Convention, Accuracy metrics, Classification, Regression

Nipun Batra

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IIT Gandhinagar

Revision: What is Machine Learning

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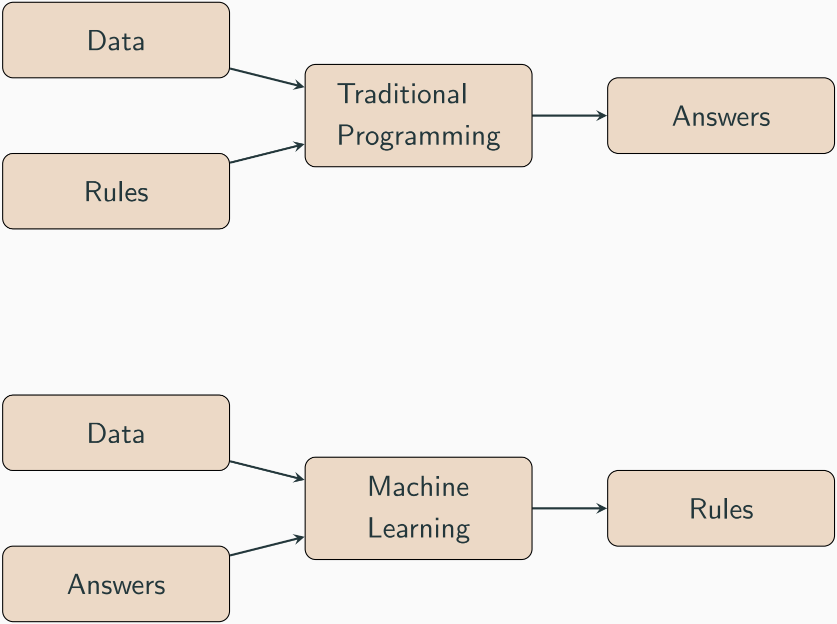
Each of the "—" can be slightly slanted. Similarly the horizontal line can be slanted. There can be some cases of 4 where the first "—" is at 45 degrees There can be some cases of 4 where the width of each stroke is different


Data
Rules
Traditional Programming
Answers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Revision: What is Machine Learning

"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.

Dataset

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

Dataset

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

- Size

Dataset

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

- Size
- Colour

Dataset

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

- Size
- Colour
- Texture

Dataset

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?

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

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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

Training Set

Colour	**Size**	**Texture**	**Condition**
Orange	Small	Smooth	Good
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The training set consists of two parts:

Training Set

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1. Features, Attributes or Covariates

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The training set consists of two parts:

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

Training Set

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
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Training Set

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

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

Training Set

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.

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

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    - Example $x_1 = \begin{bmatrix} Orange \\ Small \\ Smooth \end{bmatrix}$

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

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   - 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:

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1. Learn f: Condition $= f(\text{colour, size, texture})$

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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	?

Generalisation

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

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- Ideally - we want to predict “well” on all possible inputs. But, can we test that?

Generalisation

- 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.

Generalisation

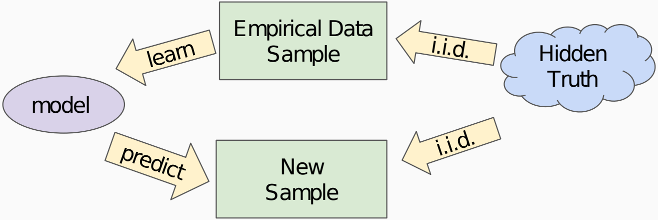

Image courtesy Google ML crash course

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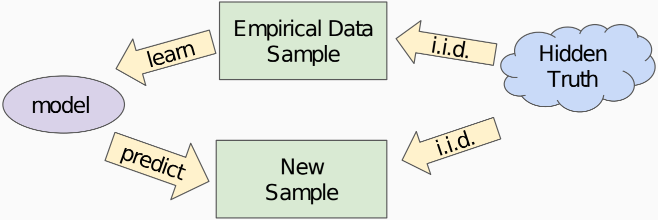

Image courtesy Google ML crash course

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

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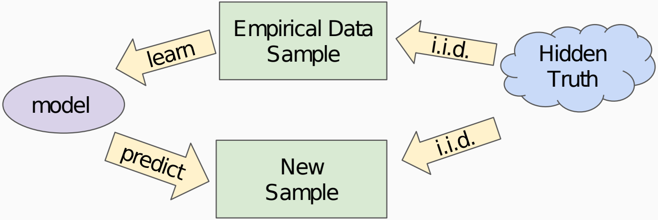

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Both the training set and the test set are samples drawn from the hidden true distribution (also sometimes called population)

More discussion later once we study bias and variance

Second ML Task: Predict energy consumption of campus

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

Answer:

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

Answer:

- # People (More people $\implies$ More Energy)
- Temperature (Higher Temp. $\implies$ Higher Energy)

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

Classification v/s Regression

- Classification

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    - Output variable is discrete

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    - Will I get a loan? (Yes, No)

Classification v/s Regression

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

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    - Output variable is continuous

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- Classification
  - Output variable is discrete
  - i.e. $y_i \in \{1, \cdots C\}$
  - 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 v/s Regression

- Classification
  - Output variable is discrete
  - i.e. $y_i \in \{1, \cdots C\}$
  - Examples - Predicting:
    - Will I get a loan? (Yes, No)
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  - Examples - Predicting:
    - How much energy will campus consume?

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

$$\begin{array}{cc} \text{Prediction } (\hat{y}) & \text{Ground Truth } (y) \\ \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix} & \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Bad} \end{pmatrix} \end{array}$$

Ground Truth: From the actual training set
Prediction: Made by the model

Accuracy

$$\begin{array}{cc} & \text{Prediction } (\hat{y}) \\ \checkmark & \\ \checkmark & \\ & \\ & \\ \checkmark & \end{array}\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix} \qquad \begin{array}{c} \text{Ground Truth } (y) \end{array}\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Bad} \end{pmatrix}$$

Accuracy

$$
\begin{array}{cc}
\text{Prediction } (\hat{y}) & \text{Ground Truth } (y) \\
\begin{array}{c} \checkmark \\ \checkmark \\ \\ \\ \checkmark \end{array}
\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix}
&
\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Bad} \end{pmatrix}
\end{array}
$$

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

Types of Data: Imbalanced Classes

$$
\begin{array}{r}
\text{1 sample } \{ \\
\text{100 samples } \left\{ \begin{array}{l} \\ \\ \\ \\ \end{array} \right.
\end{array}
\begin{pmatrix} \text{Bad} \\ \text{Good} \\ \text{Good} \\ \dots \\ \text{Good} \end{pmatrix}
$$

Imbalanced Classes

Types of Data: Imbalanced Classes

$$\begin{array}{r} \text{1 sample} \left\{ \vphantom{\text{Bad}} \right. \\ \text{100 samples} \left\{ \begin{array}{c} \\ \\ \\ \\ \end{array} \right. \end{array} \begin{pmatrix} \text{Bad} \\ \text{Good} \\ \text{Good} \\ \dots \\ \text{Good} \end{pmatrix} \qquad \text{Imbalanced Classes}$$

Cases for this:

- Cancer Screening
- Planet Detection

Accuracy Metrics: Precision

$$
\begin{array}{ll}
 & \text{Prediction } (\hat{y}) \\
\begin{array}{l} \rightarrow \checkmark \\ \rightarrow \checkmark \\ \rightarrow \\ \rightarrow \\ \end{array} & \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix}
\end{array}
\qquad
\begin{array}{c}
\text{Ground Truth } (y) \\
\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Good} \end{pmatrix}
\end{array}
$$

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

"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

$$
\begin{array}{ccc}
 & \text{Prediction } (\hat{y}) & \text{Ground Truth } (y) \\
\begin{array}{l} \rightarrow \checkmark \\ \rightarrow \checkmark \\ \rightarrow \\ \rightarrow \\ \end{array} & \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix} & \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Good} \end{pmatrix}
\end{array}
$$

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"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

$$
\begin{array}{cc}
 & \text{Prediction } (\hat{y}) \\
\begin{array}{c} \rightarrow \checkmark \\ \rightarrow \checkmark \\ \\ \\ \rightarrow \end{array} &
\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix}
\end{array}
\qquad
\begin{array}{c}
\text{Ground Truth } (y) \\
\begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Good} \end{pmatrix}
\end{array}
$$

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

"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 ($n = 100$).

$$\begin{array}{c} \text{Prediction } (\hat{y}) \\ \begin{array}{r} \rightarrow \\ \\ \\ \\ \\ \end{array}\begin{pmatrix} \text{Yes} \\ \text{No} \\ \text{No} \\ \dots \\ \text{No} \end{pmatrix} \end{array} \qquad \begin{array}{c} \text{Ground Truth } (y) \\ \begin{array}{r} \\ \\ \\ \\ \rightarrow \end{array}\begin{pmatrix} \text{No} \\ \text{No} \\ \dots \\ \text{No} \\ \text{Yes} \end{pmatrix} a \end{array}$$

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

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$$\text{Accuracy} = \frac{98}{100} = 0.98 \qquad \begin{aligned} \text{Recall} &= \frac{0}{1} = 0 \\ \text{Precision} &= \frac{0}{1} = 0 \end{aligned}$$

Accuracy Metrics: Confusion Matrix

		Ground Truth	
		Yes	No
Predicted	Yes	0	1
	No	1	98

Accuracy Metrics: Confusion Matrix

		Ground Truth: Yes	Ground Truth: No
Predicted	Yes	0	1
	No	1	98

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

Accuracy Metric: Confusion Matrix

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

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

Accuracy Metric: Confusion Matrix

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Accuracy Metric: Confusion Matrix

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

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

Accuracy Metrics: F-Score

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

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

Accuracy Metrics: Matthew's Correlation Coefficient

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

Matthew's correlation coefficient =

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

Accuracy Metrics: Example

For the data given below, calculate:

$$\begin{array}{r c} & \begin{array}{cc} \text{G.T. Positive} & \text{G.T. Negative} \end{array} \\ \begin{array}{r} \text{Pred Positive} \\ \text{Pred Negative} \end{array} & \begin{pmatrix} 90 & 4 \\ 1 & 1 \end{pmatrix} \end{array}$$

Precision = ?

Recall = ?

F-Score = ?

Matthew's Coeff. = ?

Accuracy Metrics: Answer

For the same data

$$\begin{array}{r c}
 & \begin{array}{cc} \text{G.T. Positive} & \text{G.T. Negative} \end{array} \\
\begin{array}{r} \text{Pred Positive} \\ \text{Pred Positive} \end{array} & \begin{pmatrix} 90 & 4 \\ 1 & 1 \end{pmatrix}
\end{array}$$

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

Metrics for Regression MSE & MAE

$$\text{Prediction } (\hat{y}) \quad \begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix} \qquad \text{Ground Truth } (y) \quad \begin{pmatrix} 20 \\ 30 \\ 40 \\ 50 \\ 60 \end{pmatrix}$$

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

$$\text{Root Mean Square Error (RMSE)} = \sqrt{\text{MSE}}$$

Accuracy Metrics: MAE & ME

$$\text{Prediction } (\hat{y}) \quad \begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix} \qquad \text{Ground Truth} \quad \begin{pmatrix} 20 \\ 30 \\ 40 \\ 50 \\ 60 \end{pmatrix}$$

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

$$\text{Mean Error} = \frac{\sum_{i=1}^{N} \hat{y}_i - y_i}{N}$$

Accuracy Metrics: MAE & ME

$$\begin{array}{cc} \text{Prediction } (\hat{y}) & \text{Ground Truth} \\ \begin{pmatrix} 10 \\ 20 \\ 30 \\ 40 \\ 50 \end{pmatrix} & \begin{pmatrix} 20 \\ 30 \\ 40 \\ 50 \\ 60 \end{pmatrix} \end{array}$$

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

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Is there any downside with using mean error?

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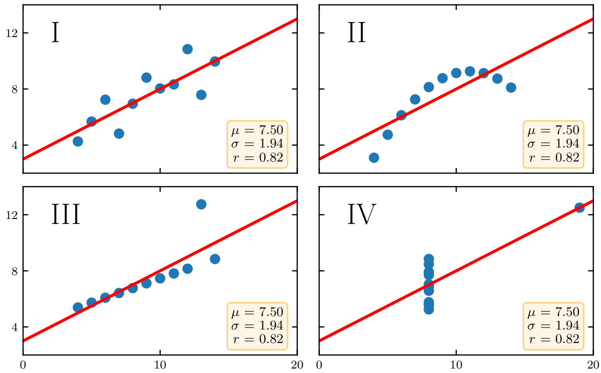
Is there any downside with using mean error?

Errors can get cancelled out

The Importance of Plotting

Notebook: anscombe.html



Anscombe's Quartet

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