Demystifying Artificial Intelligence Sorcery

(Part 2: Machine Learning)[a]

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[a]Available @ https://github.com/a-mhamdi/jlai/

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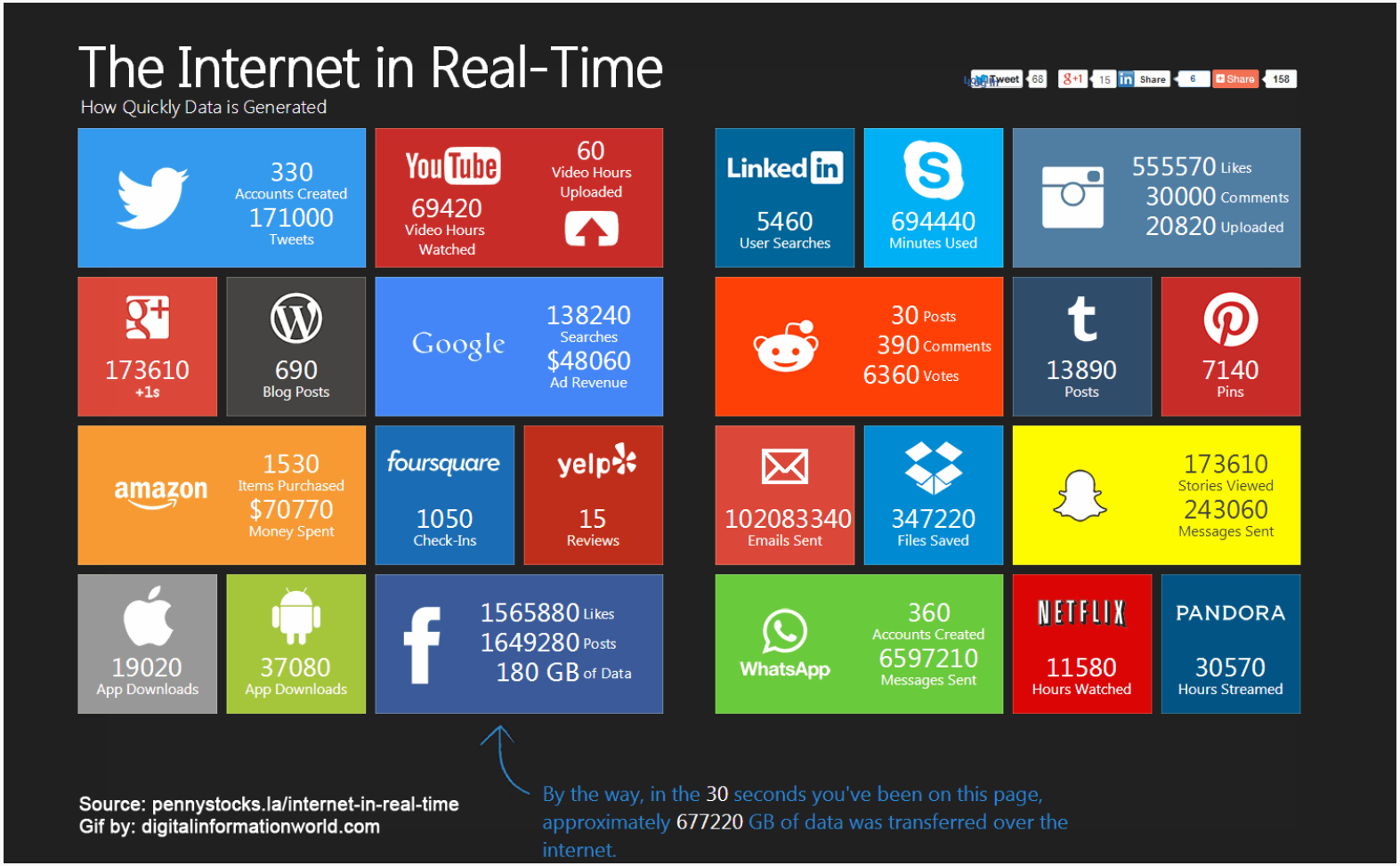
Roadmap

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

An overview

Global Data Traffic



Update on the internet in real time is available here.

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.**

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.**

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 Naqa, I. and Murphy, M. J. (2015) *What Is Machine Learning?*, pages 3–11. **Springer International Publishing.**

Debrief

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 $\mathcal{E}$.

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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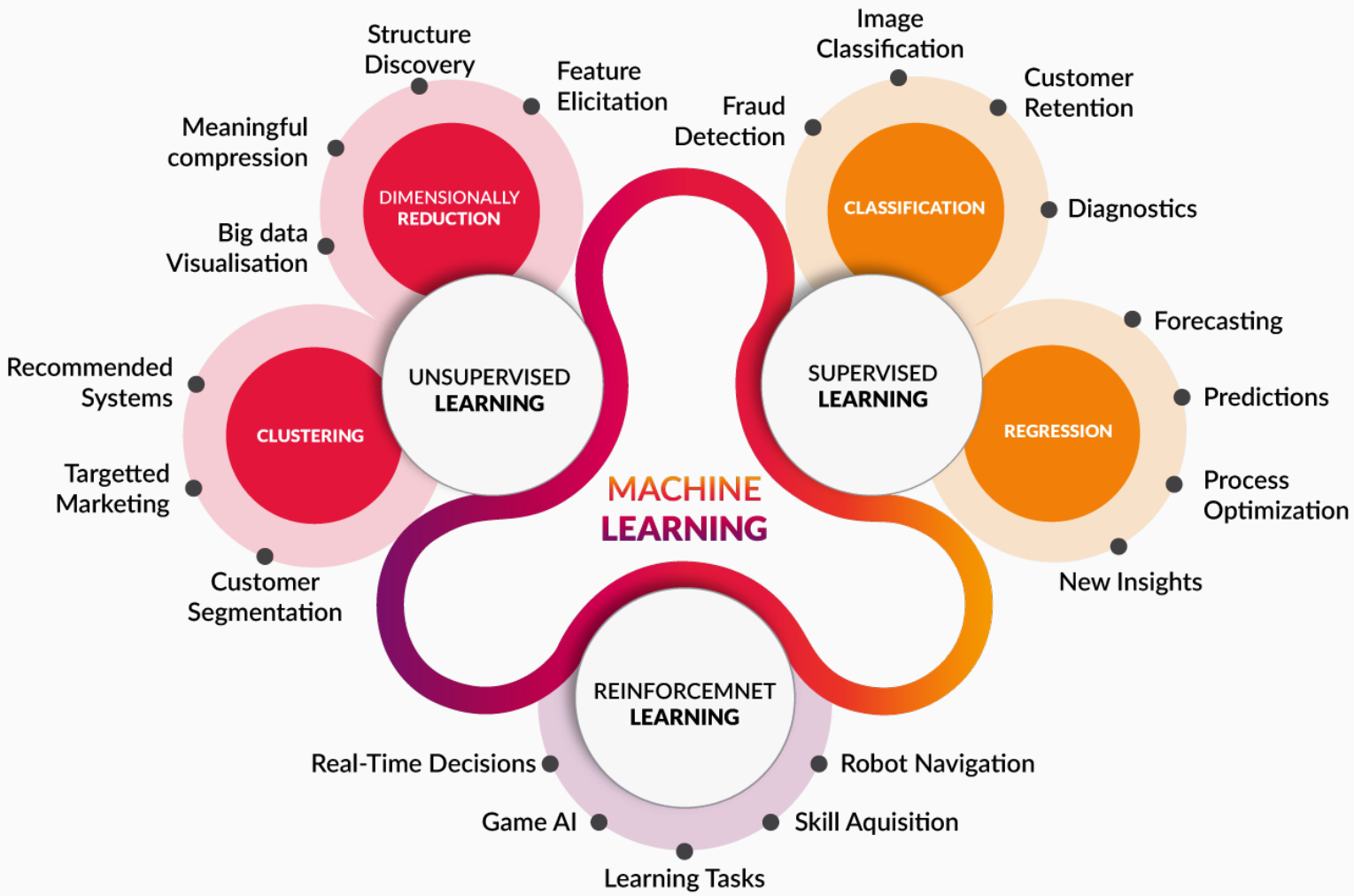
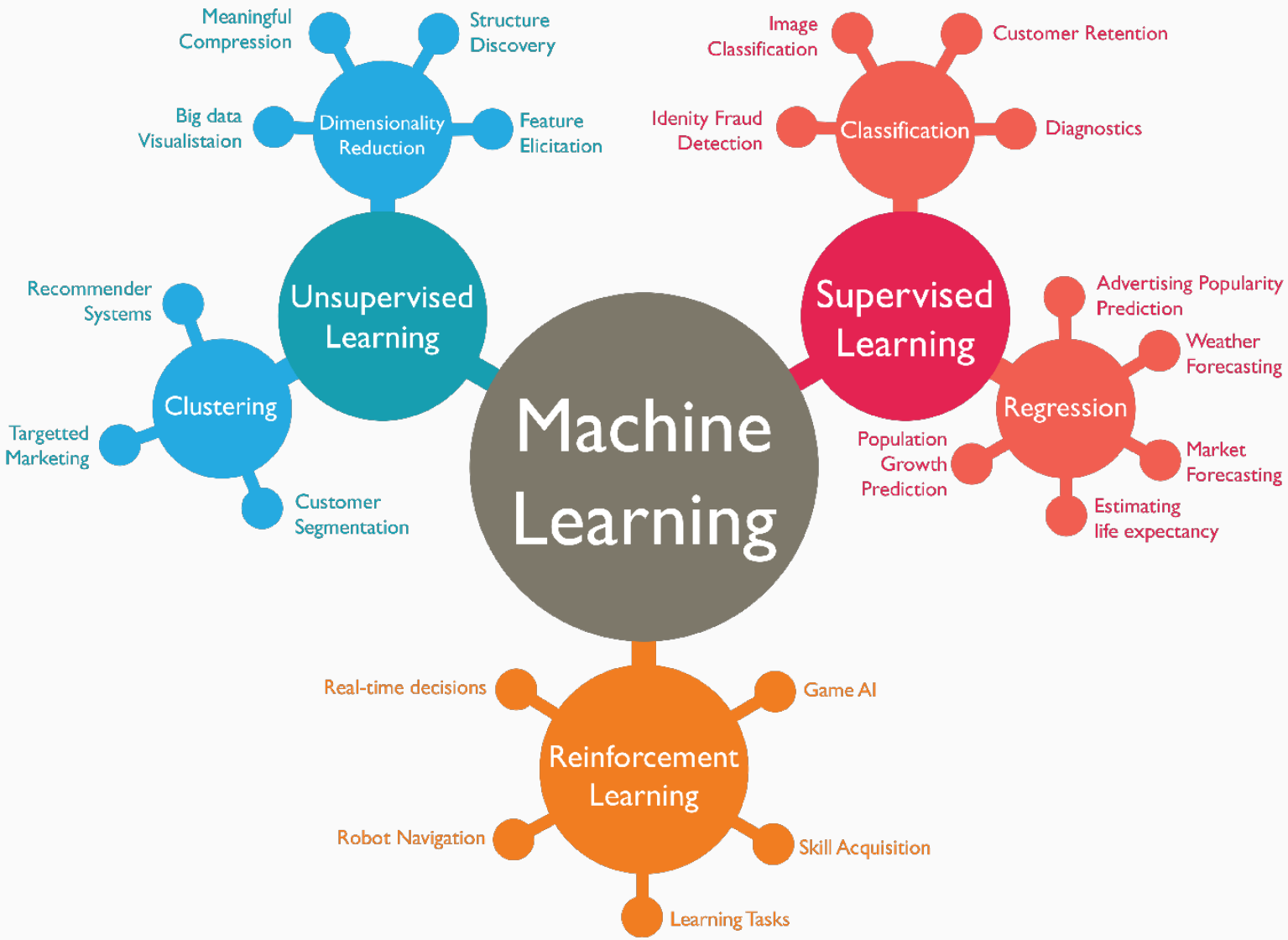
Overall Methodology

1. Define the problem;
2. Gather dataset;
3. Choose measure of success;
4. Decide evaluation protocol;
5. Prepare the data;
6. Develop a model;
7. Iterate models.

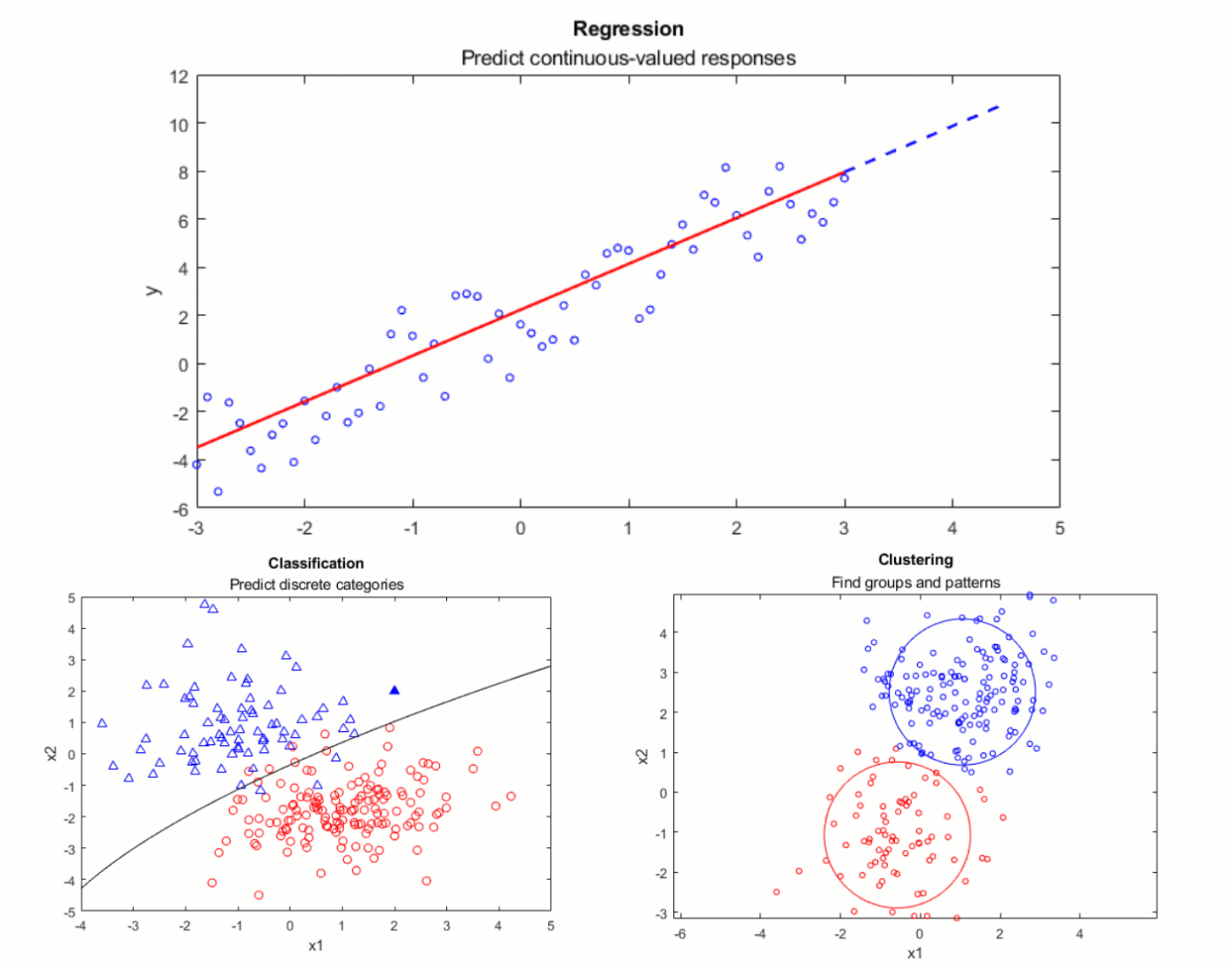


https://www.cognub.com/index.php/cognitive-platform/



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

Regression | Classification | Clustering



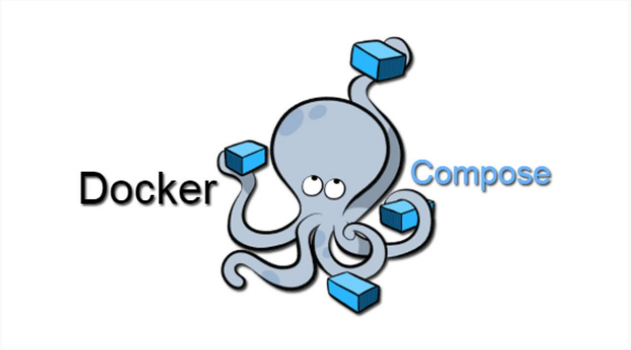
https://github.com/MathWorks-Teaching-Resources/Machine-Learning-for-Regression


REMINDER

Programming Language

julialang.org/

Development Environments

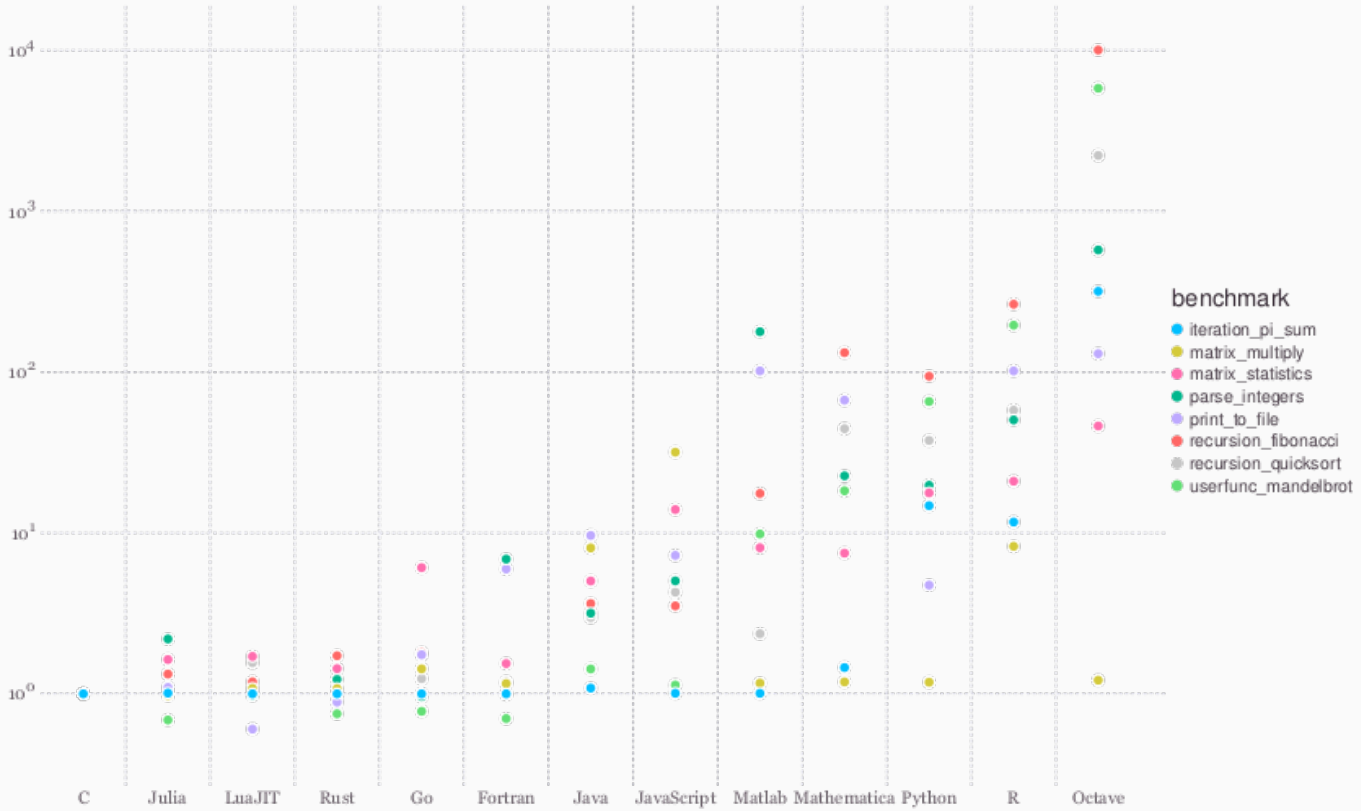


- ▲ $ docker compose up
- ▼ $ docker compose down

Julia in a Nutshell

- Fast
- Dynamic
- Reproducible
- Composable
- General
- Open Source

Julia Micro-Benchmarks (1/2)



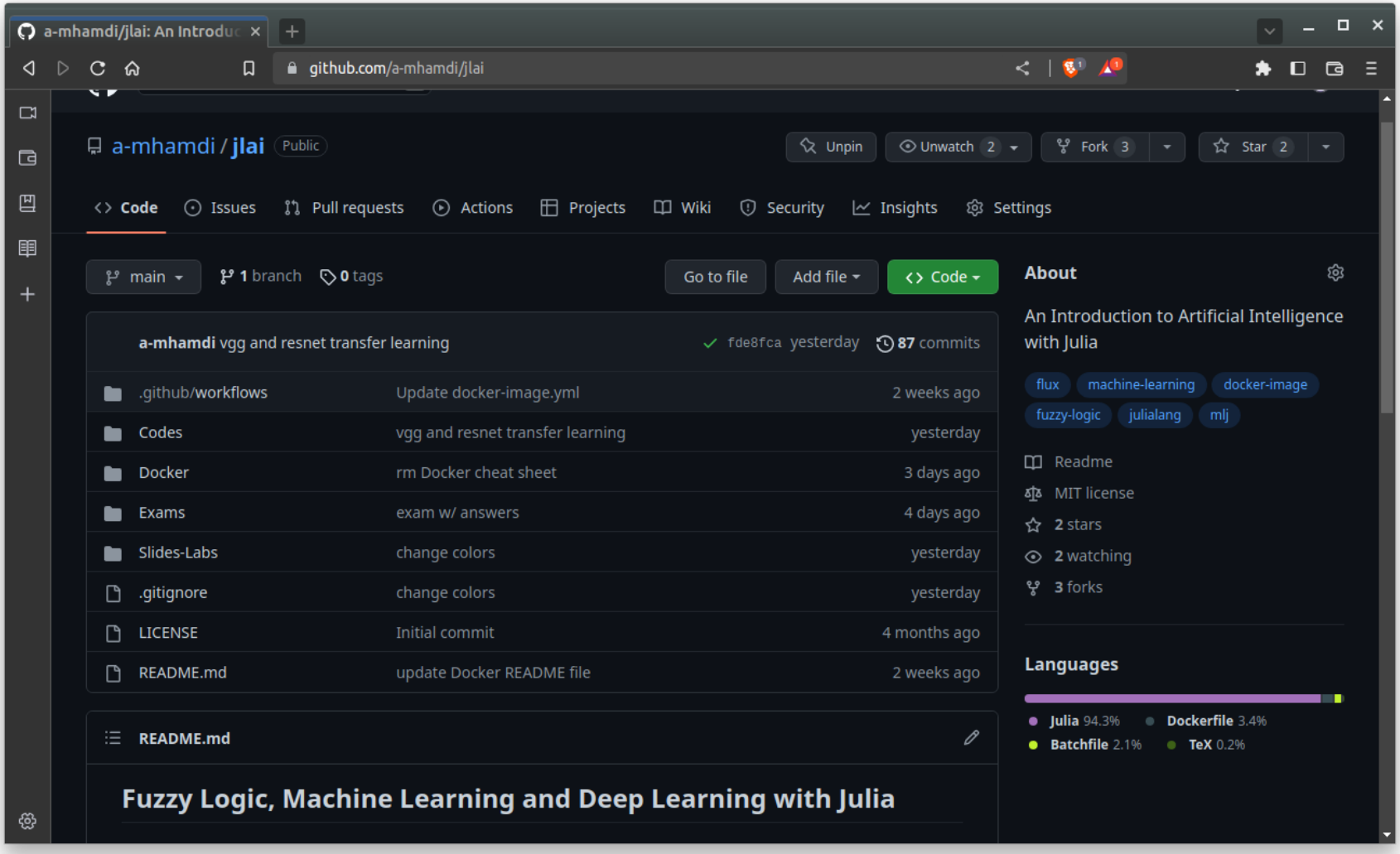
https://julialang.org/benchmarks

Julia Micro-Benchmarks (2/2)

Geometric Means of Micro-Benchmarks by Language

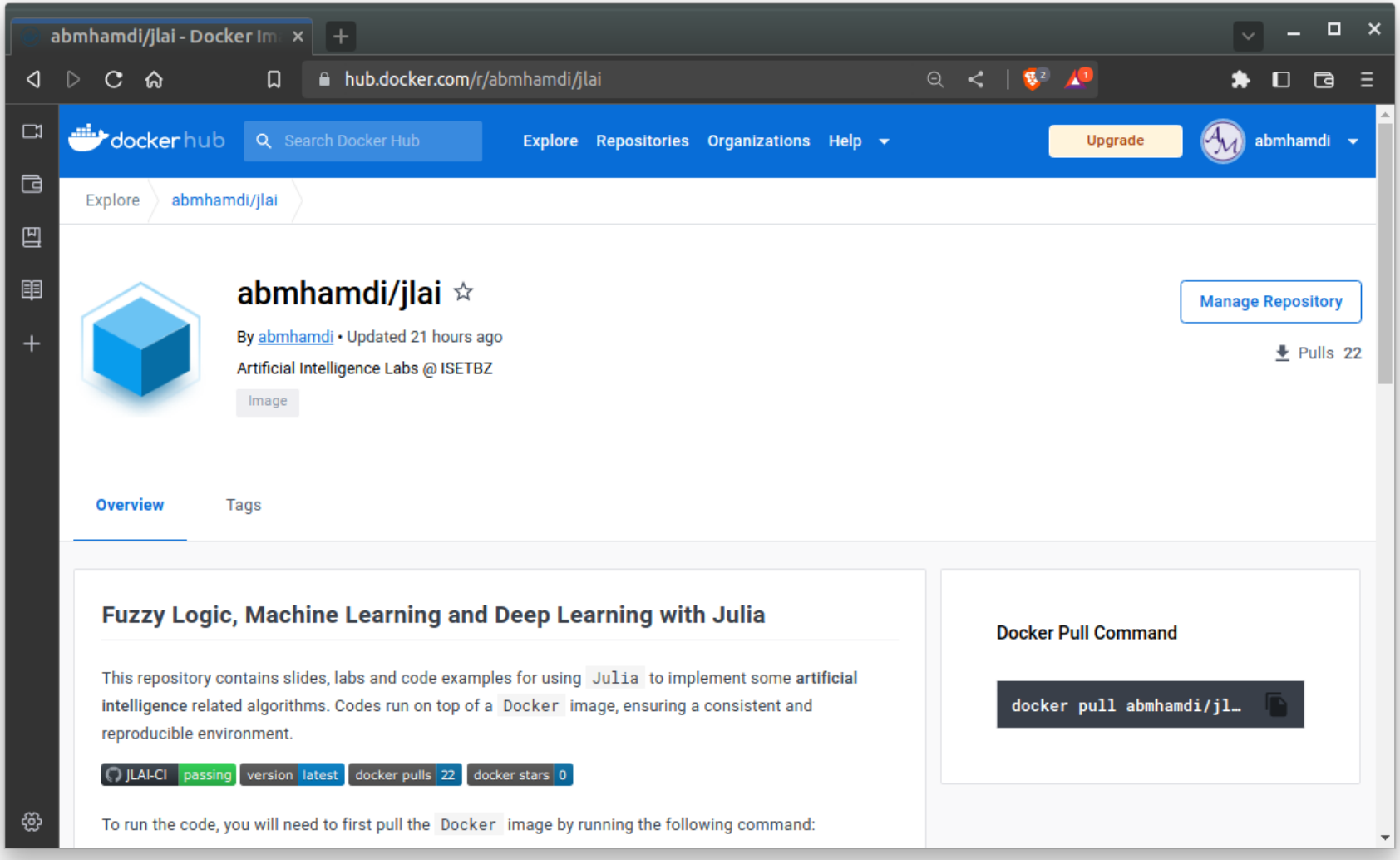
1	C	1.0
2	Julia	1.17006
3	LuaJIT	1.02931
4	Rust	1.0999
5	Go	1.49917
6	Fortran	1.67022
7	Java	3.46773
8	JavaScript	4.79602
9	Matlab	9.57235
10	Mathematica	14.6387
11	Python	16.9262
12	R	48.5796
13	Octave	338.704

Source Control Management (SCM)



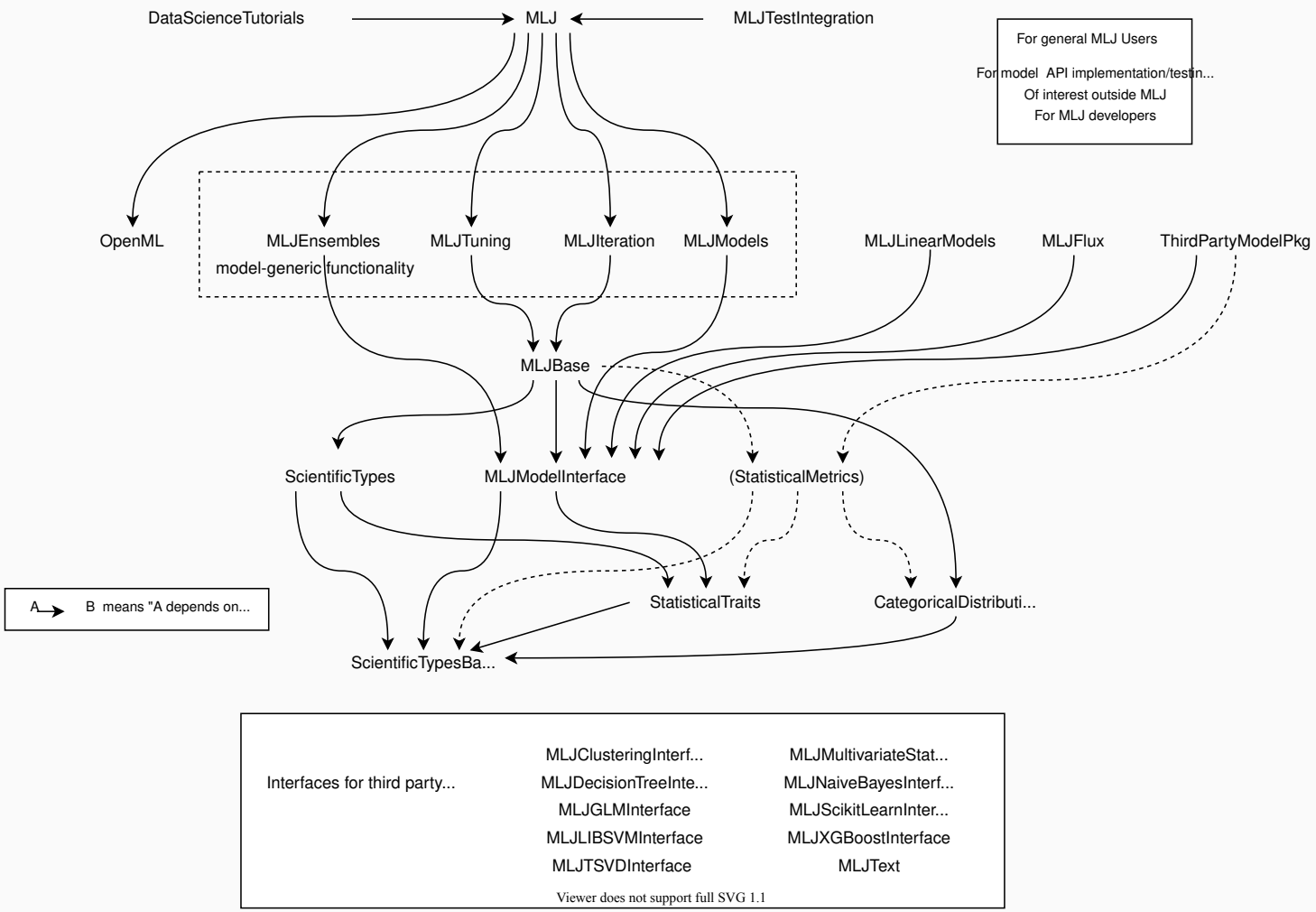
https://github.com/a-mhamdi/jlai

Continuous Integration (CI)



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

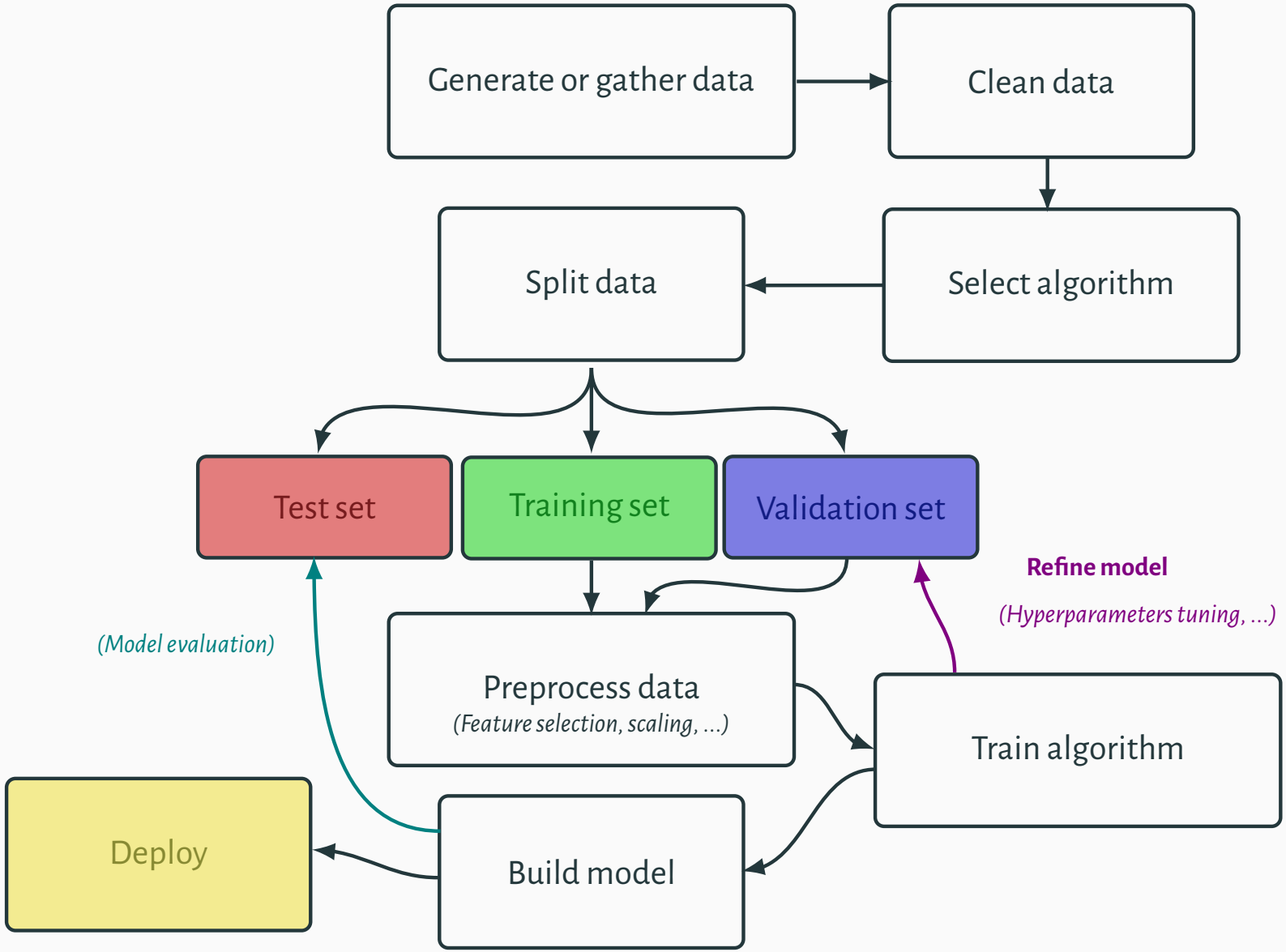
A Machine Learning Framework for Julia



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

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.

Data Preprocessing

Why?

- 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

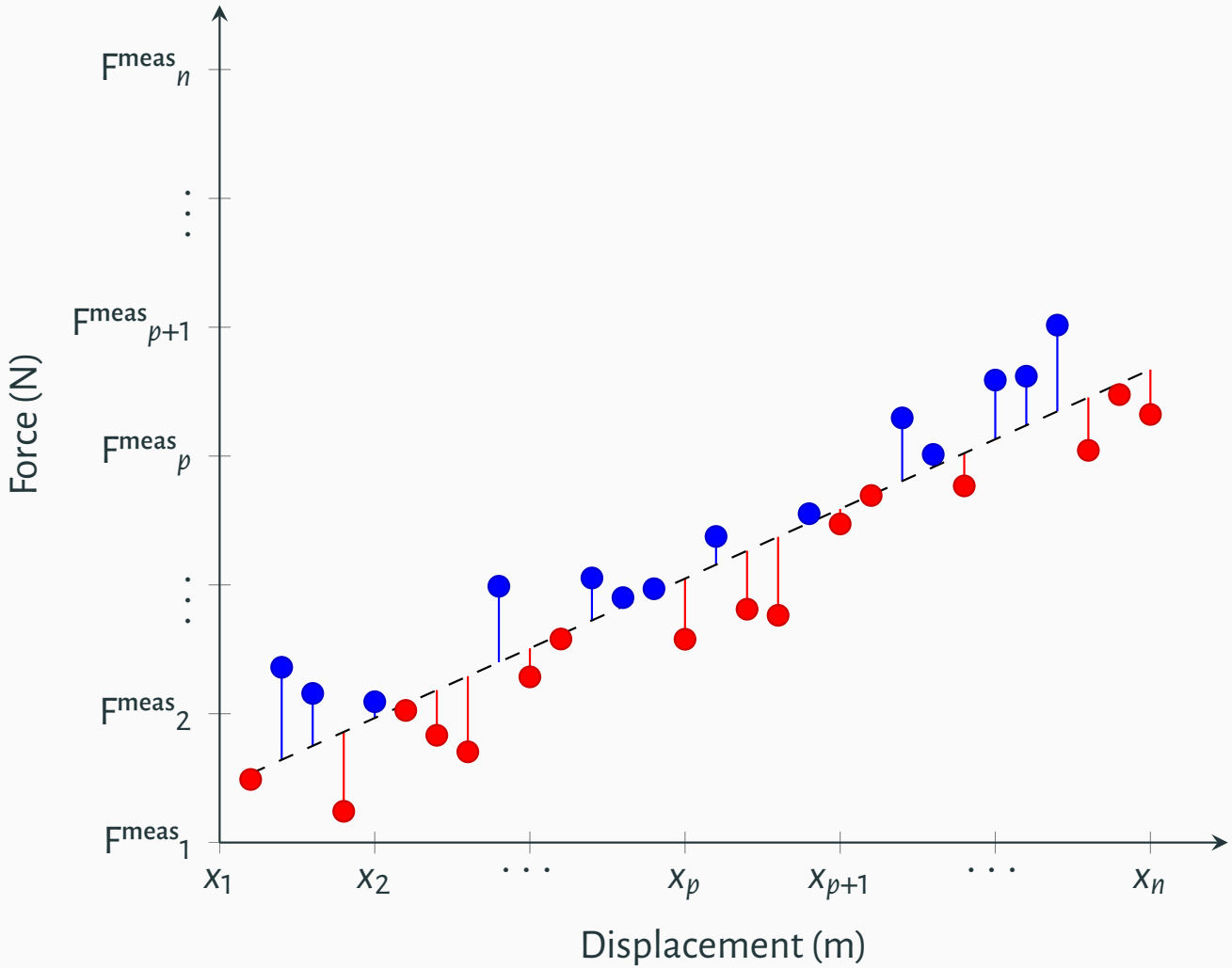
Feature Scaling

Normalization	**Standardization** *(Standardizer)*
$X \triangleq \frac{X - \text{minimum}(X)}{\text{maximum}(X) - \text{minimum}(X)}$	$X \triangleq \frac{X - \mu}{\sigma}$
▲ No assumption on data distribution	▲ More recommended when following normal distribution

Data Preprocessing Template

Code Snippet

Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *ml-workflows.jl*


F^{meas}_n
F^{meas}_{p+1}
F^{meas}_p
F^{meas}_2
F^{meas}_1
Force (N)
x_1
x_2
x_p
x_{p+1}
x_n
Displacement (m)

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)*:

$$F = kx \tag{1}$$

Restoring force is proportional to displacement.

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

x_i	x_1	$\cdots$	x_p	$\cdots$	x_n
$\mathrm{F}^{\mathrm{meas}}{}_i$	$\mathrm{F}^{\mathrm{meas}}{}_1$	$\cdots$	$\mathrm{F}^{\mathrm{meas}}{}_p$	$\cdots$	$\mathrm{F}^{\mathrm{meas}}{}_n$

$$\begin{aligned} \mathrm{F}^{\mathrm{meas}}{}_i &= \mathrm{F}_i + \varepsilon_i \\ &= kx_i + \varepsilon_i, \end{aligned} \tag{2}$$

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:

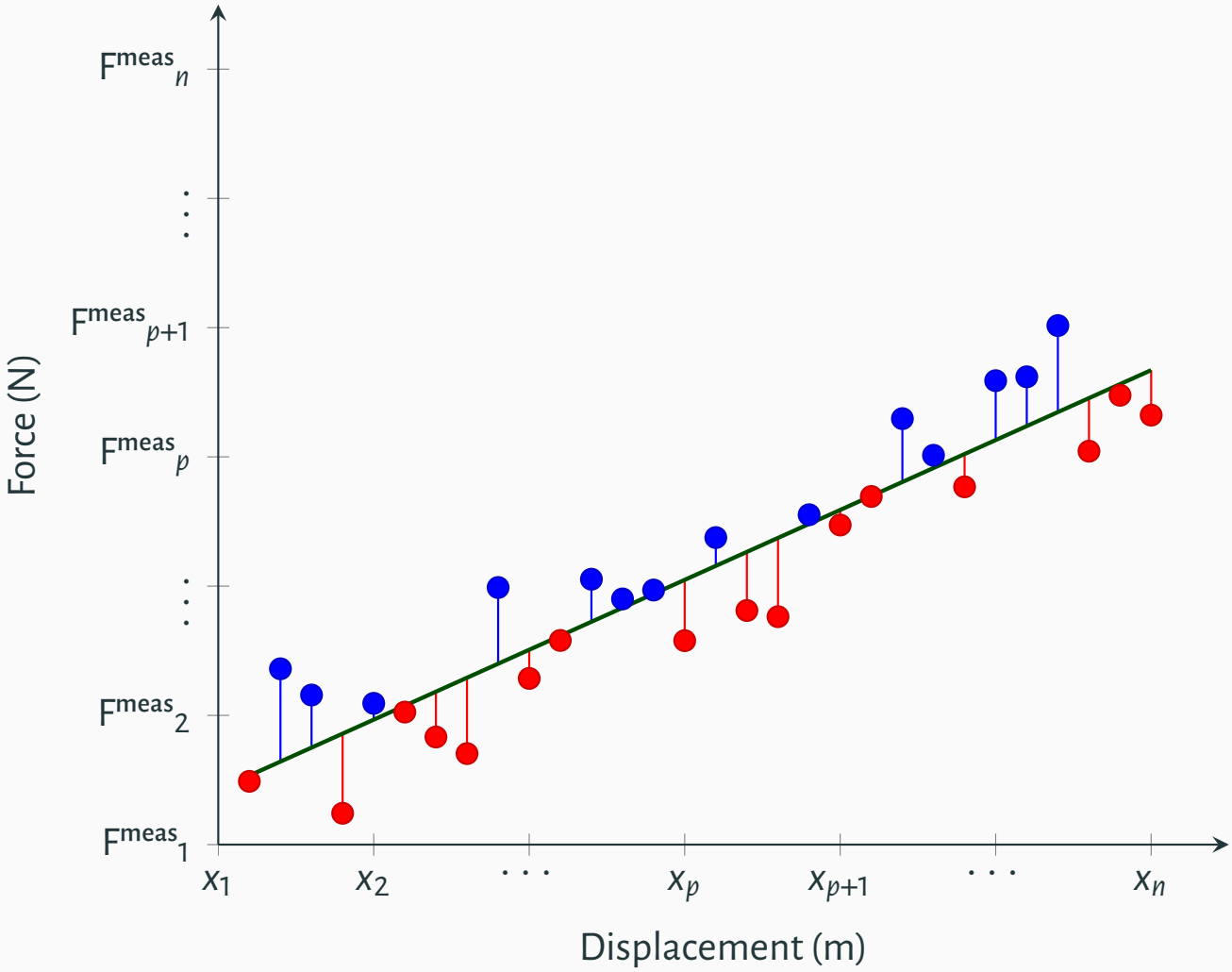
$$\begin{aligned} \mathcal{J} &= \sum_{i=1}^{n} \varepsilon_i^2 \\ &= \sum_{i=1}^{n} \left(\mathrm{F}^{\mathrm{meas}}{}_i - kx_i\right)^2 \end{aligned}$$

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

$$2 \sum_{i=1}^{n} \left({F^{meas}}_i - k x_i \right) \sum_{i=1}^{n} \frac{\partial \left({F^{meas}}_i - k x_i \right)}{\partial k} = 0$$

$$\sum_{i=1}^{n} \left({F^{meas}}_i - k x_i \right) \sum_{i=1}^{n} x_i = 0$$

$$\sum_{i=1}^{n} {F^{meas}}_i \, x_i = k \sum_{i=1}^{n} x_i^2 \iff \boxed{\hat{k} = \frac{\sum_{i=1}^{n} {F^{meas}}_i \, x_i}{\sum_{i=1}^{n} x_i^2}}$$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Force (N)
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x_n
Displacement (m)

Simple Linear Regression

Code Snippet

Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *simple-regression-∗.jl*

This example consists on determining the unknown couple $(y_0,\ v_0)$ of a mobile solid. We assume that the trajectory is linear. The mathematical model that relates the position y to time t is given by this equation:

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

Table 2: Measurements of position y

t_k	t_1	$\cdots$	t_p	$\cdots$	t_n
$y^{meas}{}_k$	$y^{meas}{}_1$	$\cdots$	$y^{meas}{}_p$	$\cdots$	$y^{meas}{}_n$

$$\begin{aligned} y^{meas}{}_k &= y_k + \varepsilon_k \\ &= y_0 + v_0 t_k + \varepsilon_k, \end{aligned} \tag{5}$$

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

In order to estimate the values taken by the couple $\begin{bmatrix} y_0, & v_0 \end{bmatrix}^T$, we consider the quadratic criterion again, as follows:

$$\begin{aligned} \mathcal{J} &= \sum_{k=1}^{n} \varepsilon_k^2 \\ &= \varepsilon^T \times \varepsilon \end{aligned}$$

The vector ε is set by $\varepsilon_k, \ \forall k \geq 1$:

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

$$\frac{\partial \mathcal{J}}{\partial \begin{bmatrix} y_0 \\ \\ v_0 \end{bmatrix}} = 0 \tag{6}$$

Multiple Linear Regression

Code Snippet

Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *multivariable-regression.jl*

Consider the following multivariable equation:

$$y = \theta_1 x_{(1)} + \theta_2 x_{(2)} + \cdots + \theta_m x_{(m)} \tag{7}$$

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

$$y_k = \theta_1 x_{(1,k)} + \theta_2 x_{(2,k)} + \cdots + \theta_m x_{(m,k)} + \varepsilon_k \tag{8}$$

We denote hereafter by θ the vector $\begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_m \end{bmatrix}$. The function y_k becomes:

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

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

$$y = H\theta + \varepsilon,$$

where $y^T = [y_1,\, y_2,\, \cdots,\, y_n]$, $X = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{bmatrix}$, and $\varepsilon^T = [\varepsilon_1,\, \varepsilon_2,\, \cdots,\, \varepsilon_n]$.

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

$$\begin{aligned} \mathcal{J} &= \sum_{k=1}^{n} \varepsilon_k^2 \\ &= \varepsilon^T \varepsilon \end{aligned}$$

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 θ:

$$\frac{\partial \mathcal{J}}{\partial \theta} = \frac{\partial \left(\varepsilon^T \varepsilon\right)}{\partial \theta} \tag{9}$$

$$\frac{\partial \left(\varepsilon^T \varepsilon\right)}{\partial \theta} = 2 \left(\frac{\partial \varepsilon}{\partial \theta}\right)^T \varepsilon \tag{10}$$

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

$$\frac{\partial \varepsilon}{\partial \theta} = -X \tag{11}$$

$$\begin{aligned}\frac{\partial J}{\partial \theta} &= 2(-X)^T (y - X\theta) \\ &= 0\end{aligned}$$

The vector $\hat{\theta}$ is given by $\hat{\theta} = \left(X^T X\right)^{-1} X^T y$

$X^T X$ **is not invertible (singular/degenerate)**

▼ Redundant Features

Some features are linearly dependent, i.e, $\exists$ some $x_p \propto$ some x_l for instance x_p in feet and x_l in m.

▼ Too many features

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

▲ Delete some features

▲ Add extra observations

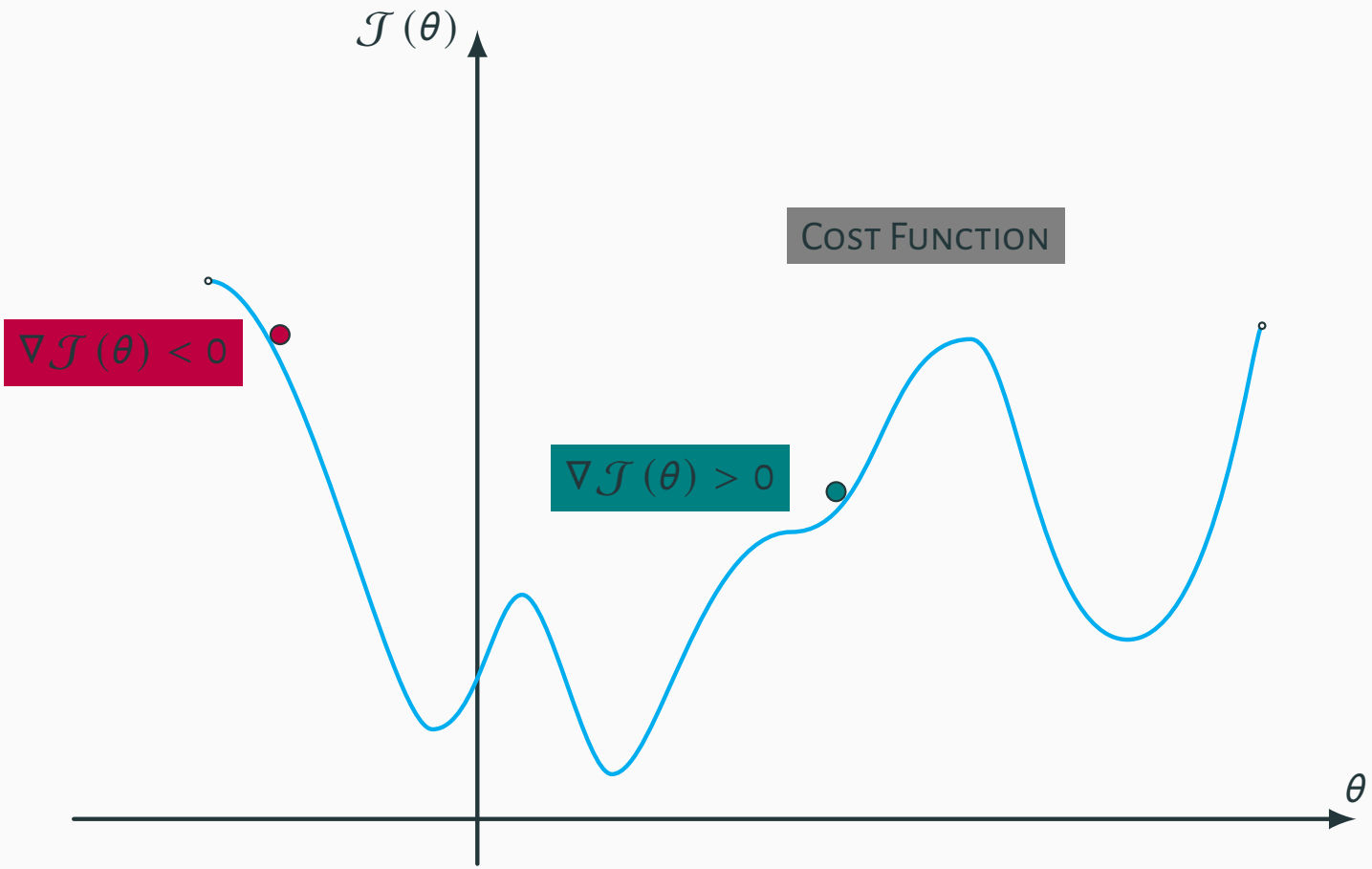
▲ Use regularization: $\underbrace{\lambda \sum_{i=1}^{m} |\theta_i|}_{\text{Ridge}}$ $\underbrace{\frac{1}{2}\lambda \sum_{i=1}^{m} \theta_i^2}_{\text{Lasso}}$ $\underbrace{r\lambda \sum_{i=1}^{m} |\theta_i| + \frac{(1-r)}{2}\lambda \sum_{i=1}^{m} \theta_i^2}_{\text{Elastic net}}$

Polynomial Regression

Code Snippet

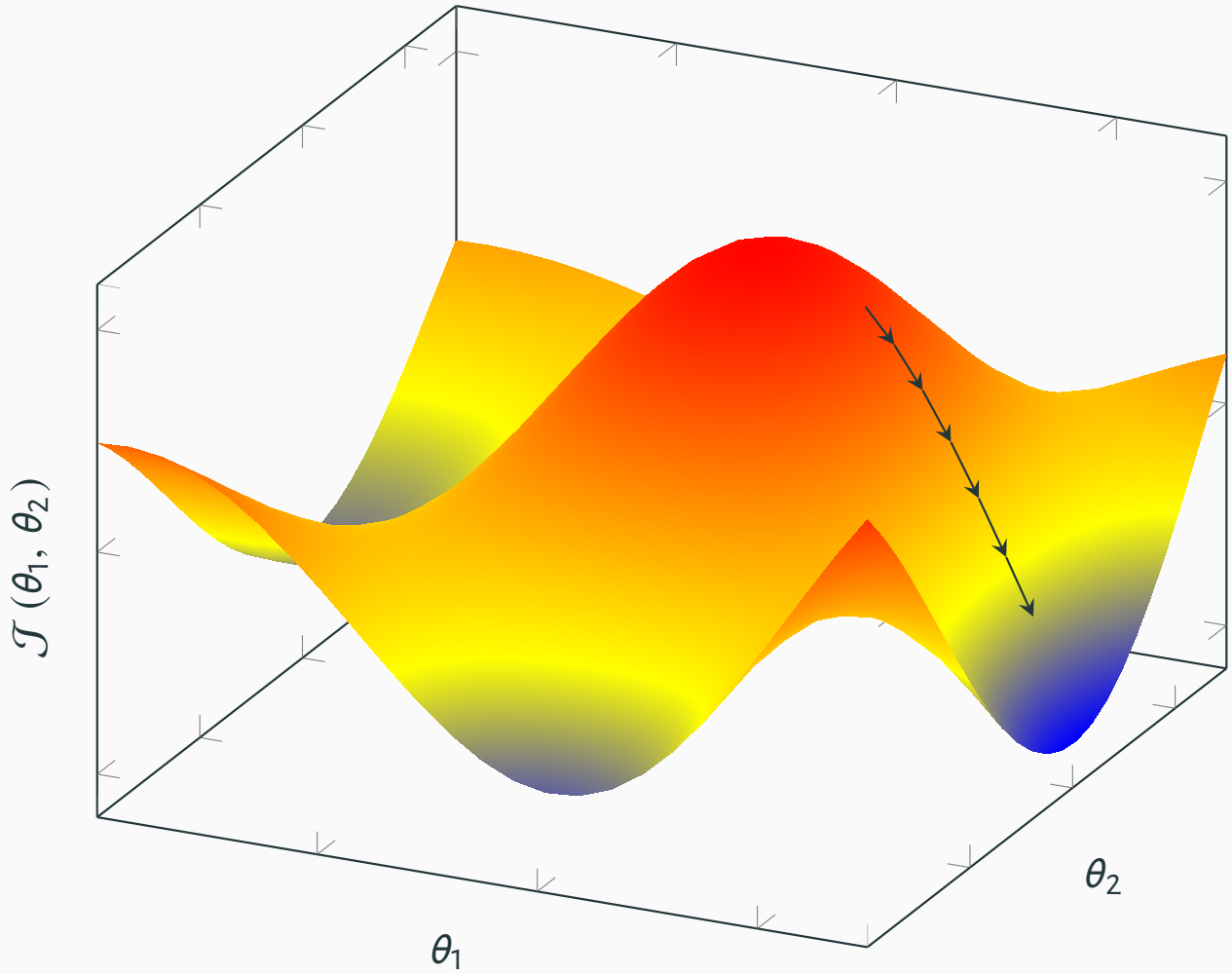
Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *polynomial-regression.jl*

Gradient Descent (1/3)



$$\underbrace{\theta}_{\text{New value}} \triangleq \underbrace{\theta}_{\text{Old value}} - \overbrace{\alpha}^{\text{Weighting factor}} \underbrace{\nabla \mathcal{J}(\theta)}_{\text{Gradient term is steepest ascent}}$$

Gradient Descent (2/3)



① Start with some random values of θ_1 and θ_2

② Keep changing θ_1 and θ_2 to reduce $\mathcal{J}(\theta_1, \theta_2)$ until we hopefully end up at minimum

Gradient Descent (3/3)

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

Recall that $\mathcal{J} = 1/2n \sum_{k=1}^{n} (y_k - h_\theta(x_k))^2 \implies \frac{\partial \mathcal{J}}{\partial \theta_i} = -1/n \sum_{k=1}^{n} (y_k - h_\theta(x_k))\, x_{(i,k)}$

$$\theta_i \triangleq \theta_i + \alpha \frac{1}{n} \sum_{k=1}^{n} (y_k - h_\theta(x_k))\, x_{(i,k)}$$

$$\theta_1 \triangleq \theta_1 + \alpha \frac{1}{n} \sum_{k=1}^{n} (y_k - h_\theta(x_k))\, x_{(1,k)} \qquad \theta_2 \triangleq \theta_2 + \alpha \frac{1}{n} \sum_{k=1}^{n} (y_k - h_\theta(x_k))\, x_{(2,k)}$$

$$\vdots$$

$$\theta_m \triangleq \theta_m + \alpha \frac{1}{n} \sum_{k=1}^{n} (y_k - h_\theta(x_k))\, x_{(m,k)}$$

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 θ_0, θ_1.

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

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

① Normal Equation

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

② Stochastic Gradient Descent

k	1	2	3	4	5
y	14	38	54	76	95
$h_\theta(x_k)$	1	13.63	330.999	−9894.410	734688.376
$\hat{\theta} = \begin{bmatrix} \hat{\theta}_1 \\ \\ \hat{\theta}_2 \end{bmatrix}$	$\begin{bmatrix} 1.13 \\ \\ 0.5 \end{bmatrix}$	$\begin{bmatrix} 1.374 \\ \\ 6.592 \end{bmatrix}$	$\begin{bmatrix} -1.396 \\ \\ -131.907 \end{bmatrix}$	$\begin{bmatrix} 98.308 \\ \\ 7345.901 \end{bmatrix}$	$\begin{bmatrix} -7247.626 \\ \\ -727247.475 \end{bmatrix}$

GD in action

Code Snippet

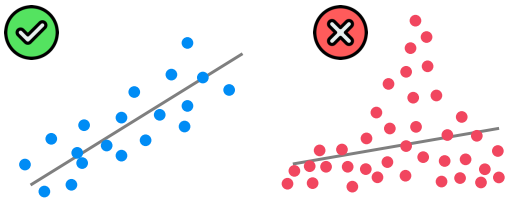
```julia
X = [1 0; 1 25; 1 50; 1 75; 1 100] # Features
y = [14, 38, 54, 76, 95] # Target

alpha, n, theta = 0.01, 5, [1; .5]
J = []
for k in 1:5
    h_th = X[k, :]' * theta
    println("h_th is $(h_th)")
    cost = (y[k] - h_th)^2
    push!(J, cost);
    theta += alpha * (y[k] - h_th) * X[k, :]
    println("theta is $(theta)")
end
```

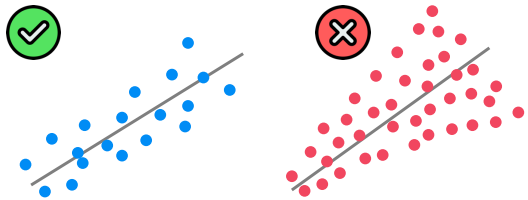
Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *gradient-descent.jl*

Assumptions of Linear Regression

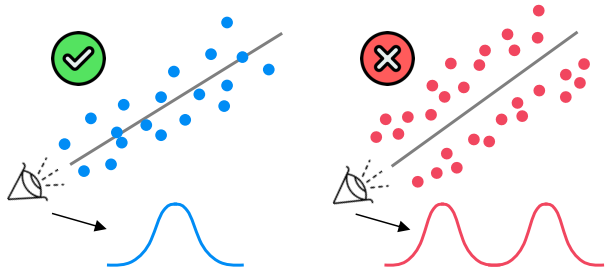
1. Linearity
(Linear relationship between Y and each X)



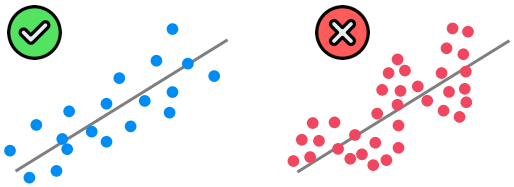
2. Homoscedasticity
(Equal variance)



3. Multivariate Normality
(Normality of error distribution)



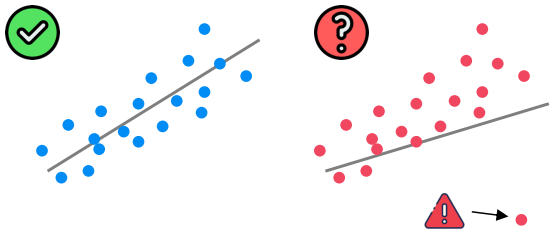
4. Independence
(of observations. Includes “no autocorrelation”)



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

$X_1 \not\sim X_2$ $X_1 \sim X_2$

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



▶ Source

Evaluation metrics (1/2)

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

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

👍 *A lower **MAE** indicates a better fit of the model to the data.*

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

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

👍 *A lower **RMSE** indicates a better fit of the model to the data.*

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.

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

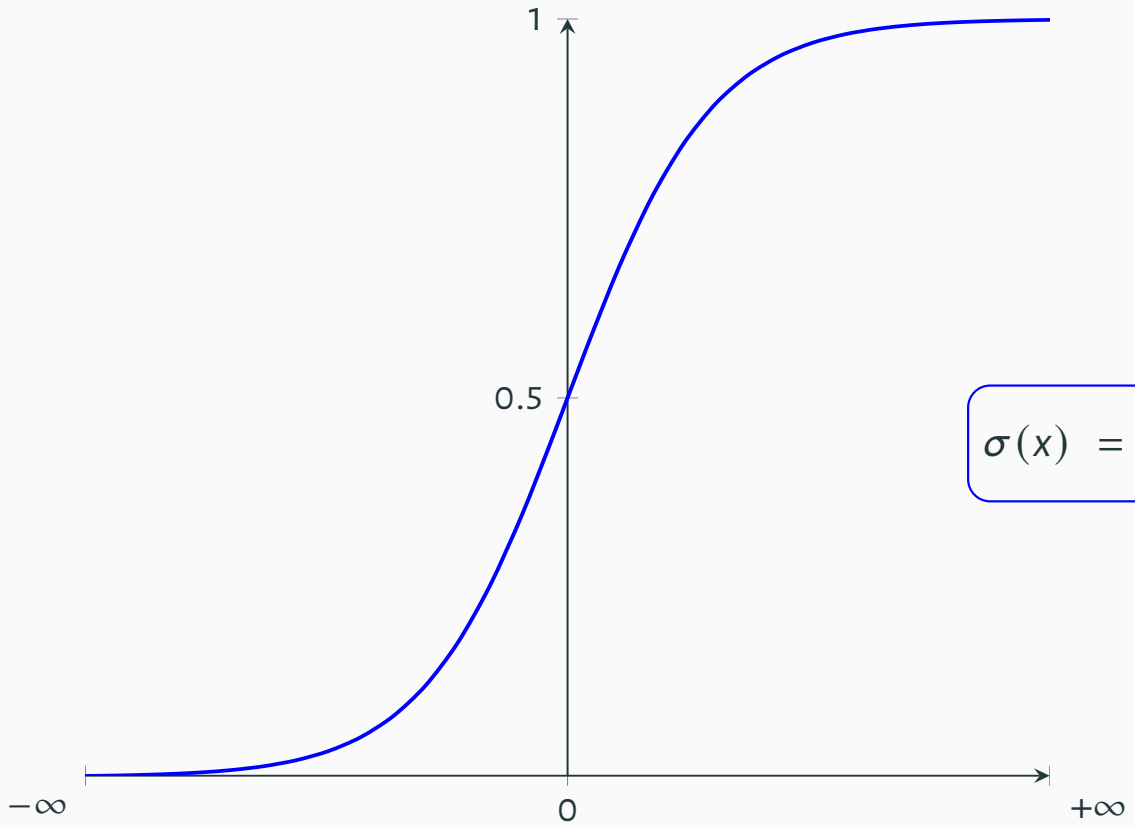
👍 1 *indicates that the model explains* ***ALL*** *the variance in the dependent variable*

👎 0 *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.

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

Logistic or S-shaped function σ



$$\sigma(x) = \frac{1}{1+e^{-x}}$$

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

Decision boundary

$$y = \sigma\left(\theta_1 x_{(1)} + \theta_2 x_{(2)} + \cdots + \theta_m x_{(m)}\right)$$

$$y = \frac{1}{1 + \mathrm{e}^{-x^T\theta}}$$

Hypothesis

$$h_\theta(x) = \frac{1}{1 + \mathrm{e}^{-x^T\theta}} \qquad h_\theta(x_k) = \frac{1}{1 + \mathrm{e}^{-x_k^T\theta}}$$

Cost function

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

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

Gradient Descent

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

Generalizing $\mathcal{J}$ yields: $\mathcal{J} = -\frac{1}{n}\sum_{k=1}^{n}\left(y_k \ln\left(h_\theta(x_k)\right) + (1-y_k)\ln\left(1-h_\theta(x_k)\right)\right)$

$$\Longrightarrow \quad \frac{\partial \mathcal{J}}{\partial \theta_i} = -\frac{1}{n}\sum_{k=1}^{n}\left(y_k - h_\theta(x_k)\right)x_{(i,k)}$$

$$\theta_i \triangleq \theta_i + \alpha\frac{1}{n}\sum_{k=1}^{n}\left(y_k - h_\theta\left(x_k\right)\right)x_{(i,k)}$$

$$\theta_1 \triangleq \theta_1 + \alpha\frac{1}{n}\sum_{k=1}^{n}\left(y_k - h_\theta\left(x_k\right)\right)x_{(1,k)} \qquad \theta_2 \triangleq \theta_2 + \alpha\frac{1}{n}\sum_{k=1}^{n}\left(y_k - h_\theta\left(x_k\right)\right)x_{(2,k)}$$

$$\vdots$$

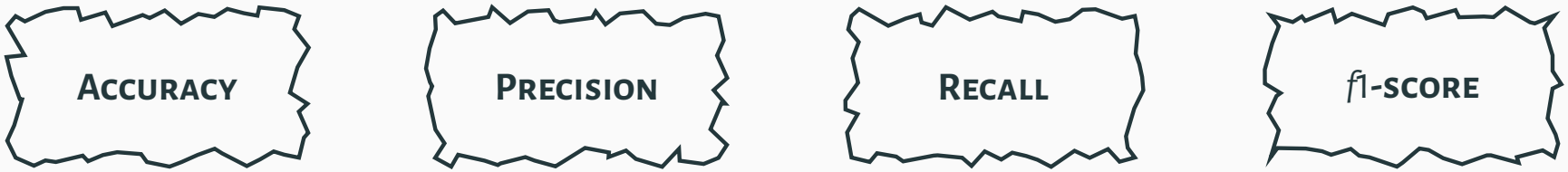
$$\theta_m \triangleq \theta_m + \alpha\frac{1}{n}\sum_{k=1}^{n}\left(y_k - h_\theta\left(x_k\right)\right)x_{(m,k)}$$

Logistic Regression

Code Snippet

Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *logistic-regression.jl*

Evaluation metrics



Accuracy denotes the ratio of how much we got right over all cases.

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

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

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

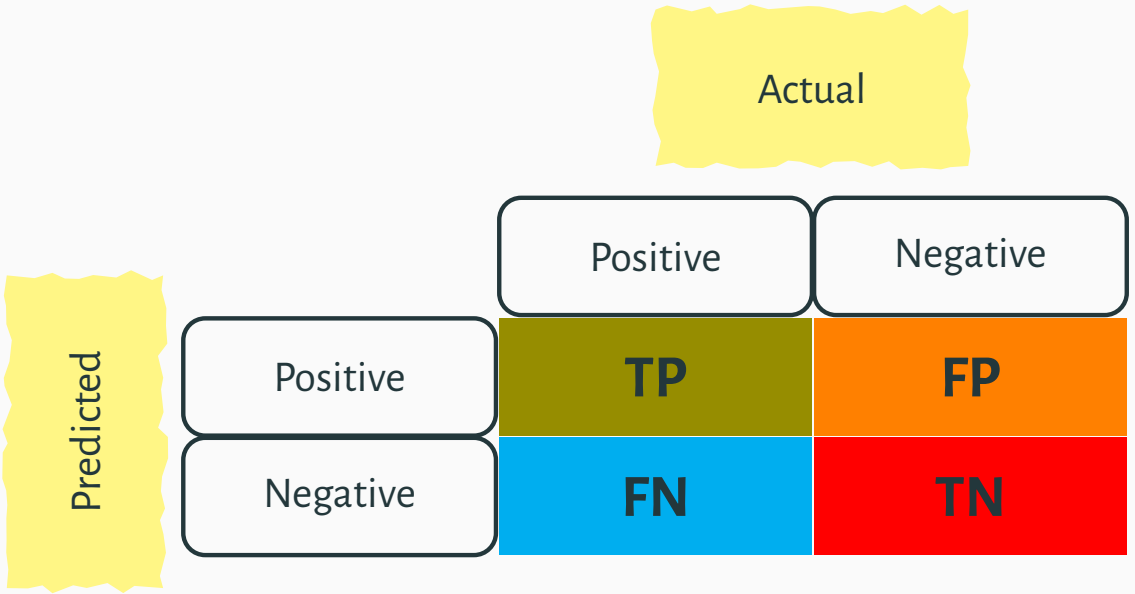
Recall is the ratio of how much positives we got right over all actual positive cases:

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

$f1 - \text{score}$ denotes the *Harmonic Mean of Precision & Recall*

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

Confusion Matrix



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

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

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

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

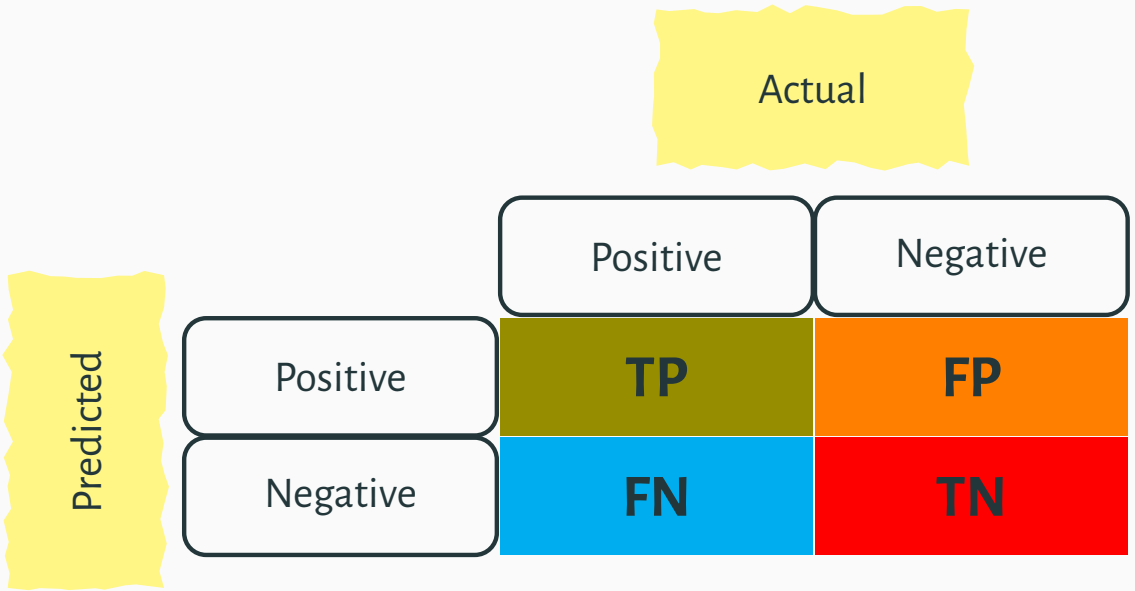
183	141
13	663

$Accuracy = 0.846$
$Precision = 0.565$
$Recall = 0.934$
$f1 - score = 0.704$

320	20
43	538

$Accuracy = 0.932$
$Precision = 0.941$
$Recall = 0.882$
$f1 - score = 0.910$

Confusion Matrix



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Evaluation Metrics

Follow up

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

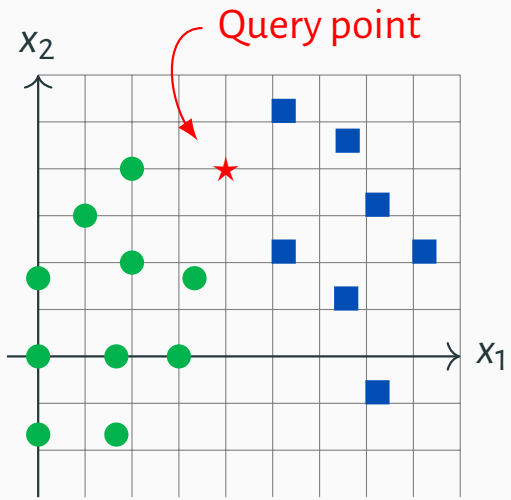
Case #1: Prioritize *Precision* over *Recall*, *e.g.*, $\beta = 0.5$

- 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 (1/6)



Minkowski distance

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

Manhattan distance (p=1)

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

Euclidean distance (p=2)

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

k-Nearest Neighbors (2/6)

- 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**

k-Nearest Neighbors (3/6)

Task #3
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 $P(5,\ 5)$?

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

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

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

```
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))
end

dds(1, 6) # Point `A`
dds(2, 6) # Point `B`
```

k-Nearest Neighbors (4/6)

Task #4[1]

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_1	F_2	F_3	F_4	F_5	F_6	F_7	F_8
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: $\frac{1}{d^2}$. We take 3 neighbors, what is the color of U? Compare your results to those in question 2.

k-Nearest Neighbors (5/6)

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

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

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

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

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

k-Nearest Neighbors (6/6)

```
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))
end

dds(2, 6) # Fruit `F_1`
dds(5, 6) # Fruit `F_2`
```

[1] From Prof. Winston's book

k-NN

Code Snippet

Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *knn.jl*

Rule of Thumb to Choose k

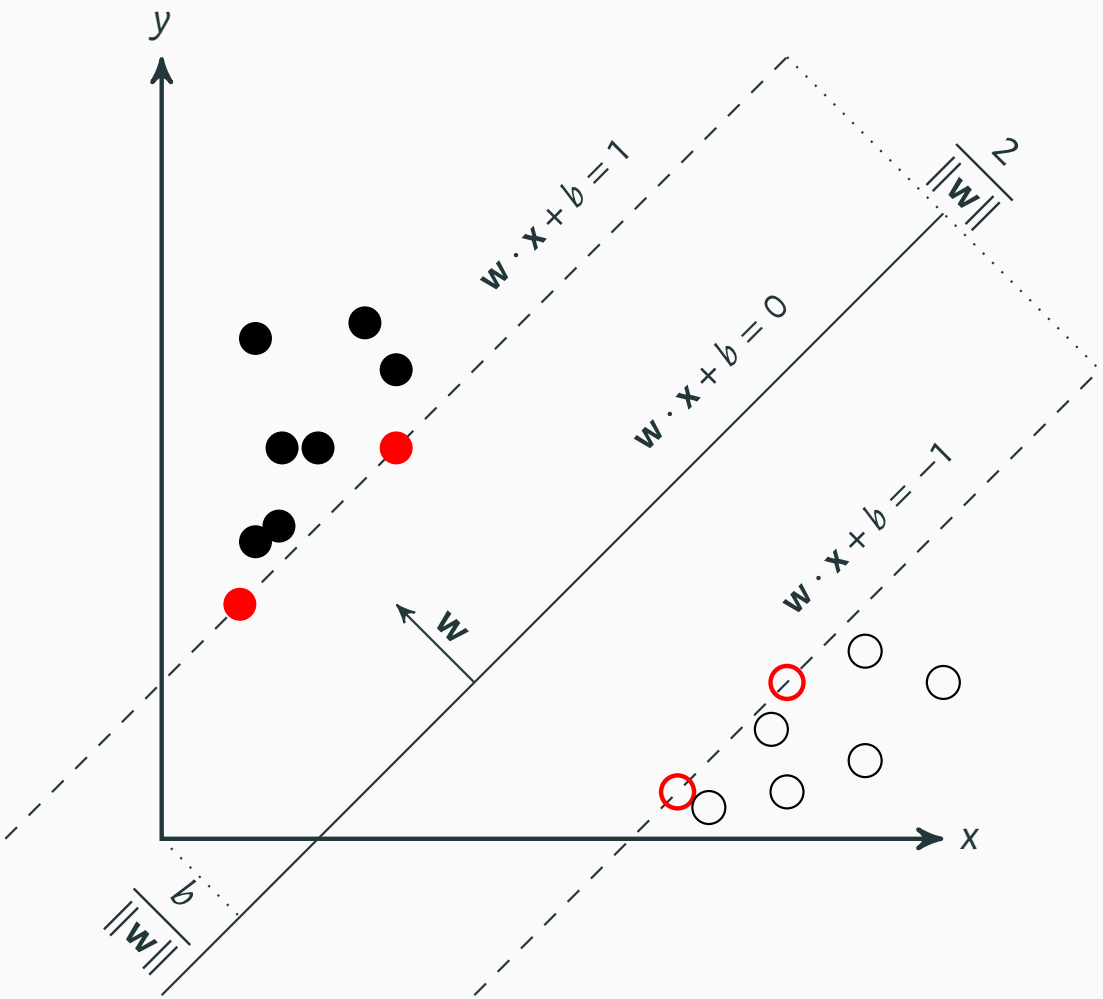
k **is even** if the number of classes is odd

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.

Support Vector Machine (SVM)



SVM for Classification

Code Snippet

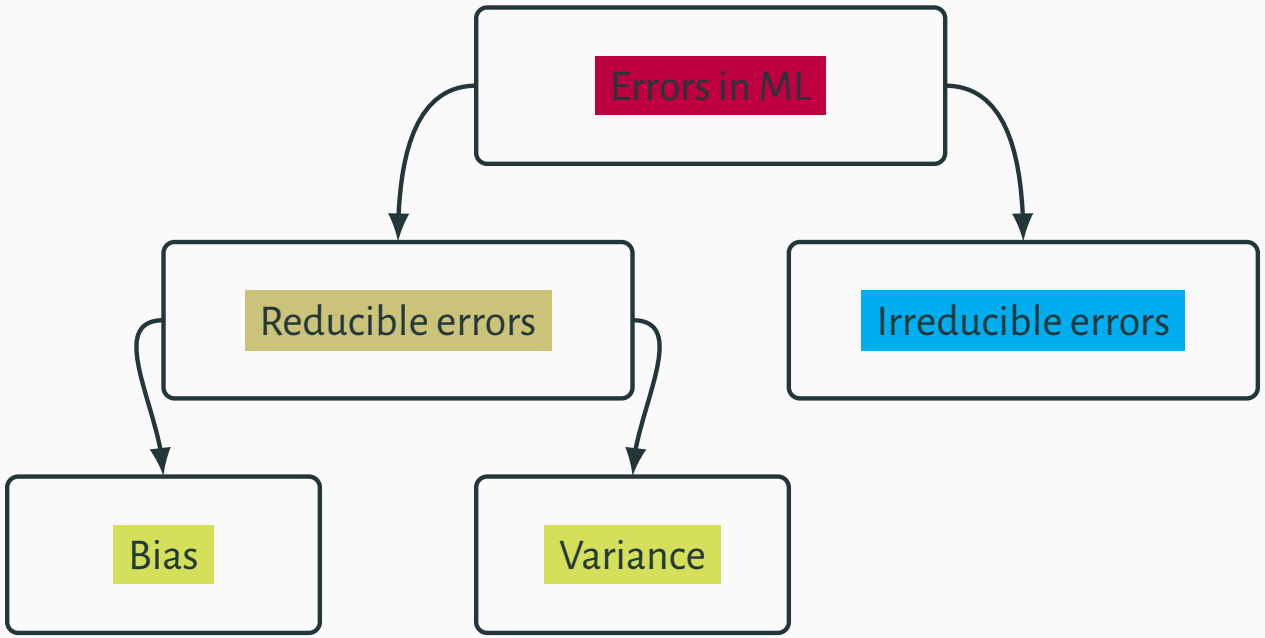
Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *svc.jl*

Summary

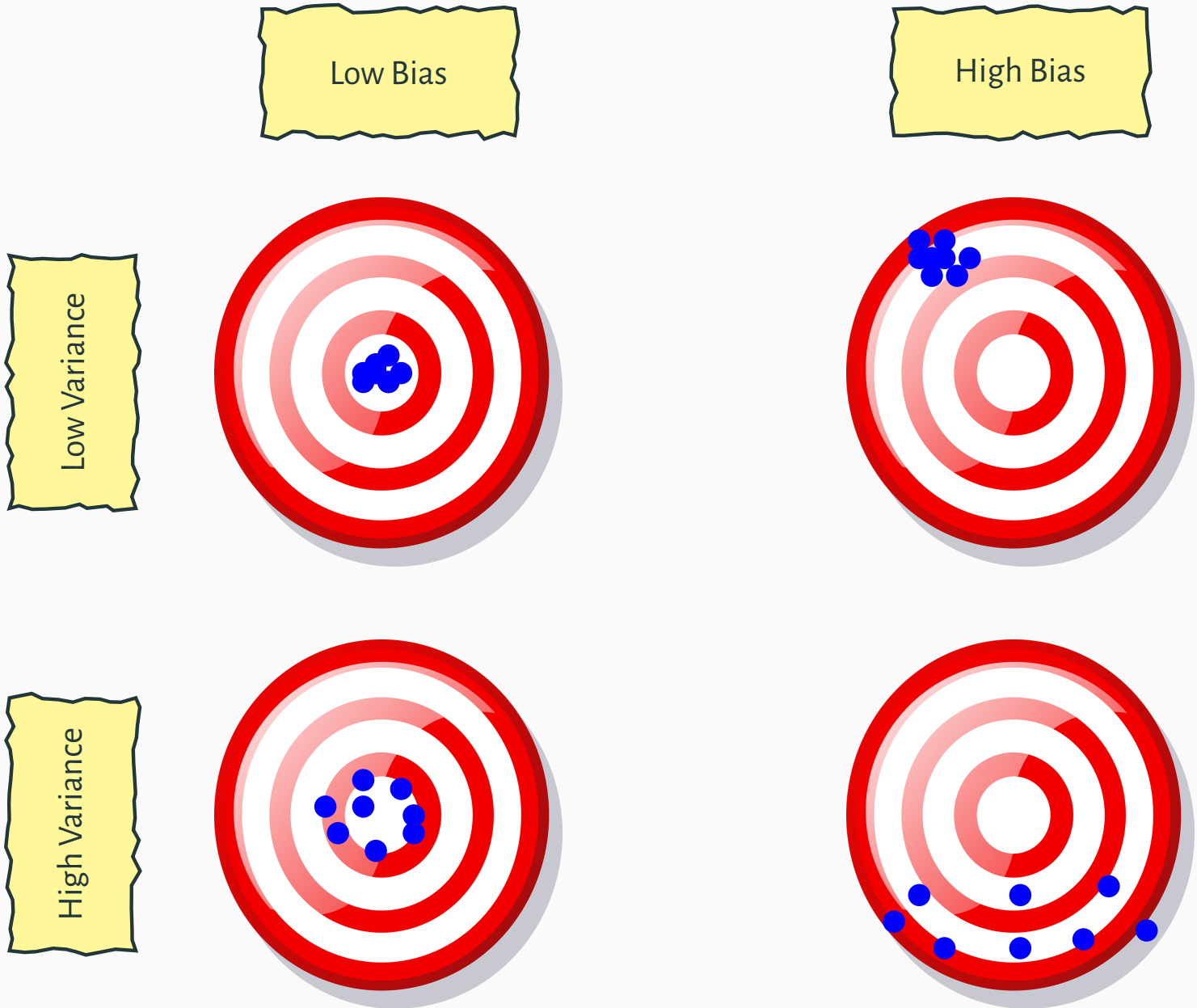
Method		Pros		Cons
Logistic Regression	▲	Probabilistic	▼	Almost linearly separable data
k-NN	▲	Fast and efficient	▼	# of neighbors k
			▼	Detecting outliers[2]
SVM	▲	Memory efficient	▼	Kernel's choice
	▲	Versatile	▼	Large datasets
	▲	Noise and outliers	▼	Overlapping classes
	▲	High dimension	▼	Interpretability
Naive Bayes	▲	Simplicity and efficiency	▼	Independence between features
	▲	High dimension	▼	$\exists$ of irrelevant features
Decision Tree	▲	Interpretability	▼	Overfitting
	▲	Numerical and categorical data	▼	Unstable
	▲	Robust to outliers	▼	Continuous variables
	▲	High accuracy	▼	# of input features
Random Forest	▲	Less prone to overfitting	▼	Computation
	▲	High dimension	▼	Interpretability

[2] Points that differ significantly from the rest of the data points.

Errors in ML


Errors in ML
Reducible errors
Irreducible errors
Bias
Variance

Bias-variance tradeoff



Unsupervised Learning

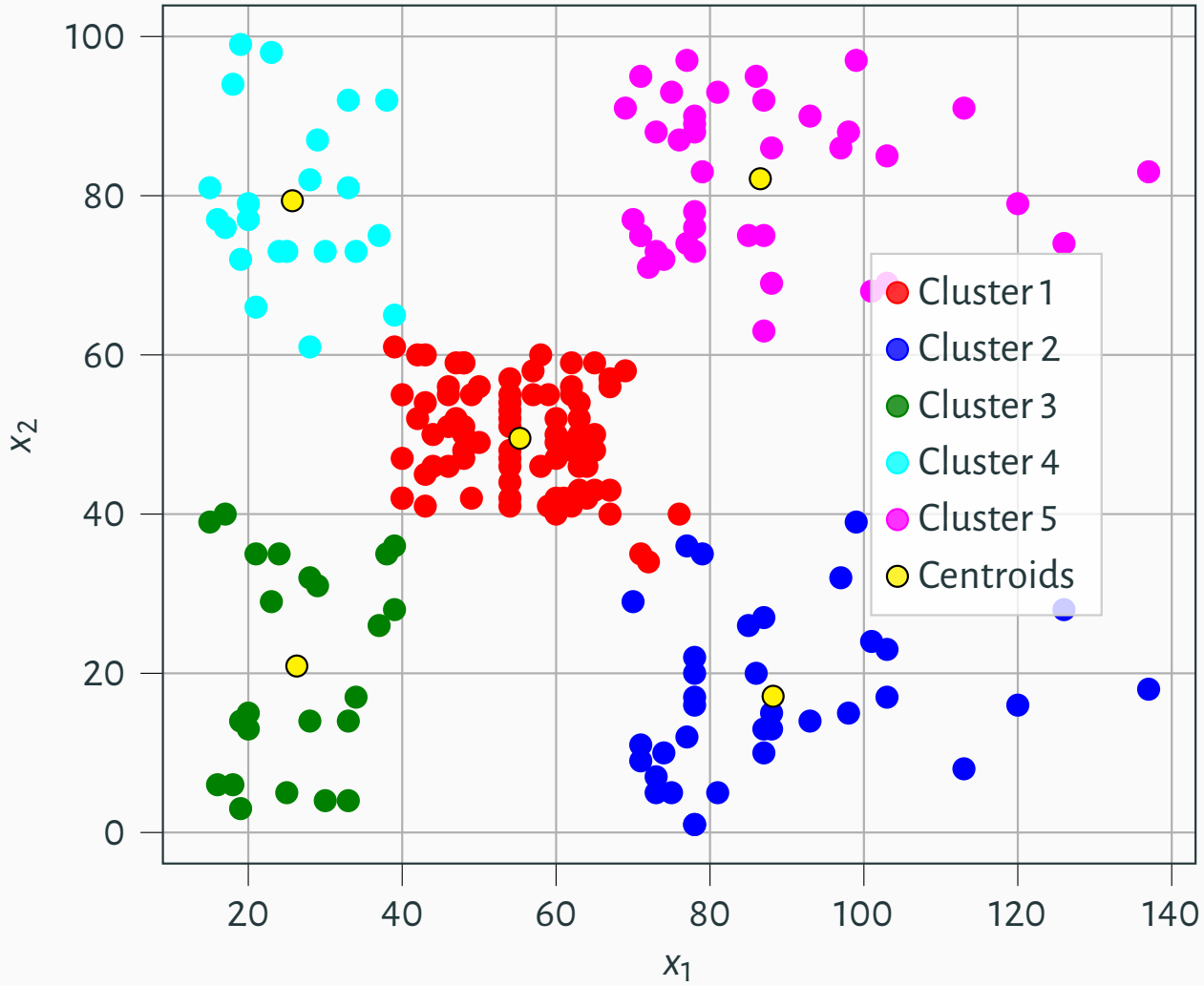
K-Means Clustering (1/3)

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.

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;
3: 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**

Task #5[3]

Of the following examples, which would you address using an unsupervised learning 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
3. 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.

[3] From 'Machine Learning' course on 'Coursera'

Task #5[3]

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

1. Given email labeled as spam/not spam, learn a spam filter
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Task #6[4]

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

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

- 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

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

[4]Credit: Shokoufeh Mirzaei, PhD

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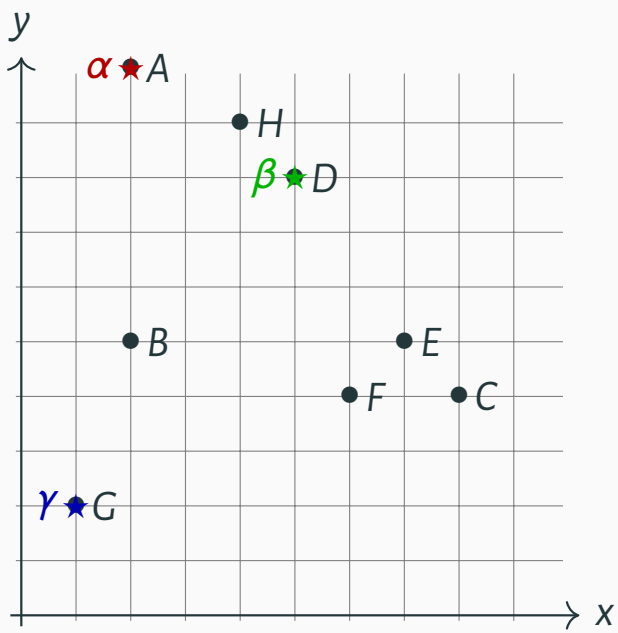

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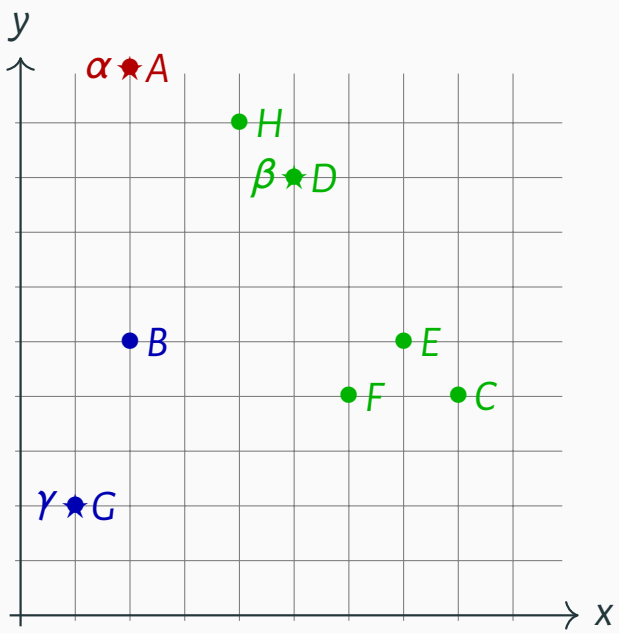
Point	$\alpha(2,\ 10)$	$\beta(5,\ 8)$	$\gamma(1,\ 2)$	#
$A(2,\ 10)$	0	5	9	1
$B(2,\ 5)$	5	6	4	3
$C(8,\ 4)$	12	7	9	2
$D(5,\ 8)$	5	0	10	2
$E(7,\ 5)$	10	5	9	2
$F(6,\ 4)$	10	5	7	2
$G(1,\ 2)$	9	10	0	3
$H(4,\ 9)$	3	2	10	2



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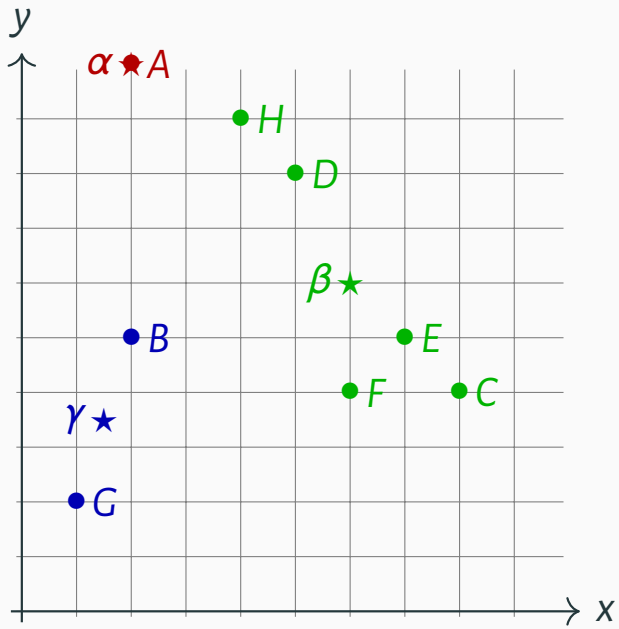
$F(6,\ 4)$	10	5	7	2
$G(1,\ 2)$	9	10	0	3
$H(4,\ 9)$	3	2	10	2
	$\alpha(2,\ 10)$	$\beta(6,\ 6)$	$\gamma(1.5,\ 3.5)$	



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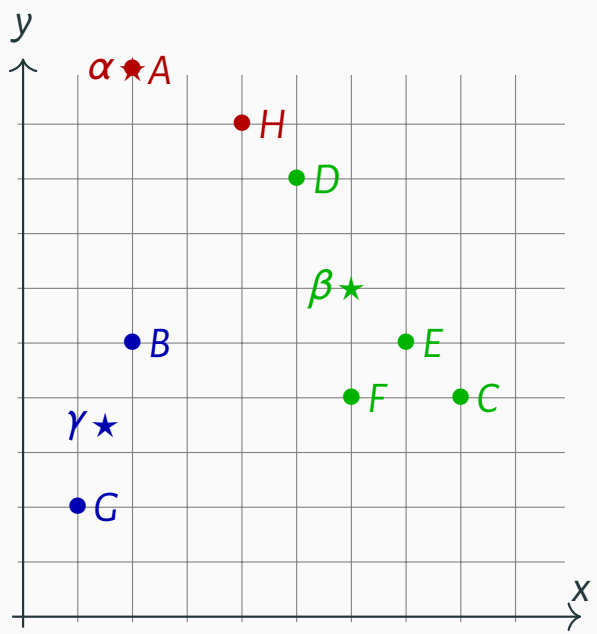
$F(6,\ 4)$	10	2	5	2
$G(1,\ 2)$	9	9	2	3
$H(4,\ 9)$	3	5	8	1



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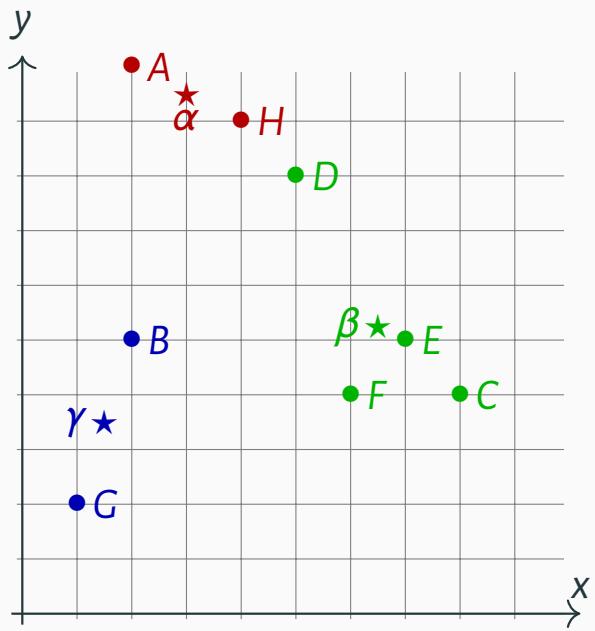
- The distance between two points: $M(x_m,\ y_m)$ and $N(x_n,\ y_n)$ is defined as

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

Point	$\alpha(2,\ 10)$	$\beta(6,\ 6)$	$\gamma(1.5,\ 3.5)$	#
$A(2,\ 10)$	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
	$\alpha(3,\ 9.5)$	$\beta(6.5,\ 5.25)$	$\gamma(1.5,\ 3.5)$	



[4]Credit: Shokoufeh Mirzaei, PhD

Task #6[4]

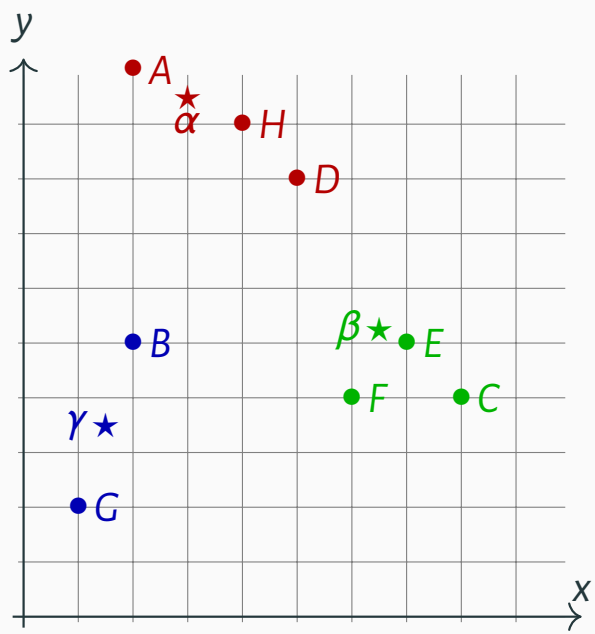
Use *K*-Means algorithm to cluster the following eight points intro three clusters:

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

- 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

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

Point	$\alpha(3,\ 9.5)$	$\beta(6.5,\ 5.25)$	$\gamma(1.5,\ 3.5)$	#
$A(2,\ 10)$	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



[4]Credit: Shokoufeh Mirzaei, PhD

Task #6[4]

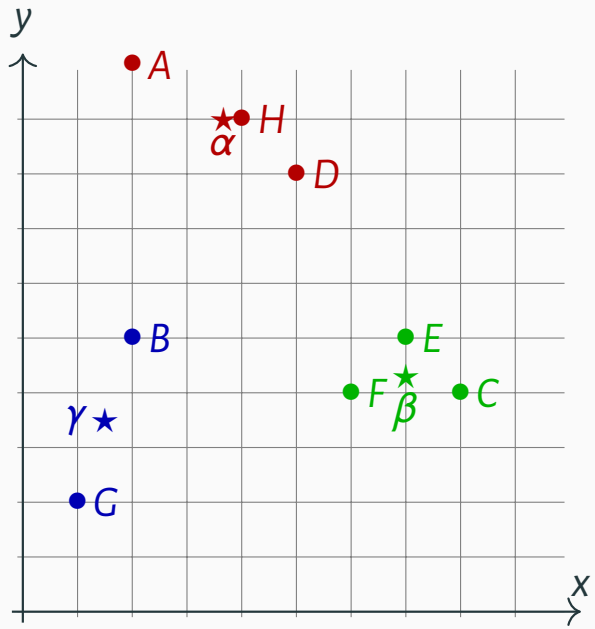
Use *K*-Means algorithm to cluster the following eight points intro three clusters:

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

- 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

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

Point	$\alpha(3,\ 9.5)$	$\beta(6.5,\ 5.25)$	$\gamma(1.5,\ 3.5)$	#
$A(2,\ 10)$	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
	$\alpha(3.67,\ 9)$	$\beta(7,\ 4.3)$	$\gamma(1.5,\ 3.5)$	



[4]Credit: Shokoufeh Mirzaei, PhD

Task #6[4]

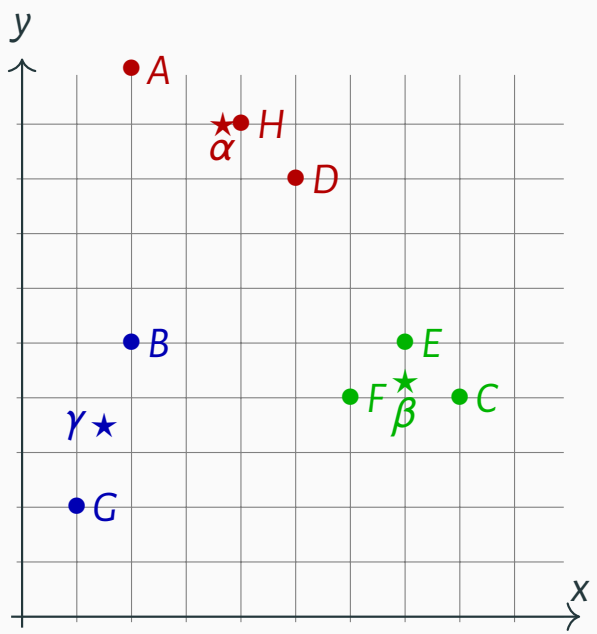
Use *K*-Means algorithm to cluster the following eight points intro three clusters:

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

- 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

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

Point	$\alpha(3.67,\ 9)$	$\beta(7,\ 4.3)$	$\gamma(1.5,\ 3.5)$	#
$A(2,\ 10)$	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



[4]Credit: Shokoufeh Mirzaei, PhD

Task #6[4]

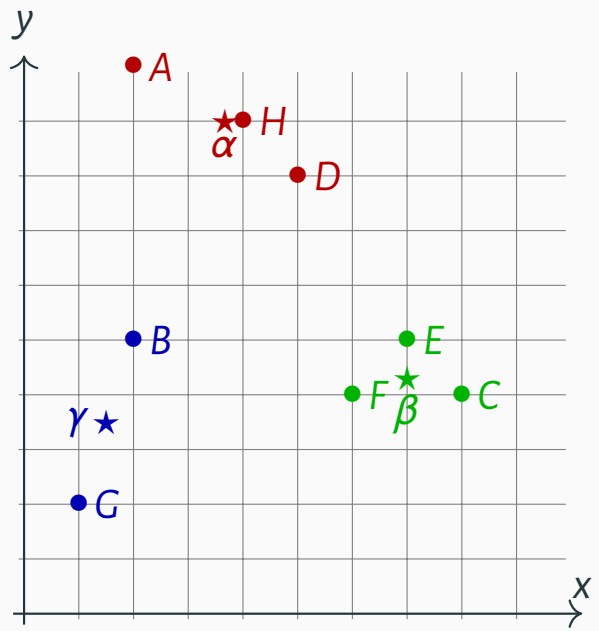
Use *K*-Means algorithm to cluster the following eight points intro three clusters:

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

- 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

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

Point	$\alpha(3.67,\ 9)$	$\beta(7,\ 4.3)$	$\gamma(1.5,\ 3.5)$	#
$A(2,\ 10)$	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
	$\alpha(3.67,\ 9)$	$\beta(7,\ 4.3)$	$\gamma(1.5,\ 3.5)$	



[4]Credit: Shokoufeh Mirzaei, PhD

K-Means

Code Snippet

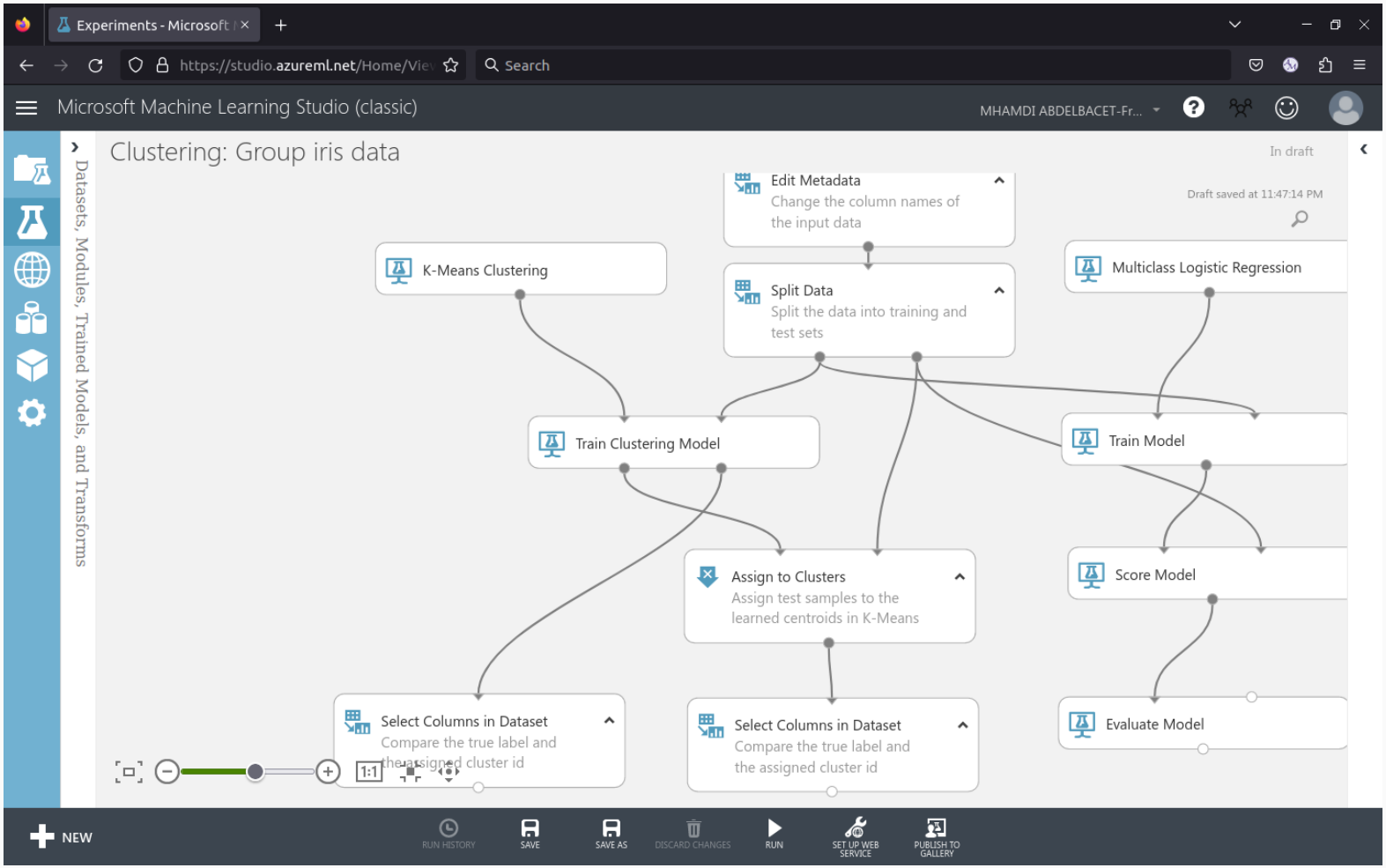
Code is available at https://github.com/a-mhamdi/jlai/
⟶ *Codes* ⟶ *Julia* ⟶ *Part-2* ⟶ *kmeans.jl*

Complementary Lab. Project

On the day of assignment, you will be informed about the **dataset to consider**, **specific features to keep**, and **name of machine learning model to build**. You will be asked to:

① conduct the experiment successfully *(pipeline, featurization, split, etc.)*;

② deploy a fully functional web service app that meets the given specifications.



https://studio.azureml.net/

ML Landscape through Quizzes

Knowledge Check

https://app.wooclap.com/RAIAS2

Link Bundle

https://karpathy.ai/

https://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

http://yann.lecun.com/

https://www.ibm.com/downloads/cas/GB8ZMQZ3

https://www.hackingnote.com/

https://stanford.edu/ shervine/teaching/

https://machinelearningmastery.com/

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[ENM15] I. El Naqa and M. J. Murphy. "What Is Machine Learning?" In: *Machine Learning in Radiation Oncology: Theory and Applications*. Ed. by I. El Naqa, R. Li, and M. J. Murphy. Cham: Springer International Publishing, 2015, pp. 3–11. DOI: 10.1007/978-3-319-18305-3_1.

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Further Reading (2/2)

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[Woj12] J. Wojtusiak. "Machine Learning". In: *Encyclopedia of the Sciences of Learning*. Springer US, 2012, pp. 2082–2083. DOI: 10.1007/978-1-4419-1428-6_1927.