# Tutorial Introduction

## *Machine Learning for Materials Science*

Adalberto Fazzio, Marcio Costa, Antonio C M Padilha, Gabriel R Schleder

SBF Autumn Meeting - 26 may 2019

*Tutorial Website*

*https://github.com/gschleder/MLtutorial*

Universidade Federal do ABC

CNPEM
Brazilian Center for Research in Energy and Materials

LNNano
Brazilian Nanotechnology National Laboratory

MINISTRY OF SCIENCE, TECHNOLOGY, INNOVATION AND COMMUNICATION

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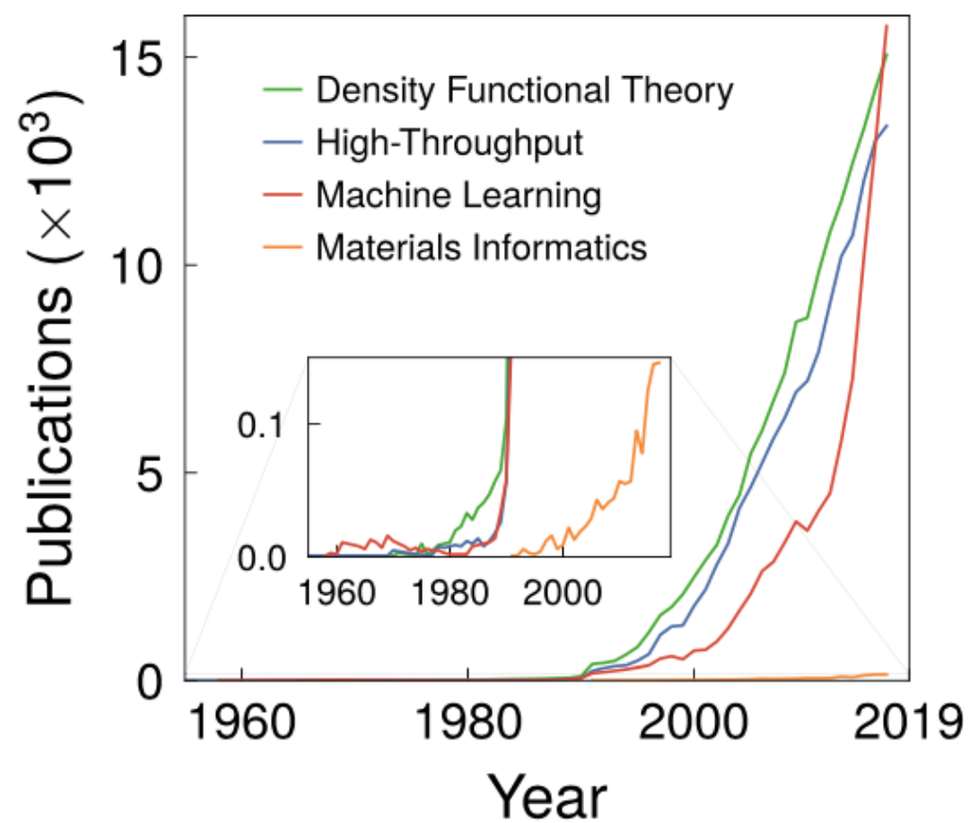
JPhys Materials

**TOPICAL REVIEW**

## From DFT to machine learning: recent approaches to materials science–a review

**Gabriel R Schleder[1,2,3], Antonio C M Padilha[2], Carlos Mera Acosta[1,2], Marcio Costa[2] and Adalberto Fazzio[1,2,3]**

[1] Center for Natural and Human Sciences, Federal University of ABC, 09210-580, Santo André, São Paulo, Brazil
[2] Brazilian Nanotechnology National Laboratory/CNPEM, 13083-970, Campinas, São Paulo, Brazil
[3] Authors to whom any correspondence should be addressed.



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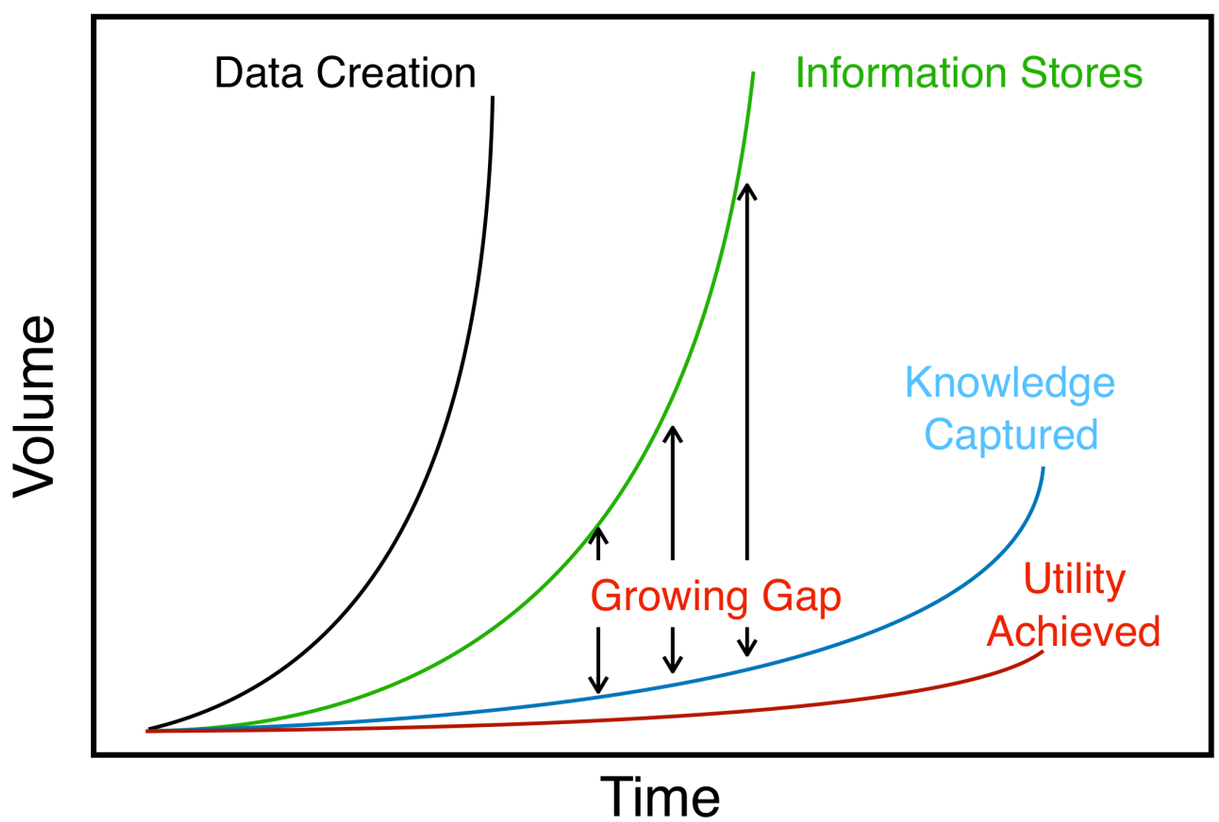


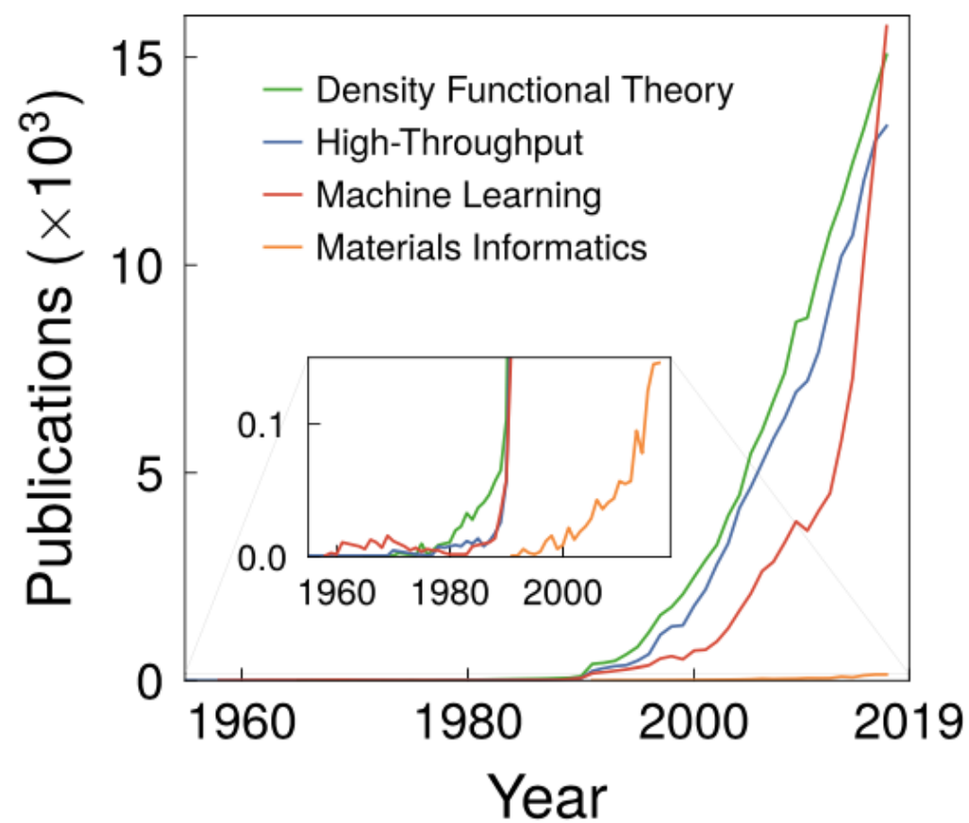

# Banking System



Question : How to decide whether to lend money?

# Banking System



## Question : How to decide whether to lend money?

## Banking

| Label | X1 | X2 | X3 | X4 | Xn |
|---|---|---|---|---|---|
| John | | | | | |

# Banking System



## Question : How to decide whether to lend money?

## Banking

| Label | X1 | X2 | X3 | X4 | Xn |
|---|---|---|---|---|---|
| John | Income | | | | |

# Banking System



## Question : How to decide whether to lend money?

## Banking

| Label | X1 | X2 | X3 | X4 | Xn |
|---|---|---|---|---|---|
| John | Income | Age | | | |

# Banking System



## Question : How to decide whether to lend money?

## Banking

| Label | X1 | X2 | X3 | X4 | Xn |
|---|---|---|---|---|---|
| John | Income | Age | Morgatge | | |

# Banking System



## Question : How to decide whether to lend money?

## Banking

| Label | X1 | X2 | X3 | X4 | Xn |
|---|---|---|---|---|---|
| John | Income | Age | Morgatge | Education | |

# Banking System



## Question : How to decide whether to lend money?

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| Label | X1 | X2 | X3 | X4 | Xn |
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| John | Income | Age | Morgatge | Education | ? |

# Banking System



## Question : How to decide whether to lend money?

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| Label | X1 | X2 | X3 | X4 | Xn |
|---|---|---|---|---|---|
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John's fingerprint!!

# Banking System



## Question : How to decide whether to lend money?

### Banking

| Label | X1 | X2 | X3 | X4 | Xn |
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John's fingerprint!!

### Material Science

| Label | X1 | X2 | X3 | X4 | Xn |
|---|---|---|---|---|---|
| Bi-BCC | IE | EA | HOMO | LUMO | ? |

# Banking System



Question : How to decide whether to lend money?

Banking

| Label | X1 | X2 | X3 | X4 | Xn |
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| John | Income | Age | Morgatge | Education | ? |

John's fingerprint!!

The bank has a large database of past loans

# Banking System



Question : How to decide whether to lend money?

Banking

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|---|---|---|---|---|---|
| John | Income | Age | Morgatge | Education | ? |

John's fingerprint!!

The bank has a large database of past loans

Can we use the historical data to predict the new loan?

# What is Machine Learning?

We would like to analyze and understand the output "P"( Property) on the input "X"(fingerprint).

$$\mathbf{P} = \mathbf{f}(\mathbf{X})$$

- How to predict property P?
- Discover the function $f(\mathbf{X})=P$
  - **X**: known (input) variables, easily obtained

# What is Machine Learning?



We would like to analyze and understand the output "P"( Property) on the input "X"(fingerprint).

$$\mathbf{P} = \mathbf{f}(\mathbf{X})$$

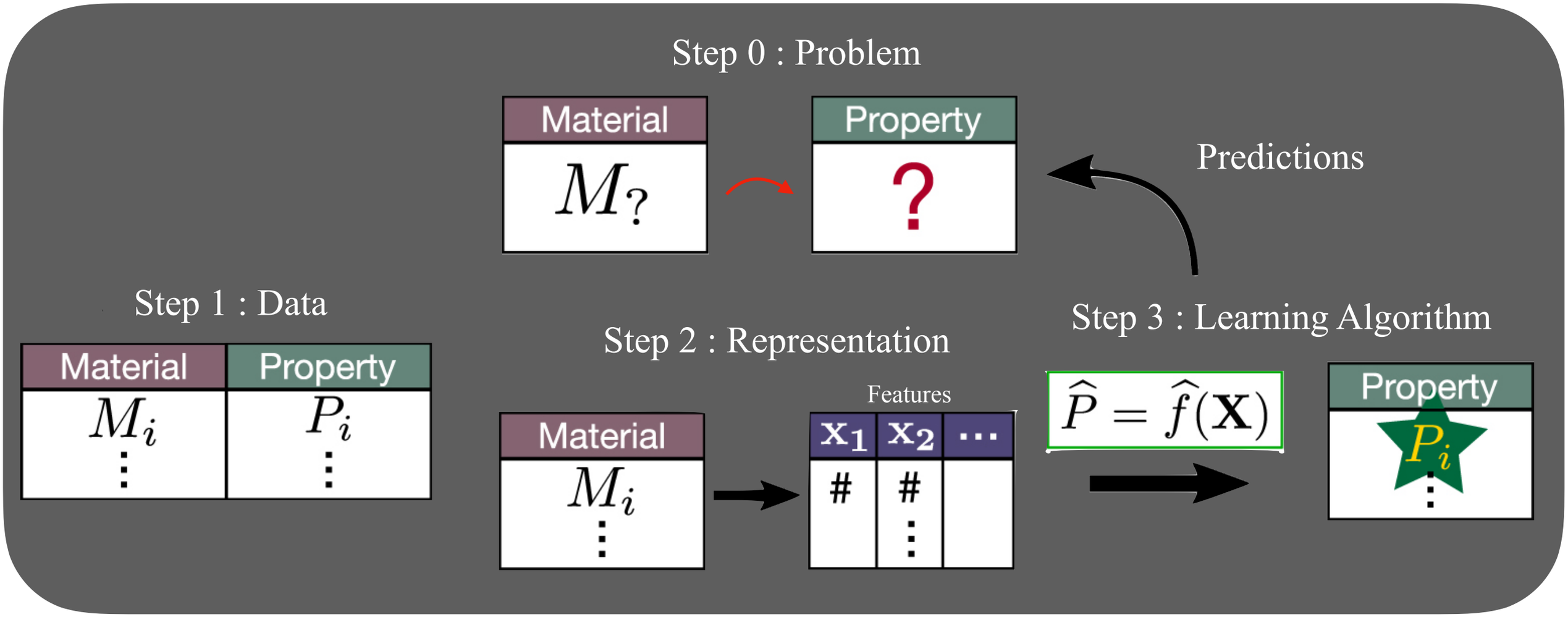
- How to predict property P?
- Discover the function $f(\mathbf{X})=P$
  - **X**: known (input) variables, easily obtained
  - Ideally, $f(\mathbf{X})$ has physical meaning

# What is Machine Learning?

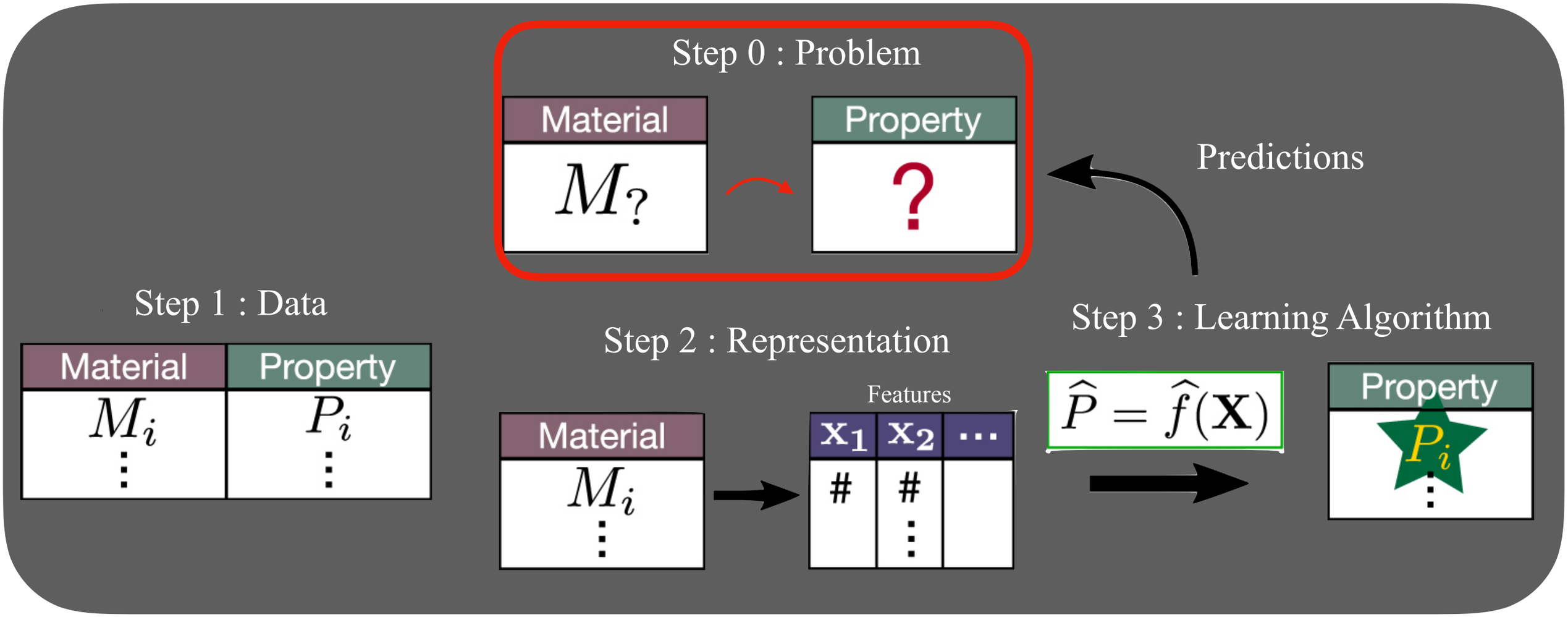


Machine learning can be defined as a class of methods for automated data analysis, which are capable of detecting patterns in data. These extracted patterns can be used to predict unknown data or to assist in decision-making processes under uncertainty.

# Machine Learning Workflow



# Machine Learning Workflow



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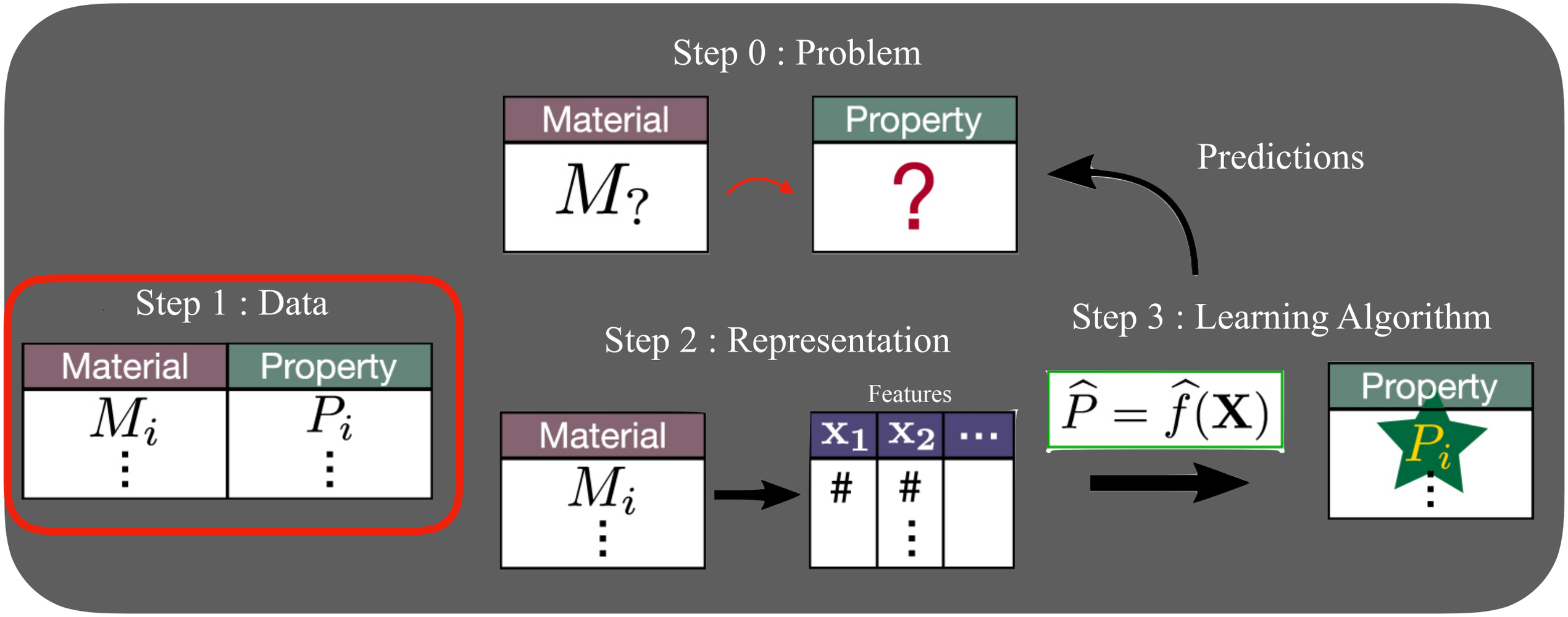

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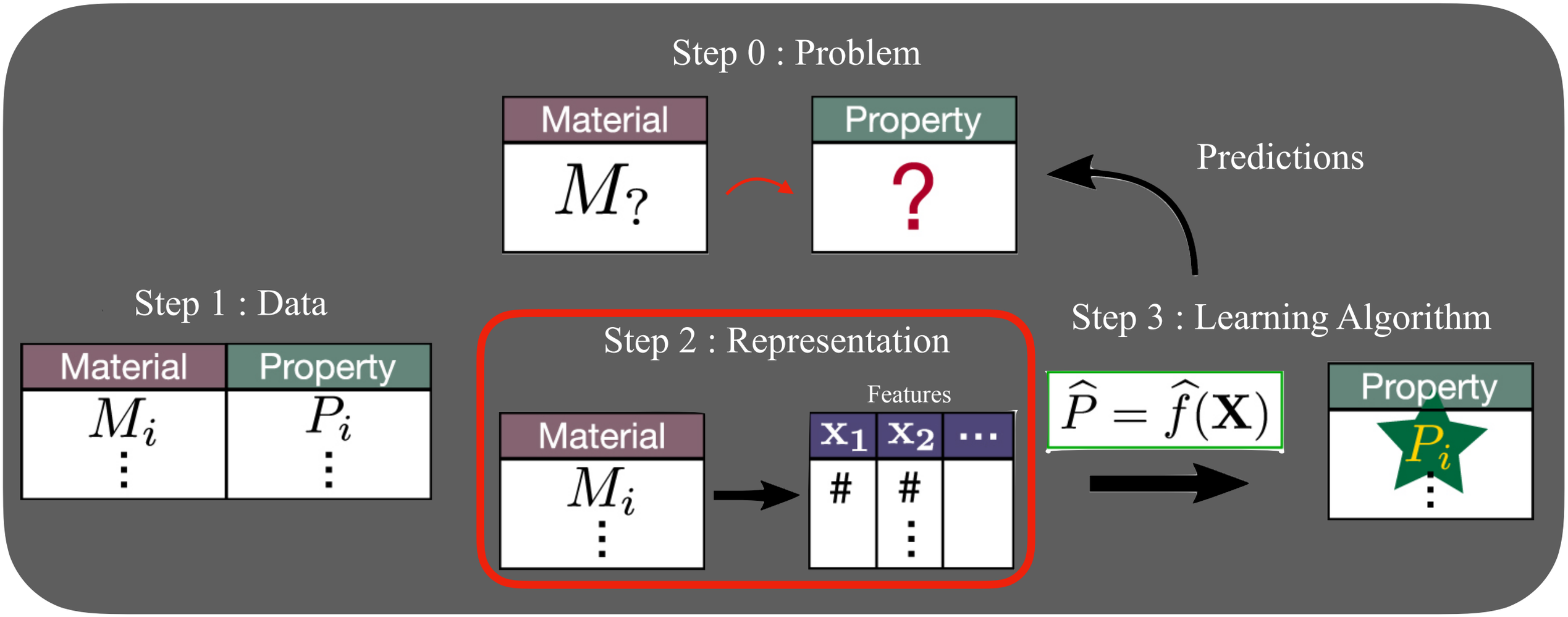

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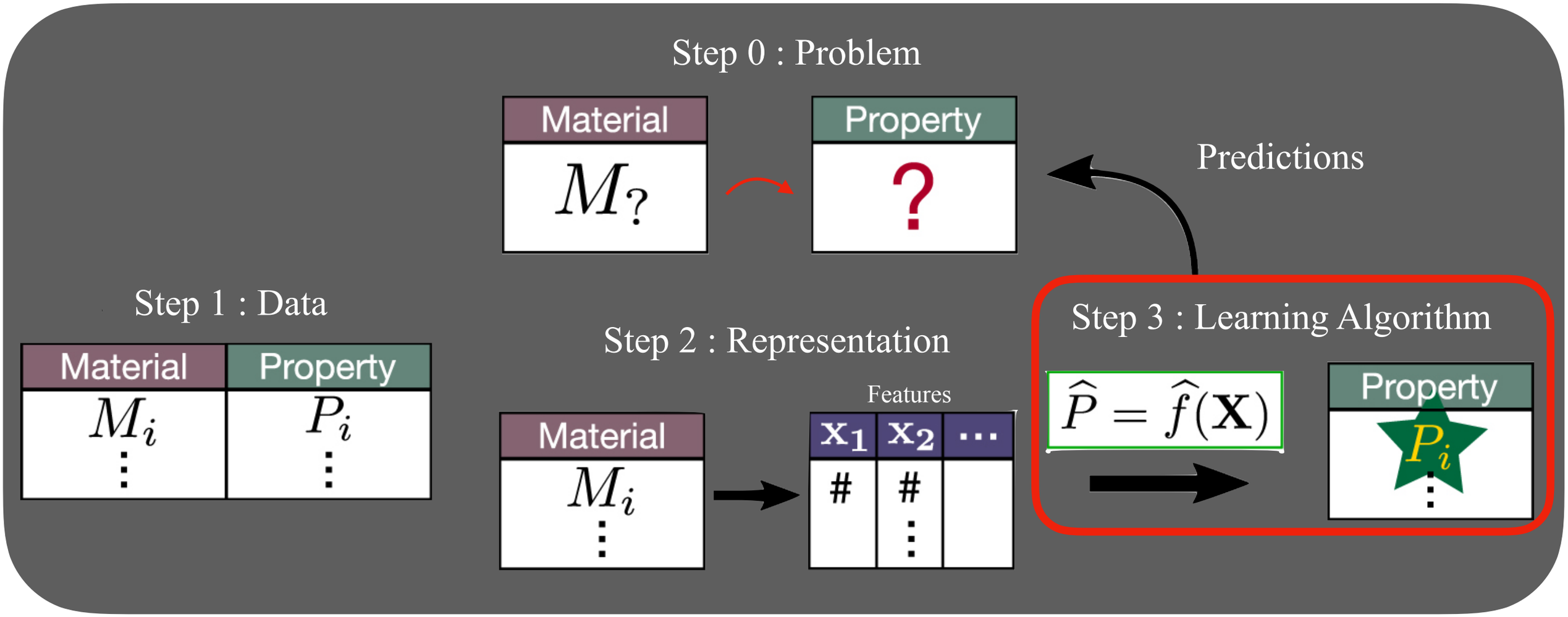
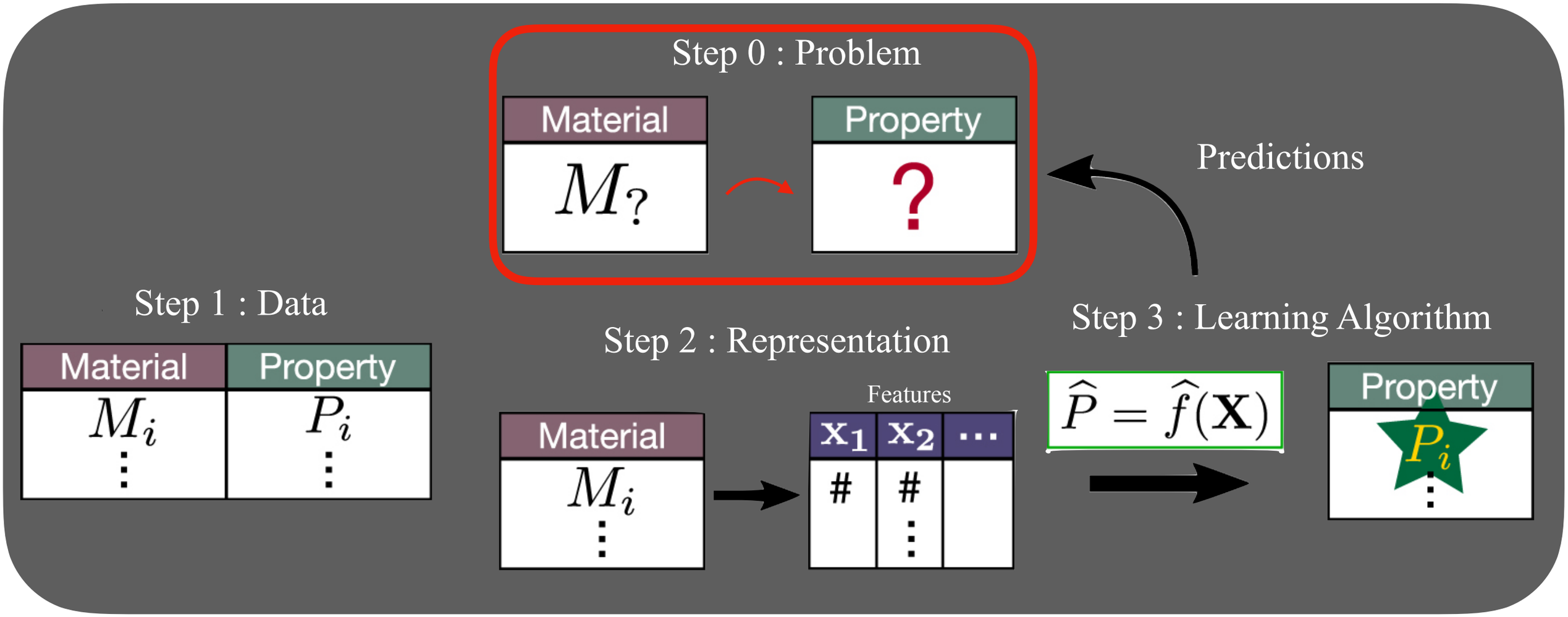


# Step 0 : Problem



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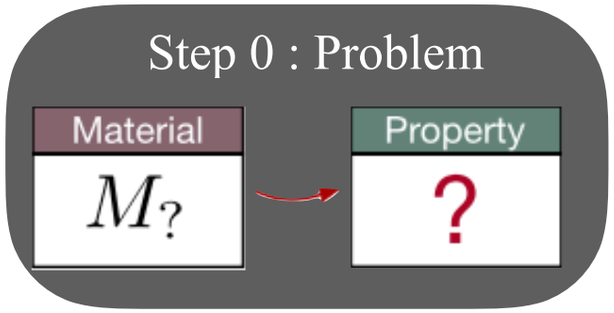

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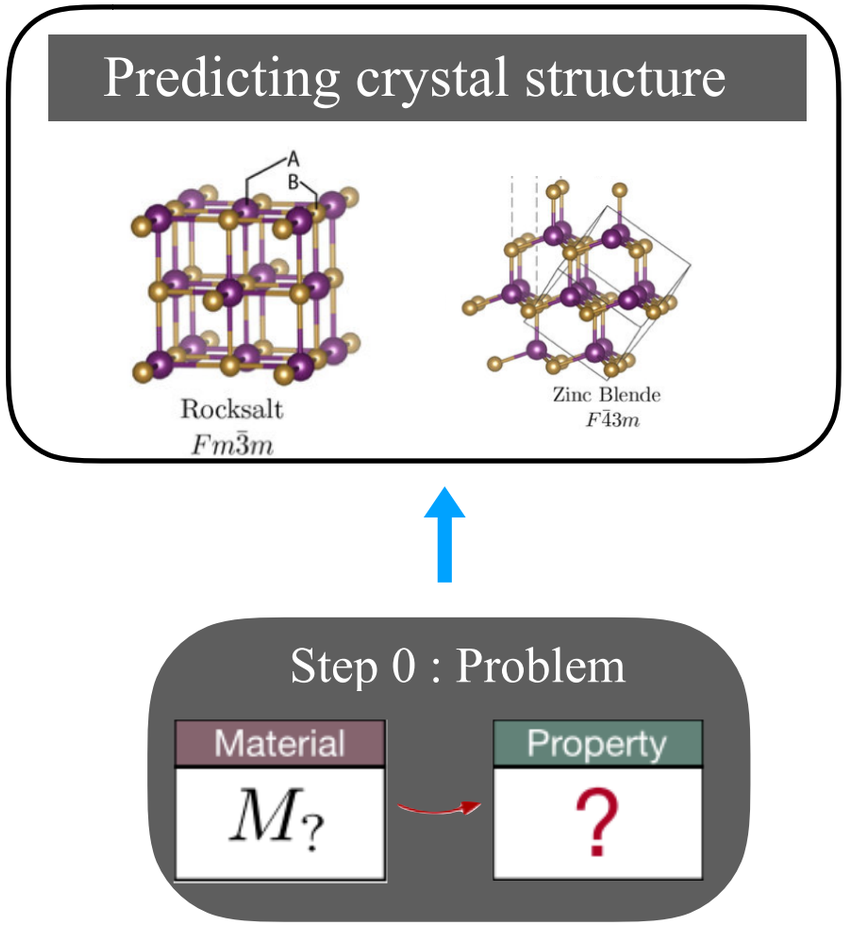
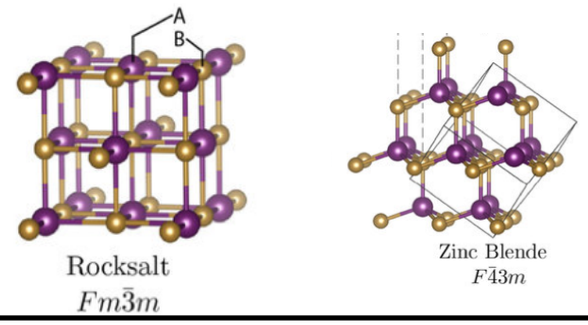
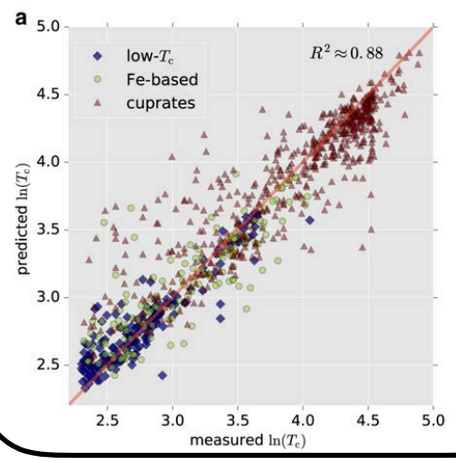


# Step 0 : Problem

## Predicting crystal structure




## Superconductivity

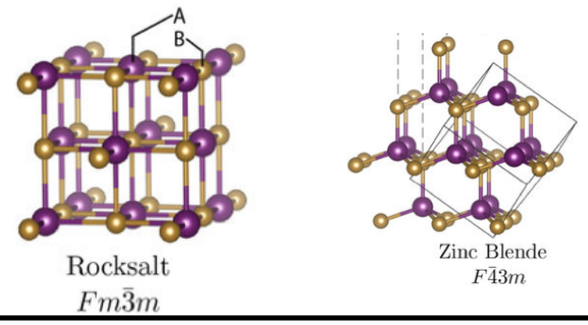



## Step 0 : Problem

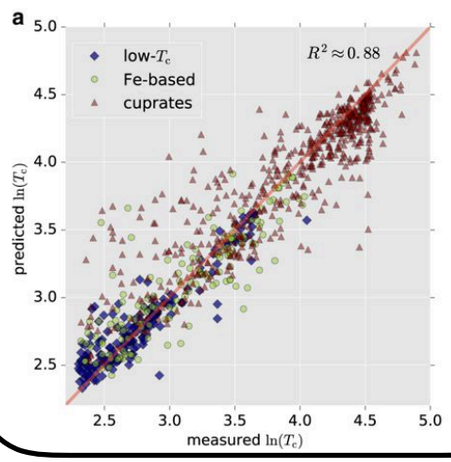
| Material | Property |
|---|---|
| $M_?$ | ? |

# Step 0 : Problem

## Predicting crystal structure




## Superconductivity

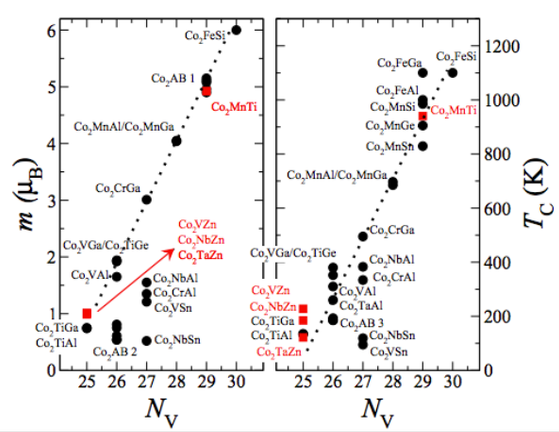



## Step 0 : Problem

Material: $M_?$

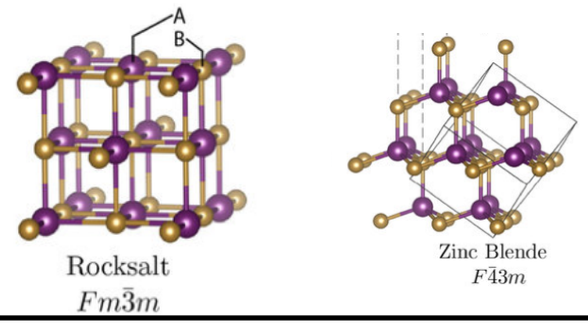
Property: ?

## Magnetic Materials



# Step 0 : Problem

## Predicting crystal structure

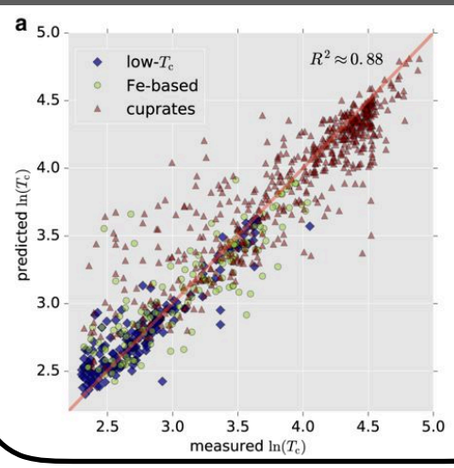



## Step 0 : Problem

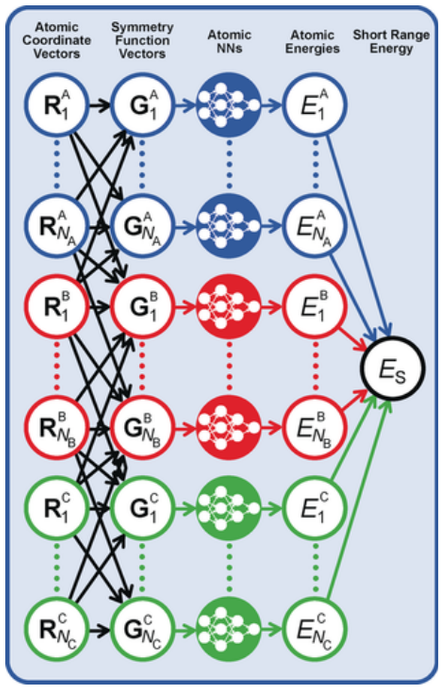
Material: $M_?$

Property: ?

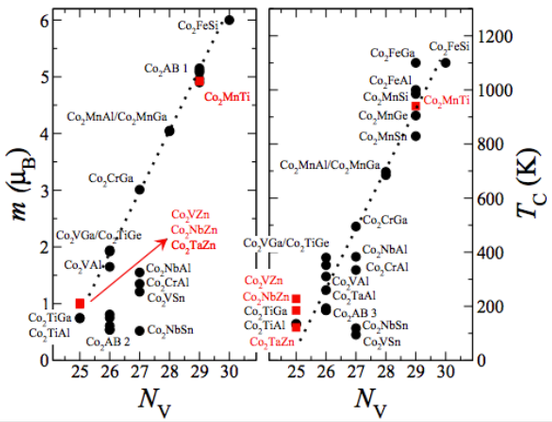
## Superconductivity




## Atomistic Potentials



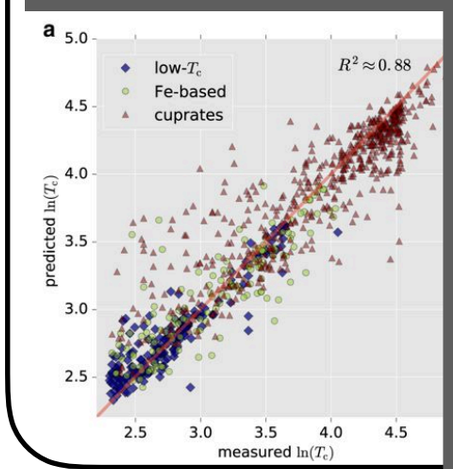

## Magnetic Materials



# Step 0 : Problem

- Predicting crystal structure
- Formation energy
- Atomistic potentials
- Electronic properties : bandgap
- Electronic properties : conductivity
- Metal / Insulator?
- Permanent Magnets

Superconductiv

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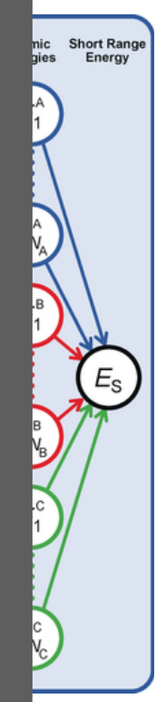


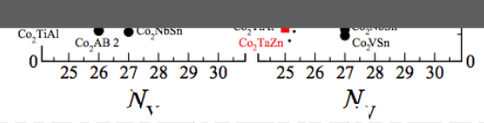

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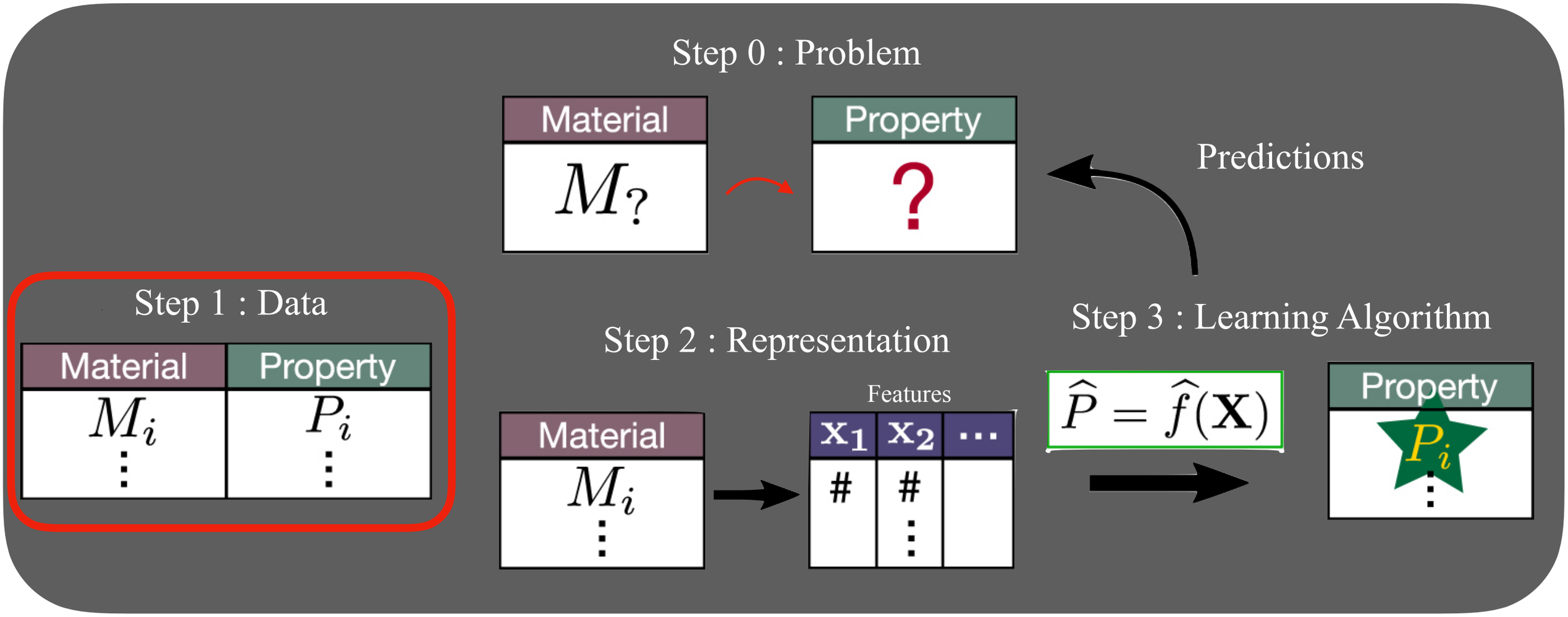
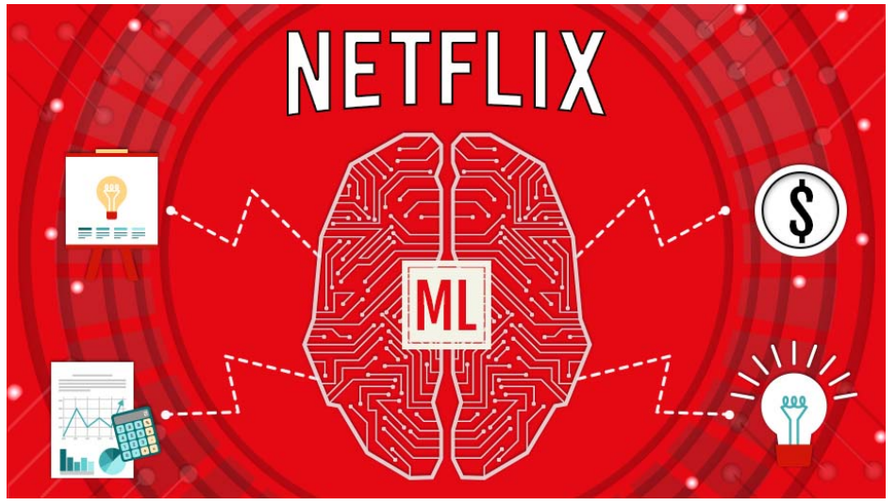


# Step 0 : Problem

Pharmaceutical

Social




Step 1 : Data

| Material | Property |
|---|---|
| $M_i$ | $P_i$ |
| $\vdots$ | $\vdots$ |

Materials Science

MP

NOMAD

ICSD

AFLOW

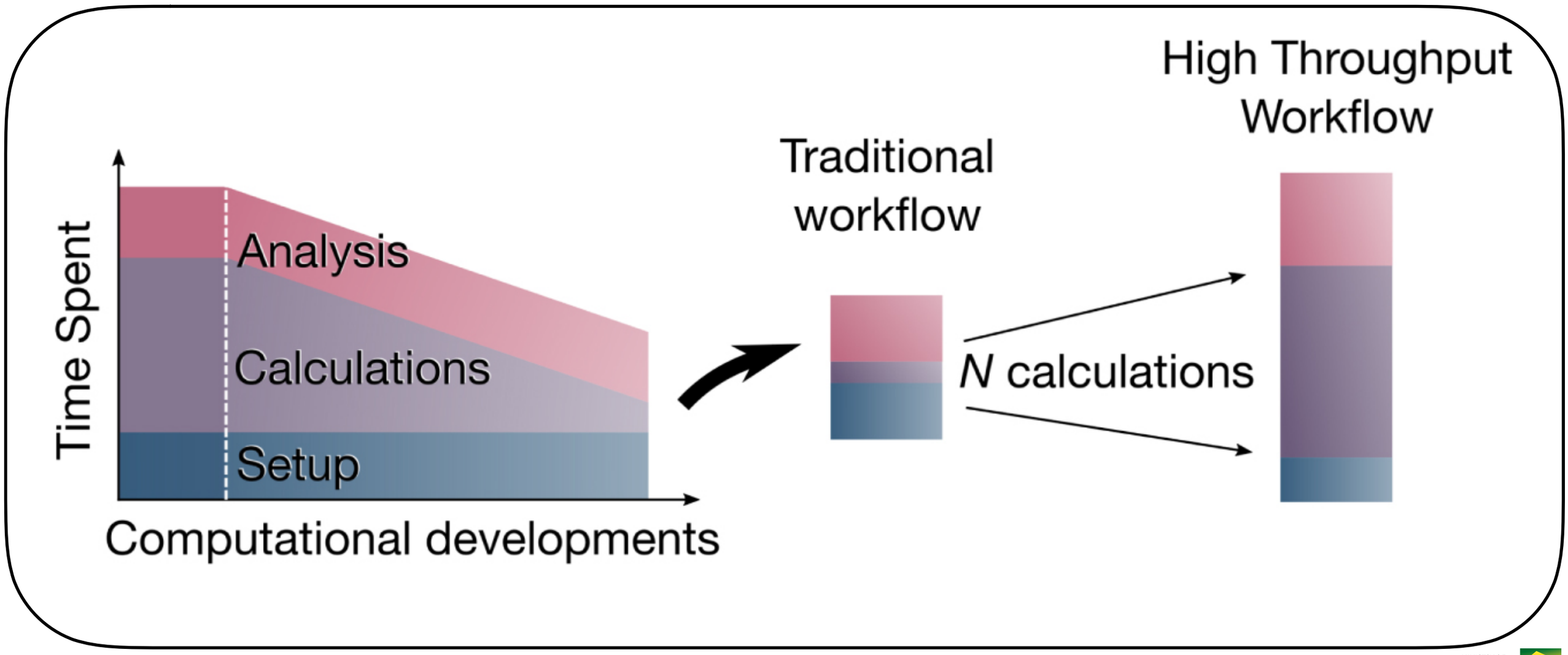
Automatic - FLOW for Materials Discovery

# Step 1 : Data

Step 1 : Data

| Material | Property |
| --- | --- |
| $M_i$ | $P_i$ |
| ⋮ | ⋮ |

## High Throughput (HT) calculations



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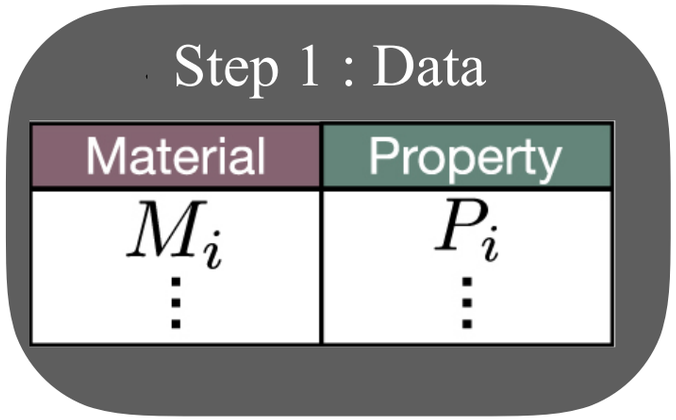
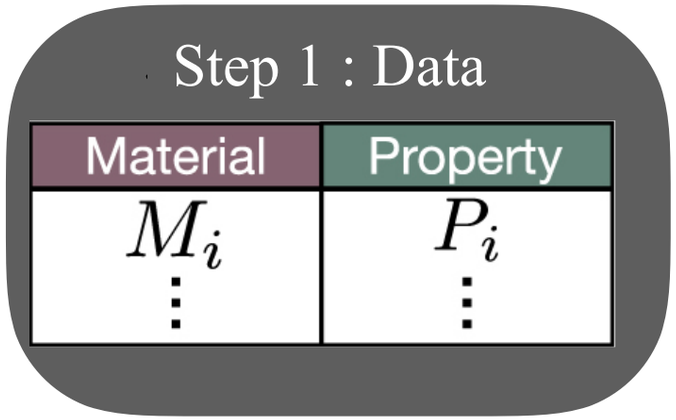



## Material Science Databases

**HT databases**

| | | | |
|---|---|---|---|
| ICSD | Inorganic experimental | http://www2.fiz-karlsruhe.de/icsd_home.html | [152] |
| COD | Organic and Inorganic experimental | http://crystallography.net | [153] |
| AFLOWlib | Multi-purpose repository | http://aflowlib.org/ | [148] |
| Materials Project | Multi-purpose repository | https://materialsproject.org/ | [149] |
| OQDM | Multi-purpose repository | http://oqmd.org/ | [150] |
| CMR | Multi-purpose (3D and 2D materials) repository | https://cmr.fysik.dtu.dk/ | [154] |
| OMDB | Organic materials database | https://omdb.mathub.io/ | [155] |
| MaterialsWeb | 2D materials (derived from Materials Project) | https://materialsweb.org/twodmaterials | [156] |
| JARVIS-DFT | 2D materials | https://ctcms.nist.gov/~knc6/JVASP.html | [157, 158] |
| NOMAD | Multiple source repository | https://repository.nomad-coe.eu/ | |
| Materials Cloud | Multiple source repository | https://materialscloud.org/discover | [3] |
| Citrination | Multiple source (experimental and theoretical) repository | https://citrination.com | [159] |
| Clean Energy Project | Multiple source repository for solar cells | | [160] |
| C2DB | 2D materials (derived from CMR) | https://cmr.fysik.dtu.dk/c2db/c2db.html | [161] |

# Step 1 : Data

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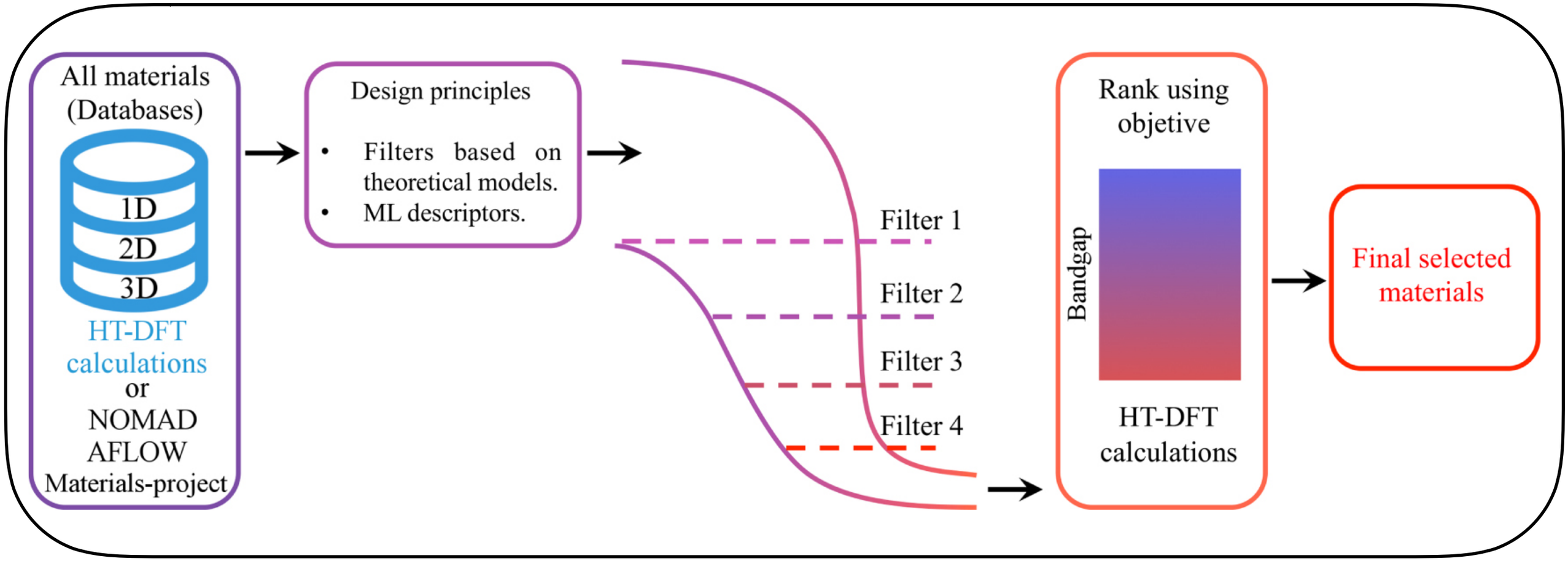
| ⋮ | ⋮ |



# Step 1 : Data

Step 1 : Data

| Material | Property |
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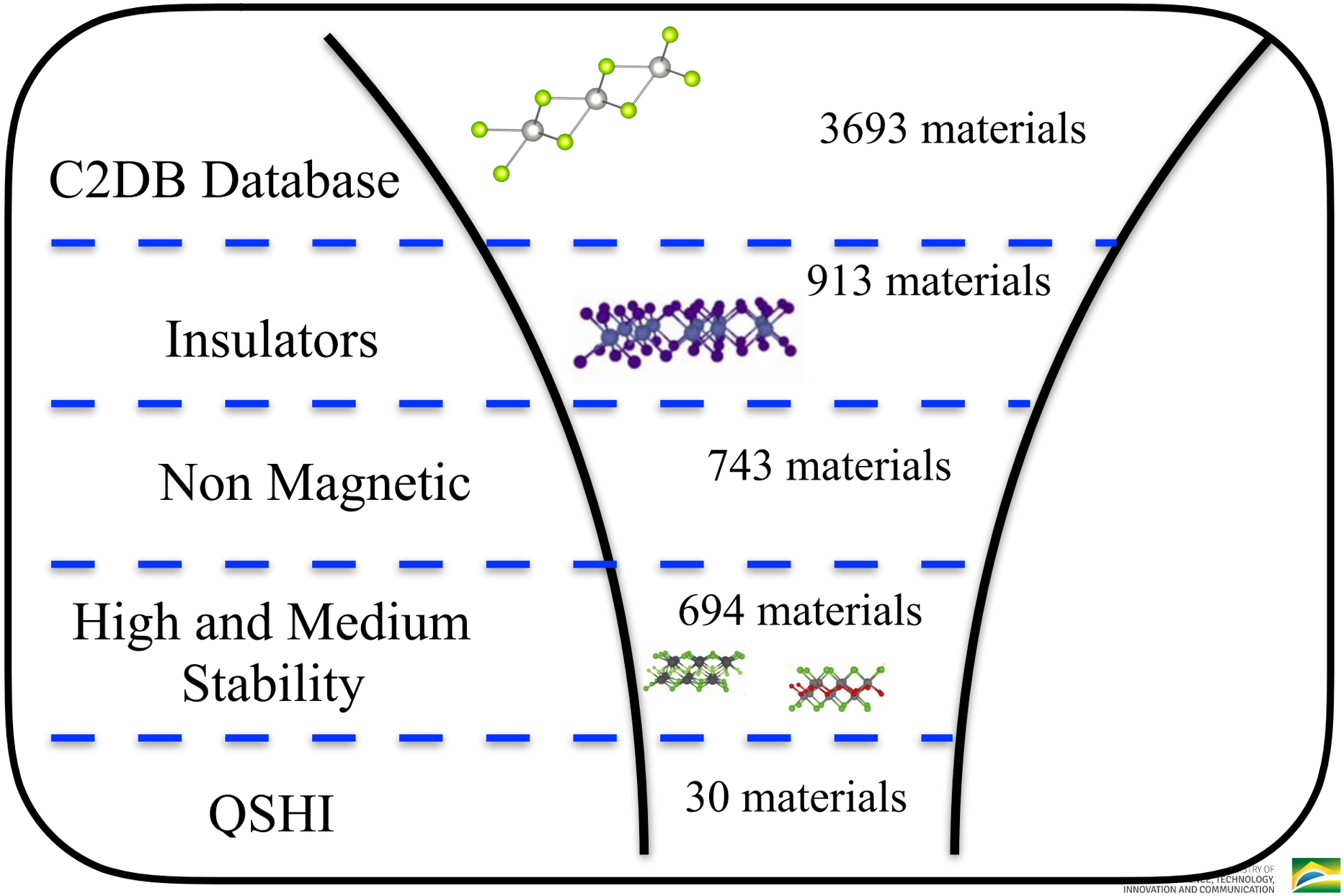

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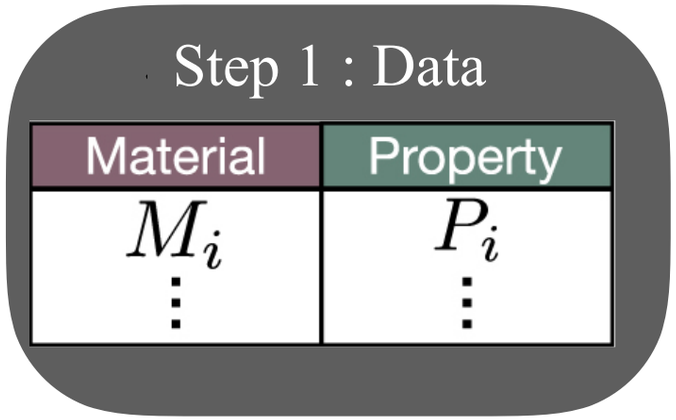
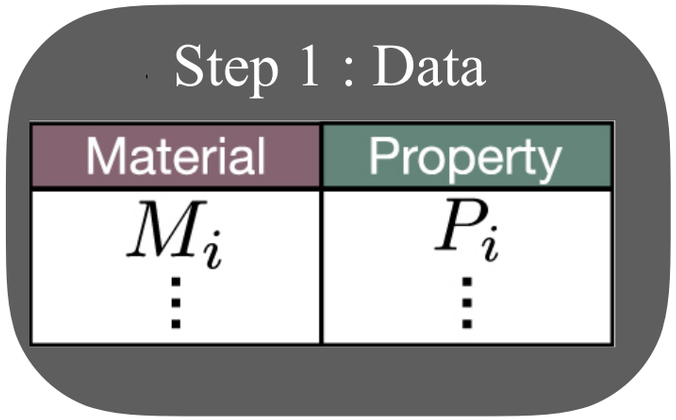



## Packages for HT and screening

**HT Codes and tools**

| | | | |
|---|---|---|---|
| ASE | Complete package for HT | https://wiki.fysik.dtu.dk/ase/ | [162] |
| Pymatgen | Complete package for HT | http://pymatgen.org/ | [163] |
| AiiDA | Framework for HT | http://aiida.net/ | [164] |
| AFLOW$\pi$ | Framework for HT | http://aflowlib.org/src/aflowpi/index.html | [165] |
| Atomate | Complete package for HT | https://atomate.org/ | [166] |
| Pylada | Framework for HT | http://pylada.github.io/pylada/ | |
| MPInterfaces | Framework for interfaces HT | http://henniggroup.github.io/MPInterfaces/ | [167] |
| Imeall | Atomistic properties of grain boundaries | https://github.com/Montmorency/imeall | [168] |
| FireWorks | Framework for HT | https://materialsproject.github.io/fireworks/ | [169] |

# Step 1 : Data

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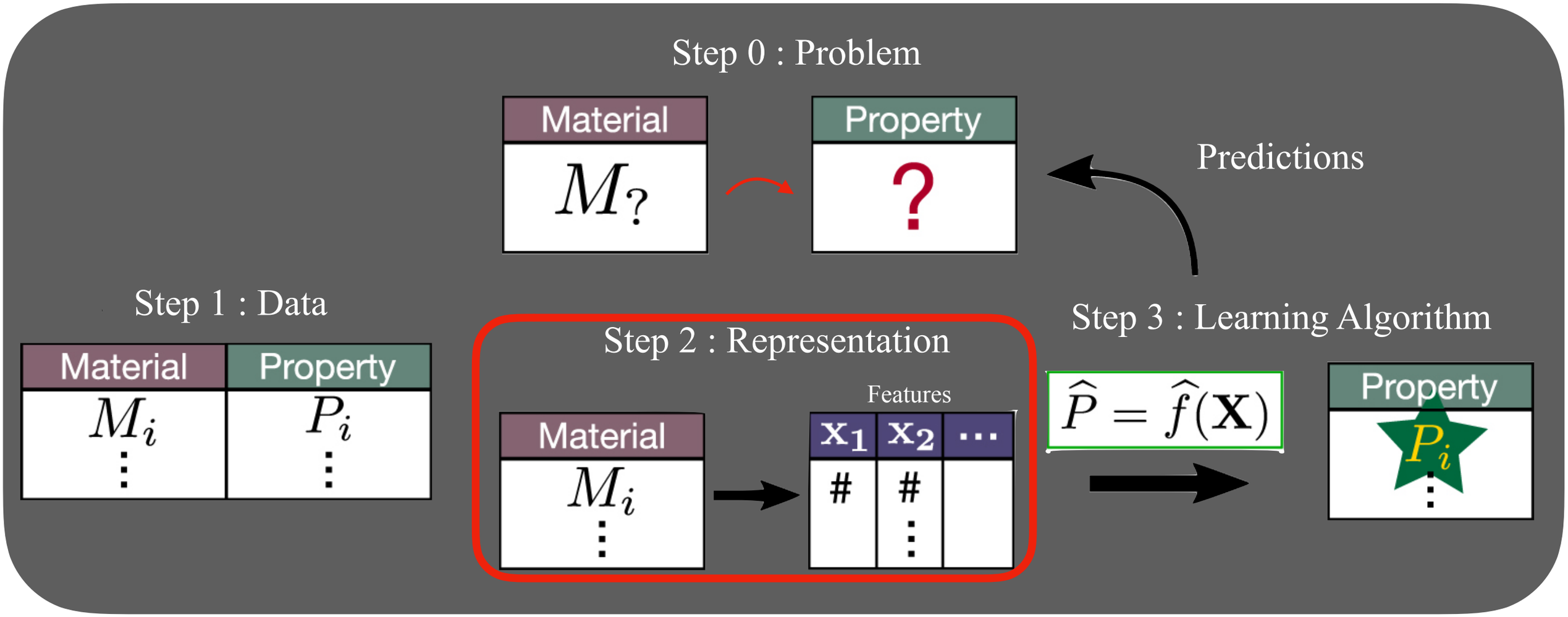
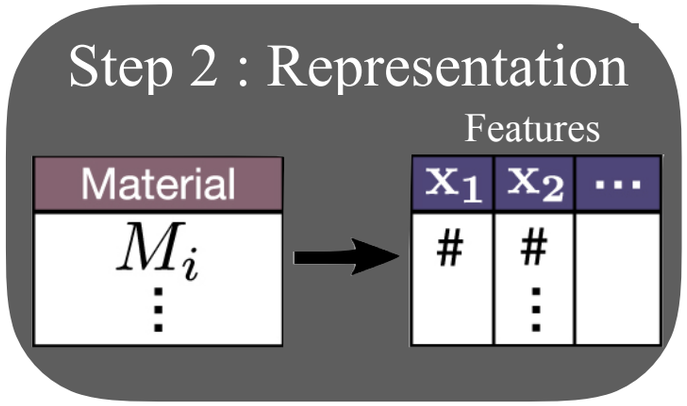
| AFLOW$\pi$ | Framework for HT | http://aflowlib.org/src/aflowpi/index.html | [165] |
| Atomate | Complete package for HT | https://atomate.org/ | [166] |
| Pylada | Framework for HT | http://pylada.github.io/pylada/ | |
| MPInterfaces | Framework for interfaces HT | http://henniggroup.github.io/MPInterfaces/ | [167] |
| Imeall | Atomistic properties of grain boundaries | https://github.com/Montmorency/imeall | [168] |
| FireWorks | Framework for HT | https://materialsproject.github.io/fireworks/ | [169] |

# Step 2 : Representation

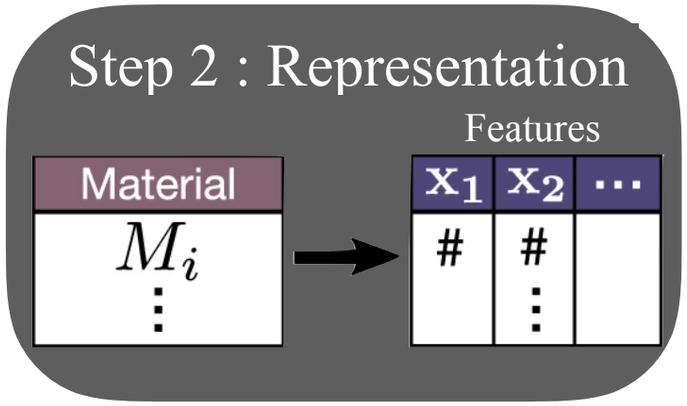


# Step 2 : Representation




i) Complete
ii) Unique
iii) Discriminative
iv) Efficient and Simple

# Step 2 : Representation




PRL **114,** 105503 (2015) PHYSICAL REVIEW LETTERS week ending 13 MARCH 2015

**Big Data of Materials Science: Critical Role of the Descriptor**

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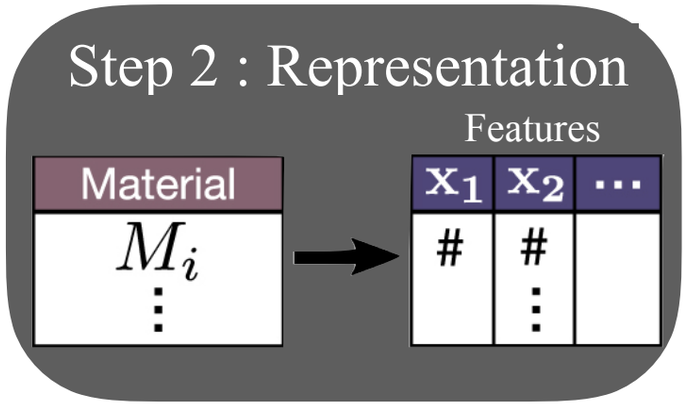
(Received 14 April 2014; revised manuscript received 20 October 2014; published 10 March 2015)

| $Z_A$ | A | IP [eV] | EA [eV] | EN = −1/2(EA+IP) [eV] | Highest occ. KS level [eV] | Lowest unocc. KS level [eV] | $r_s$ [Å] | $r_p$ [Å] | $r_d$ [Å] |
|---|---|---|---|---|---|---|---|---|---|
| 3 | Li | -5.329 | -0.698 | 3.014 | -2.874 | -0.978 | 1.652 | 1.995 | 6.930 |
| 4 | Be | -9.459 | 0.631 | 4.414 | -5.600 | -2.098 | 1.078 | 1.211 | 2.877 |
| 5 | B | -8.190 | -0.107 | 4.149 | -3.715 | 2.248 | 0.805 | 0.826 | 1.946 |
| 6 | C | -10.852 | -0.872 | 5.862 | -5.416 | 1.992 | 0.644 | 0.630 | 1.631 |
| 7 | N | -13.585 | -1.867 | 7.726 | -7.239 | 3.057 | 0.539 | 0.511 | 1.540 |
| ⋮ | | | | | | | | | |
| 50 | Sn | -7.043 | -1.039 | 4.041 | -3.866 | 0.008 | 1.057 | 1.344 | 2.030 |
| 51 | Sb | -8.468 | -1.847 | 5.158 | -4.991 | 0.105 | 1.001 | 1.232 | 2.065 |
| 52 | Te | -9.867 | -2.666 | 6.266 | -6.109 | 0.099 | 0.945 | 1.141 | 1.827 |
| 53 | I | -11.257 | -3.513 | 7.385 | -7.236 | 0.213 | 0.896 | 1.071 | 1.722 |
| 55 | Cs | -4.006 | -0.570 | 2.288 | -2.220 | -0.548 | 2.464 | 3.164 | 1.974 |
| 56 | Ba | -5.516 | 0.278 | 2.619 | -3.346 | -2.129 | 2.149 | 2.632 | 1.351 |

# Step 2 : Representation

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**X1**

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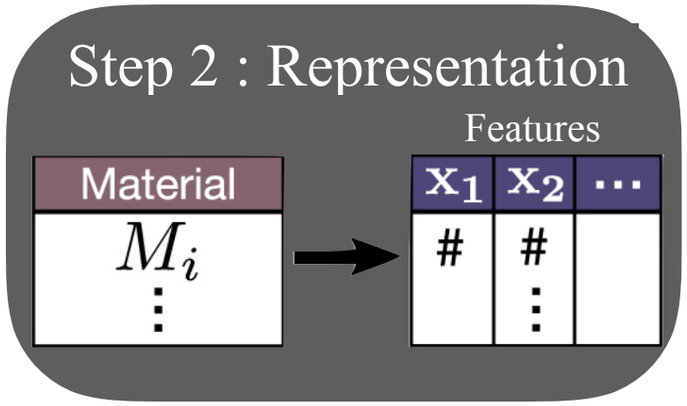


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**X1 X2**

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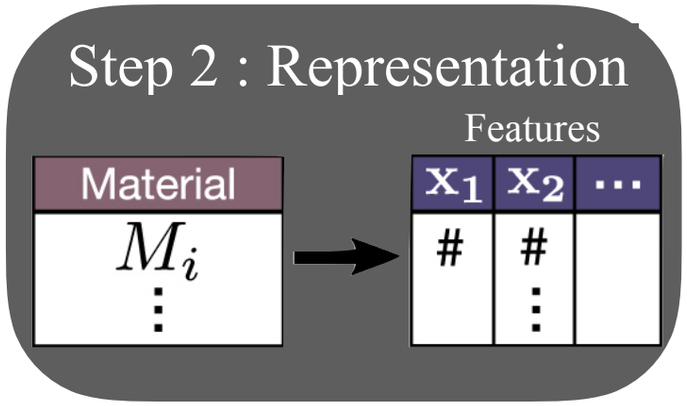


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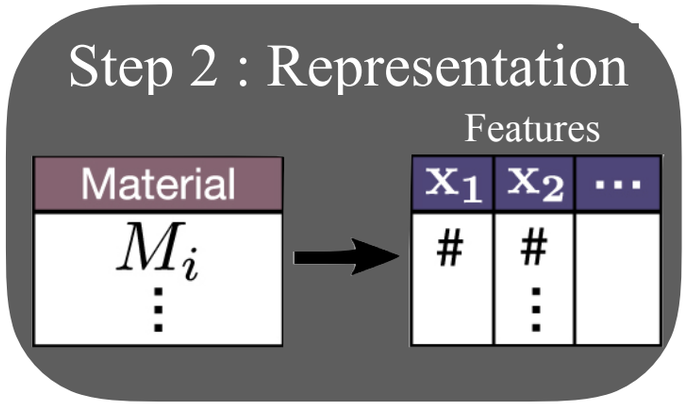


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| X1 | X2 | X3 | X4 | X5 | X6 | X7 | X8 | X9 | X10 |
|---|---|---|---|---|---|---|---|---|---|
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**Feature space**

**(*Fingerprint*)**

# Step 2 : Representation

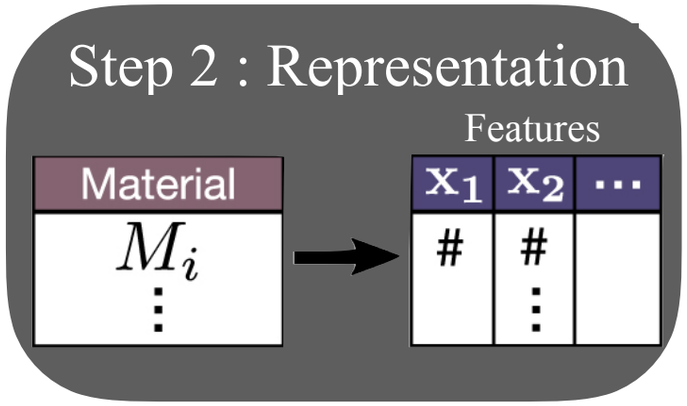


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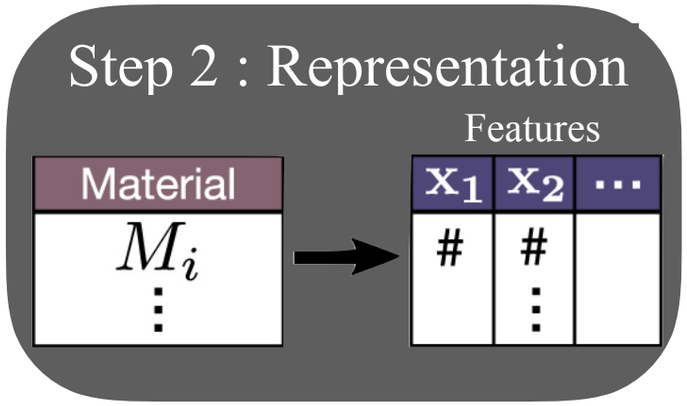
TABLE I. Dependence of the metal-insulator classification descriptors on the prototypes of training binary materials.

| prototypes | #materials | primary features | descriptor | classification accuracy |
|---|---|---|---|---|
| NaCl | 132 | $IE_A$, $IE_B$, $\chi_A$, $\chi_B$, $r_{\mathrm{covA}}$, $r_{\mathrm{covB}}$, $EA_A$, $EA_B$, $v_A$, $v_B$, $d_{AB}$ | $d_1 := \frac{IE_A IE_B (d_{AB} - r_{\mathrm{covA}})}{\exp(\chi_A)\sqrt{r_{\mathrm{covB}}}}$ | 100% |
| NaCl, CsCl, ZnS, $CaF_2$, $Cr_3Si$ | 217 | $IE_A$, $IE_B$, $\chi_A$, $\chi_B$, $r_{\mathrm{covA}}$, $r_{\mathrm{covB}}$, $d_{AB}$, $CN_A$, $CN_B$ | $d_1 := \frac{IE_B d_{AB}^2}{\chi_A r_{\mathrm{covA}}^2 \sqrt{CN_B}}$, $d_2 := \frac{IE_A^2 r_{\mathrm{covB}} \log(IE_A) \lvert r_{\mathrm{covA}} - r_{\mathrm{covB}} \rvert}{CN_B}$ | 100% |
| NaCl, CsCl, ZnS, $CaF_2$, $Cr_3Si$, SiC, $TiO_2$, ZnO, FeAs, NiAs | 260 | $IE_A$, $IE_B$, $\chi_A$, $\chi_B$, $r_{\mathrm{covA}}$, $r_{\mathrm{covB}}$, $d_{AB}$, $CN_A$, $CN_B$ | $d_1 := \frac{d_{AB}/r_{\mathrm{covA}} - \chi_A/\chi_B}{\exp(CN_B/IE_B)}$, $d_2 := \frac{r_{\mathrm{covA}}^3 d_{AB} IE_B}{\lvert \chi_B/\chi_A - \lvert CN_B - CN_A \rvert \rvert}$ | 99.6%[a] |
| NaCl, CsCl, ZnS, $CaF_2$, $Cr_3Si$, SiC, $TiO_2$, ZnO, FeAs, NiAs | 260 | $IE_A$, $IE_B$, $\chi_A$, $\chi_B$, $x_A$, $x_B$, $V_{\mathrm{cell}}/\sum V_{\mathrm{atom}}$ | $d_1 := \frac{V_{\mathrm{cell}}}{\sum V_{\mathrm{atom}}} \frac{\sqrt{\chi_B}}{\chi_A}$, $d_2 := \frac{IE_A IE_B}{\exp(V_{\mathrm{cell}}/\sum V_{\mathrm{atom}})}$ | 99.6%[a] |
| NaCl, CsCl, ZnS, $CaF_2$, $Cr_3Si$, SiC, $TiO_2$, ZnO, FeAs, NiAs, $Al_2O_3$, $La_2O_3$, $Th_3P_4$, $ReO_3$, $ThH_2$ | 299 | $IE_A$, $IE_B$, $\chi_A$, $\chi_B$, $x_A$, $x_B$, $V_{\mathrm{cell}}/\sum V_{\mathrm{atom}}$ | $d_1 := \frac{x_B}{\sum V_{\mathrm{atom}}/V_{\mathrm{cell}}} \frac{IE_B \sqrt{\chi_B}}{\chi_A}$, $d_2 := \chi_A^2 \lvert \lvert 1 - 2x_A \rvert - x_A^2 \frac{\chi_B}{\chi_A} \rvert$ | 99.0%[b] |

Runhai Ouyang, *et. al.* Phys. Rev. Mat. **2**, 083802 (2018).

# Step 2 : Representation




## Atomic properties

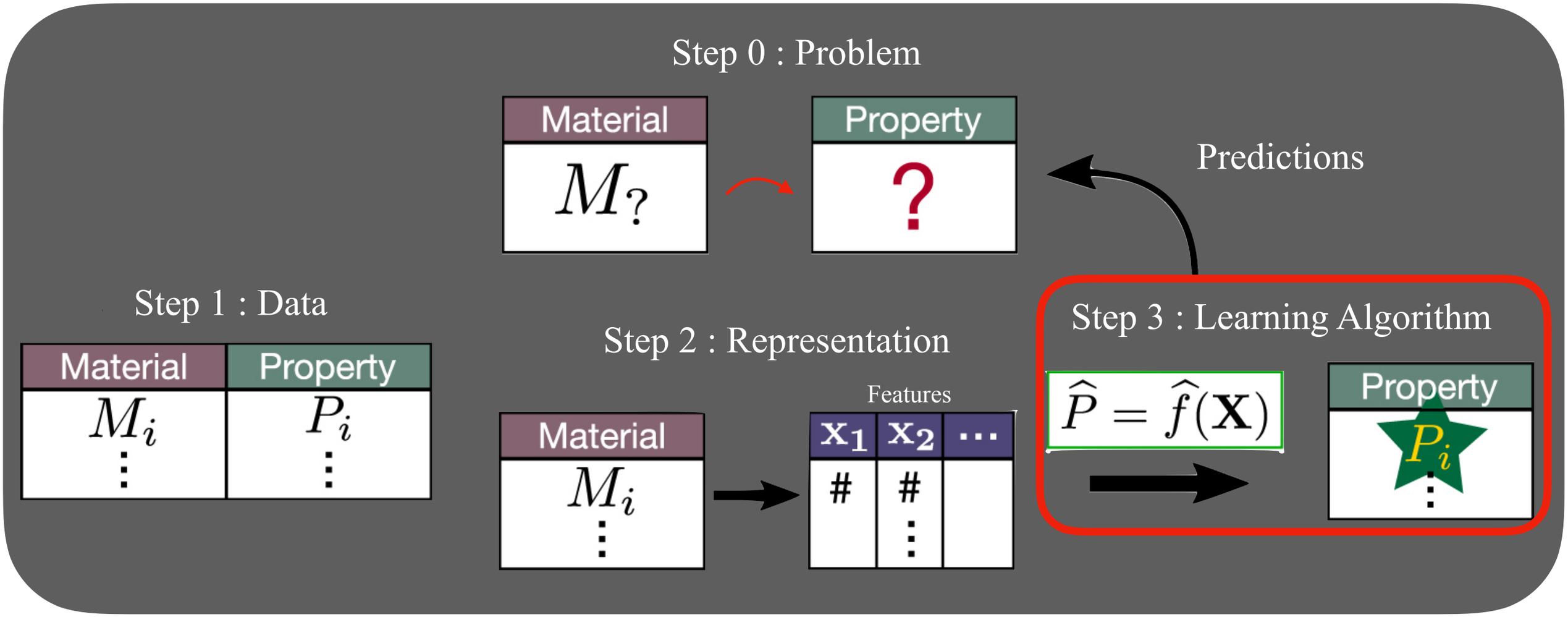
Z
EA
$r_p$
$r_s$
LUMO
HOMO
IP

## Operations

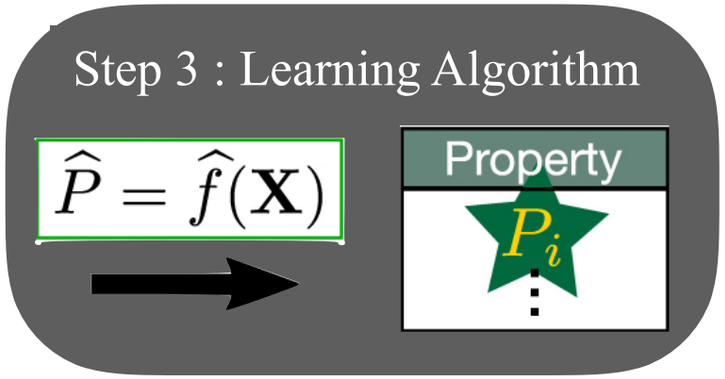
+
*
ln
-
/
$(\ )^2$
Exp.
$(\ )^3$

## Feature Space

$H_{ks}(A)+H_{ks}(B)+\ldots$
$L_{ks}(A)+L_{KS}(B)+\ldots$
$r_s(A)+r_s(B)+..$
$(r_s(A))^2,(L_{ks}(A))^2$
$(IP(A))^2/r_S(A) +r_s(B)$
……..


Step 0 : Problem
Material
$M_?$
Property
?
Predictions
Step 1 : Data
Material
Property
$M_i$
$P_i$
Step 2 : Representation
Material
$M_i$
Features
$x_1$
$x_2$
...
#
#
Step 3 : Learning Algorithm
$\widehat{P} = \widehat{f}(\mathbf{X})$
Property
$P_i$

# Step 3 : Learning Algorithms




- Unsupervised
  - Principal component analysis (PCA)
  - Clustering

- Supervised
  - Linear Regression
  - Logistic Regression
  - Naïve Bayes
  - K-NN
  - Decision Trees

# Step 3 : Learning Algorithms

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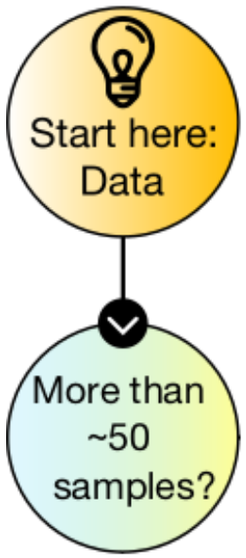

# Step 3 : Learning Algorithms

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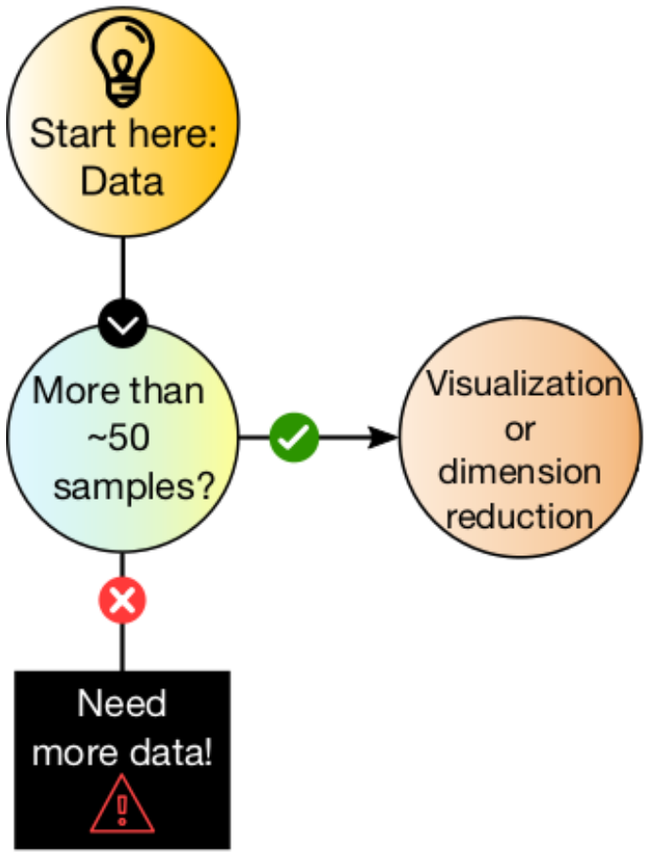

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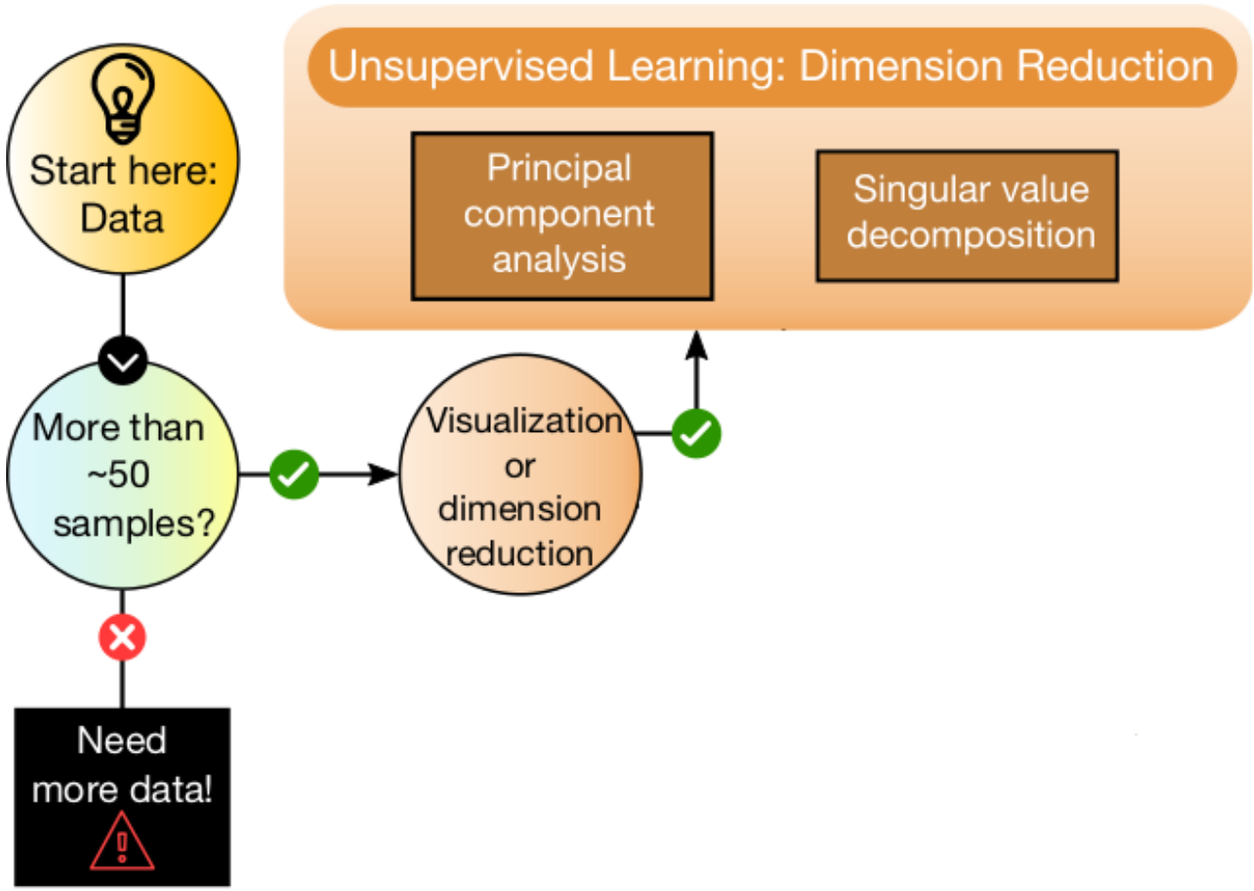

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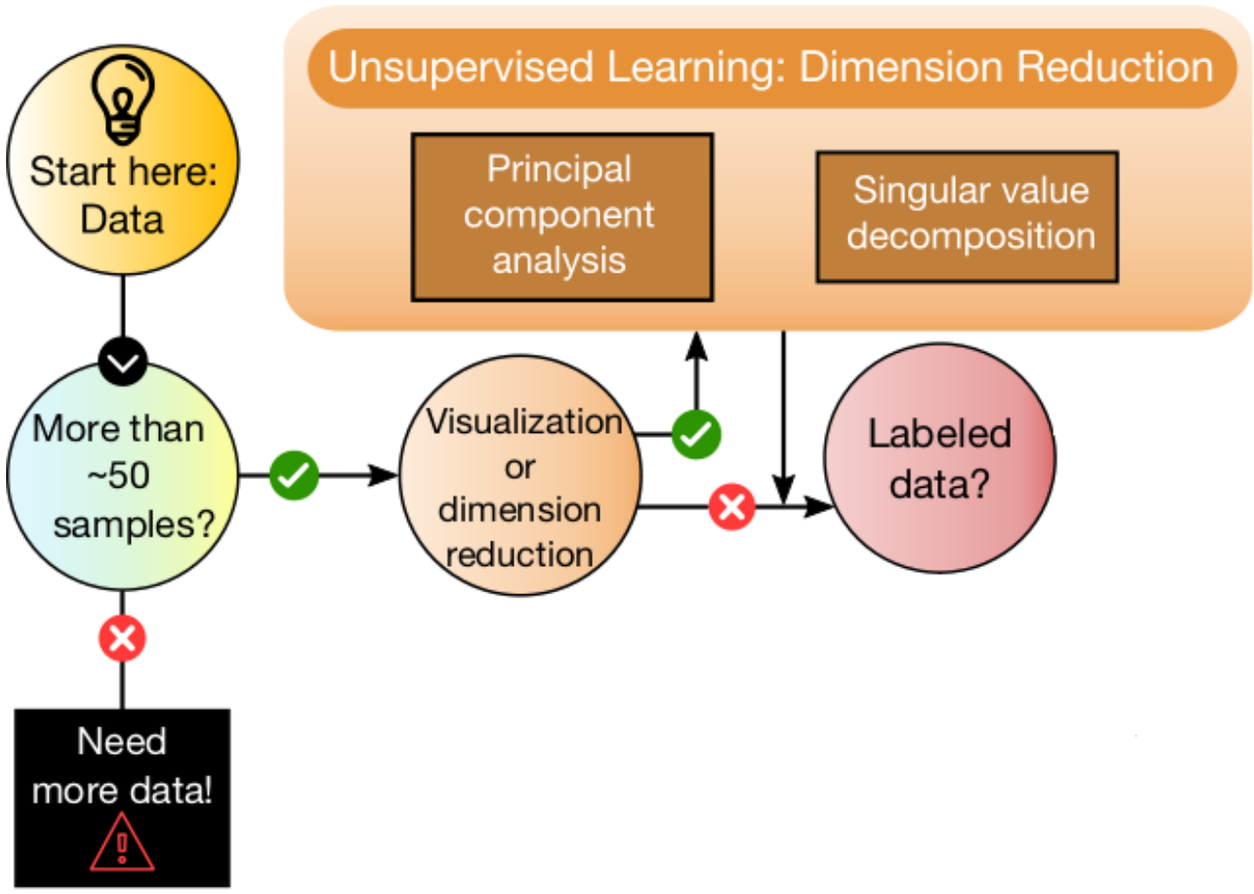

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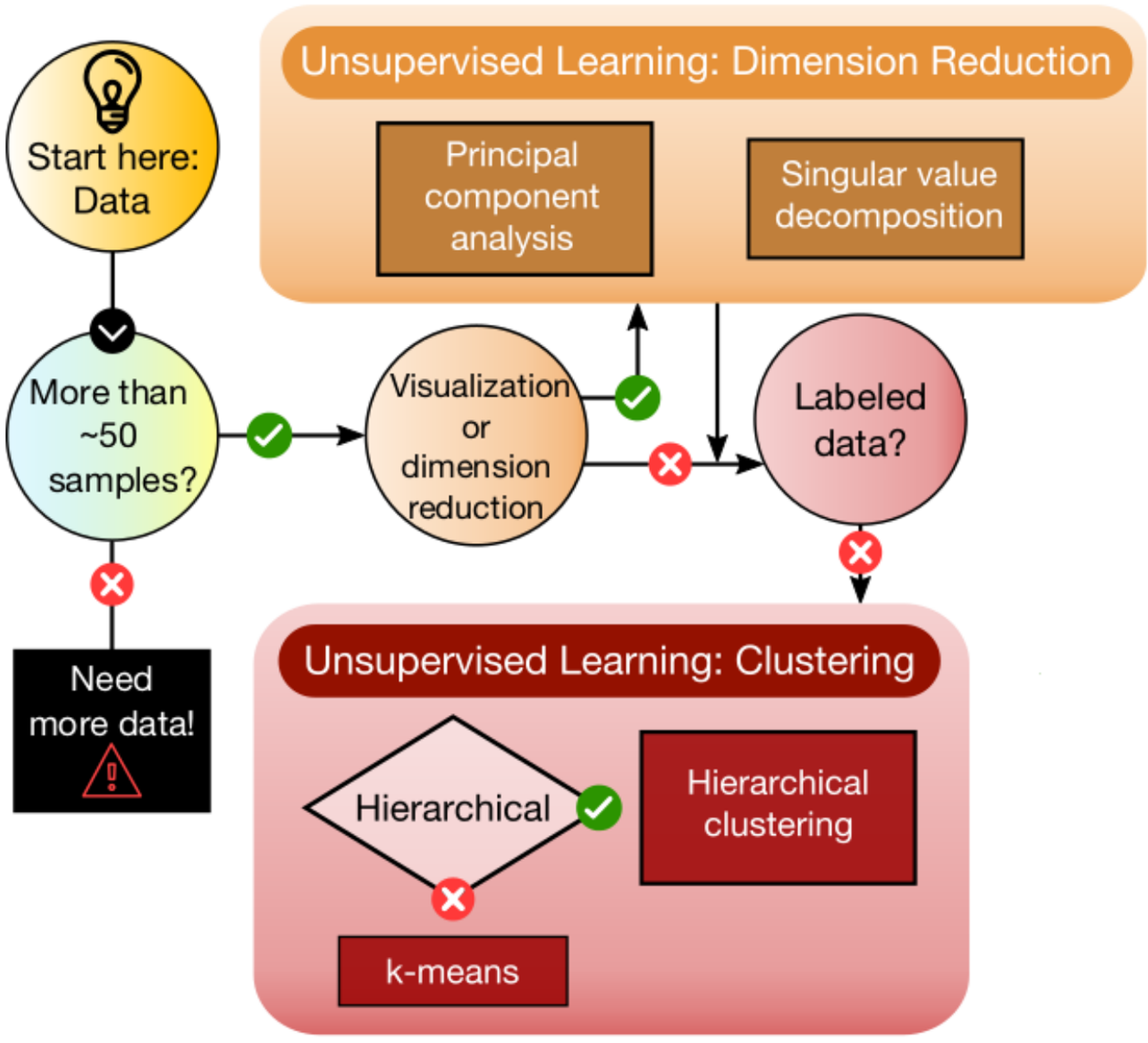

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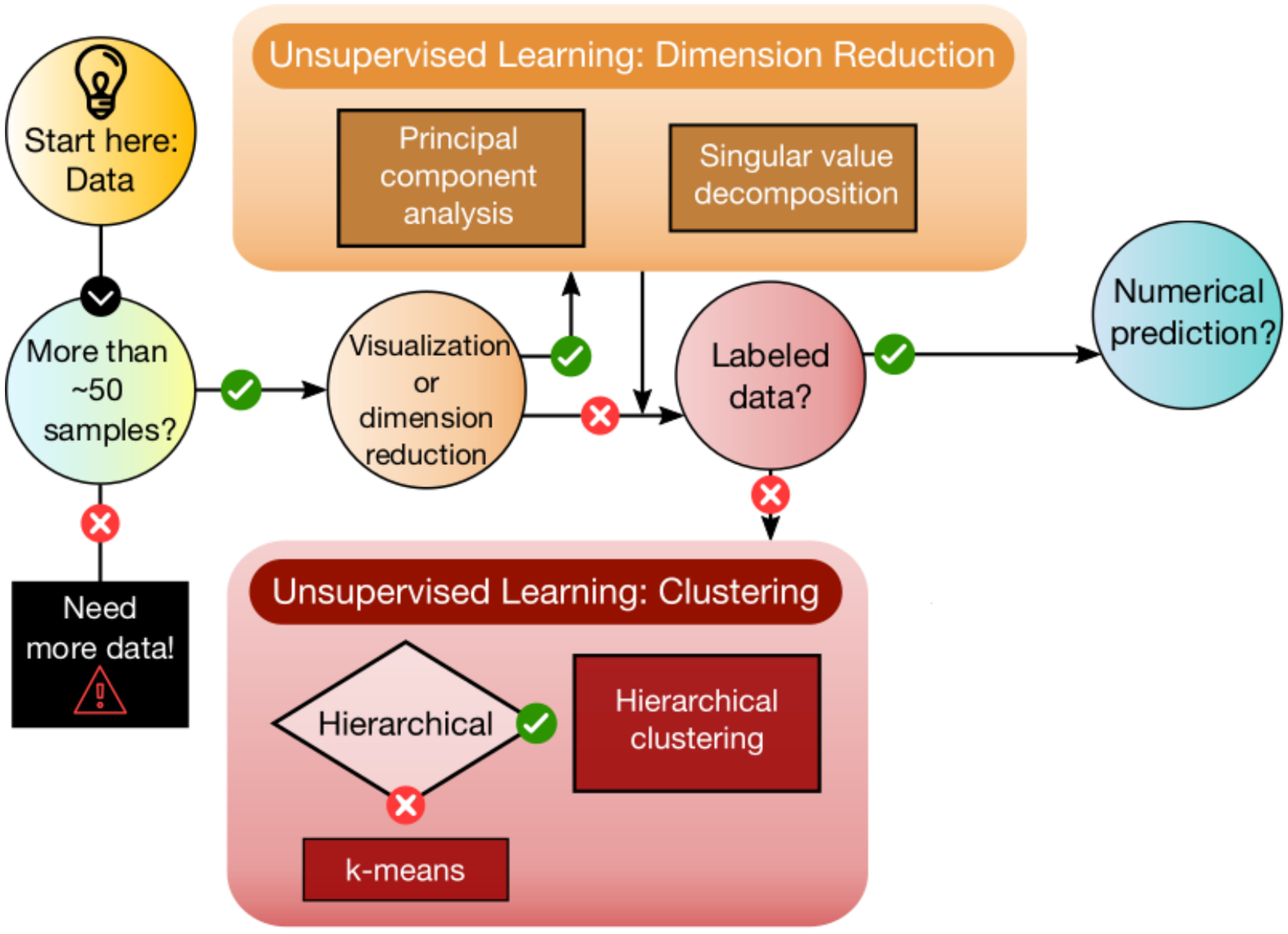
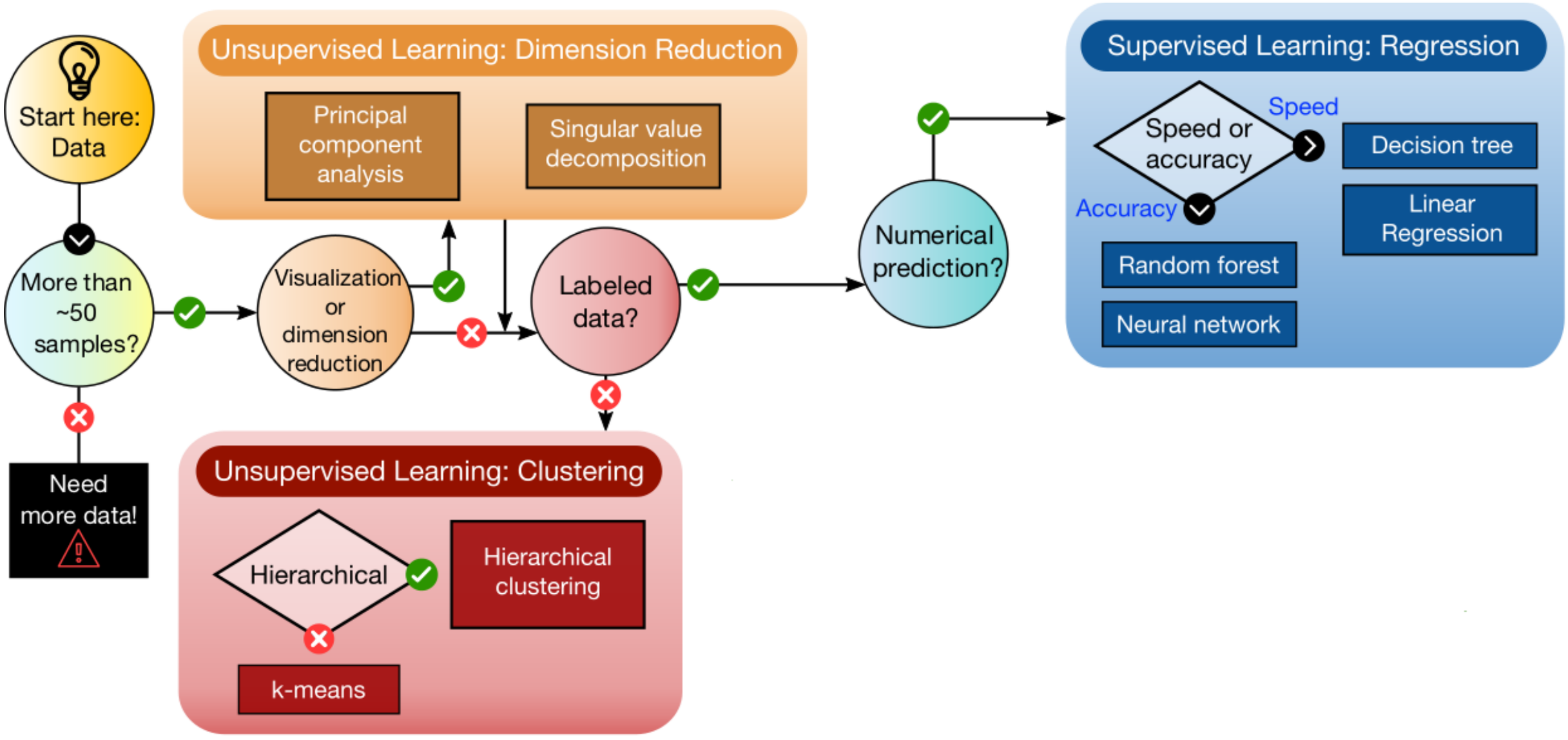
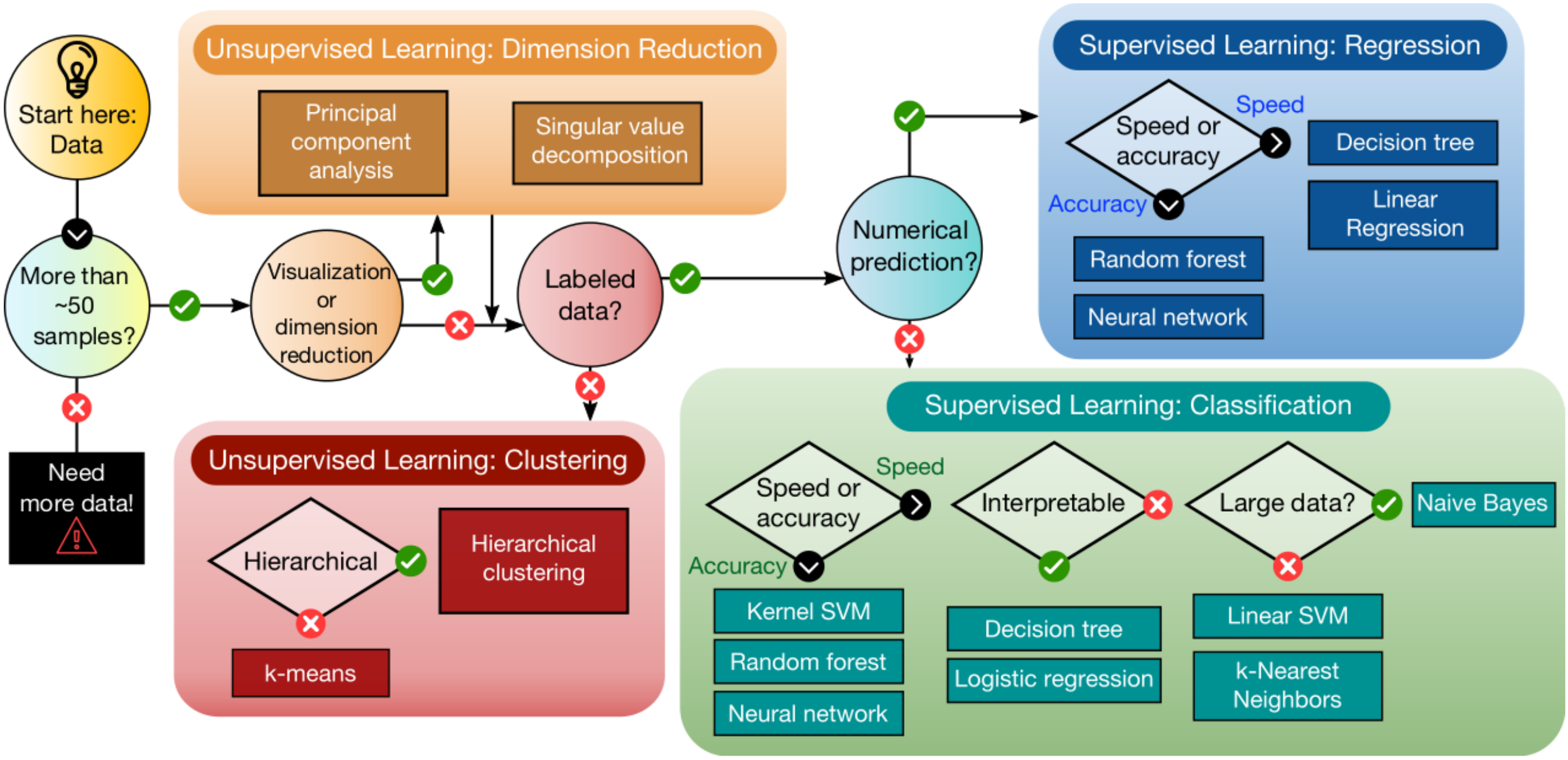


# Step 3 : Learning Algorithms



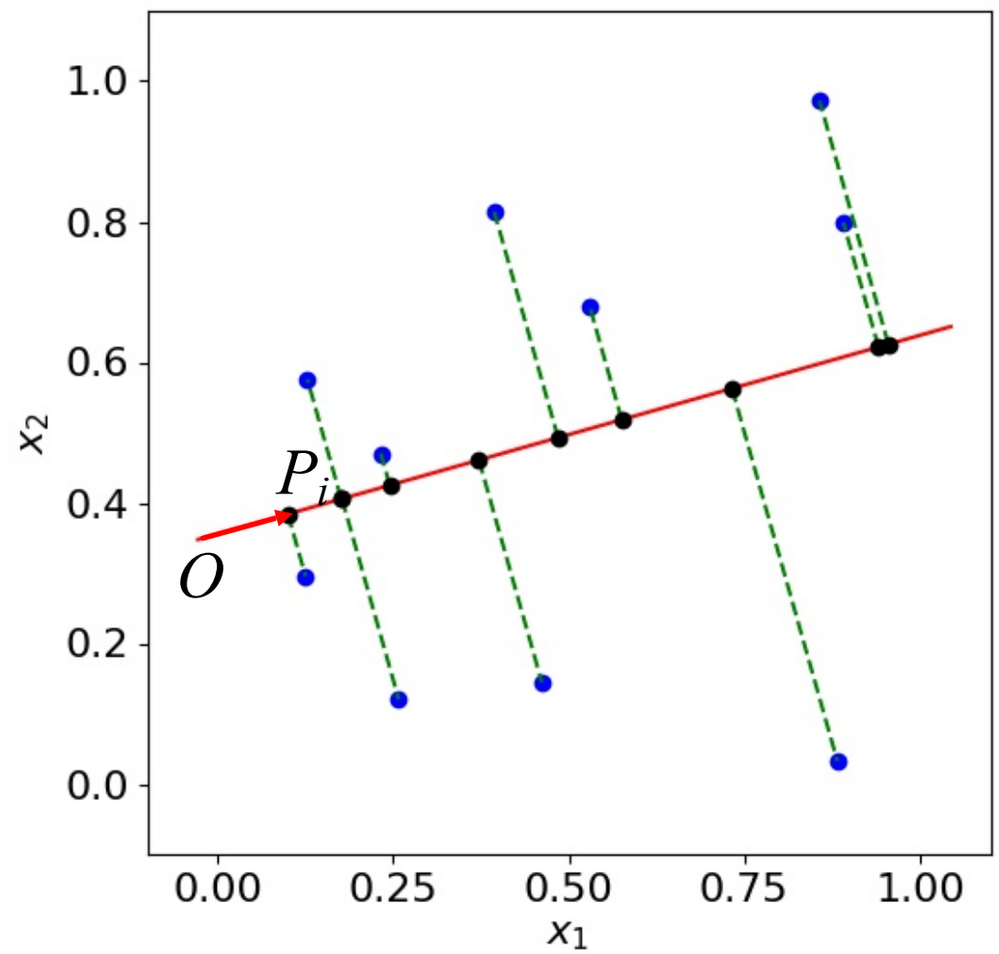
# Step 3 : Learning Algorithms



# Step 3 : Learning Algorithms (unsupervised)



## Principal component Analysis (PCA)

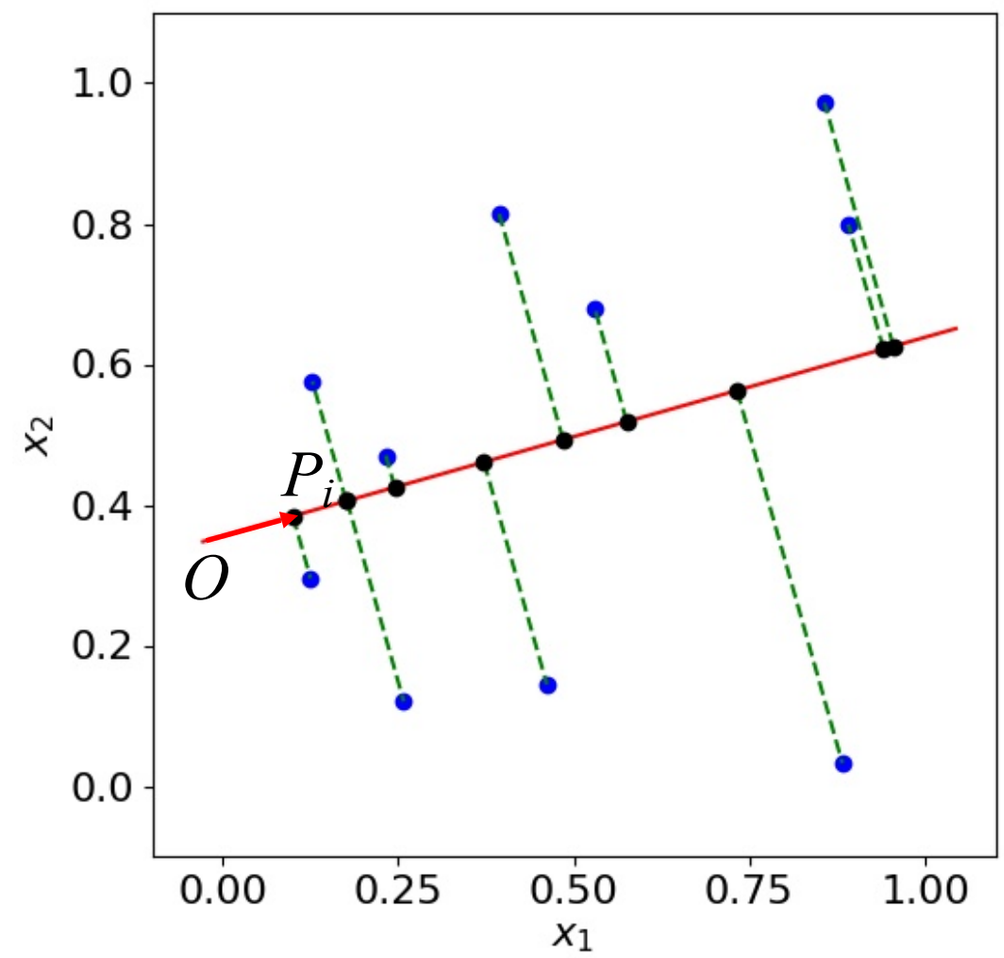


# Step 3 : Learning Algorithms (unsupervised)



## Principal component Analysis (PCA)

$$X = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & & \vdots \\ x_{p1} & x_{p2} & \dots & x_{pn} \end{pmatrix}$$



# Step 3 : Learning Algorithms (unsupervised)



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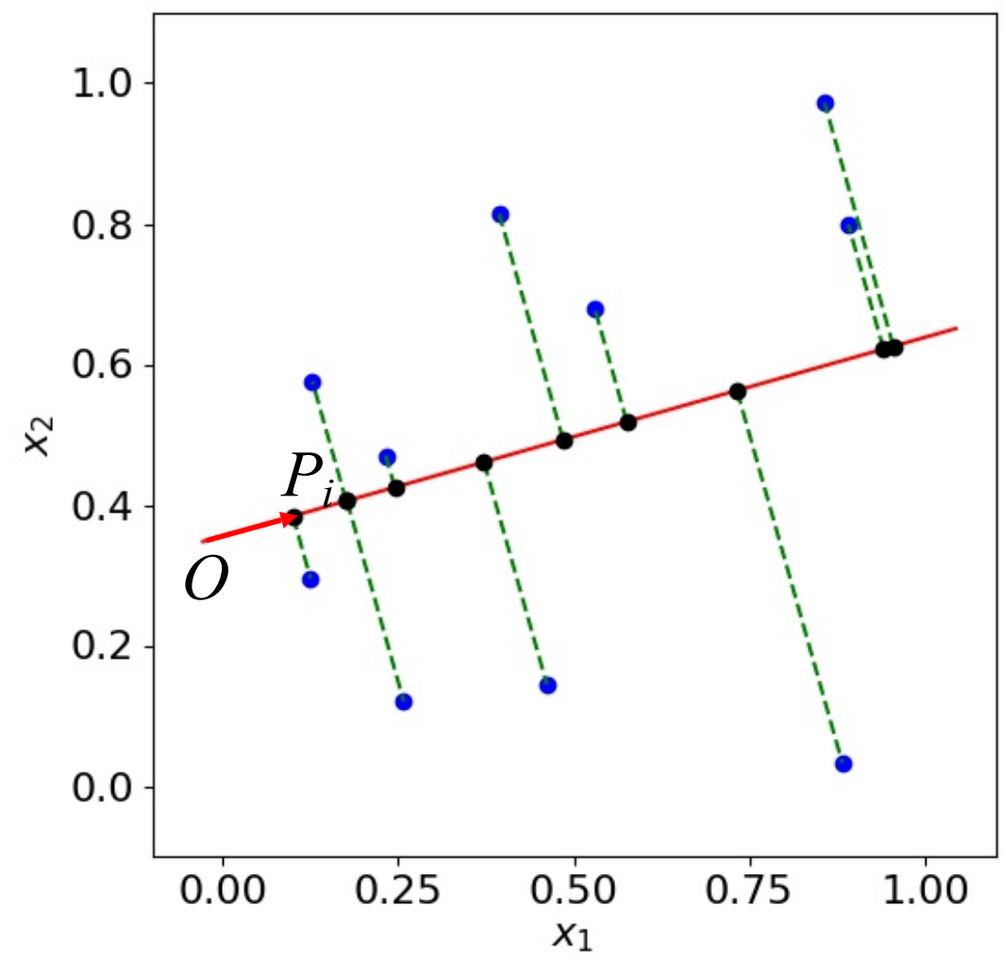

# Step 3 : Learning Algorithms (unsupervised)



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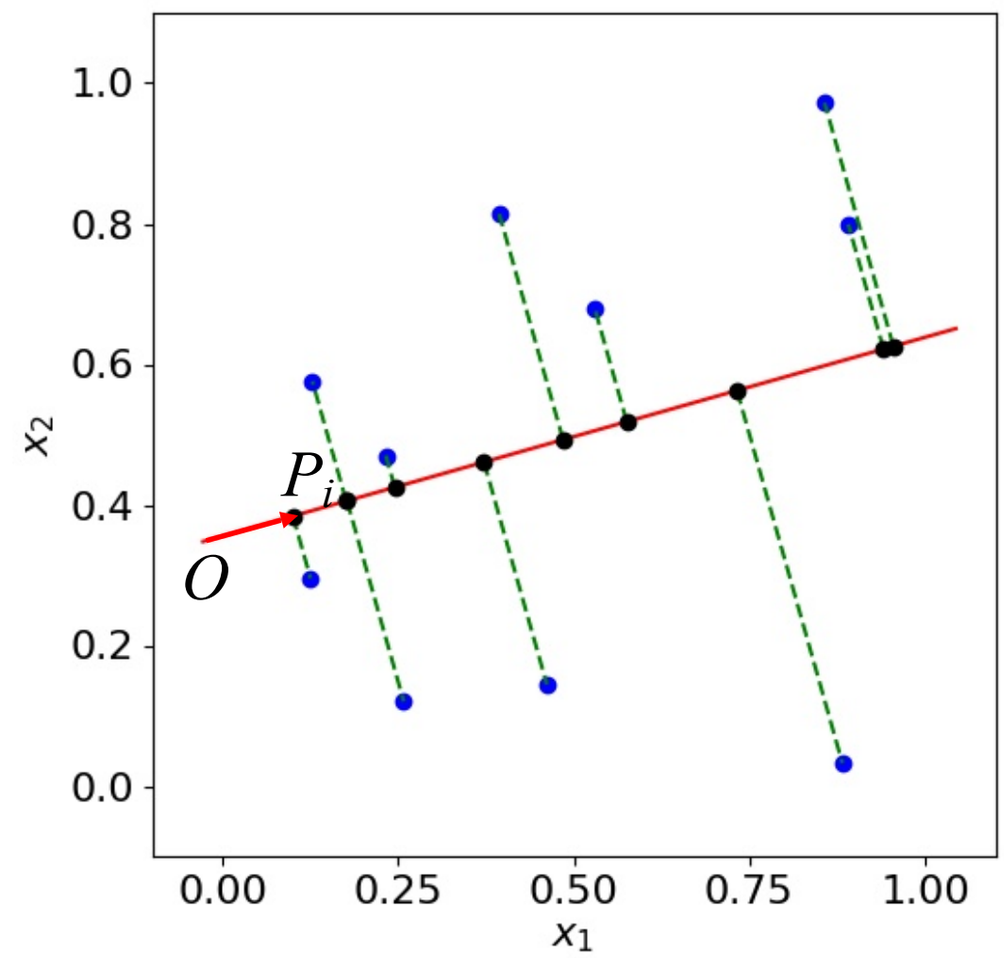
$$\sum_i \overline{OP_i}^2 = \sum_i c_i^T \cdot c_i = u^T X^T X u = u^T A u$$



# Step 3 : Learning Algorithms (unsupervised)



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maximze it!

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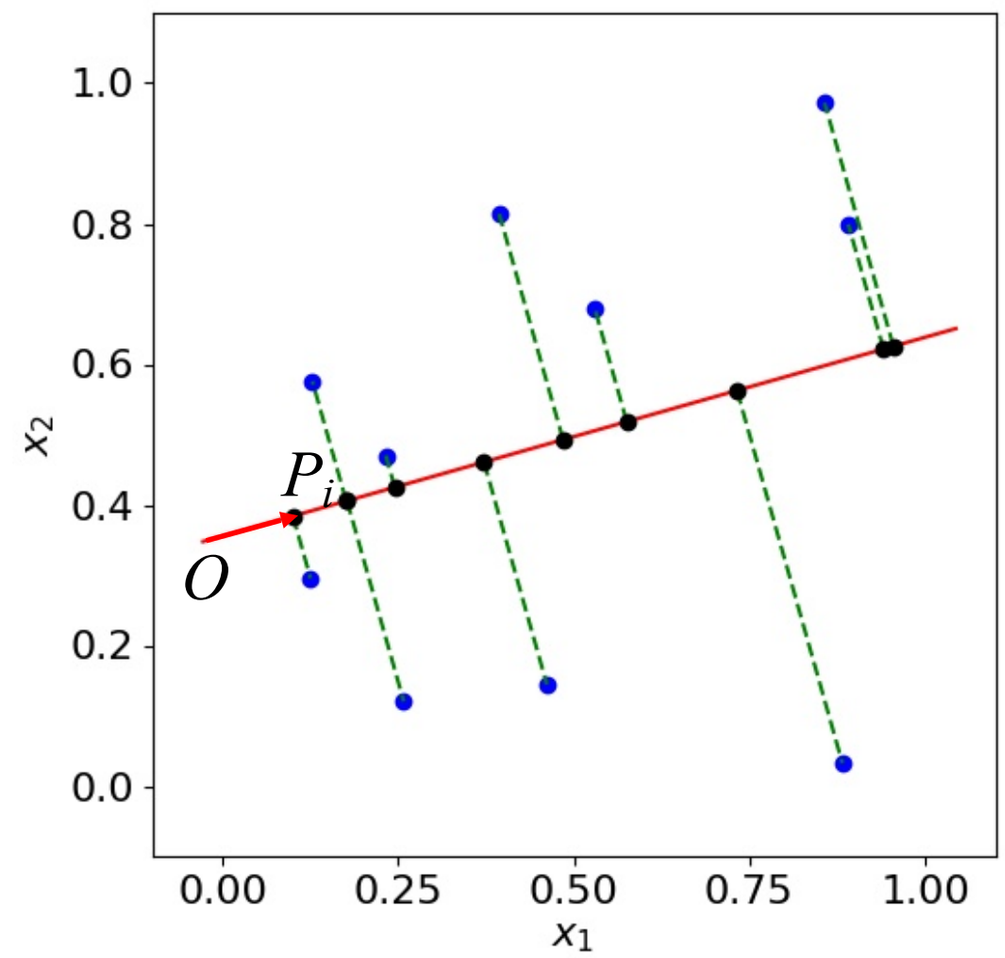

# Step 3 : Learning Algorithms (unsupervised)



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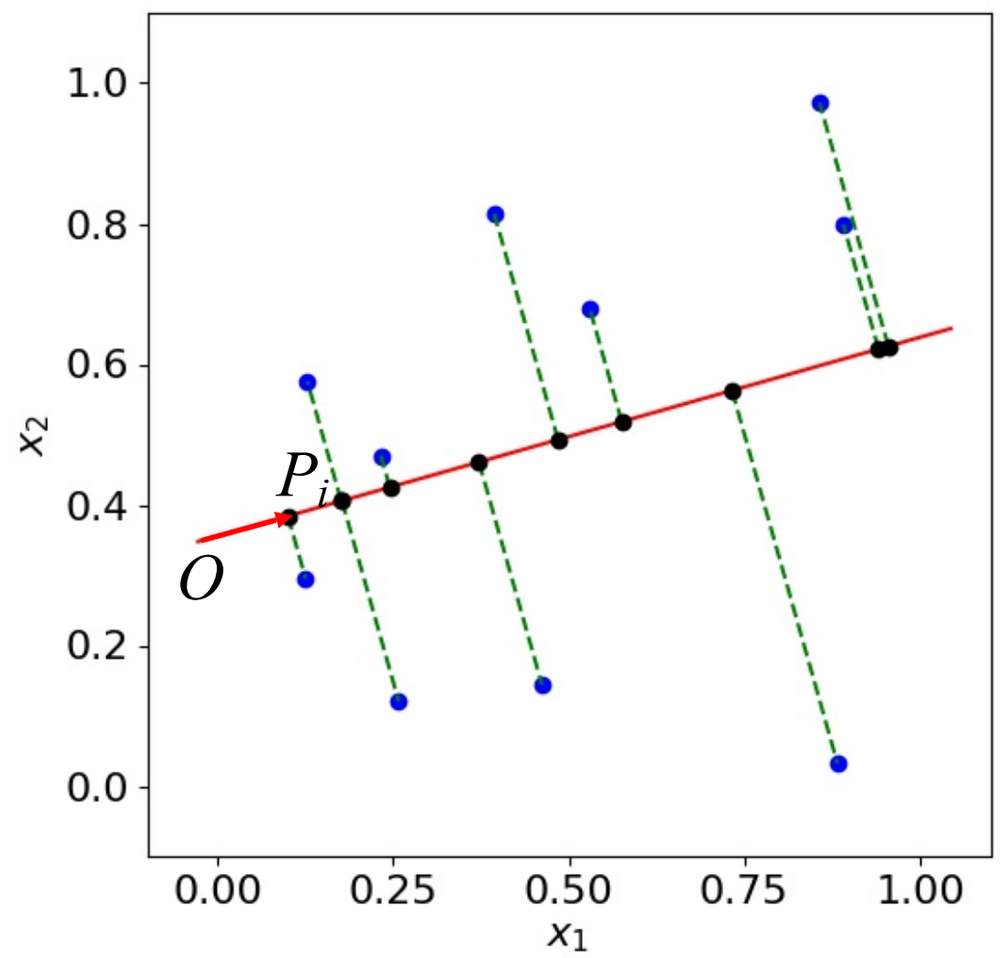

# Step 3 : Learning Algorithms (unsupervised)



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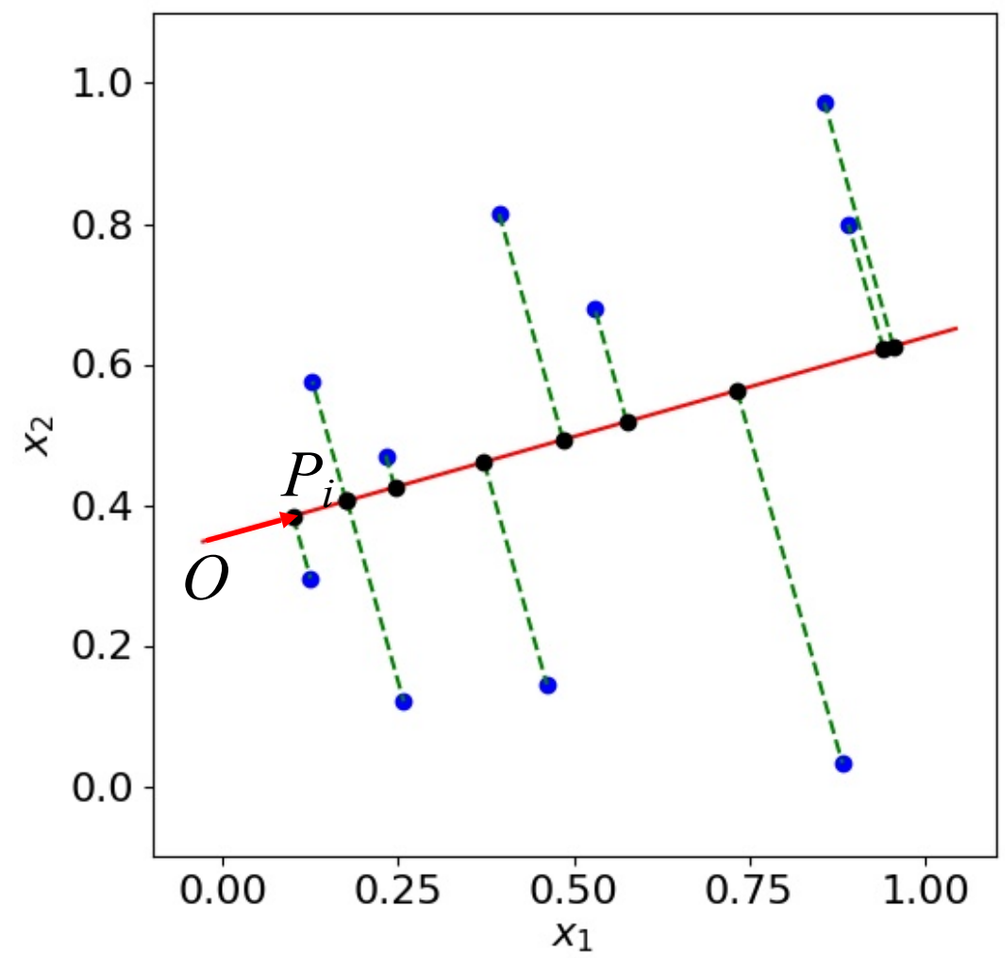
$$\sum_i \overline{OP_i}^2 = \sum_i c_i^T \cdot c_i = u^T X^T X u = u^T A u$$

$$A u_i = \lambda u_i \qquad\qquad U^T A U = \Lambda$$

Eigenvalues: variance
Eigenvectors: corresponding direction



# Step 3 : Learning Algorithms (unsupervised)



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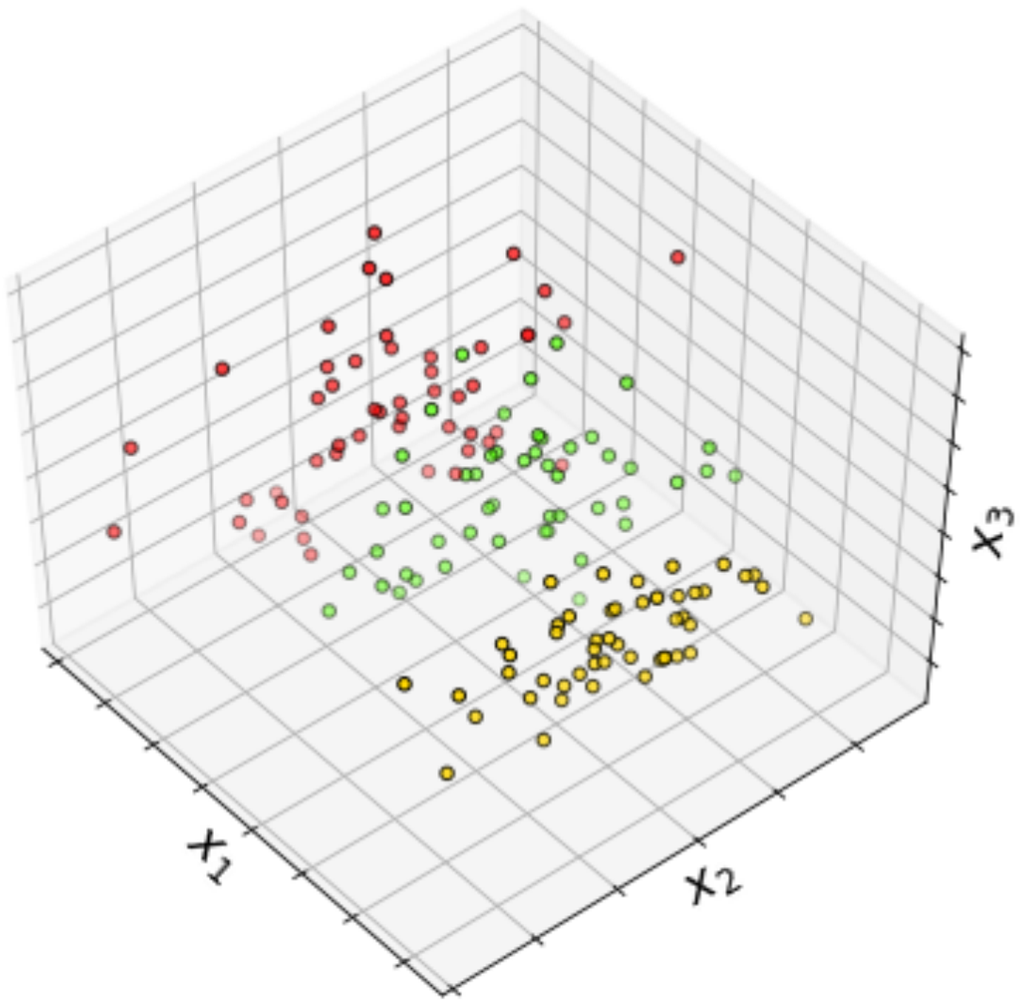
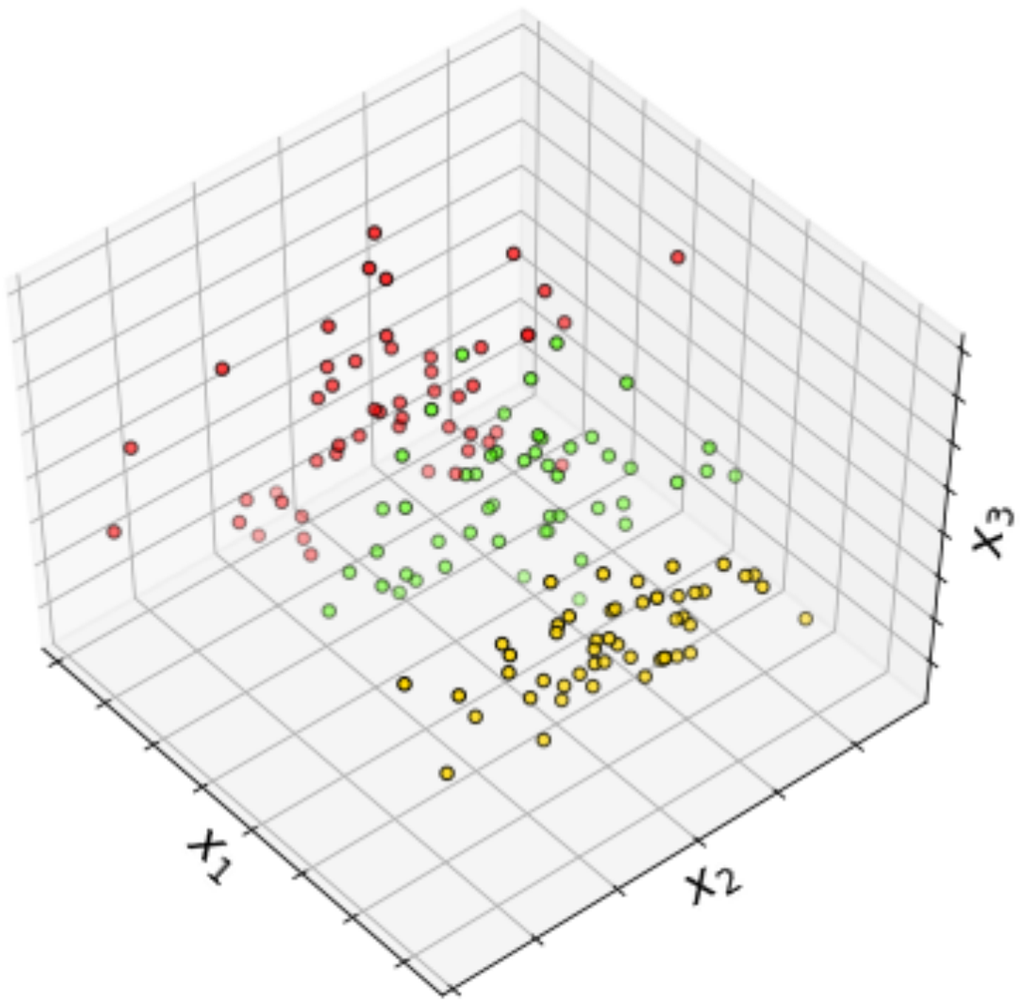
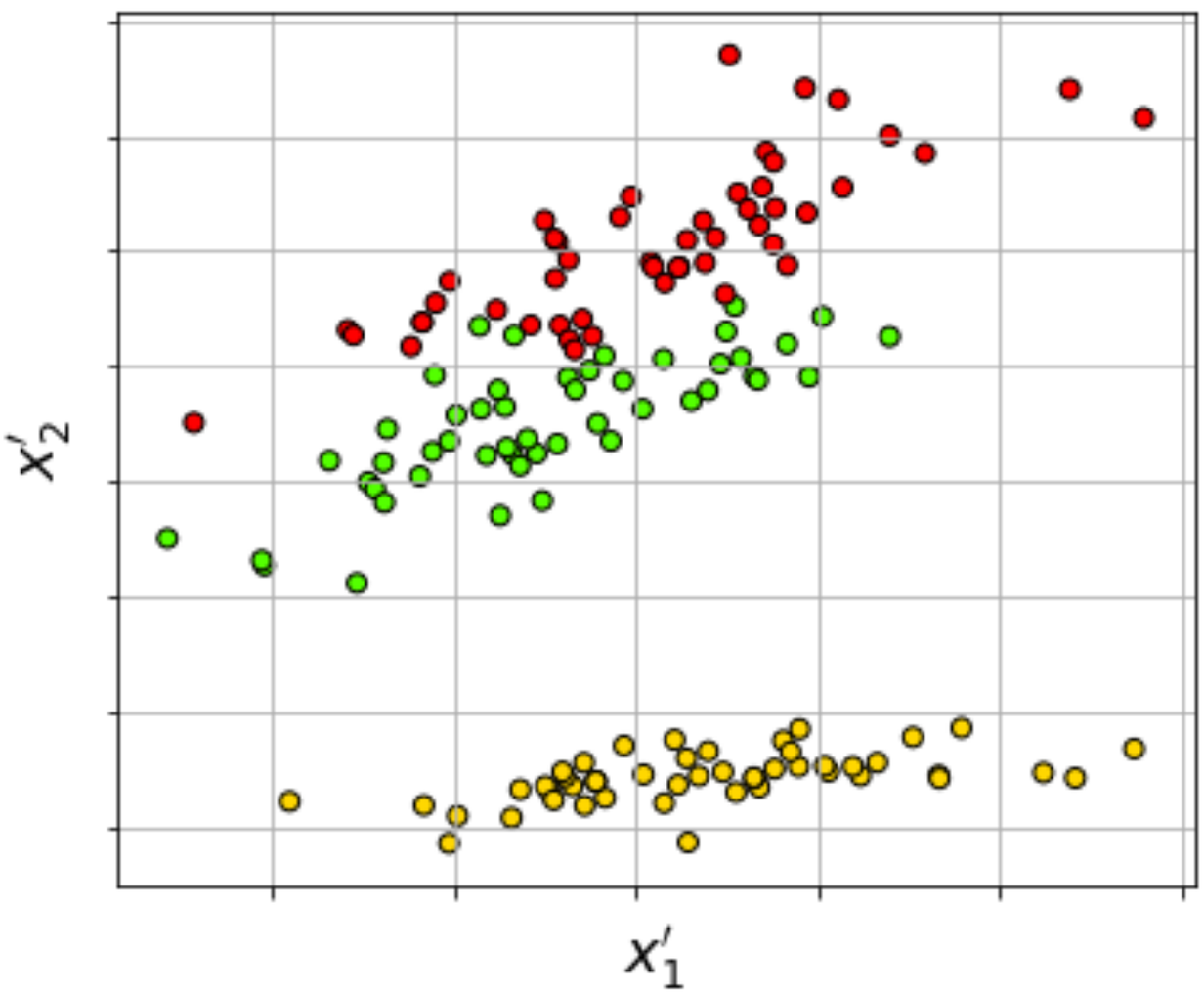


# Step 3 : Learning Algorithms (unsupervised)



## Principal component Analysis (PCA)



# Step 3 : Learning Algorithms (unsupervised)



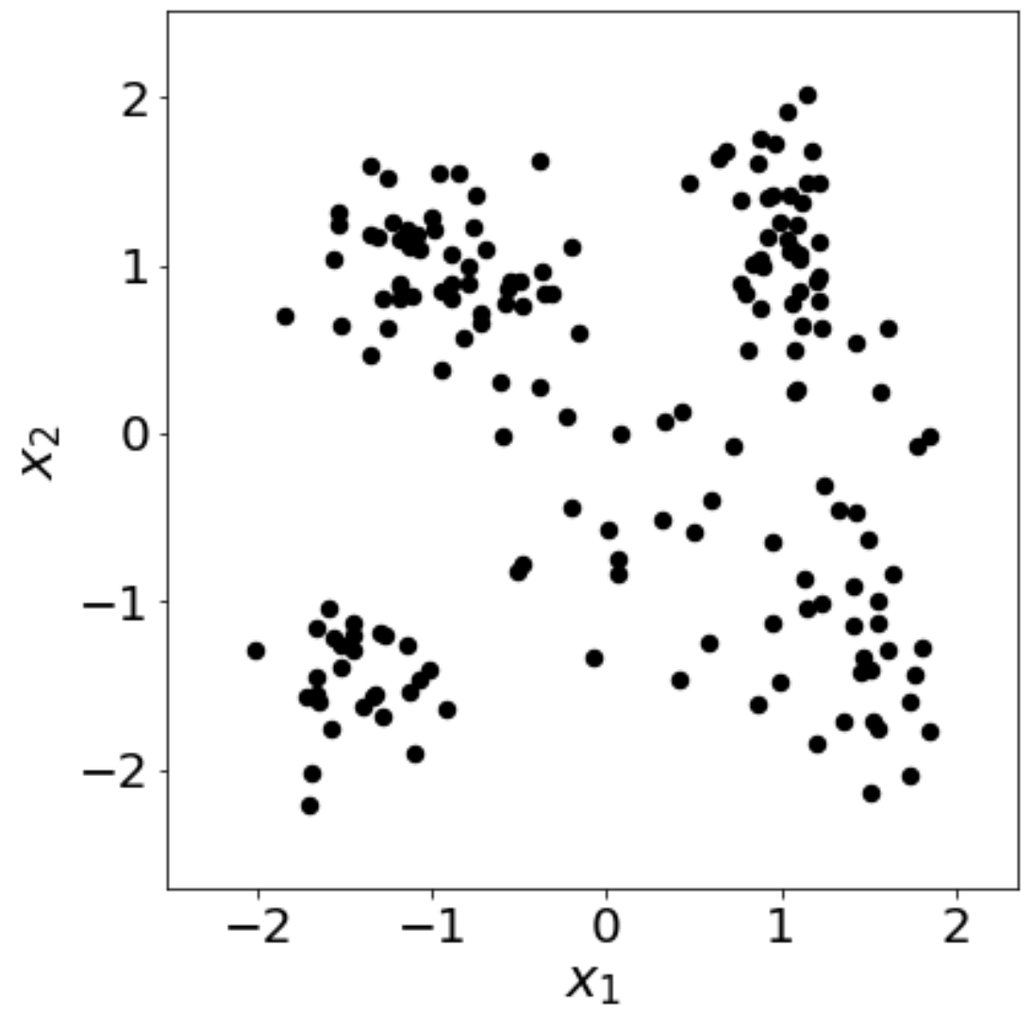
## Clustering

# Step 3 : Learning Algorithms (unsupervised)



## Clustering

- k-means



# Step 3 : Learning Algorithms (unsupervised)



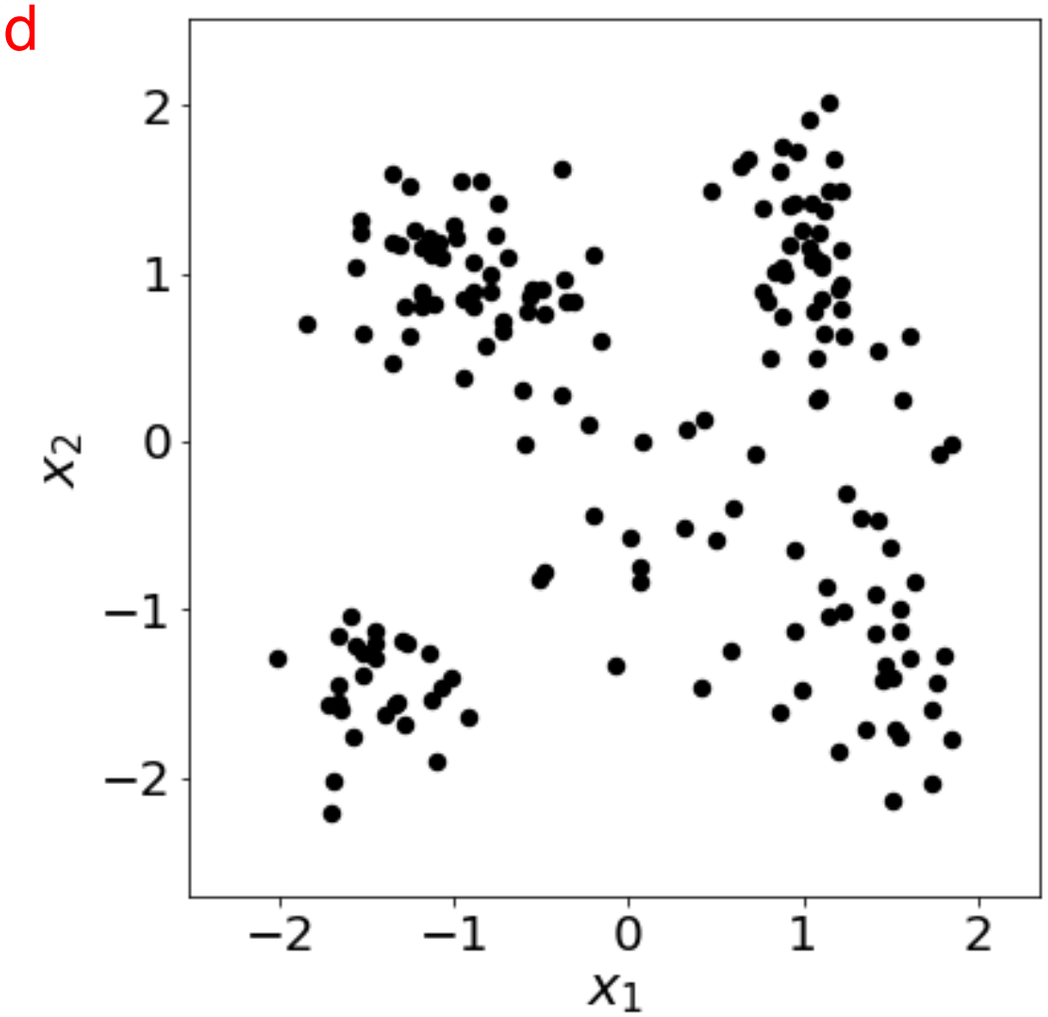
## Clustering

- k-means

i) Assign labels according to closest centroid

$$y_t^{(i)} = \text{argmin}_j \|\mathbf{x}^{(i)} - \boldsymbol{\mu}_t^{(j)}\|_p$$

$$\|\mathbf{x} - \boldsymbol{\mu}\|_p = \left[\sum_j (x_j - \mu_j)^p\right]^{\frac{1}{p}}$$



# Step 3 : Learning Algorithms (unsupervised)



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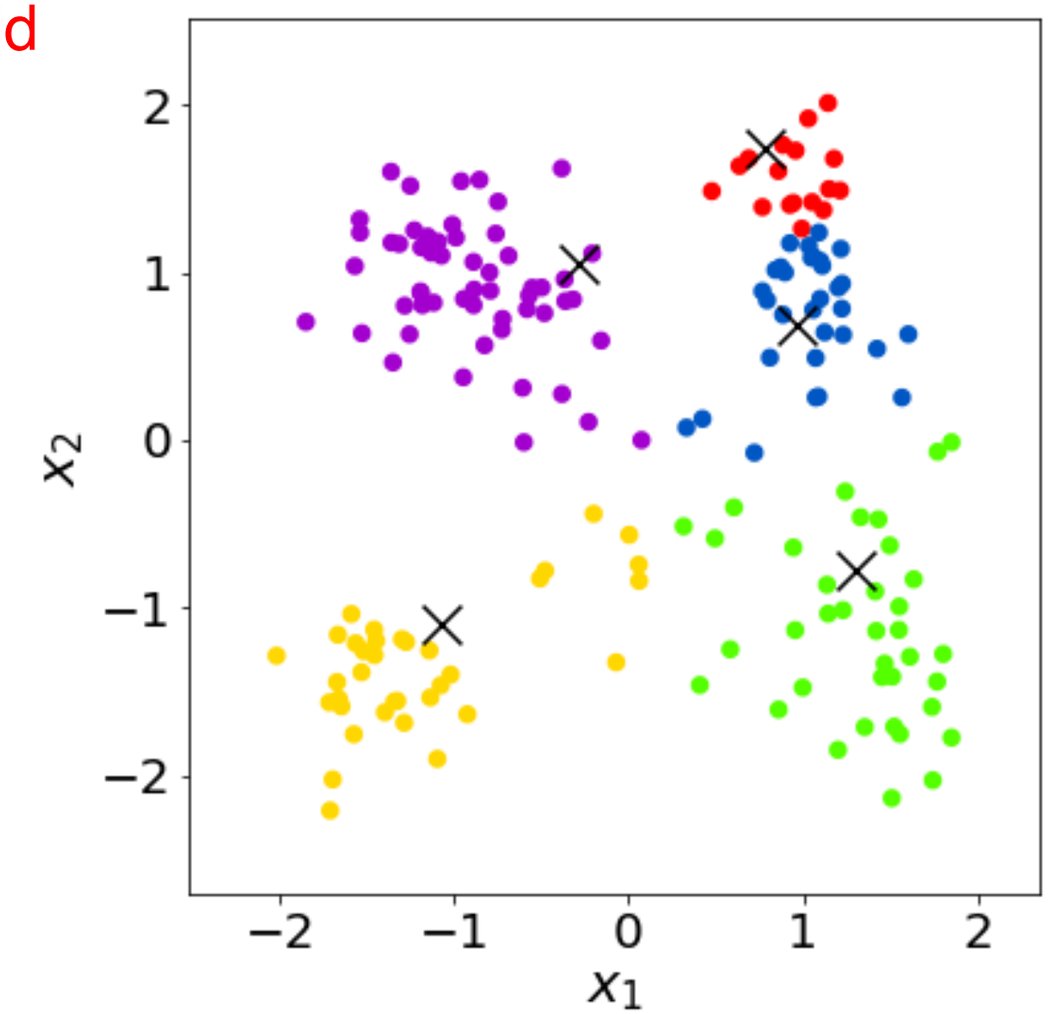

# Step 3 : Learning Algorithms (unsupervised)



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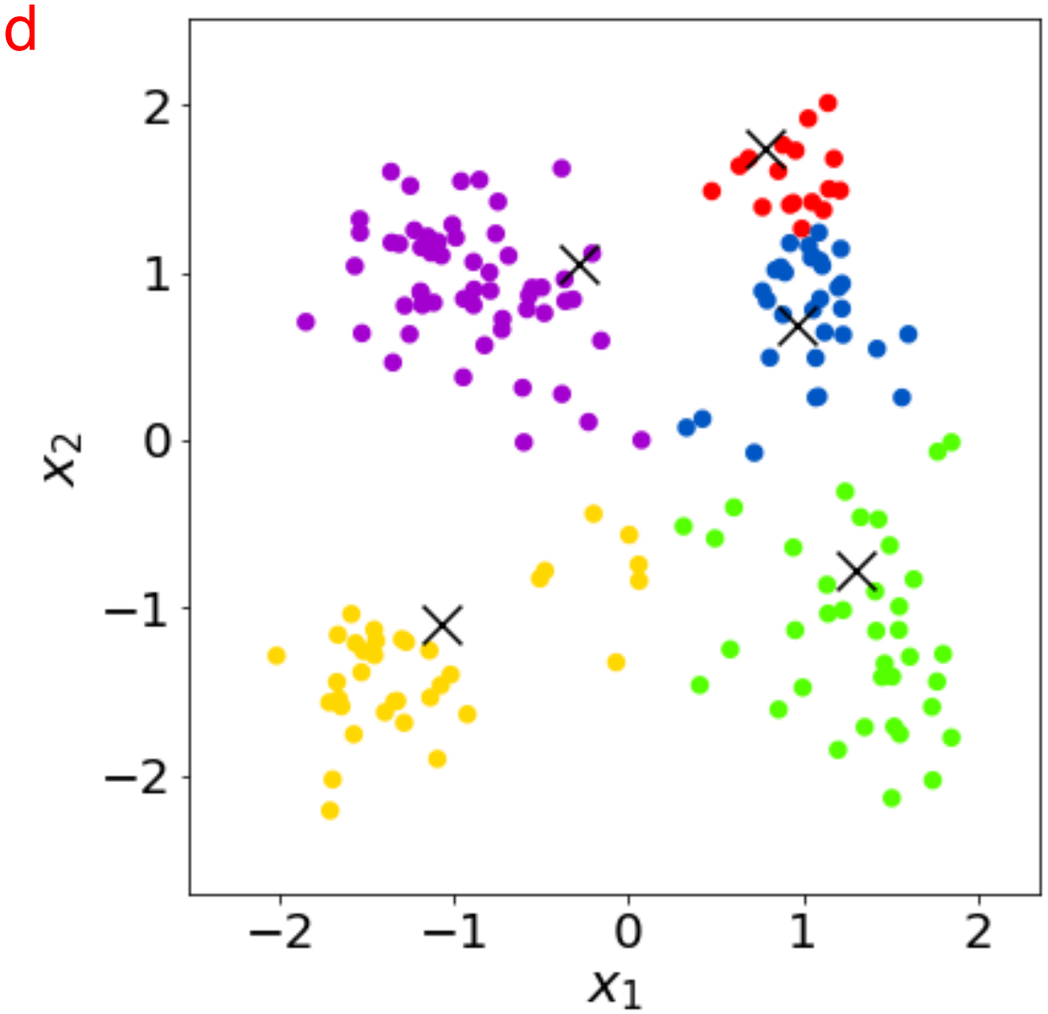


ii) Update centroid's coords

$$\boldsymbol{\mu}_{t+1}^{(j)} = \frac{1}{n_j} \sum_i \mathbf{x}^{(i)} \delta_{y_t^{(i)},j}$$

# Step 3 : Learning Algorithms (unsupervised)



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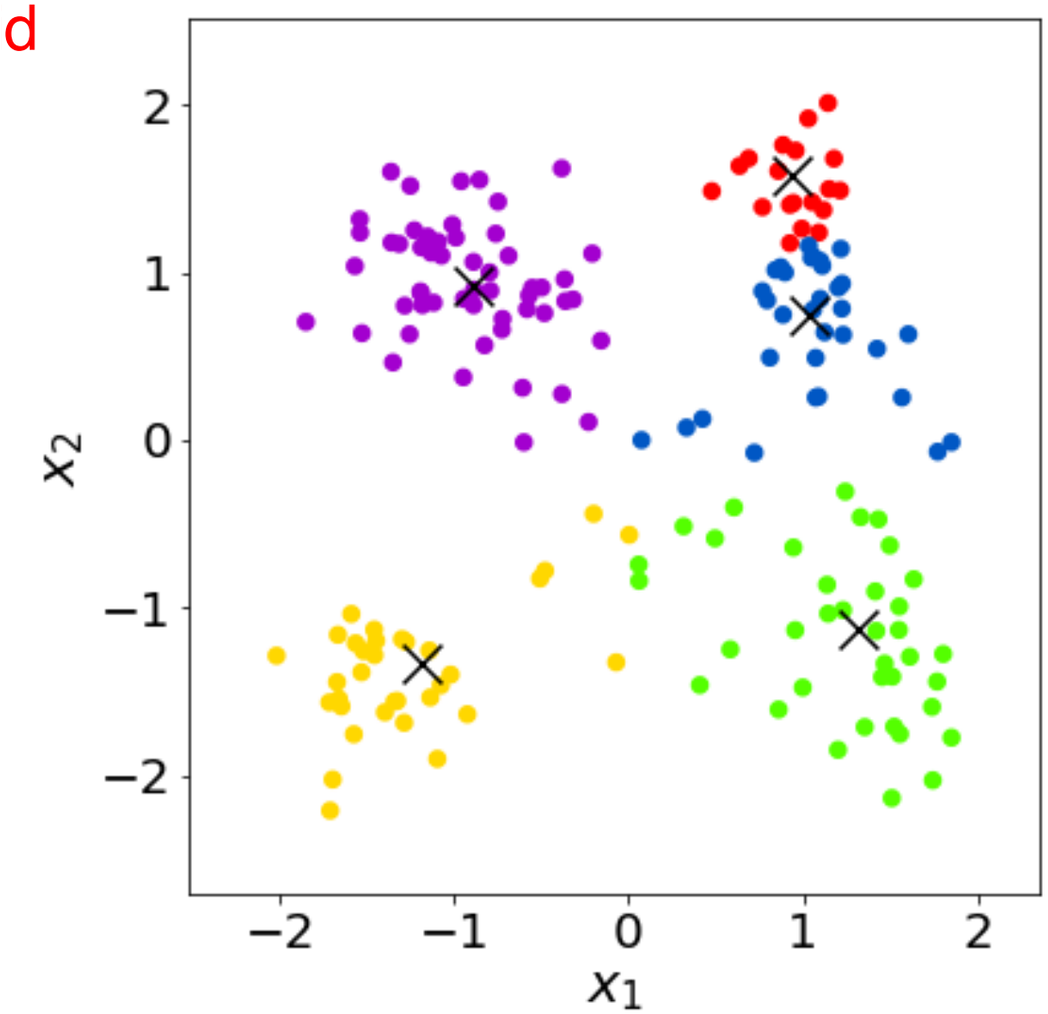


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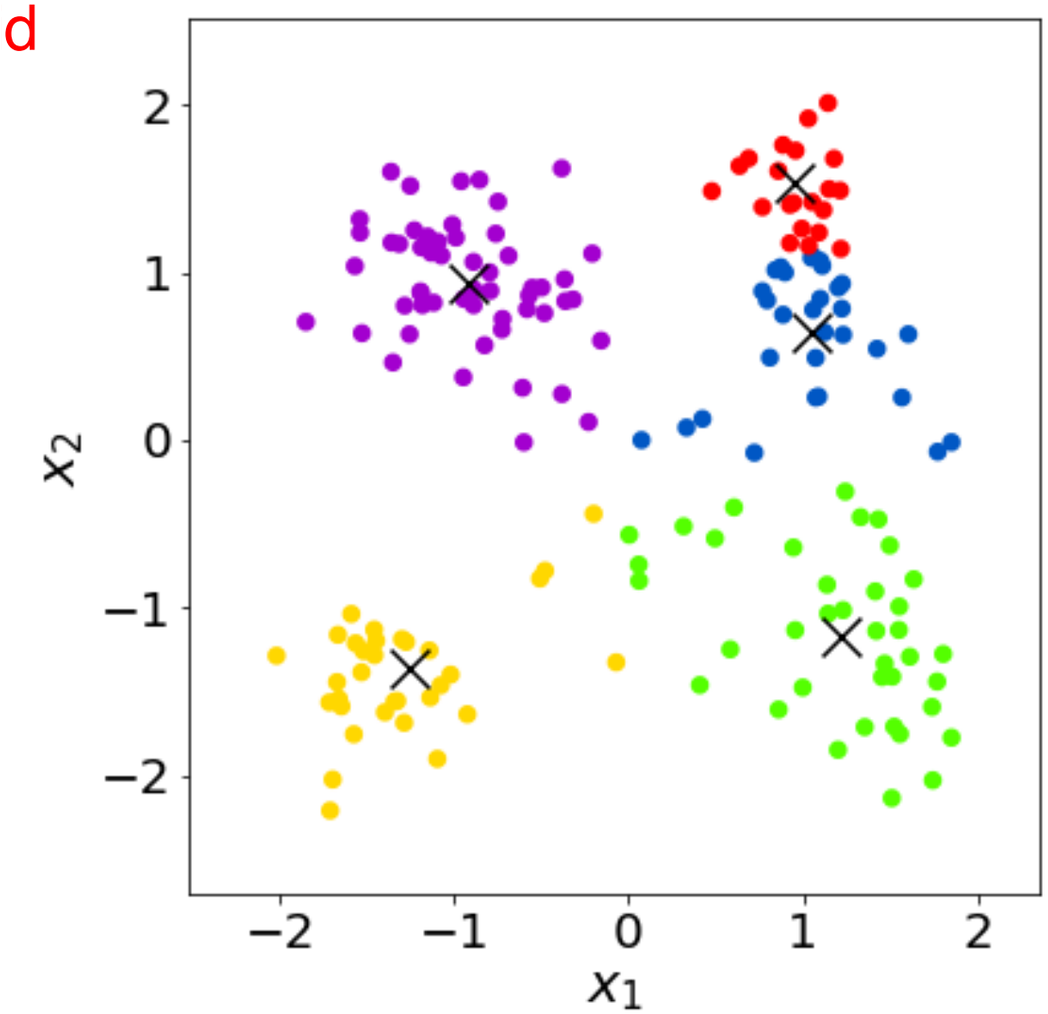


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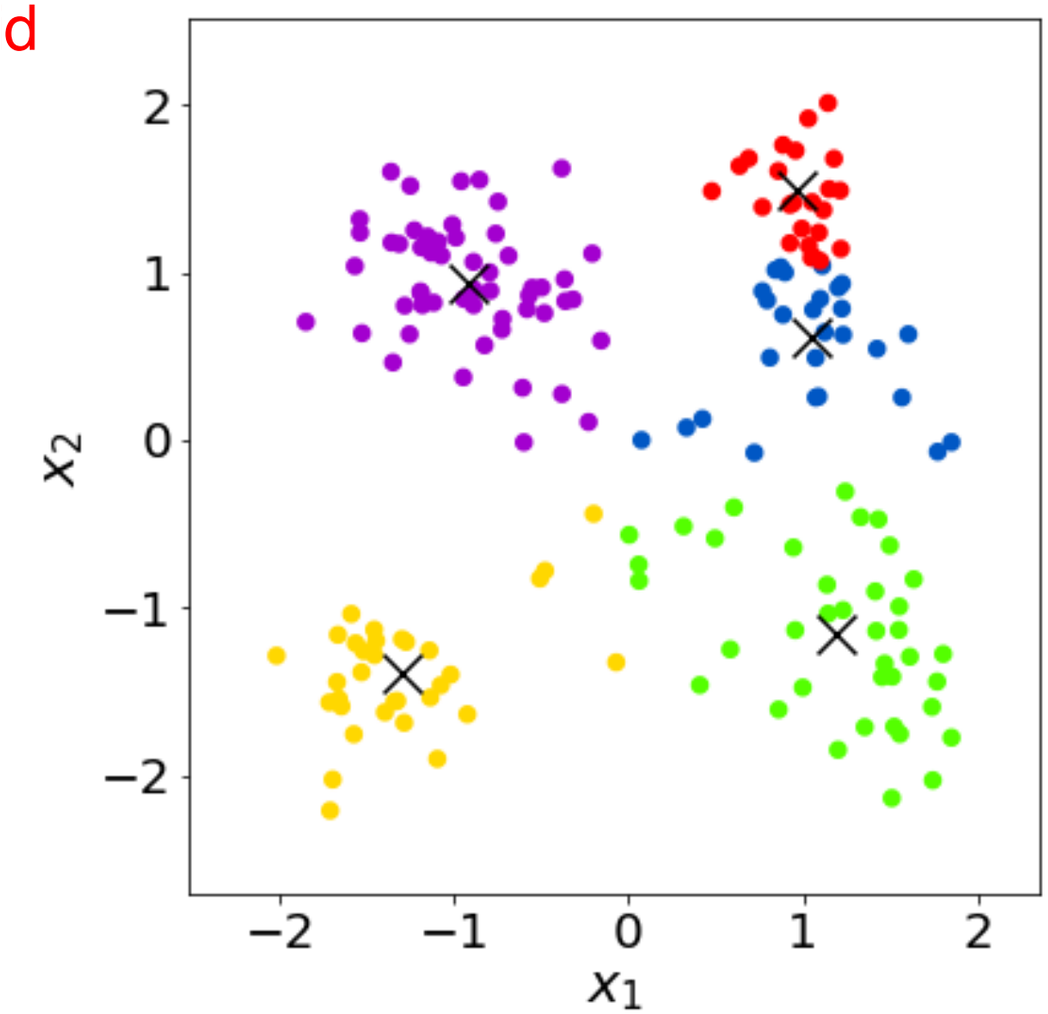


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# Step 3 : Learning Algorithms (unsupervised)



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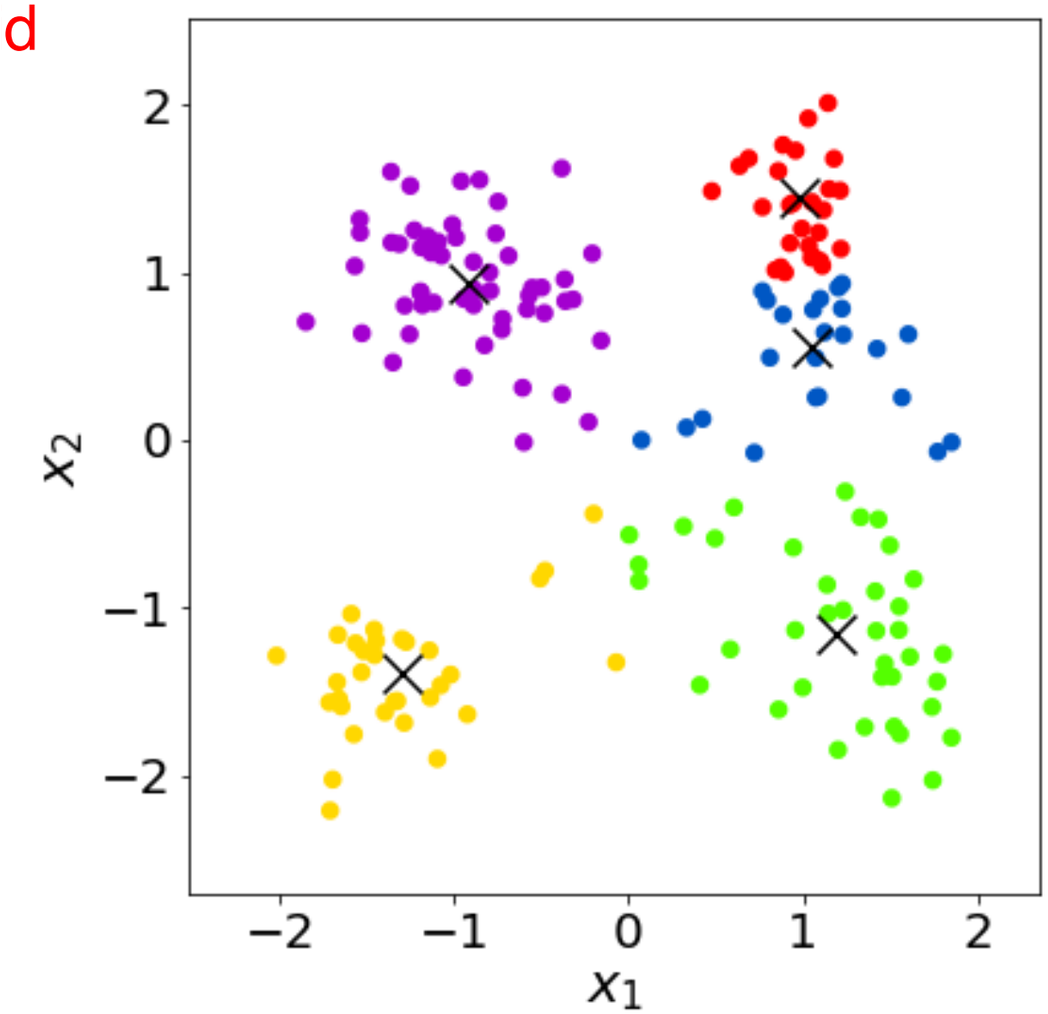


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# Step 3 : Learning Algorithms (unsupervised)



## Clustering

- hierarchical clustering

# Step 3 : Learning Algorithms (unsupervised)



## Clustering

- hierarchical clustering

  i) Start with one cluster for each data point

  ii) Merge clusters based on similarity

$$d(A, B) = \min_{\mathbf{x} \in A, \mathbf{y} \in B} \|\mathbf{x} - \mathbf{y}\|_p$$

# Step 3 : Learning Algorithms (unsupervised)



## Clustering

- hierarchical clustering

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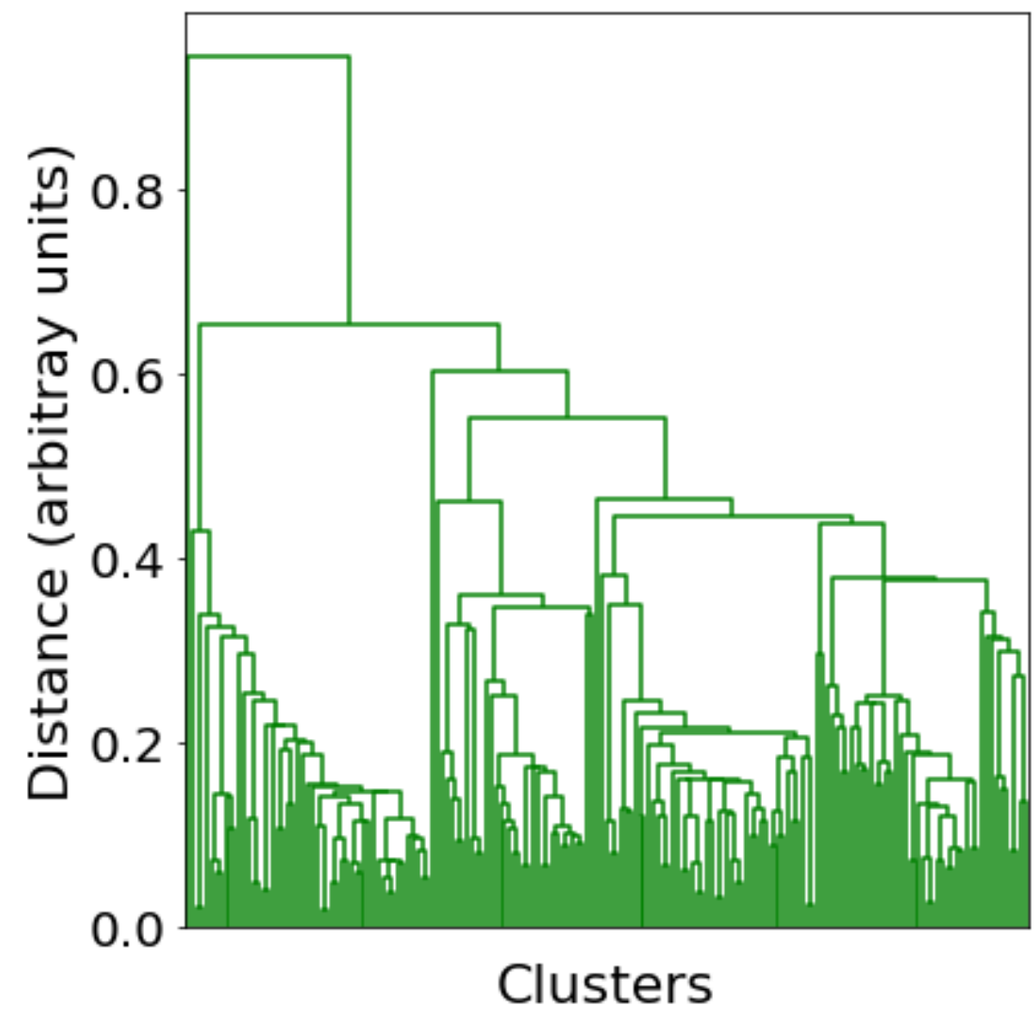
$$d(A, B) = \min_{\mathbf{x} \in A, \mathbf{y} \in B} \|\mathbf{x} - \mathbf{y}\|_p$$

iii) Stop when there's only one big cluster



# Step 3 : Learning Algorithms (unsupervised)



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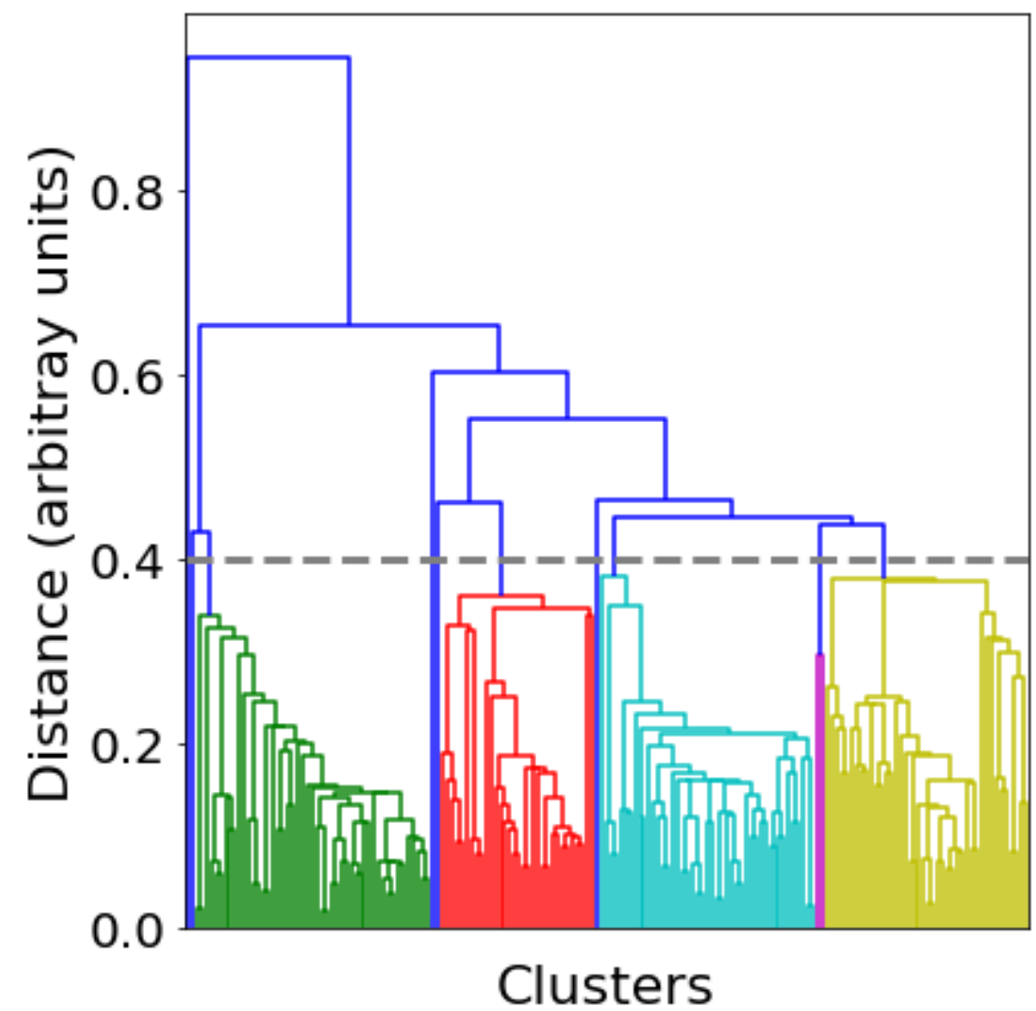
iii) Stop when there's only one big cluster

iv) Choose a cutting line (number of clusters)




**d = 0.4**
**N = 10**

# Step 3 : Learning Algorithms (unsupervised)



## Clustering

- hierarchical clustering

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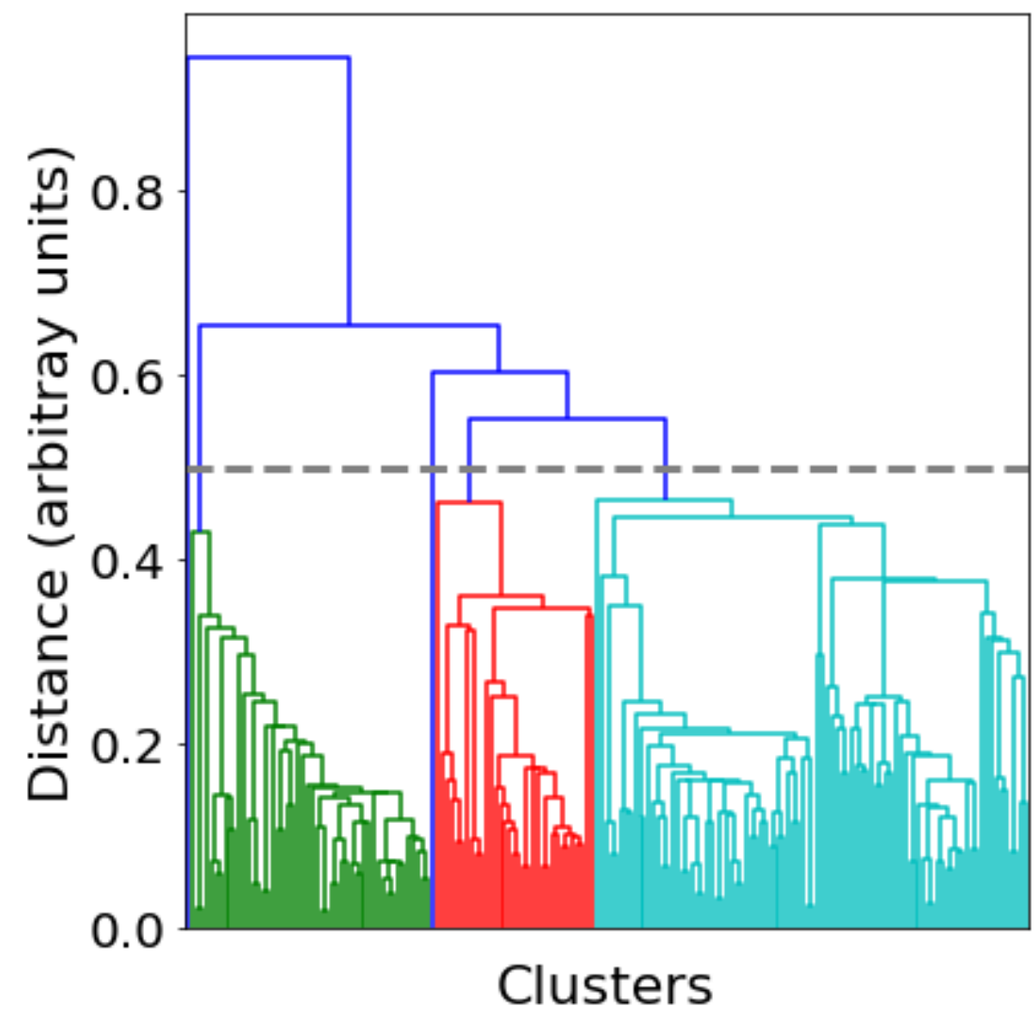


**d = 0.5**
**N = 5**

# Step 3 : Learning Algorithms (unsupervised)



## Clustering

- hierarchical clustering

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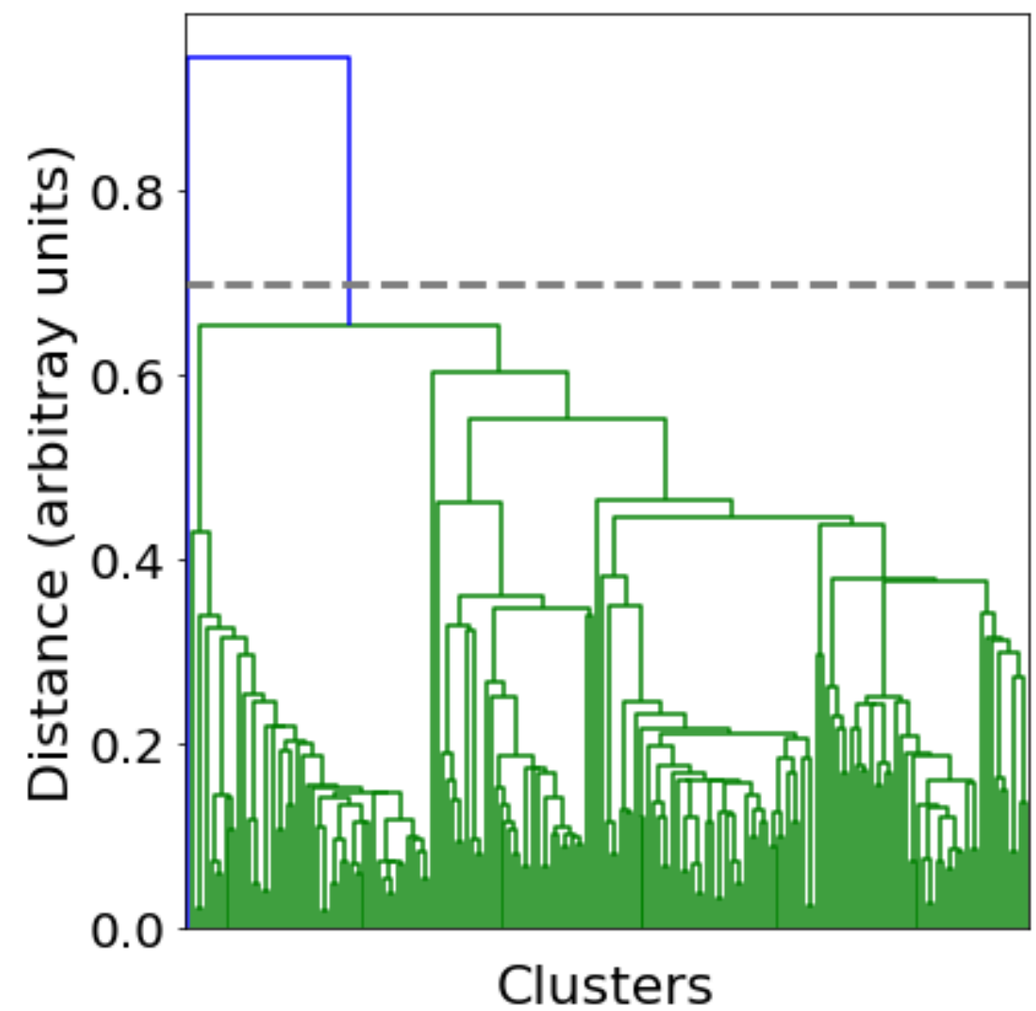


**d = 0.7**
**N = 2**

# Step 3 : Learning Algorithms (supervised)



## Linear Regression

# Step 3 : Learning Algorithms (supervised)



## Linear Regression

Function fitting: $\hat{y}^{(i)} = \boldsymbol{\theta}^T \mathbf{x}^{(i)} = x_0^{(i)}\theta_0 + x_1^{(i)}\theta_1 + \ldots$

# Step 3 : Learning Algorithms (supervised)



## Linear Regression

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# Step 3 : Learning Algorithms (supervised)



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Training = Minimize Cost function

$$J(\boldsymbol{\theta}) = \sum_{i=1}^{n} L[\hat{y}^{(i)}(\mathbf{x}^{(i)}, \boldsymbol{\theta}), y^{(i)}] = \frac{1}{2}\sum_{i=1}^{n}(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2$$

# Step 3 : Learning Algorithms (supervised)

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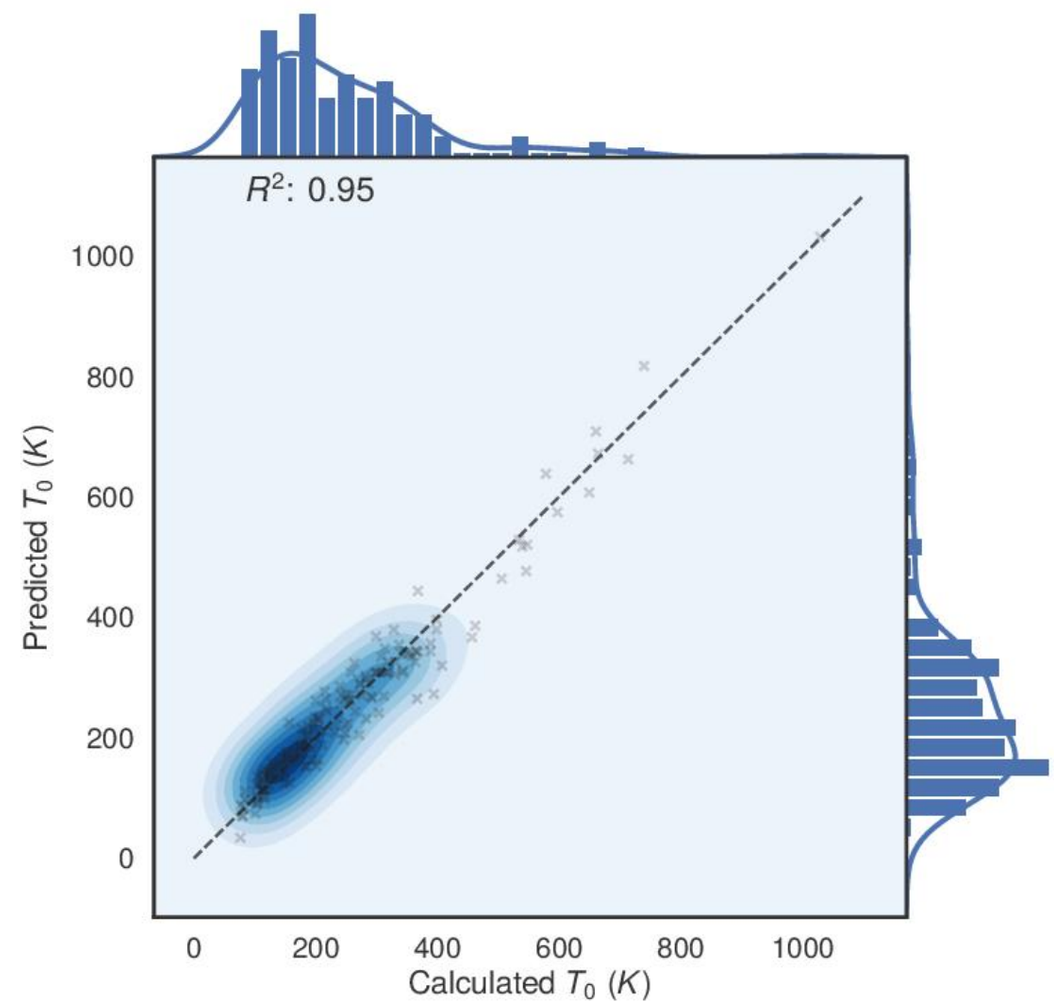

# Step 3 : Learning Algorithms (supervised)

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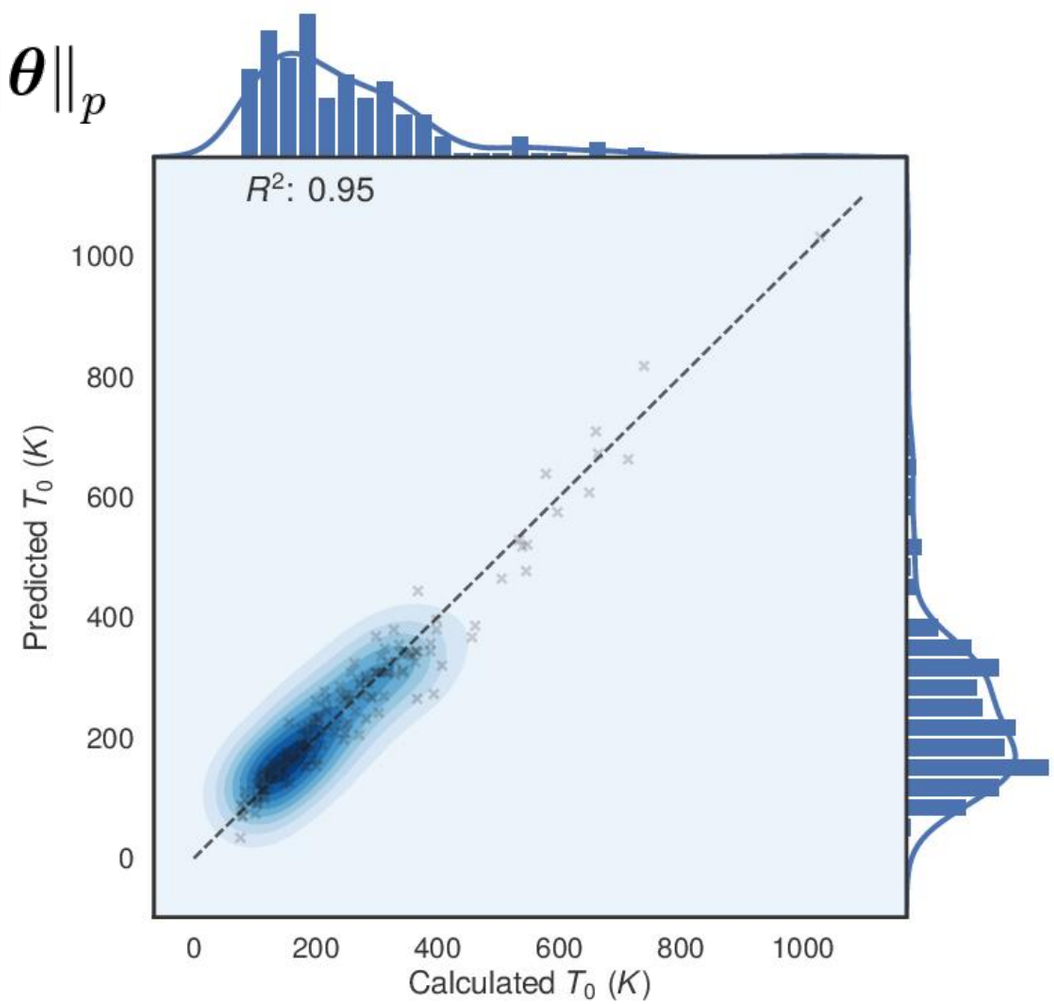

# Step 3 : Learning Algorithms (supervised)

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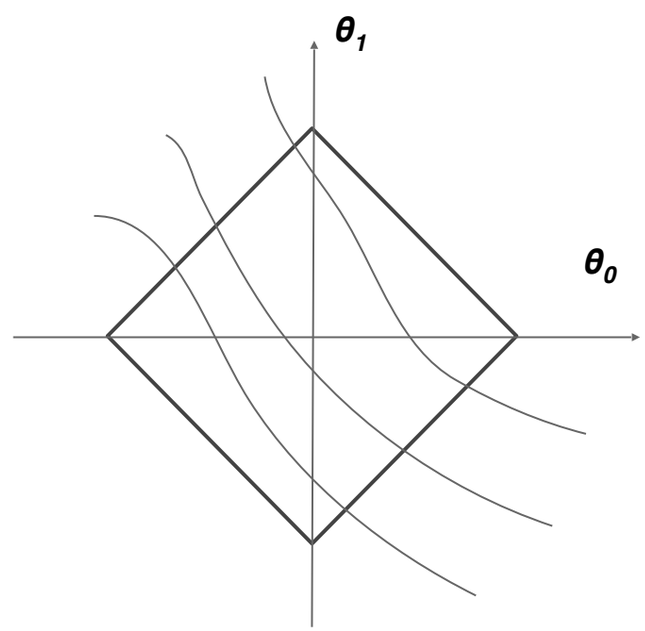


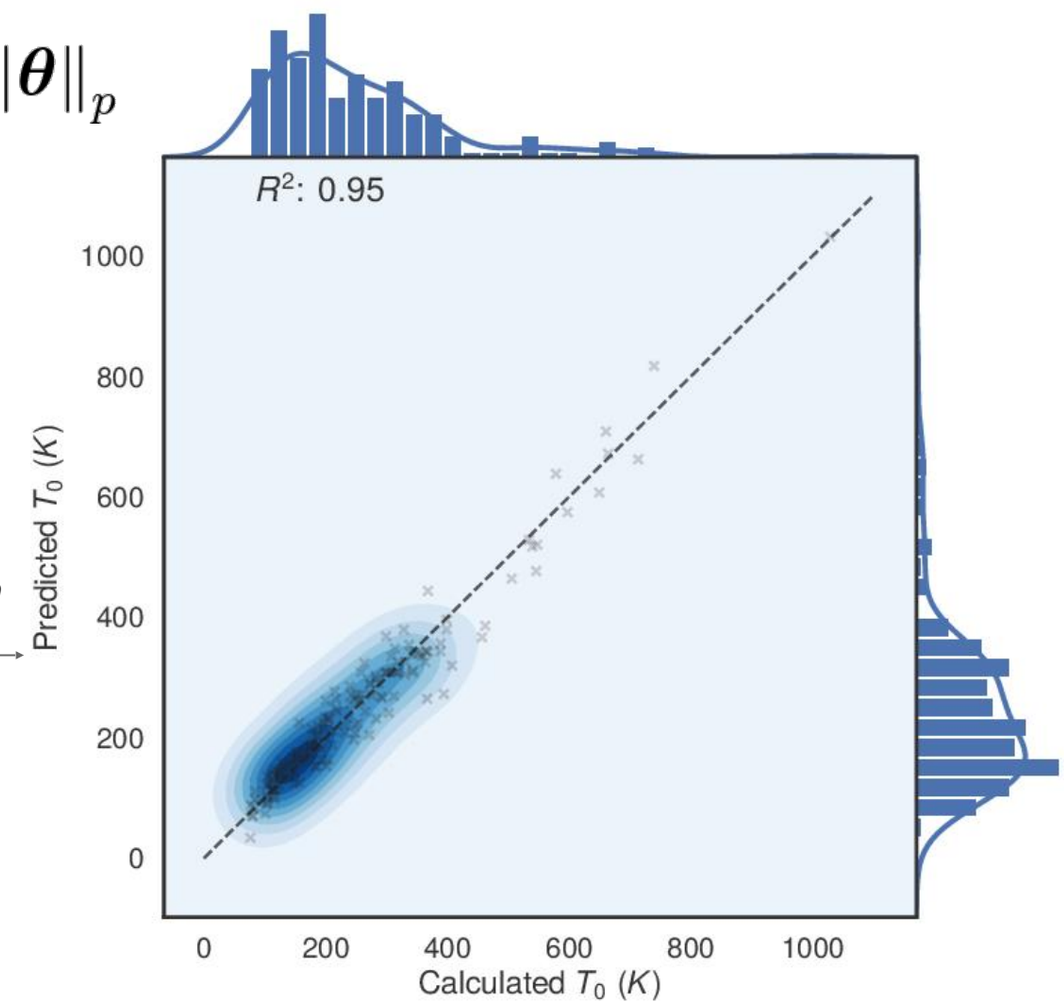

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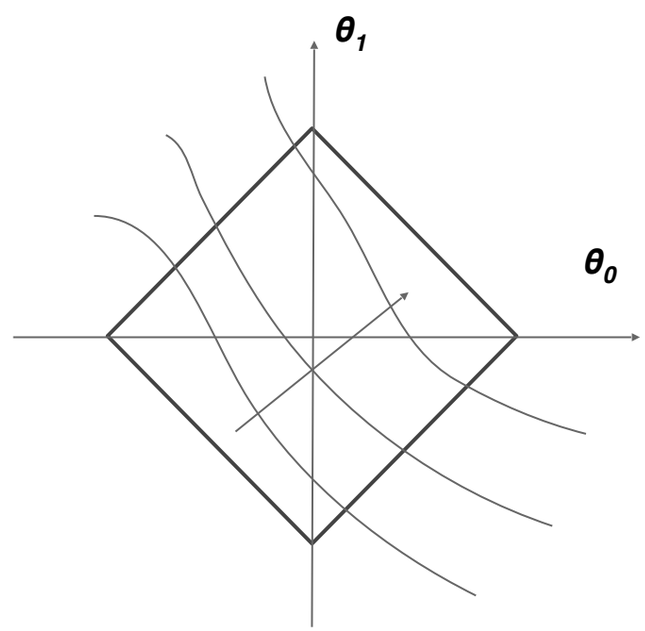
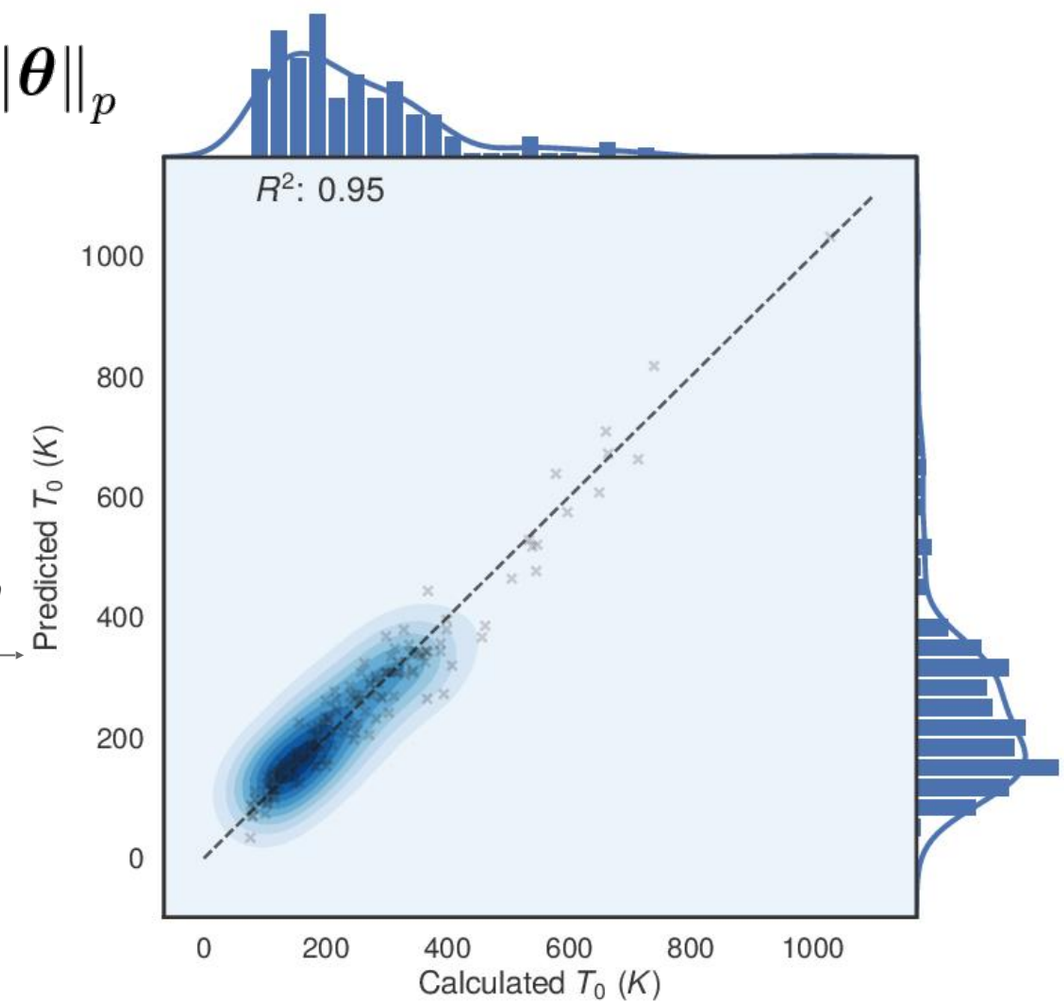


# Step 3 : Learning Algorithms (supervised)

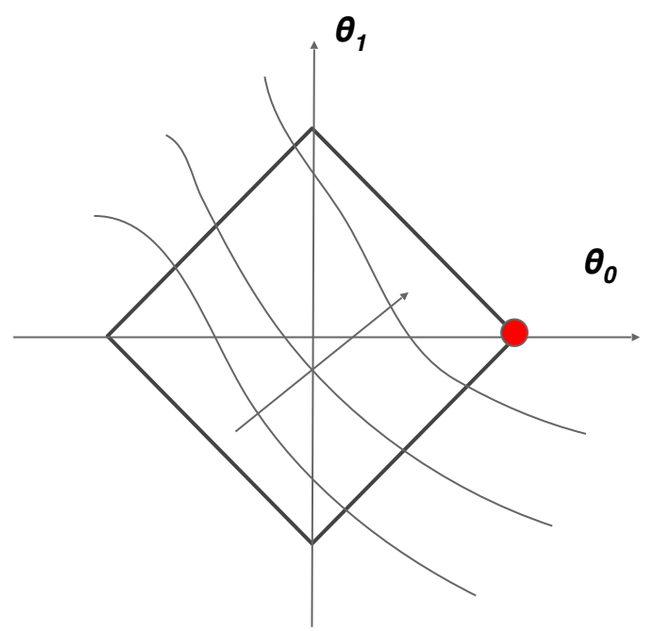
## Linear Regression

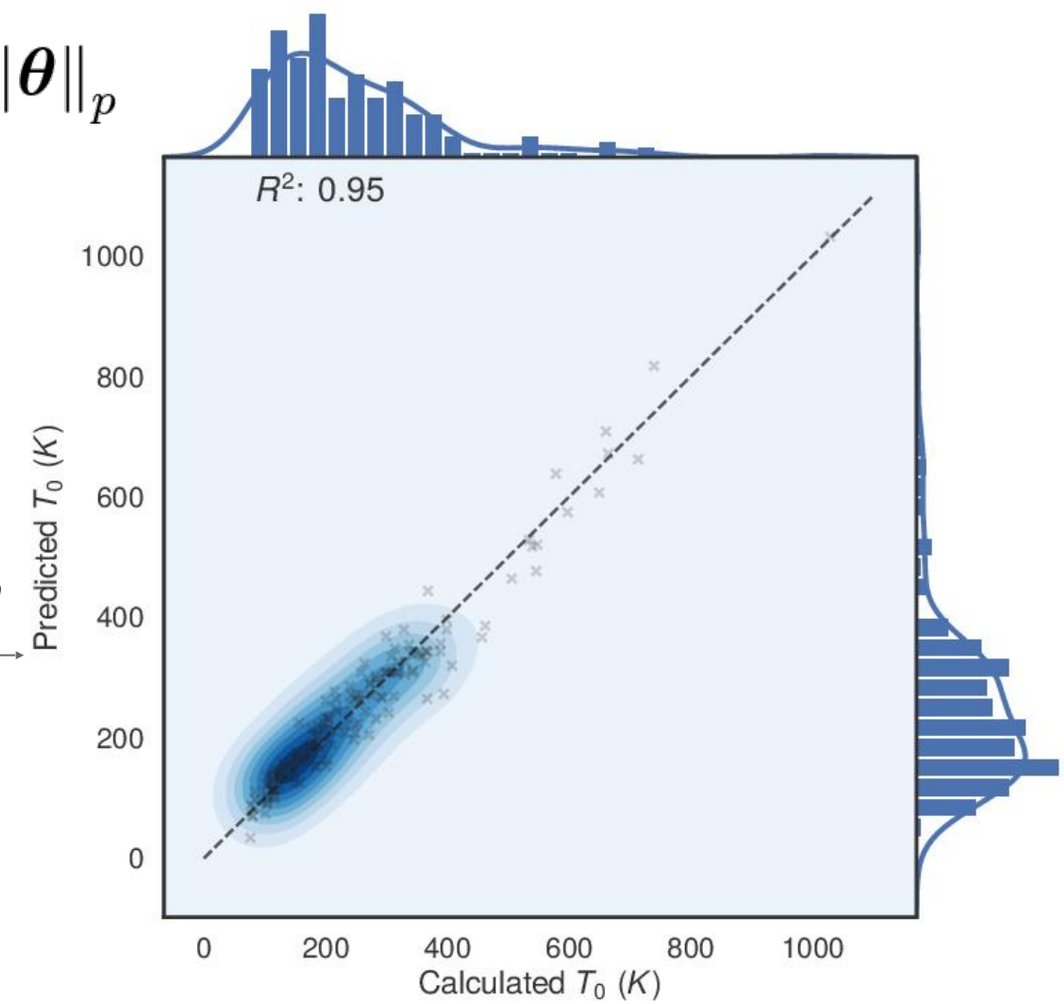
Function fitting: $\hat{y}^{(i)} = \boldsymbol{\theta}^T \mathbf{x}^{(i)} = x_0^{(i)}\theta_0 + x_1^{(i)}\theta_1 + \ldots$

Training = Minimize Cost function

$$J(\boldsymbol{\theta}) = \sum_{i=1}^{n} L[\hat{y}^{(i)}(\mathbf{x}^{(i)}, \boldsymbol{\theta}), y^{(i)}] = \frac{1}{2}\sum_{i=1}^{n}(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)})^2 + \lambda \left\|\boldsymbol{\theta}\right\|_p$$

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



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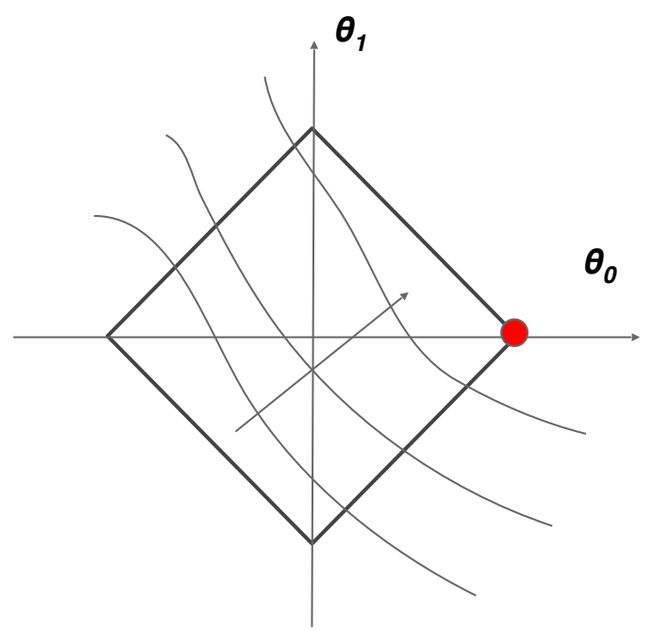
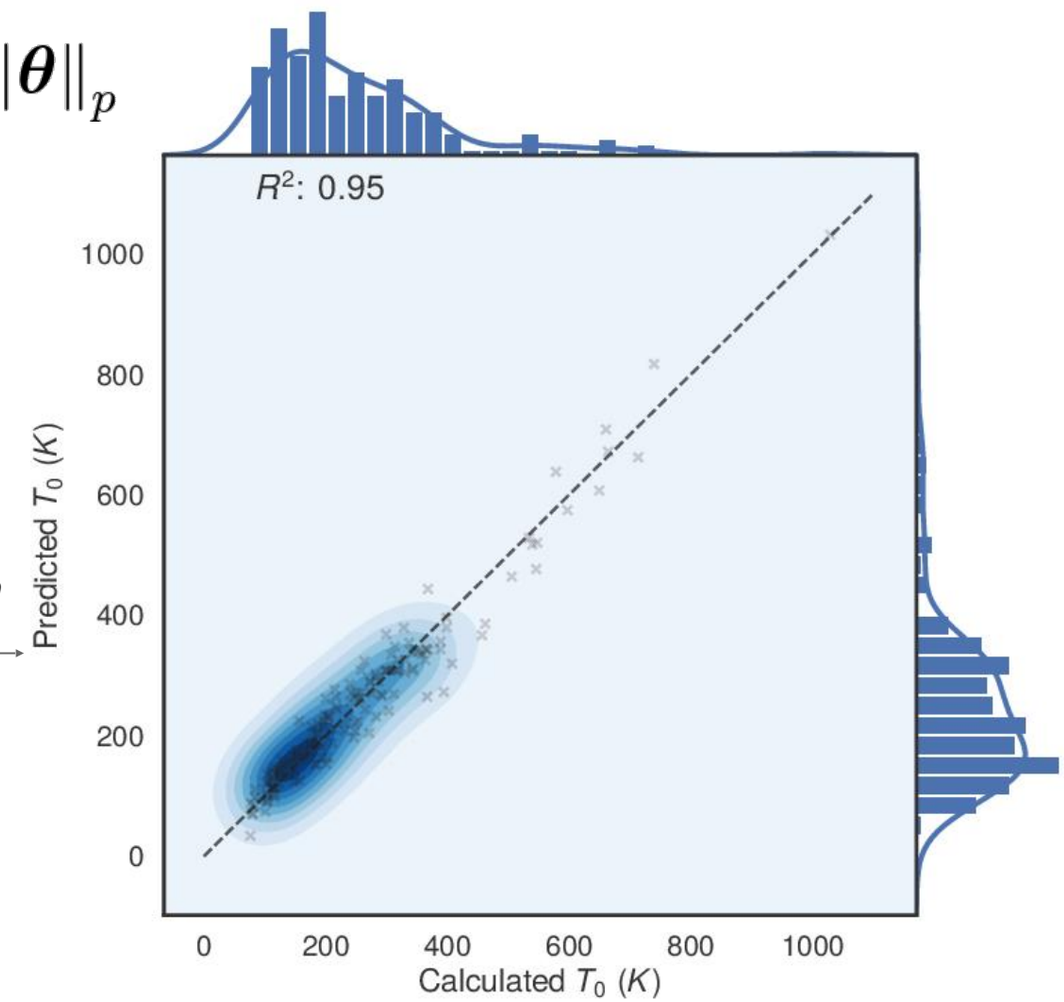
$$\boldsymbol{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

$$\text{MAE} = \frac{1}{n}\sum_{i}^{n}|y_i - \hat{y}_i|$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i}(y_i - \hat{y}_i)^2}$$

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} = 1 - \frac{\sum_i (y_i - \hat{y})^2}{\sum_i (y_i - \bar{y})^2}$$



# Step 3 : Learning Algorithms (supervised)



## Logistic Regression

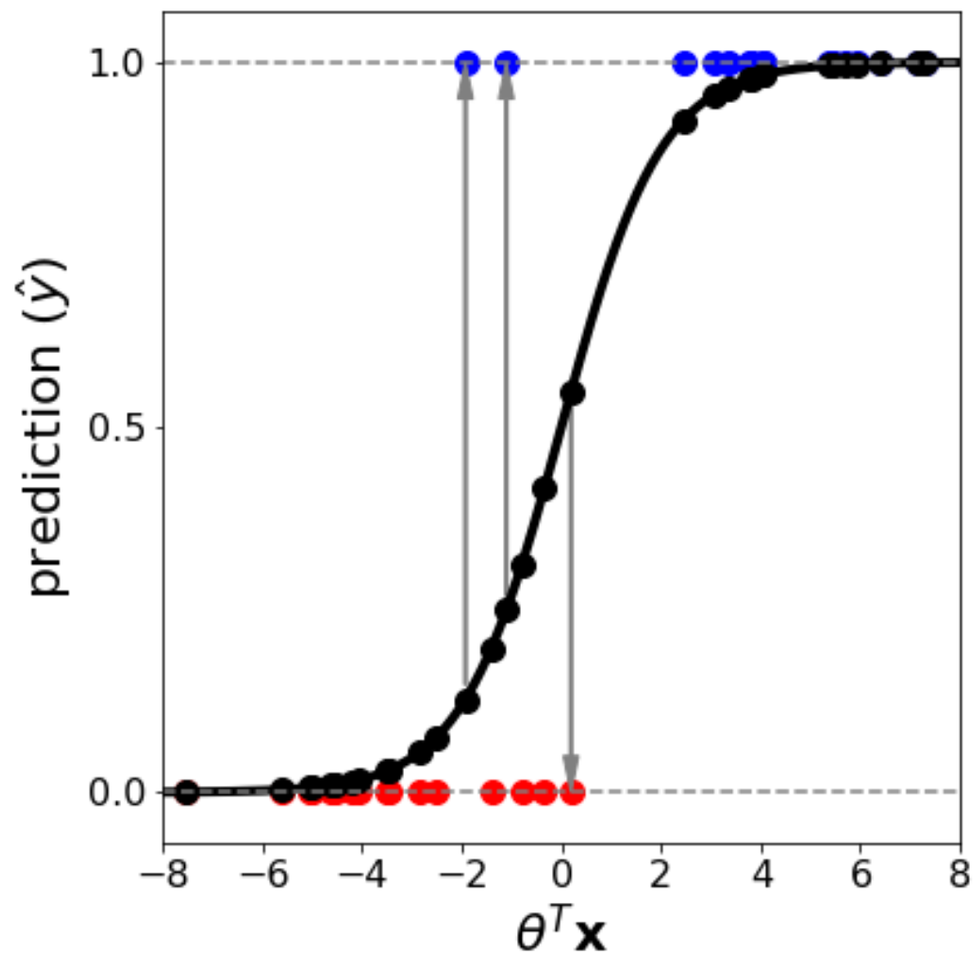
# Step 3 : Learning Algorithms (supervised)



## Logistic Regression

- Predictions: sigmoid

$$\hat{y} = \sigma(\boldsymbol{\theta}^T \mathbf{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^T \mathbf{x}}}$$



# Step 3 : Learning Algorithms (supervised)



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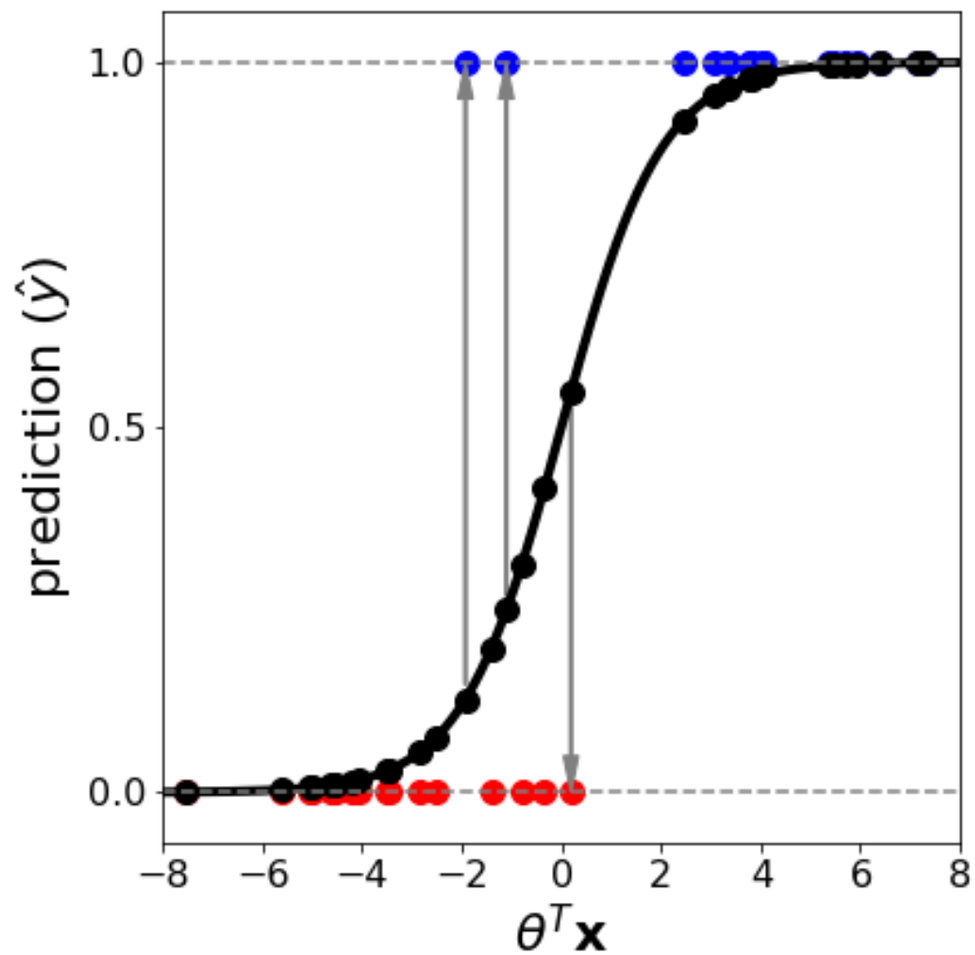

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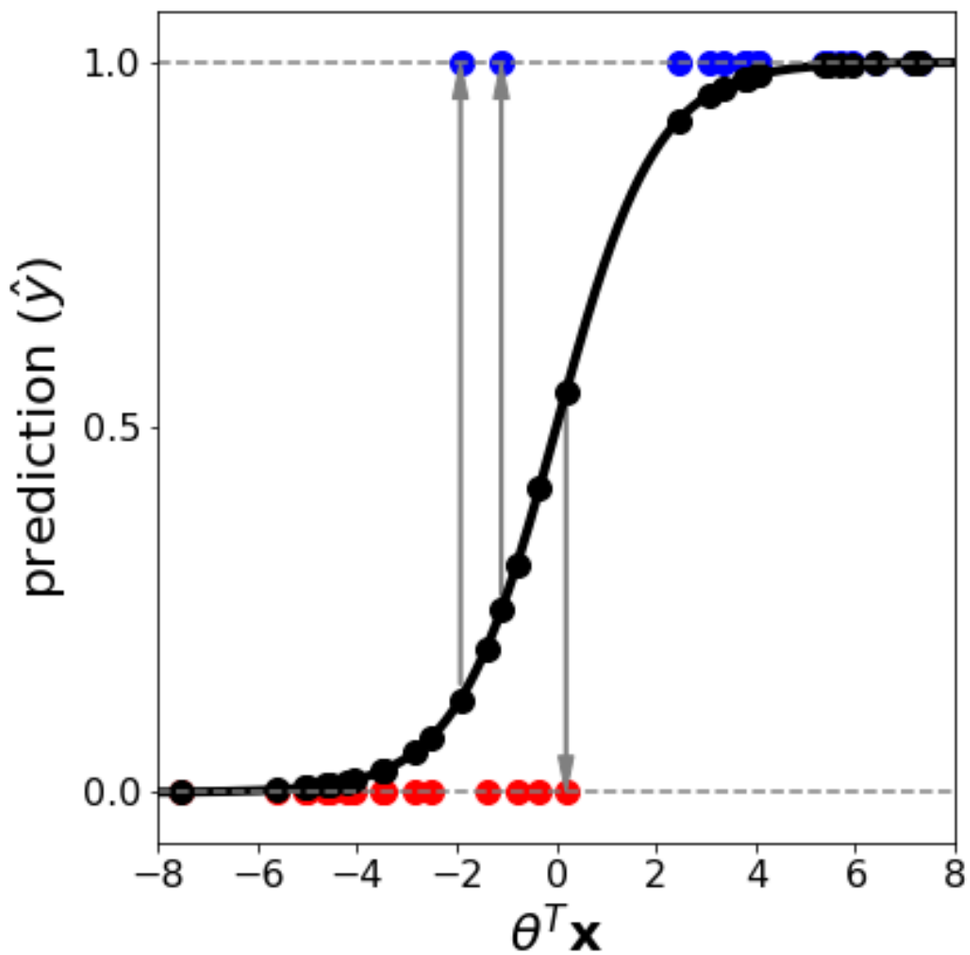
$$TPR = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{FP + TN}$$



# Step 3 : Learning Algorithms (supervised)



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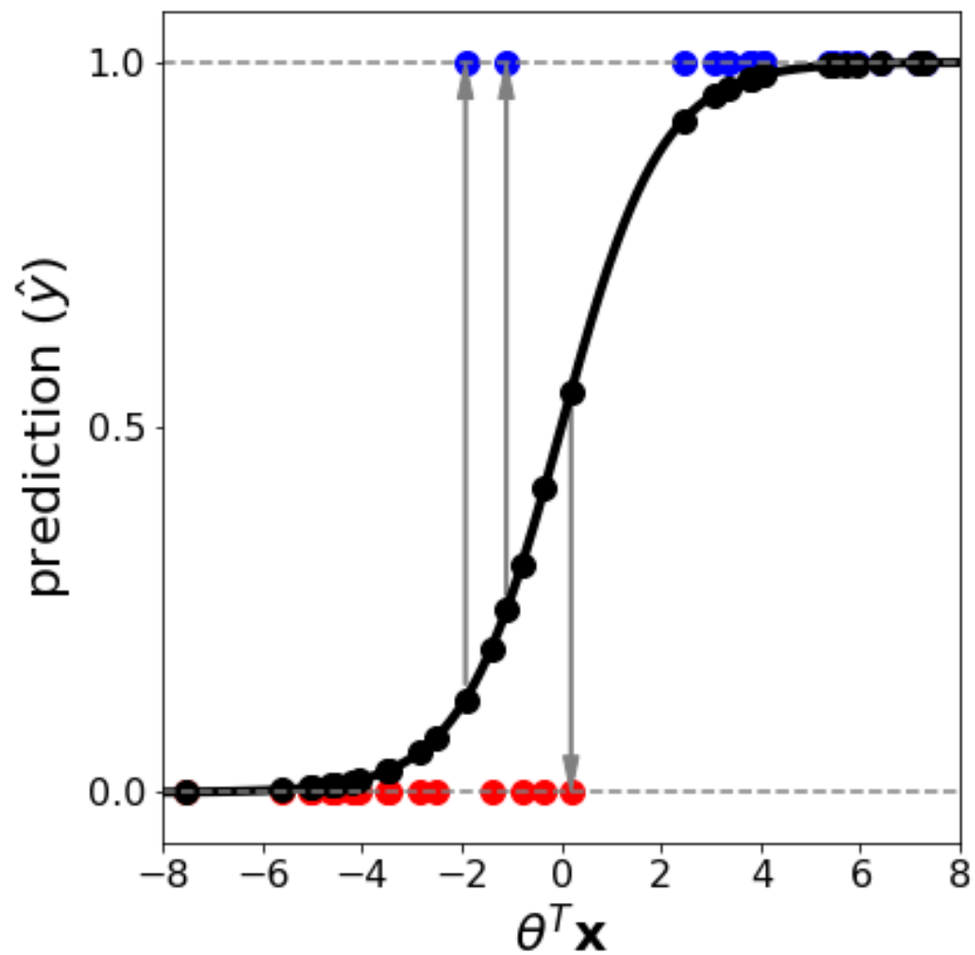


$$TPR = \frac{TP}{TP + FN}$$

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| | |
|---|---|
| TP | FP |
| FN | TN |

# Step 3 : Learning Algorithms (supervised)



## Naïve Bayes

$$P(y|\boldsymbol{x}) = \frac{P(\boldsymbol{x}|y)P(y)}{P(\boldsymbol{x})}$$

# Step 3 : Learning Algorithms (supervised)



## Naïve Bayes

Naïve = conditionally independent features

$$P(y|\boldsymbol{x}) = \frac{P(\boldsymbol{x}|y)P(y)}{P(\boldsymbol{x})} = \frac{\prod_j P(x_j|y)p(y)}{\prod_j P(x_j)}$$

# Step 3 : Learning Algorithms (supervised)



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$$P(y = \text{banana}|\text{long, sweet})$$

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$$P(y = \text{banana}|\text{long, sweet})$$

| Fruit | Long ($x_1$) | Sweet ($x_2$) | Yellow ($x_3$) |
|---|---|---|---|
| Orange | 0 | 1 | 0 |
| Banana | 1 | 0 | 1 |
| Banana | 1 | 1 | 1 |
| Mango | 1 | 1 | 0 |

# Step 3 : Learning Algorithms (supervised)

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$$P(y = \text{banana}|\text{long, sweet})$$

| Label | Long | ! Long | Sweet | ! Sweet | Yellow | ! Yellow | Total |
|---|---|---|---|---|---|---|---|
| B | 400 | 100 | 350 | 150 | 450 | 50 | 500 |
| O | 0 | 300 | 150 | 150 | 300 | 0 | 300 |
| M | 100 | 100 | 150 | 50 | 50 | 150 | 200 |
| Total | 500 | 500 | 650 | 350 | 800 | 200 | 1000 |

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priors

$$P(Y = B) = 500/1000 = 0.50$$
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likelihoods (Banana)

$$P(x_1 = \text{long}|Y = B) = 400/500 = 0.80$$
$$P(x_2 = \text{sweet}|Y = B) = 350/500 = 0.70$$
$$P(x_3 = \text{yellow}|Y = B) = 450/500 = 0.90$$

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evidence

$$P(x_1 = \text{long}) = 500/1000 = 0.50$$
$$P(x_2 = \text{sweet}) = 650/1000 = 0.65$$
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$$= \frac{0.8 \times 0.7 \times 0.1}{\quad}$$

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# Step 3 : Learning Algorithms (supervised)



## K-NN

Simply calculate distances to N nearest neighbors

# Step 3 : Learning Algorithms (supervised)



## K-NN

Simply calculate distances to N nearest neighbors

$$d(\mathbf{x}, \mathbf{x}^{(i)}) = \|\mathbf{x} - \mathbf{x}^{(i)}\|_p$$

$$\|\mathbf{x} - \boldsymbol{\mu}\|_p = \left[\sum_j (x_j - \mu_j)^p\right]^{\frac{1}{p}}$$

# Step 3 : Learning Algorithms (supervised)



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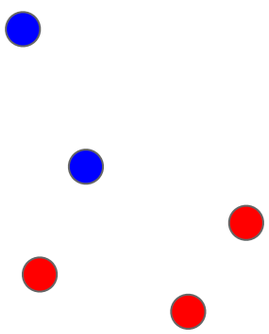

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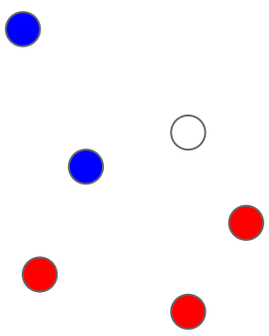

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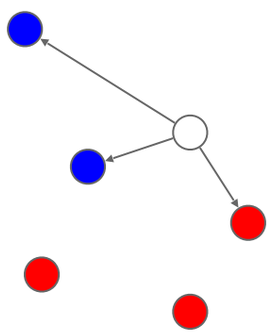

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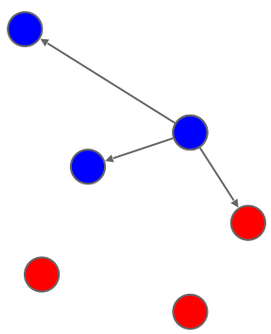

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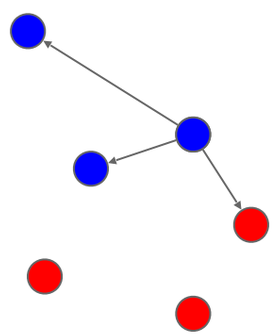

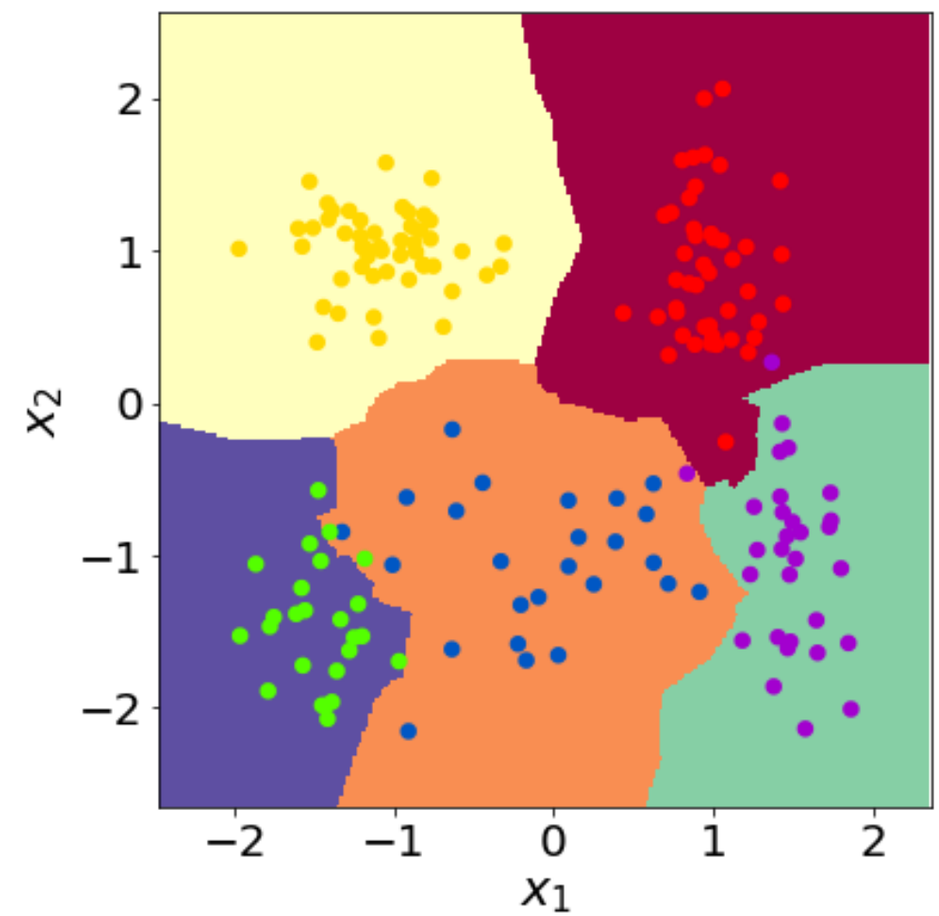

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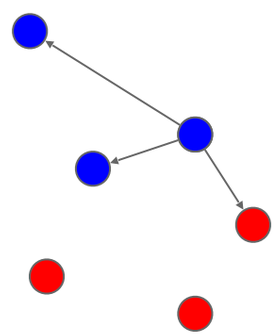
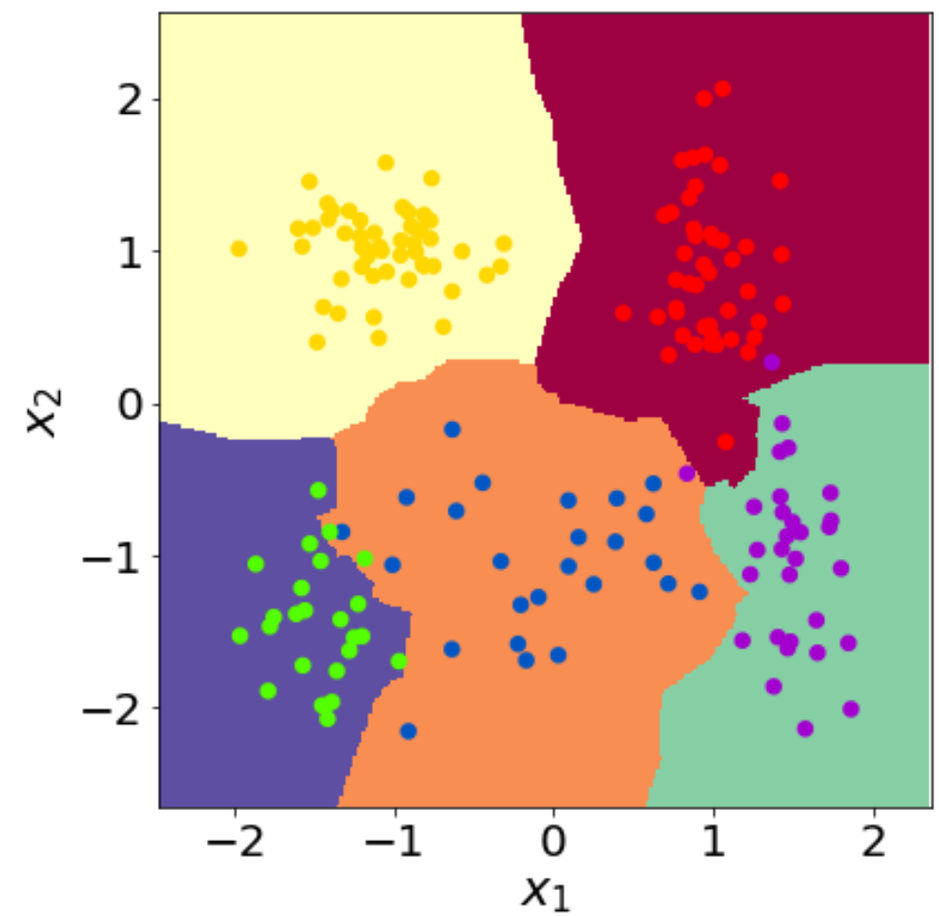
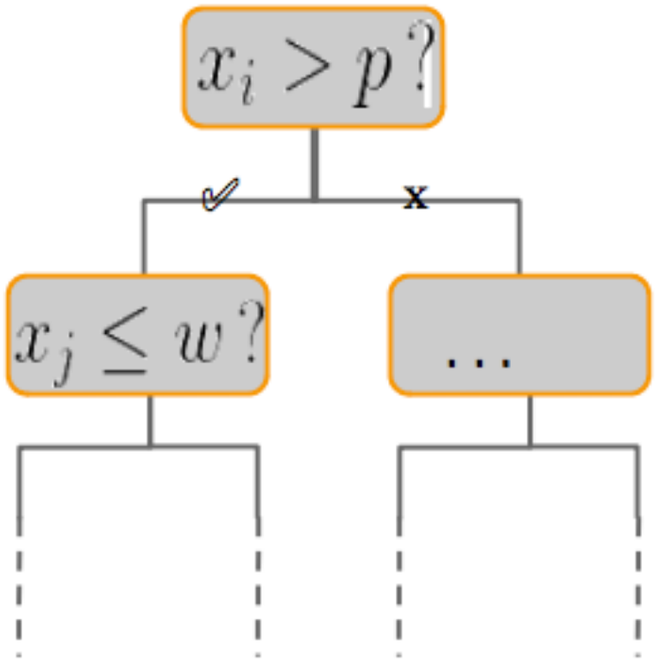





No training required: instance-based algorithm

# Decision Trees

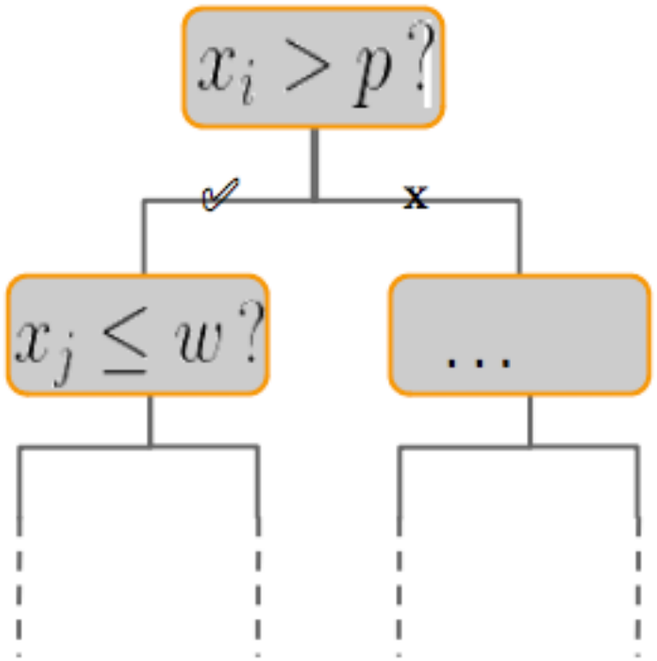


# Step 3 : Learning Algorithms (supervised)



## Decision Trees

- CART - Classification



# Step 3 : Learning Algorithms (supervised)



## Decision Trees

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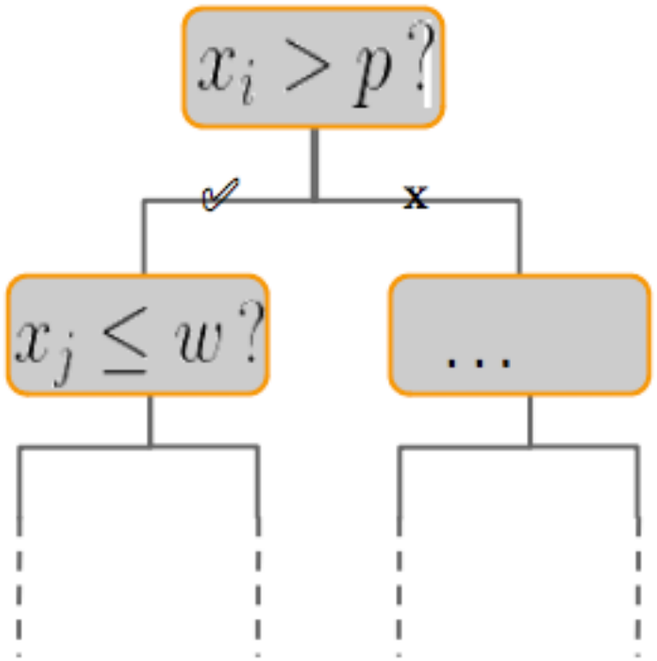
$$I_G(S) = 1 - \sum_{j=1}^{k} f_j^2$$



# Step 3 : Learning Algorithms (supervised)



## Decision Trees

- CART - Classification

minimization of GINI coefficient

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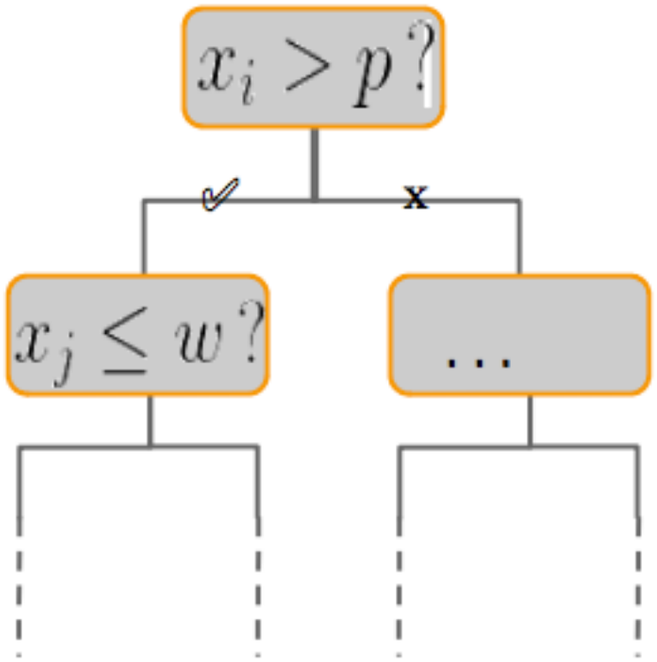

# Step 3 : Learning Algorithms (supervised)



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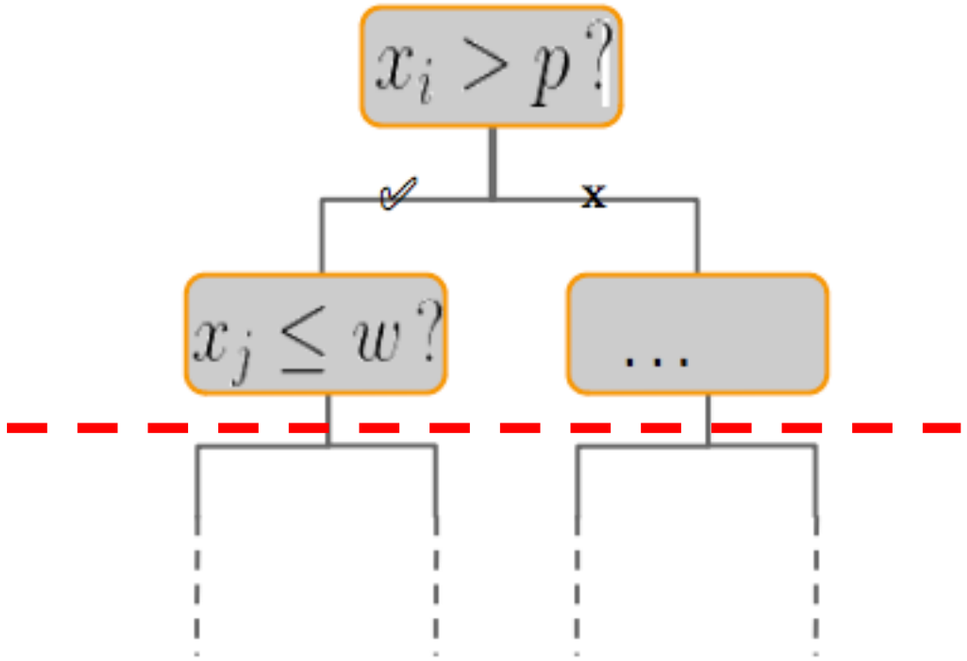

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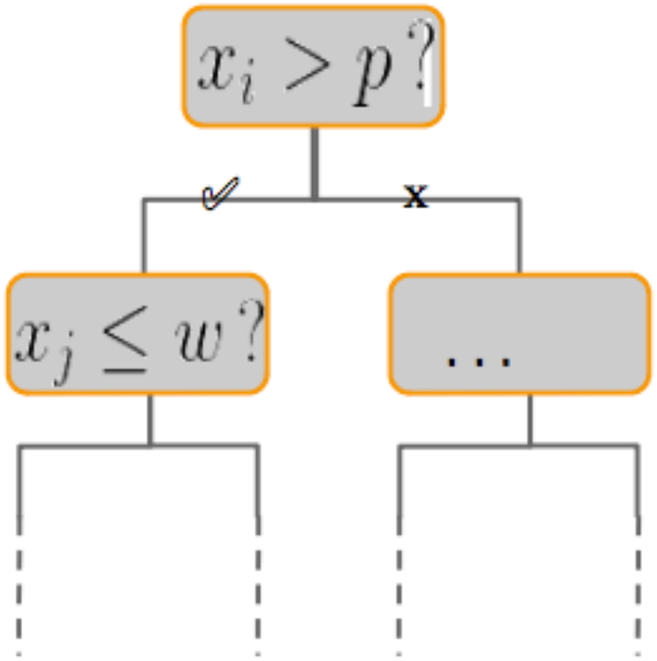


- CART - Regression

$$R(S) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

# Step 3 : Learning Algorithms (supervised)



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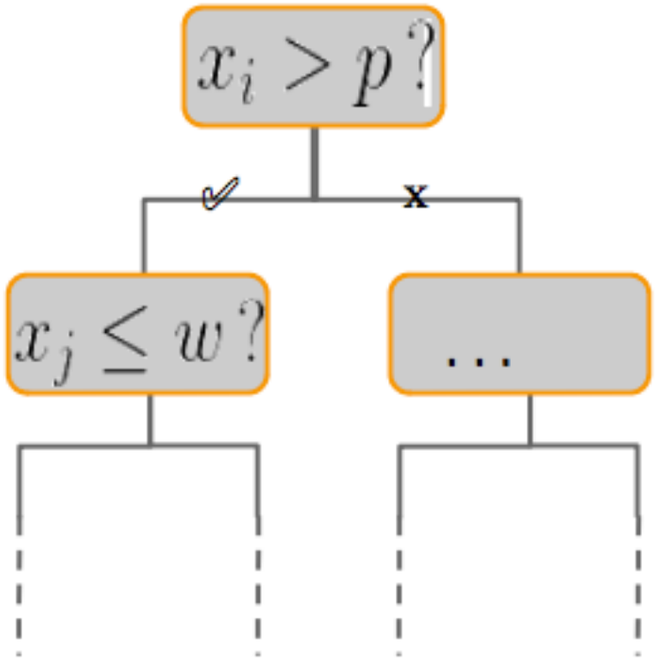


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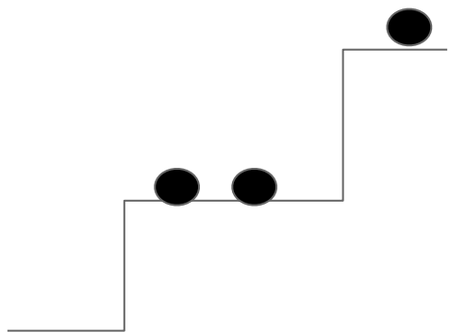

piecewise
constant function

# Step 3 : Learning Algorithms (supervised)



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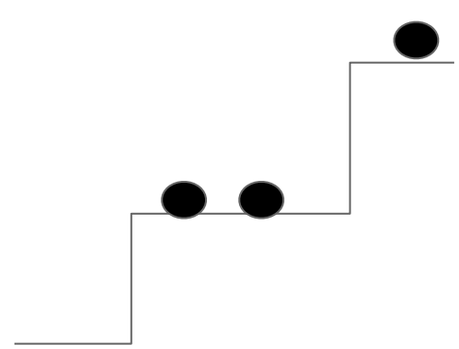

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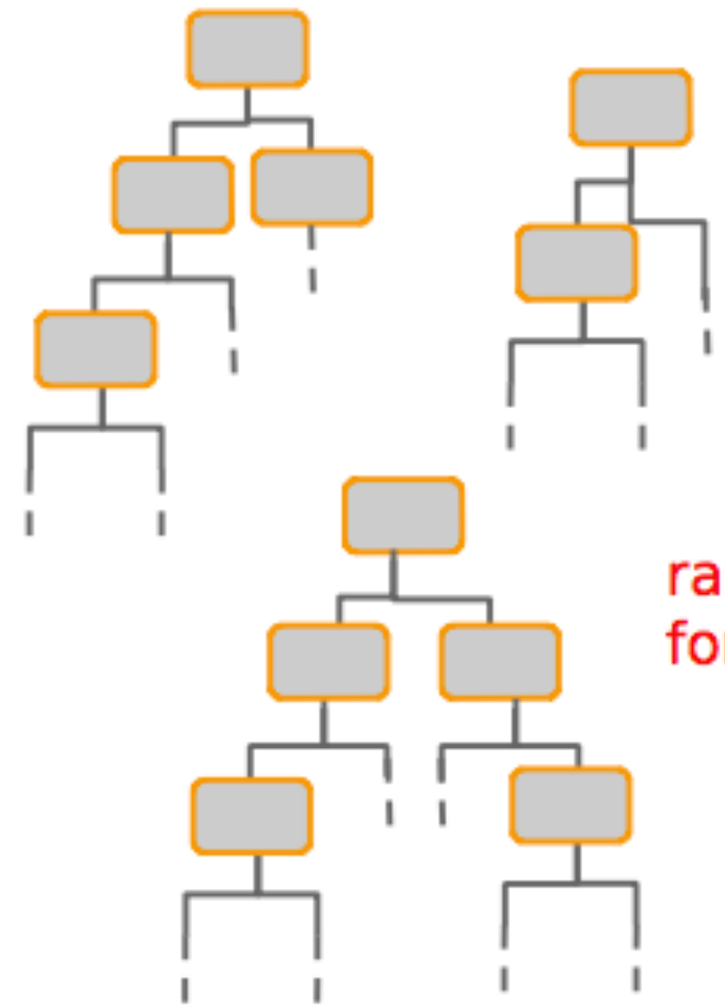

random forests

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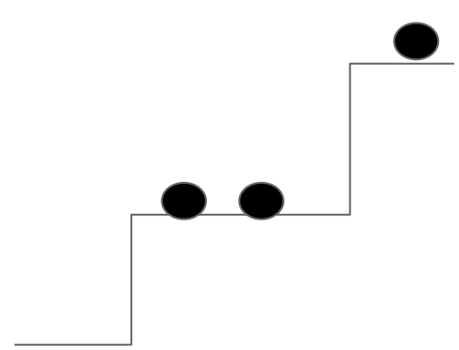

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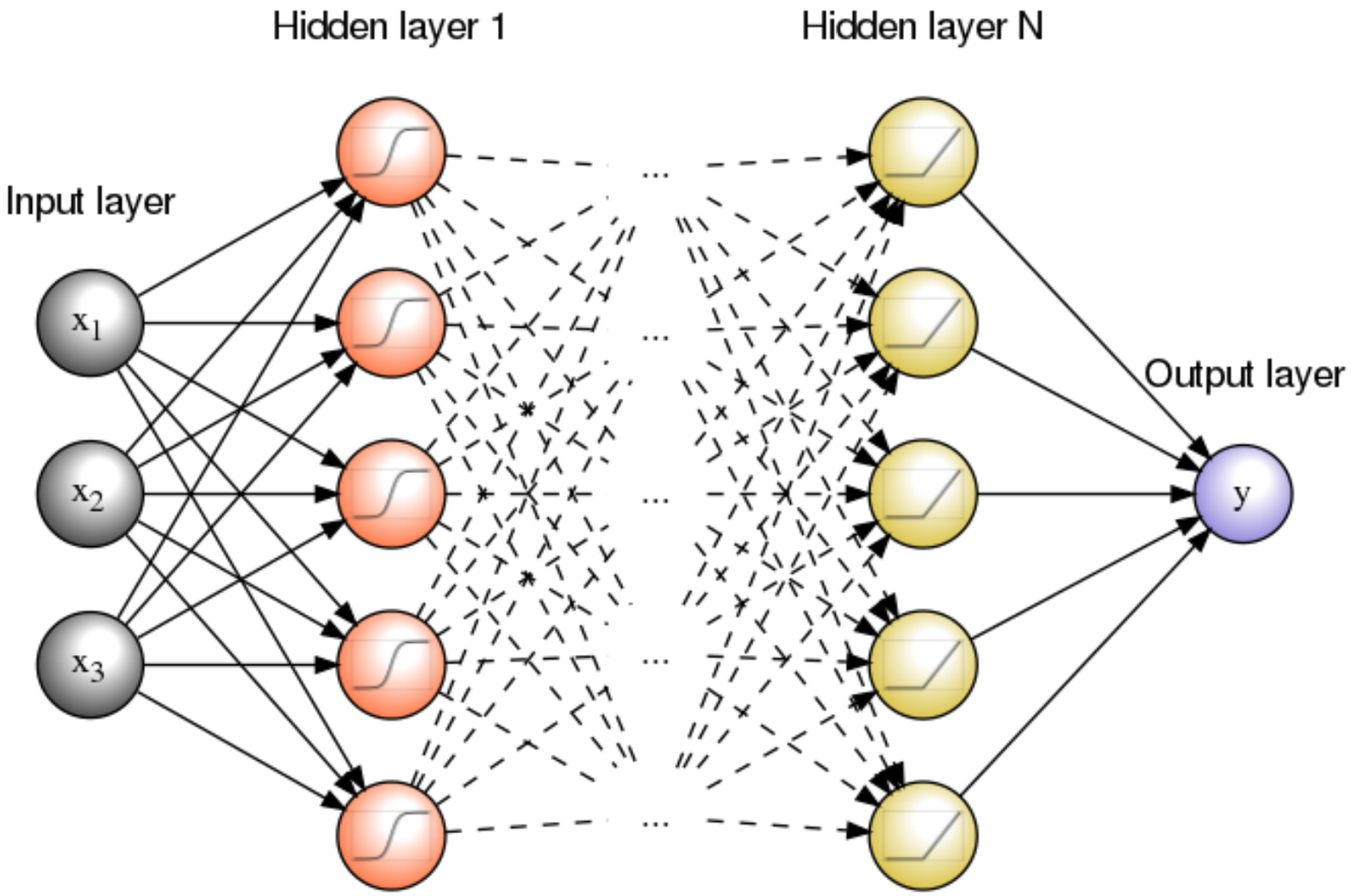
# Feed-Forward Artificial Neural Networks

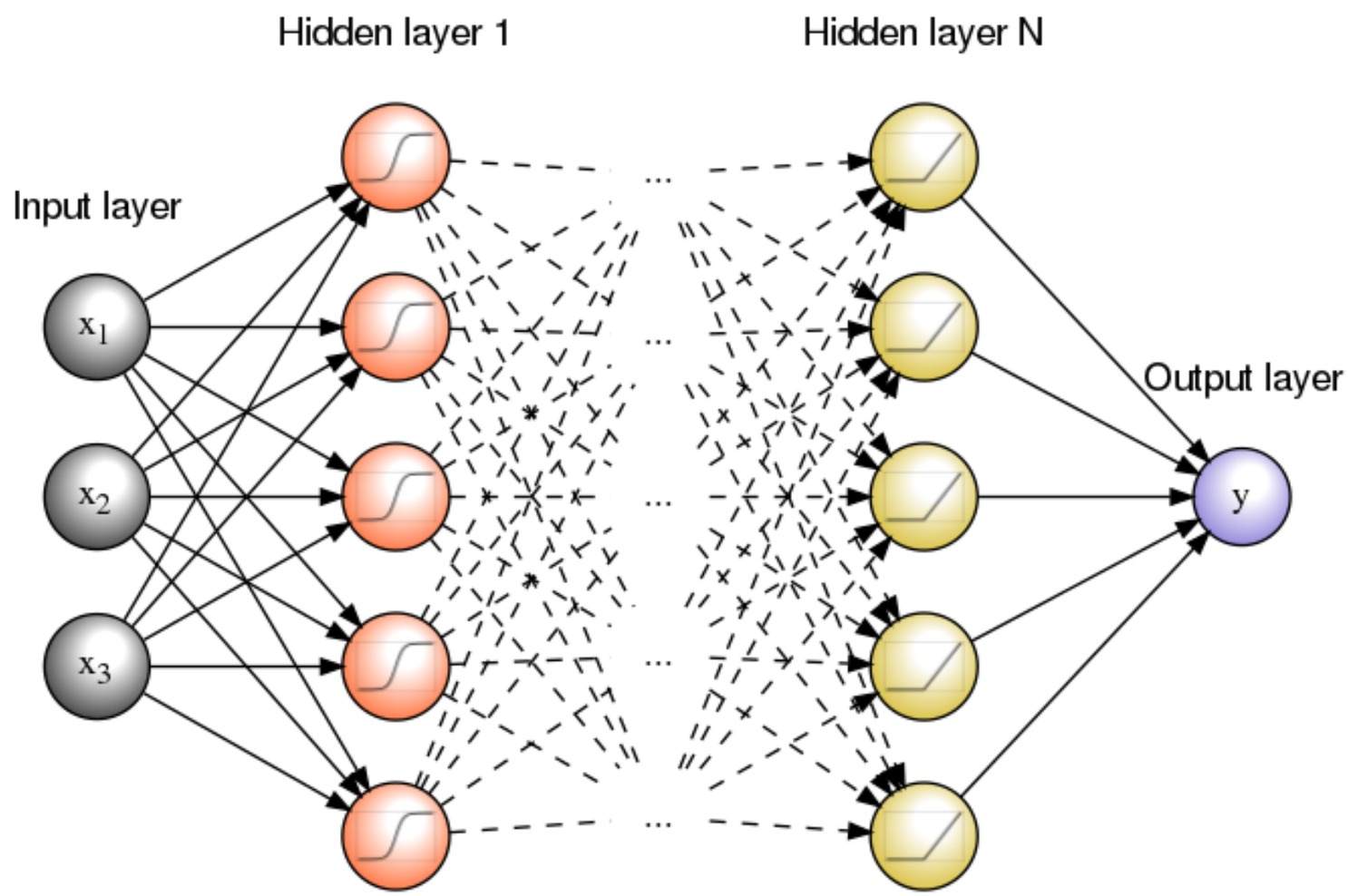


# Step 3 : Learning Algorithms (supervised)



## Feed-Forward Artificial Neural Networks

$$z_i^{(k)} = \omega_{i0}^{(k)} + \sum_j y_j^{(k-1)} \omega_{ij}^{(k)}$$



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## Feed-Forward Artificial Neural Networks

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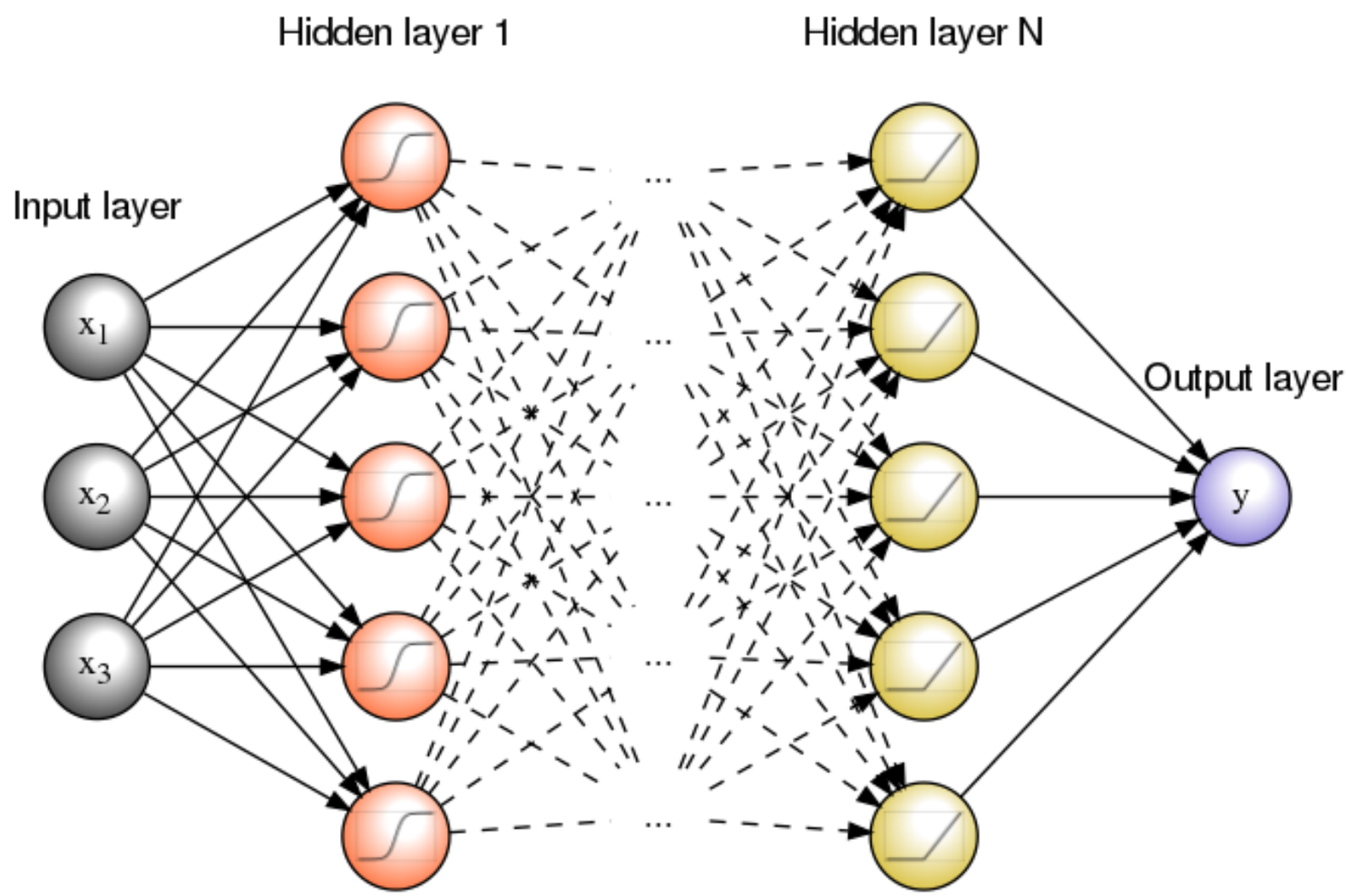

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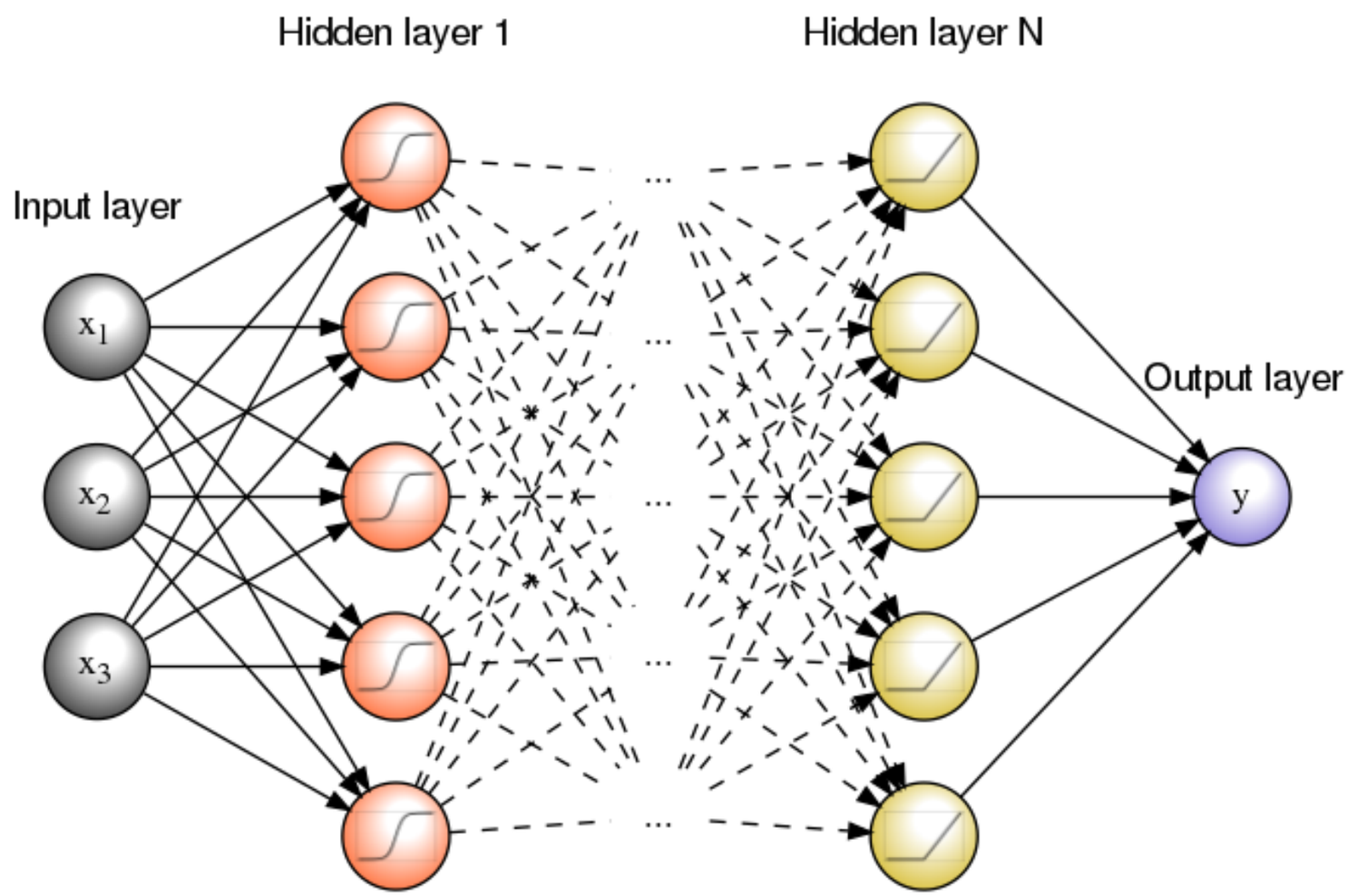

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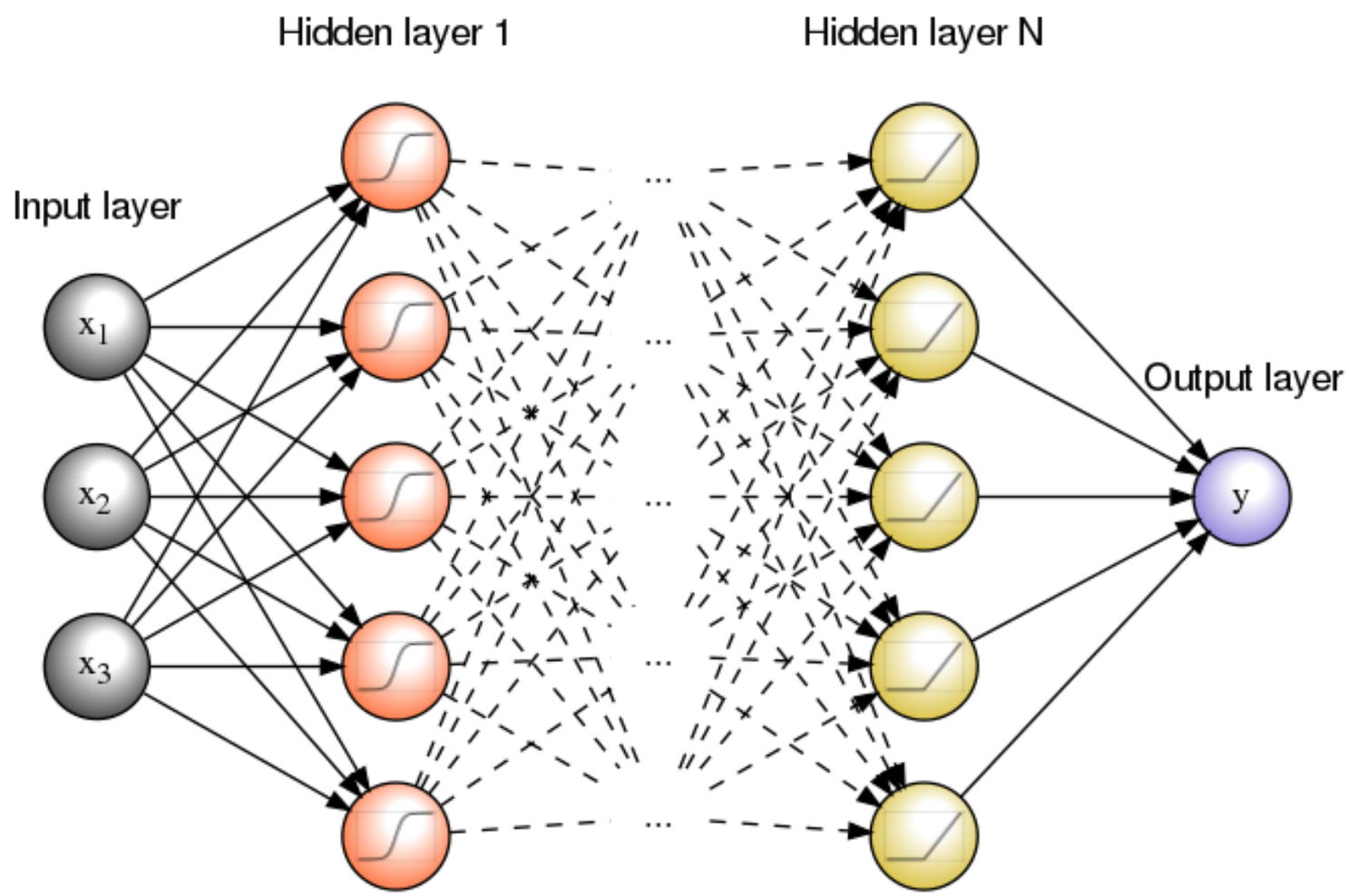

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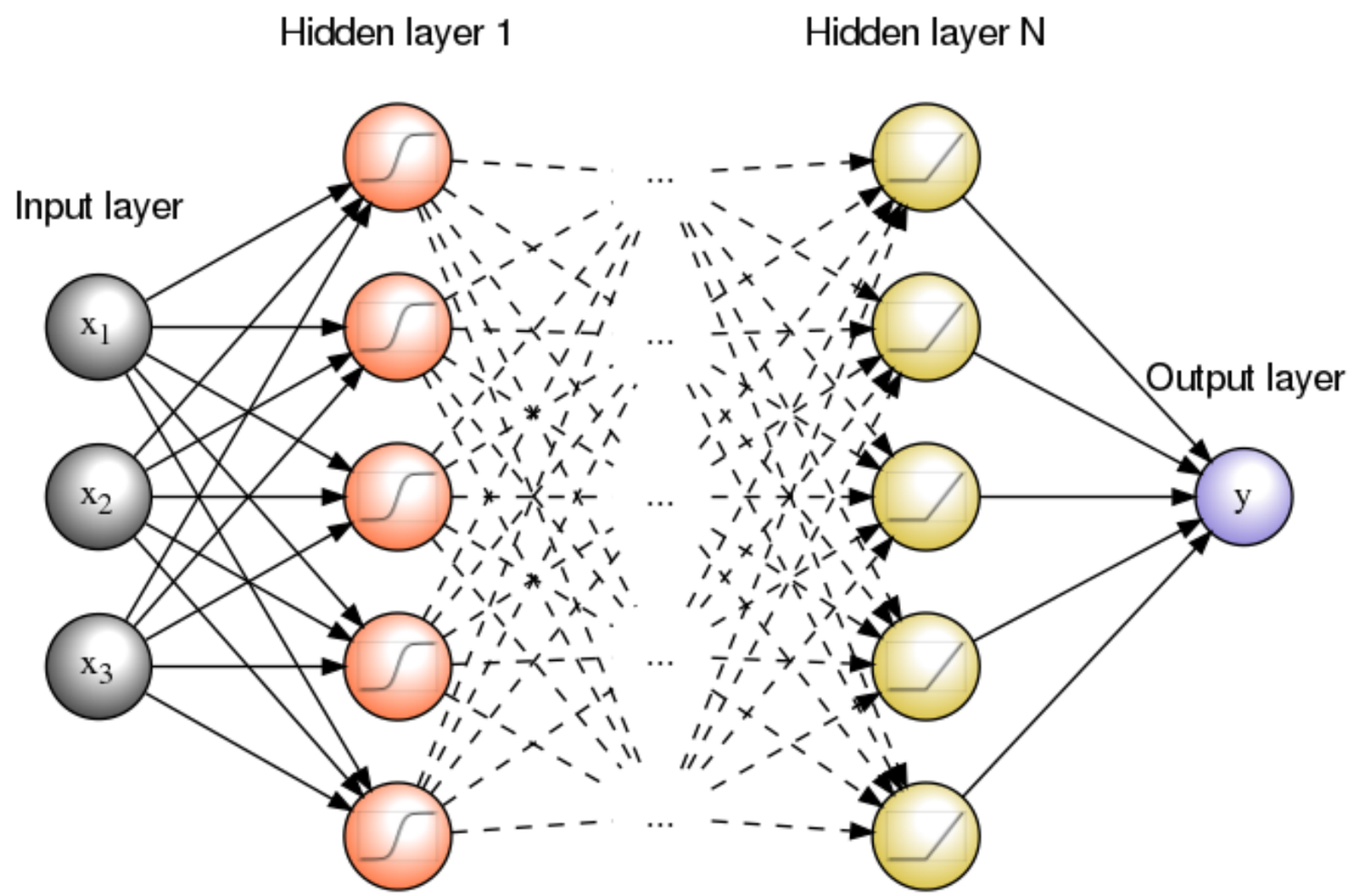


training: backpropagation

# Model Validation & Evaluation



- Train | Validation | Test split

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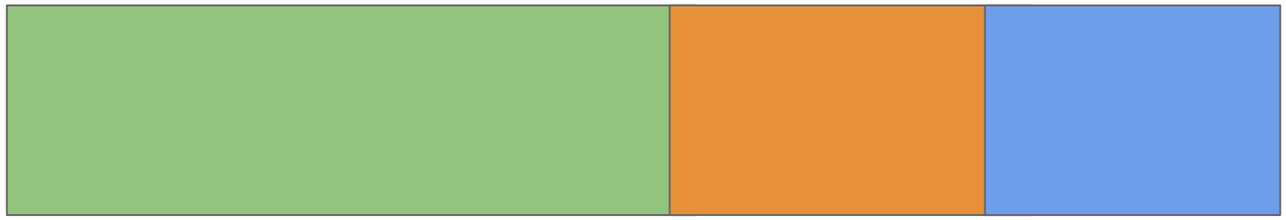

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$$E_{cv}^{K} = \frac{1}{K} \sum_{k=1}^{K} \sum_{i=1}^{n_k} L(\hat{y}_k^{(i)}, y^{(i)})$$

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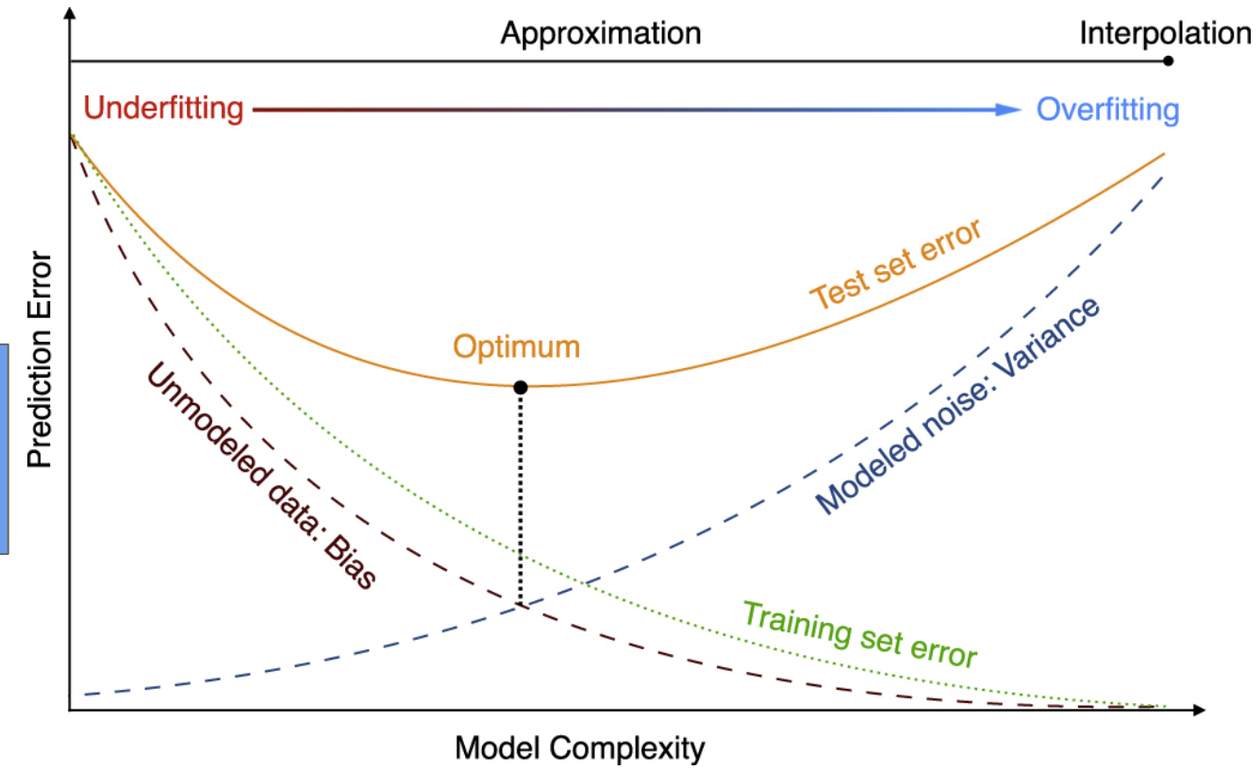


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# Acknowledgements

CNPEM
Brazilian Center for Research in Energy and Materials

LNNano
Brazilian Nanotechnology National Laboratory

UFABC

FAPESP

Tutorial Website

https://github.com/gschleder/MLtutorial