points)

Point (X, Y)	Label	Туре
(1.0, 1.0)	0	Border
(1.1, 1.1)	0	Border
(4.0, 4.0)	1	Border
(4.1, 4.1)	1	Border
(10.0, 10.0)	-1	Noise



### **PRACTICAL IMPLEMENTATION**





The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  dbscan.jl

 $\rightarrow$  Jupyter  $\rightarrow$  dbscan.ipynb

Pluto.jl 🛢



## PRINCIPAL COMPONENT ANALYSIS (PCA): OVERVIEW

PCA is a dimensionality reduction technique that transforms a high-dimensional dataset into a lower-dimensional space by identifying the directions of maximum variance.

- Reduce the number of features while retaining most of the dataset's variability.
- Identify patterns in data by capturing principal components.
- Remove redundant or irrelevant information.

#### **How PCA Works**

- 1. Standardize the dataset (mean = 0, variance = 1).
- 2. Compute the covariance matrix.
- 3. Calculate eigenvalues and eigenvectors of the covariance matrix.
- 4. Project the data onto the eigenvectors with the largest eigenvalues (principal components).

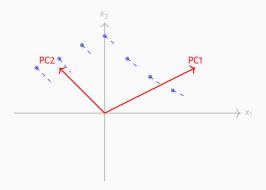
## **Applications**

- Image compression.
- Data visualization in 2D or 3D.
- Noise reduction.

### VISUALIZING PCA

#### **UNDERSTANDING PCA THROUGH A 2D EXAMPLE:**

- ▶ Dataset with two features  $(x_1, x_2)$ .
- ► PCA identifies the principal axes of variance (principal components).
- Data is projected onto these axes.



- ① PC1: Captures the most variance in the data.
- ② PC2: Captures the remaining variance, orthogonal to PC1.

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# HANDS-ON EXAMPLE (1/8)

STEP-BY-STEP PCA EXAMPLE

$$\mathbf{X} = \begin{bmatrix} 2.5 & 2.4 \\ 0.5 & 0.7 \\ 2.2 & 2.9 \\ 1.9 & 2.2 \\ 3.1 & 3.0 \\ 2.3 & 2.7 \\ 2.0 & 1.6 \\ 1.0 & 1.1 \\ 1.5 & 1.6 \\ 1.1 & 0.9 \end{bmatrix}$$

## HANDS-ON EXAMPLE (2/8)

#### STEP-BY-STEP PCA EXAMPLE

### Mean Normalization

$$\bar{X} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix} = \begin{bmatrix} 1.81 \\ 1.91 \end{bmatrix}, \quad \mathbf{X}_{normalized} = \mathbf{X} - \bar{X}$$

### Covariance Matrix

$$\mathbf{C} = \frac{1}{n-1} \mathbf{X}_{\text{normalized}}^{\mathsf{T}} \mathbf{X}_{\text{normalized}} \approx \begin{bmatrix} 0.6165 & 0.6152 \\ 0.6152 & 0.7165 \end{bmatrix}$$

## Eigenvalues and Eigenvectors

Eigenvalues: 
$$\lambda_1 \approx 1.284$$
,  $\lambda_2 \approx 0.049$ 

Eigenvectors: 
$$\mathbf{v}_1 \approx \begin{bmatrix} 0.678 \\ 0.735 \end{bmatrix}, \quad \mathbf{v}_2 \approx \begin{bmatrix} -0.735 \\ 0.677 \end{bmatrix}$$

## HANDS-ON EXAMPLE (3/8)

STEP-BY-STEP PCA EXAMPLE

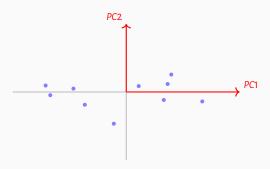
## Project Data onto Principal Components

$$= \mathbf{X}_{normalized} \mathbf{V}, \quad \therefore \quad \mathbf{Z} \approx \begin{bmatrix} 0.827 & -0.175 \\ -1.777 & 0.142 \\ 0.992 & 0.384 \\ 0.274 & 0.130 \\ 1.675 & -0.209 \\ 0.912 & 0.175 \\ -0.099 & -0.35 \\ -1.144 & 0.046 \\ -0.438 & 0.018 \\ -1.224 & -0.163 \end{bmatrix}$$

## HANDS-ON EXAMPLE (4/8)

STEP-BY-STEP PCA EXAMPLE

## Visualization of Principal Components



## **Key Observations**

- ► Most variance is along *PC*1 (horizontal axis).
- ▶ Data projected onto PC2 (vertical axis) shows minimal variance.

# HANDS-ON EXAMPLE (5/8)

#### STEP-BY-STEP PCA EXAMPLE

```
X = \Gamma
          2.5 2.4; 0.5 0.7; 2.2 2.9; 1.9 2.2; 3.1 3.0;
 2
          2.3 2.7; 2.0 1.6; 1 1.1; 1.5 1.6; 1.1 0.9
 3
 4
 5
     X = 1/10 * sum(X, dims=1) # X bar = ...
 6
     #=
     1×2 Matrix{Float64}:
     1.81 1.91
 9
     =#
10
11
     Xnorm = X . - X # X . - X bar
12
     #=
13
14
     10×2 Matrix{Float64}:
15
     0.69 0.49
      -1.31 -1.21
16
      0.39 0.99
17
      0.09 0.29
18
      1.29
            1.09
19
```

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# HANDS-ON EXAMPLE (6/8)

### STEP-BY-STEP PCA EXAMPLE

```
0.49 0.79
20
    0.19 -0.31
21
     -0.81 -0.81
22
23
     -0.31 -0.31
     -0.71 -1.01
24
     =#
25
26
     C = 1/(9)*(Xnorm'*Xnorm) # C = 1/(n-1) * ...
27
     #=
28
     2×2 Matrix{Float64}:
29
     0.616556 0.615444
30
     0.615444 0.716556
31
     =#
32
33
34
     using LinearAlgebra
     \lambda, V = eigen(C)
35
     #=
36
     Eigen{Float64, Float64, Matrix{Float64}, Vector{Float64}}
37
     values:
38
```

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## HANDS-ON EXAMPLE (7/8)

#### STEP-BY-STEP PCA EXAMPLE

```
2-element Vector{Float64}:
39
     0.04908339893832736
40
      1.2840277121727837
41
     vectors:
42
43
     2×2 Matrix{Float64}:
     -0.735179 0.677873
44
       0.677873 0.735179
45
     =#
46
47
     7 = Xnorm * V
48
     #=
49
50
     10×2 Matrix{Float64}:
      -0.175115
                   0.82797
51
      0.142857 -1.77758
52
53
      0.384375
                 0.992197
      0.130417
                 0.27421
54
      -0.209498
                  1.6758
55
      0.175282
                  0.912949
56
      -0.349825
                  -0.0991094
57
```

# HANDS-ON EXAMPLE (8/8)

#### STEP-BY-STEP PCA EXAMPLE



### **PRACTICAL IMPLEMENTATION**





The code is available @ github.com/a-mhamdi/jlai  $\rightarrow$  Codes  $\rightarrow$  Julia  $\rightarrow$  Part-2

 $\rightarrow$  Pluto  $\rightarrow$  pca.jl

 $\rightarrow$  Jupyter  $\rightarrow$  pca.ipynb

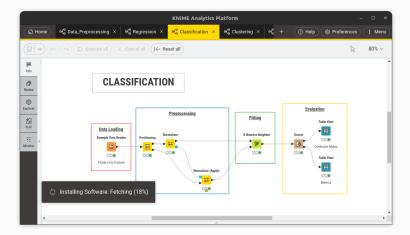
Pluto.jl 🍍



Complementary Lab. Project

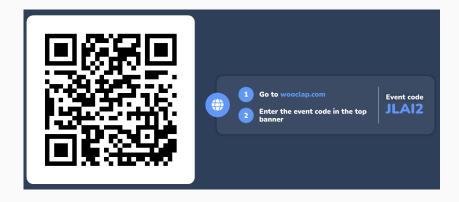
On the day of assignment, you will be informed about the **dataset to use** (*source: database*), **specific features to retain**, and the **machine learning model to implement**. You will be asked to:

- ① ETL(Extract, Transform, Load) data from a database;
- ② Build and evaluate the ML model (pipeline, featurization, split, etc.).



ML Landscape through Quizzes

## **KNOWLEDGE CHECK**



https://app.wooclap.com/JLAI2

## **FURTHER READING (1/2)**

2021, 420 pp.

## References

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