# Convention, Accuracy metrics, Classification, Regression

Nipun Batra

December 26, 2023

IIT Gandhinagar

"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

How would you program to recognise digits? Start with 4.

"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

How would you program to recognise digits? Start with 4.

Maybe 4 can be thought of as: "—" + "—" + "—" + another vertically down "—"

"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

How would you program to recognise digits? Start with 4.

Maybe 4 can be thought of as: "—" + "—" + "—" + another vertically down "—"

The heights of each of the "—" need to be similar within tolerance

"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

How would you program to recognise digits? Start with 4.

Maybe 4 can be thought of as: "—" + "—" + "—" + another vertically down "—"

The heights of each of the "—" need to be similar within tolerance Each of the "—" can be slightly slanted. Similarly the horizontal line can be slanted.

1

"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

How would you program to recognise digits? Start with 4.

Maybe 4 can be thought of as: "—" + "—" + "—" + another vertically down "—"

The heights of each of the "-" need to be similar within tolerance

Each of the "—" can be slightly slanted. Similarly the horizontal line can be slanted. There can be some cases of 4 where the first "—" is at 45 degrees

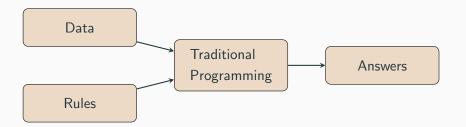
"Field of study that give computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

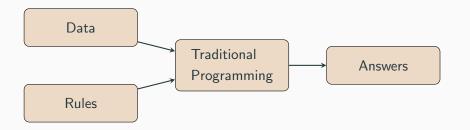
How would you program to recognise digits? Start with 4.

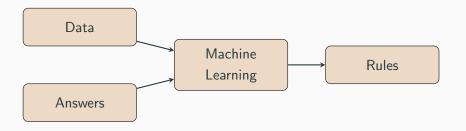
Maybe 4 can be thought of as: "—" + "—" + "—" + another vertically down "—"

The heights of each of the "-" need to be similar within tolerance

Each of the "—" can be slightly slanted. Similarly the horizontal line can be slanted. There can be some cases of 4 where the first "—" is at 45 degrees There can be some cases of 4 where the width of each stroke is different







"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E." - Tom Mitchell

# First ML Task: Grocery store tomatoes quality prediction

Problem statement: You want to predict the quality/condition of a tomato given its visual features.

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

Size

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

- Size
- Colour

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

- Size
- Colour
- Texture

Imagine you have some past data on quality of tomatoes.

Sample	Colour	Size	Texture	Condition
1	Orange	Small	Smooth	Good
2	Red	Small	Rough	Good
3	Orange	Medium	Smooth	Bad
4	Yellow	Large	Smooth	Bad

#### **Useful Features**

Is the sample number a useful feature for predicting quality of a tomato?

#### **Useful Features**

Is the sample number a useful feature for predicting quality of a tomato?

Answer: It depends! Maybe, all tomatoes received after a certain date are bad! Let us ignore that for now.

#### **Useful Features**

Is the sample number a useful feature for predicting quality of a tomato?

Answer: It depends! Maybe, all tomatoes received after a certain date are bad! Let us ignore that for now.

Let us modify our data table for now.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

7

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

The training set consists of two parts:

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

The training set consists of two parts:

1. Features, Attributes or Covariates

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

### The training set consists of two parts:

- 1. Features, Attributes or Covariates
- 2. Output or Response Variable

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

We call this matrix as  $\ensuremath{\mathcal{D}}\xspace$  , containing:

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

We call this matrix as  $\mathcal{D}$ , containing:

1. Feature matrix  $(\mathbf{X} \in \mathcal{R}^{\mathbf{N} \times \mathbf{P}})$  containing data of N samples each of which is P dimensional.

9

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

We call this matrix as  $\mathcal{D}$ , containing:

- 1. Feature matrix  $(\mathbf{X} \in \mathcal{R}^{\mathbf{N} \times \mathbf{P}})$  containing data of N samples each of which is P dimensional.
  - Thus,  $\mathbf{X} = \{x_i^T\}_{i=1}^N$  where  $x_i \in \mathcal{R}^P$

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

We call this matrix as  $\mathcal{D}$ , containing:

1. Feature matrix  $(\mathbf{X} \in \mathcal{R}^{\mathbf{N} \times \mathbf{P}})$  containing data of N samples each of which is P dimensional.

• Thus, 
$$\mathbf{X} = \{x_i^T\}_{i=1}^N$$
 where  $x_i \in \mathcal{R}^P$ 
• Example  $x_1 = \begin{bmatrix} Orange \\ Small \\ Smooth \end{bmatrix}$ 

C

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

We call this matrix as  $\mathcal{D}$ , containing:

1. Feature matrix  $(\mathbf{X} \in \mathcal{R}^{\mathbf{N} \times \mathbf{P}})$  containing data of N samples each of which is P dimensional.

• Thus, 
$$\mathbf{X} = \{x_i^T\}_{i=1}^N$$
 where  $x_i \in \mathcal{R}^P$ 
• Example  $x_1 = \begin{bmatrix} Orange \\ Small \\ Smooth \end{bmatrix}$ 

2. Output Vector  $(y \in \mathcal{R}^N)$  containing output variable for N samples.

C

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

We call this matrix as  $\mathcal{D}$ , containing:

1. Feature matrix  $(\mathbf{X} \in \mathcal{R}^{\mathbf{N} \times \mathbf{P}})$  containing data of N samples each of which is P dimensional.

• Thus, 
$$\mathbf{X} = \{x_i^T\}_{i=1}^N$$
 where  $x_i \in \mathcal{R}^P$ 

- Example  $x_1 = \begin{bmatrix} Orange \\ Small \\ Smooth \end{bmatrix}$
- 2. Output Vector  $(y \in \mathcal{R}^N)$  containing output variable for N samples.
- 3. Thus, we can also write  $\mathcal{D} = \{(x_i^T, y_i)\}_{i=1}^N$

#### **Prediction Task**

Estimate condition for unseen tomatoes (#5, 6) based on data set.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

# **Testing Set**

Testing set is similar to training set, but, does not contain labels for output variable.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

# **Prediction Task**

We hope to:

### **Prediction Task**

We hope to:

1. Learn f: Condition = f(colour, size, texture)

#### **Prediction Task**

# We hope to:

- 1. Learn f: Condition = f(colour, size, texture)
- 2. From Training Dataset

### **Prediction Task**

## We hope to:

- 1. Learn f: Condition = f(colour, size, texture)
- 2. From Training Dataset
- 3. To Predict the condition for the Testing set

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

• Q: Is predicting on test set enough to say our model generalises?

- Q: Is predicting on test set enough to say our model generalises?
- A: Ideally, no!

- Q: Is predicting on test set enough to say our model generalises?
- A: Ideally, no!
- Ideally we want to predict "well" on all possible inputs. But, can we test that?

- Q: Is predicting on test set enough to say our model generalises?
- A: Ideally, no!
- Ideally we want to predict "well" on all possible inputs. But, can we test that?
- No! Since, the test set is only a sample from all possible inputs.

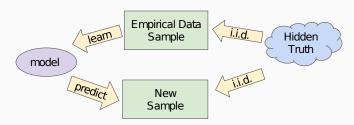


Image courtesy Google ML crash course

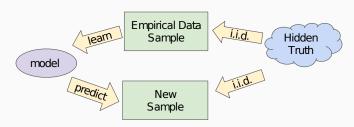


Image courtesy Google ML crash course

Both the training set and the test set are samples drawn from the hidden true distribution (also sometimes called population)

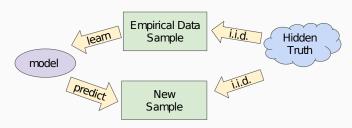


Image courtesy Google ML crash course

Both the training set and the test set are samples drawn from the hidden true distribution (also sometimes called population)

More discussion later once we study bias and variance

Question: What factors does the campus energy consumption depend on?

Answer:

Question: What factors does the campus energy consumption depend on?

#### Answer:

 • # People (More people ⇒ More Energy)

Question: What factors does the campus energy consumption depend on?

#### Answer:

- • # People (More people ⇒ More Energy)
- Temperature (Higher Temp. ⇒ Higher Energy)

Question: What factors does the campus energy consumption depend on?

#### Answer:

- # People (More people ⇒ More Energy)
- ullet Temperature (Higher Temp.  $\Longrightarrow$  Higher Energy)

# People	Temp (C)	Energy (kWh)
4000	30	30
4200	30	32
4200	35	40
3000	20	?
1000	45	?

Classification

- Classification
  - Output variable is discrete

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)
    - What is the quality of fruit? (Good, Bad)

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)
    - What is the quality of fruit? (Good, Bad)
- Regression

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)
    - What is the quality of fruit? (Good, Bad)
- Regression
  - Output variable is continuous

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)
    - What is the quality of fruit? (Good, Bad)
- Regression
  - Output variable is continuous
  - i.e.  $y_i \in \mathcal{R}$

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)
    - What is the quality of fruit? (Good, Bad)
- Regression
  - Output variable is continuous
  - i.e.  $y_i \in \mathcal{R}$
  - Examples Predicting:

- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)
    - What is the quality of fruit? (Good, Bad)
- Regression
  - Output variable is continuous
  - i.e.  $y_i \in \mathcal{R}$
  - Examples Predicting:
    - How much energy will campus consume?

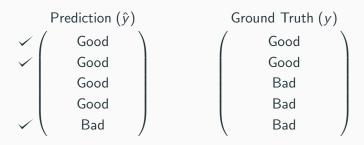
- Classification
  - Output variable is discrete
  - i.e.  $y_i \in \{1, \dots C\}$
  - Examples Predicting:
    - Will I get a loan? (Yes, No)
    - What is the quality of fruit? (Good, Bad)
- Regression
  - Output variable is continuous
  - i.e.  $y_i \in \mathcal{R}$
  - Examples Predicting:
    - How much energy will campus consume?
    - How much rainfall will fall?

### **Metrics for Classification**

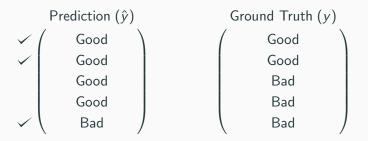
Ground Truth: From the actual training set

Prediction: Made by the model

## **Accuracy**



## **Accuracy**



$$\begin{aligned} \mathsf{Accuracy} &= \frac{||y = \hat{y}||}{||y||} \\ &= \frac{3}{5} = 0.6 \end{aligned}$$

## Types of Data: Imbalanced Classes

$$\begin{array}{c} 1 \; \mathsf{sample} \; \{ \; \left( \begin{array}{c} \mathsf{Bad} \\ \mathsf{Good} \\ \mathsf{Good} \\ \dots \\ \mathsf{Good} \end{array} \right) \\ & \mathsf{Imbalanced} \; \mathsf{Classes} \end{array}$$

## **Types of Data: Imbalanced Classes**

$$\begin{array}{c} 1 \; \mathsf{sample} \; \{ \; \left( \begin{array}{c} \mathsf{Bad} \\ \mathsf{Good} \\ \mathsf{Good} \\ \cdots \\ \mathsf{Good} \end{array} \right) \\ \\ \mathsf{Imbalanced} \; \mathsf{Classes} \end{array}$$

#### Cases for this:

- Cancer Screening
- Planet Detection

# **Accuracy Metrics: Precision**

Precision = 
$$\frac{||y = \hat{y} = Good||}{||\hat{y} = Good||} = \frac{2}{4} = 0.5$$

"the fraction of relevant instances among the retrieved instances", i.e. "out of the number of times we predict Good, how many times is the condition actually Good"

# **Accuracy Metrics: Precision**

Precision = 
$$\frac{||y = \hat{y} = Good||}{||\hat{y} = Good||} = \frac{2}{4} = 0.5$$

"the fraction of relevant instances among the retrieved instances", i.e. "out of the number of times we predict Good, how many times is the condition actually Good"

# **Accuracy Metrics: Recall**

Recall = 
$$\frac{||y = \hat{y} = \text{Good}||}{||y = \text{Good}||} = \frac{2}{3} = 0.67$$

"the fraction of the total amount of relevant instances that were actually retrieved"

# Types of Data: Imbalanced Classes

Given predictions of whether a tissue is cancerous or not (n = 100).

# **Types of Data: Imbalanced Classes**

Given predictions of whether a tissue is cancerous or not (n = 100).

$$\mbox{Accuracy} = \frac{98}{100} = 0.98 \qquad \qquad \mbox{Recall} = \frac{0}{1} = 0$$
 
$$\mbox{Precision} = \frac{0}{1} = 0$$

		Ground Truth	
		Yes	No
ted	Yes	0	1
redicted	No	1	98
Д			

		Ground Truth	
		Yes	No
ted	Yes	0	1
redicted	No	1	98
Д			

		Ground Truth	
		Yes	No
cted	Yes	True Positive	False Positive
redicted	No	False Negative	True Negative
Д			

		Ground Truth	
		Yes	No
cted	Yes	True Positive	False Positive
Predicted	No	False Negative	True Negative

$$Precision = \frac{T.P.}{T.P.+F.P.}$$

		Ground Truth	
		Yes	No
redicted	Yes	True Positive	False Positive
Predi	No	False Negative	True Negative

$$Precision = \frac{T.P.}{T.P.+F.P.}$$

		Ground Truth		
		Yes	No	
cted	Yes	True Positive	False Positive	
redicted	No	False Negative	True Negative	
Д				

$$Recall = \frac{T.P.}{T.P.+F.N.}$$

		Ground Truth		
		Yes	No	
redicted	Yes	True Positive	False Positive	
redi	No	False Negative	True Negative	
Д				

$$Recall = \frac{T.P.}{T.P.+F.N.}$$

## **Accuracy Metrics: F-Score**

		Ground Truth	
		Yes	No
ted	Yes	True Positive	False Positive
Predicted	No	False Negative	True Negative
Д			

$$F-$$
 Score =  $\frac{2 \times Precision \times Recall}{Precision + Recall}$ 

## **Accuracy Metrics: Matthew's Correlation Coefficient**

		Ground Truth	
		Yes	No
cted	Yes	True Positive	False Positive
redicted	No	False Negative	True Negative
Д			

$$\frac{\text{TP} \times \text{TN} - \text{FP} \times \text{FN}}{\sqrt{(\text{TP} + \text{FP})(\text{TP} + \text{FN})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}}$$

#### **Accuracy Metrics: Example**

For the data given below, calculate:

$$\begin{array}{cccc} & & G.T. \ Positive & G.T. \ Negative \\ Pred \ Positive & & 90 & 4 \\ Pred \ Negative & & 1 & 1 \end{array}$$

Precision = ?

Recall = ?

F-Score = ?

Matthew's Coeff. =?

## **Accuracy Metrics: Answer**

For the same data

G.T. Positive G.T. Negative Pred Positive 
$$\begin{pmatrix} 90 & 4 \\ 1 & 1 \end{pmatrix}$$

Precision = 
$$\frac{90}{94}$$
  
Recall =  $\frac{90}{91}$   
F-Score = 0.9524  
Matthew's Coeff. = 0.14

## Metrics for Regression MSE & MAE

Prediction 
$$(\hat{y})$$
 Ground Truth  $(y)$ 

$$\begin{pmatrix}
10 \\
20 \\
30 \\
40 \\
50 \\
60
\end{pmatrix}$$

Mean Squared Error (MSE) = 
$$\frac{\sum_{i=1}^{N} (\hat{y}_i - y_i)^2}{N}$$
Root Mean Square Error (RMSE) =  $\sqrt{\text{MSE}}$ 

## Accuracy Metrics: MAE & ME

Prediction 
$$(\hat{y})$$
 Ground Truth

 $\begin{pmatrix}
10 & & & \\
20 & & & \\
30 & & & \\
40 & & & \\
50 & & & & \\
60 & & & & \\
\end{pmatrix}$ 

Mean Absolute Error (ME) = 
$$\frac{\sum_{i=1}^{N} |\hat{y}_i - y_i|}{N}$$
Mean Error = 
$$\frac{\sum_{i=1}^{N} \hat{y}_i - y_i}{N}$$

## Accuracy Metrics: MAE & ME

Prediction 
$$(\hat{y})$$
 Ground Truth

 $\begin{pmatrix}
10 & & & \\
20 & & & \\
30 & & & \\
40 & & & \\
50 & & & & \\
60 & & & & \\
\end{pmatrix}$ 

Mean Absolute Error (ME) = 
$$\frac{\sum_{i=1}^{N} |\hat{y}_i - y_i|}{N}$$
Mean Error = 
$$\frac{\sum_{i=1}^{N} \hat{y}_i - y_i}{N}$$

Is there any downside with using mean error?

## Accuracy Metrics: MAE & ME

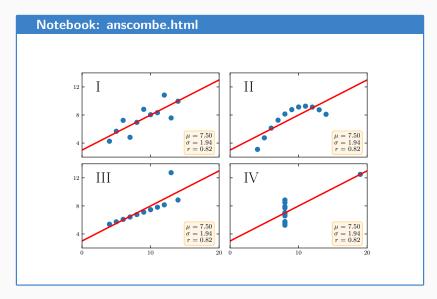
Prediction 
$$(\hat{y})$$
 Ground Truth

 $\begin{pmatrix}
10 & & & \\
20 & & & \\
30 & & & \\
40 & & & \\
50 & & & \\
60 & & & \\
\end{pmatrix}$ 

Mean Absolute Error (ME) = 
$$\frac{\sum_{i=1}^{N} |\hat{y}_i - y_i|}{N}$$
Mean Error = 
$$\frac{\sum_{i=1}^{N} \hat{y}_i - y_i}{N}$$

Is there any downside with using mean error? Errors can get cancelled out

## The Importance of Plotting



# The Importance of Plotting

Property	Value	Accross datasets
mean(X)	9	exact
mean(Y)	7.5	upto 3 decimal places
Linear regression line	y = 3.00 + 0.500x	upto 2 decimal places