Testing and Error Metrics

Machine Learning

(Largely based on slides from Luis Serrano)

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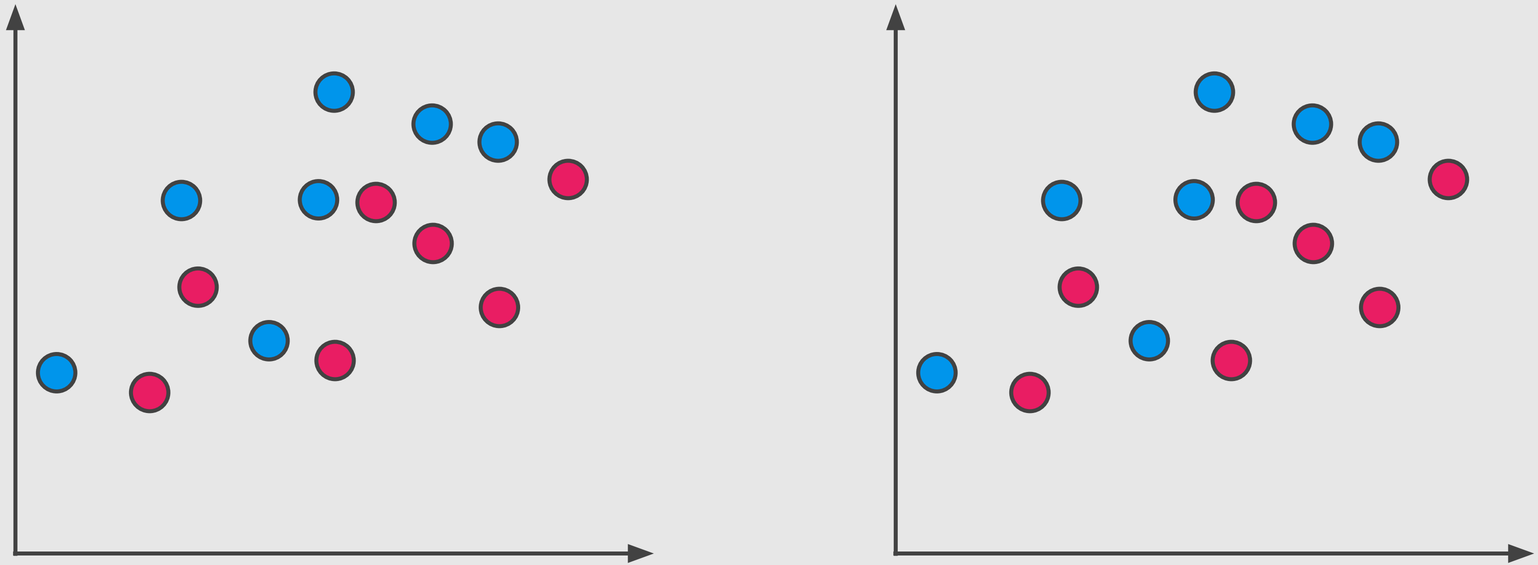
MC886, August 28, 2019

How well is my model doing?

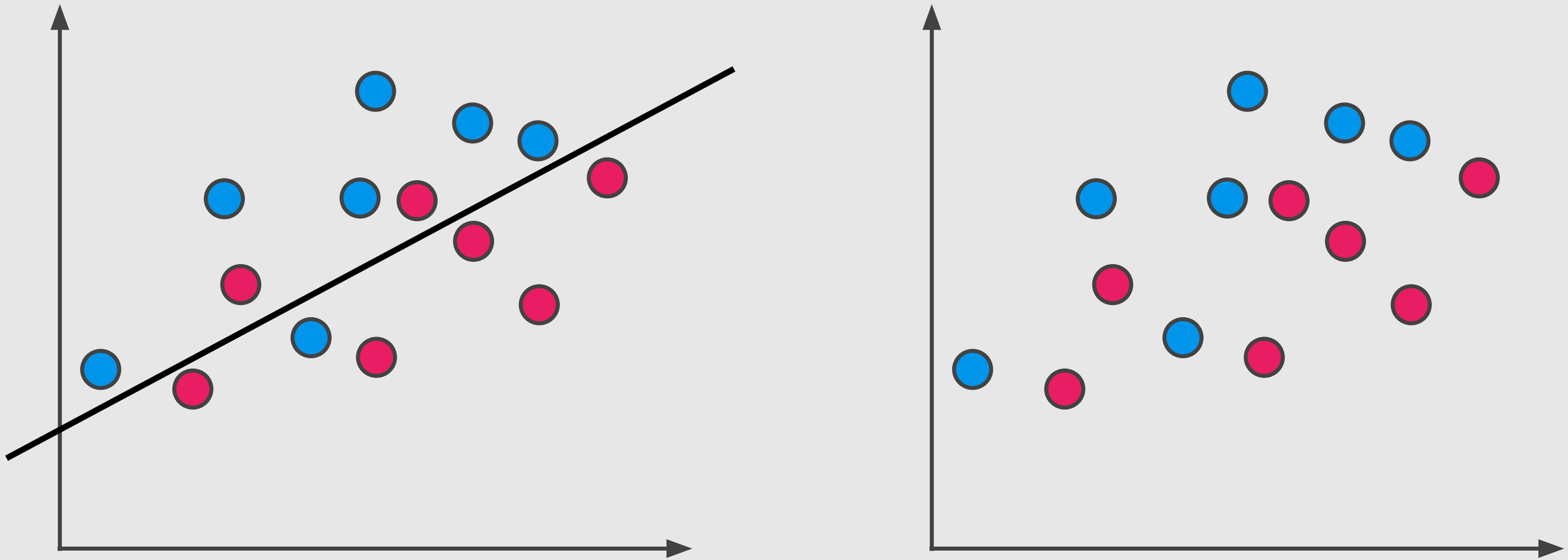
Today's Agenda

- Testing and Error Metrics
  - Training, Testing
  - Accuracy
  - Precision
  - Recall
  - F-Score

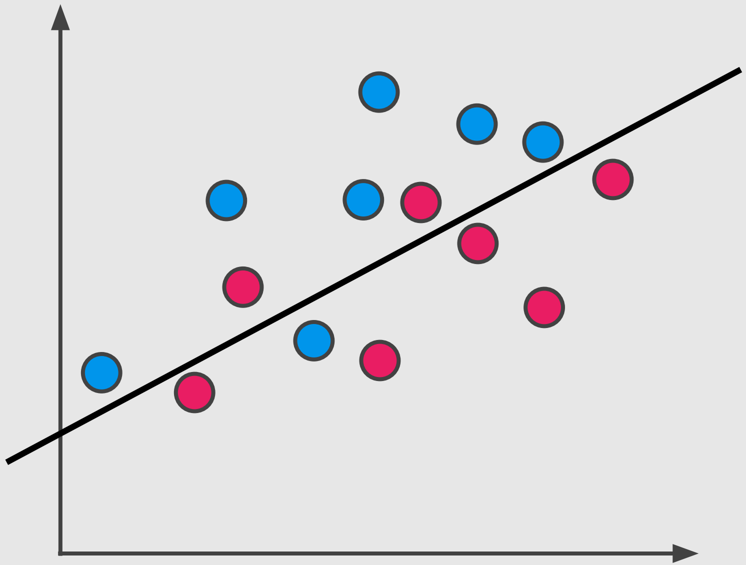
Which model is better?

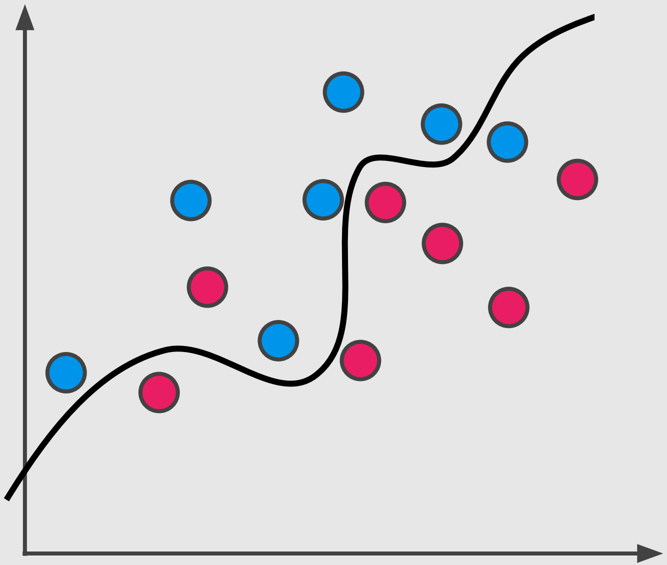


Which model is better?

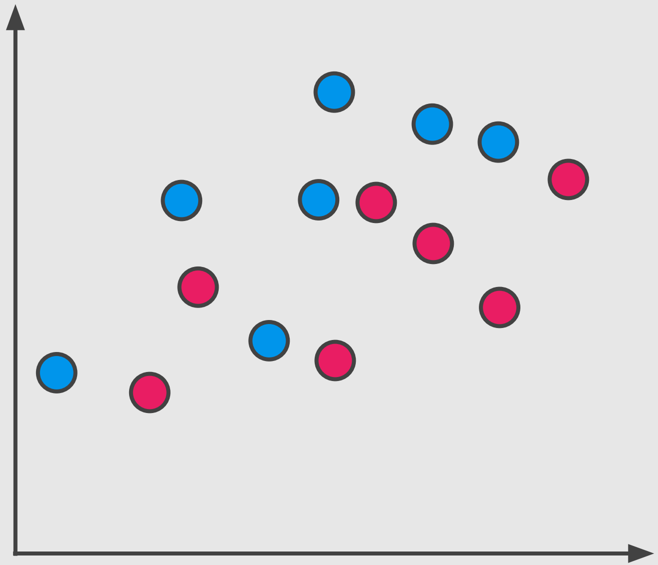


Which model is better?

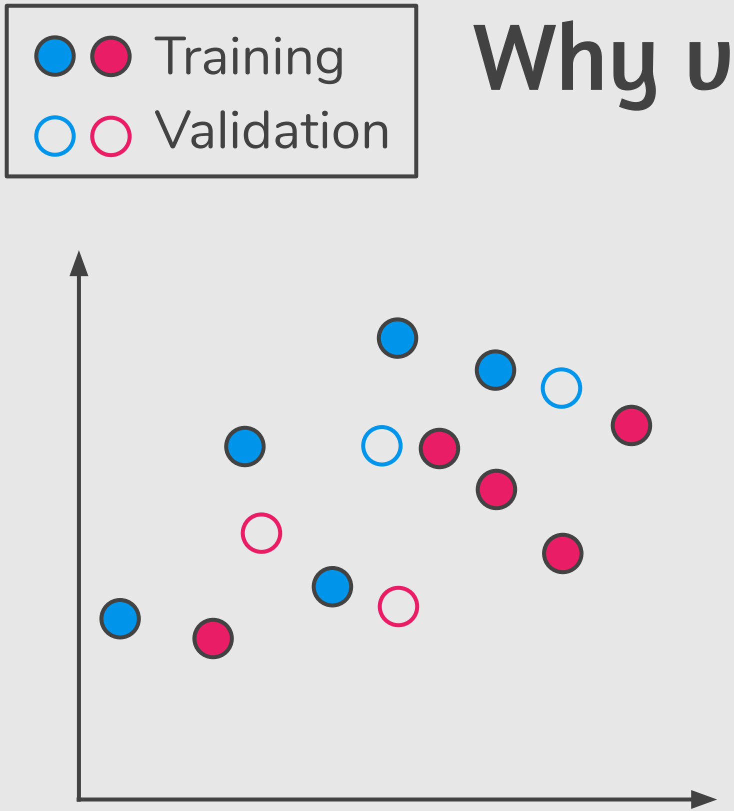




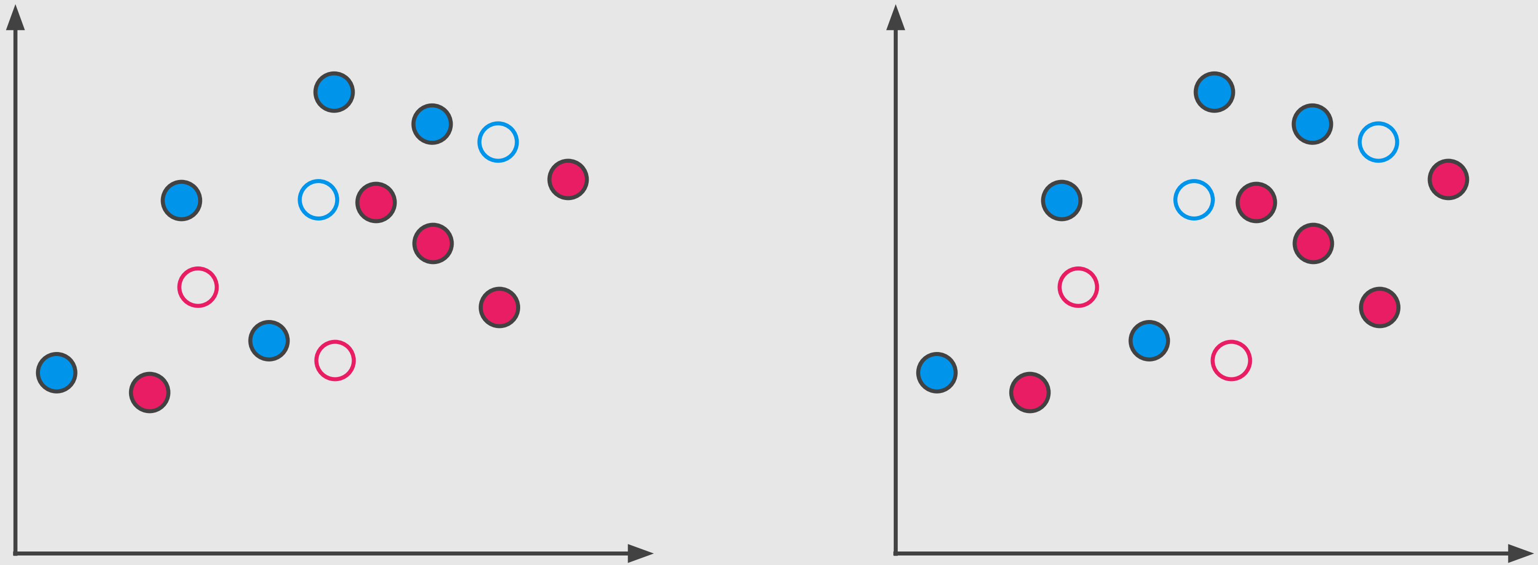
Why validating?



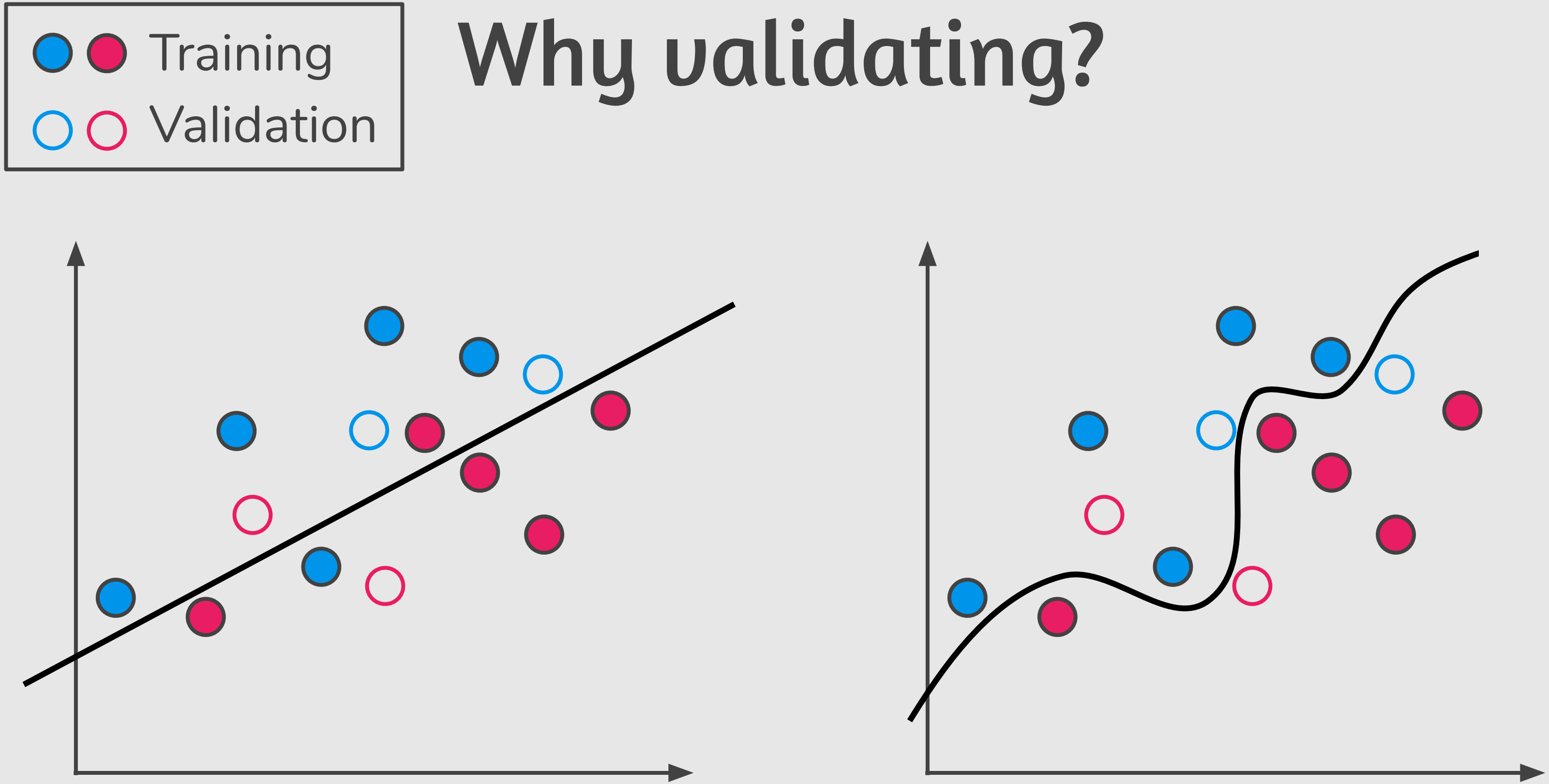
Why validating?



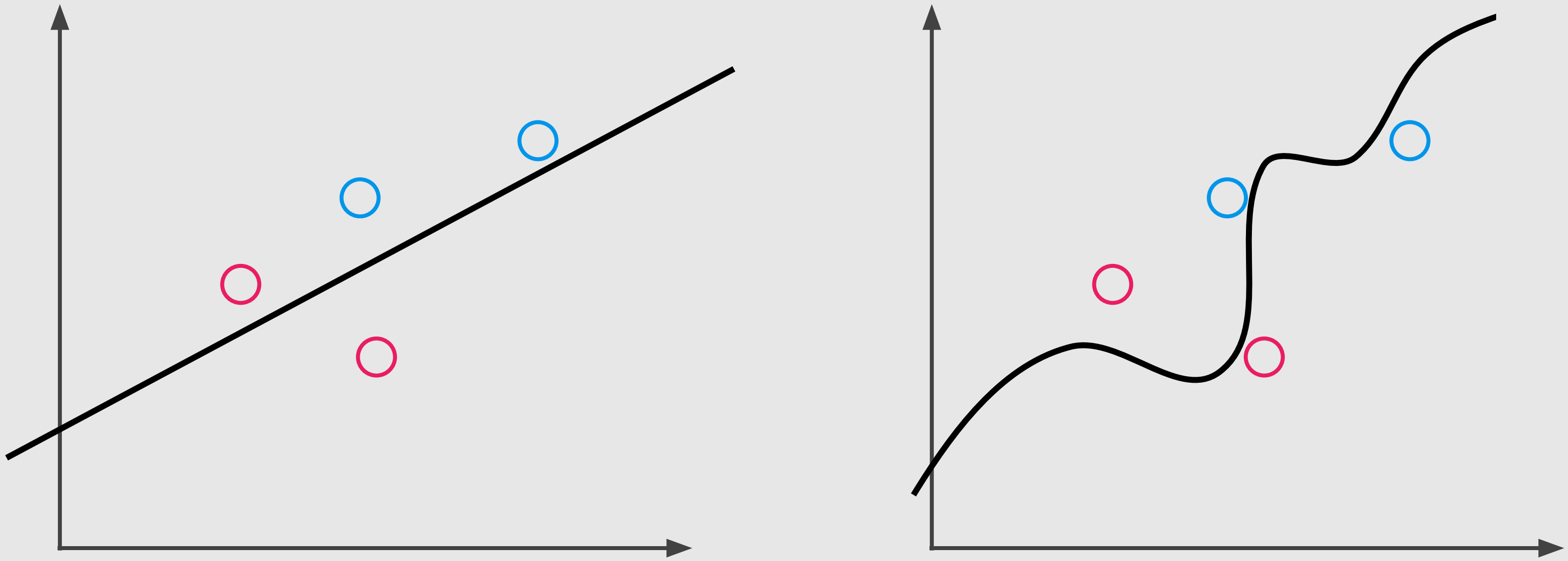
Why validating?



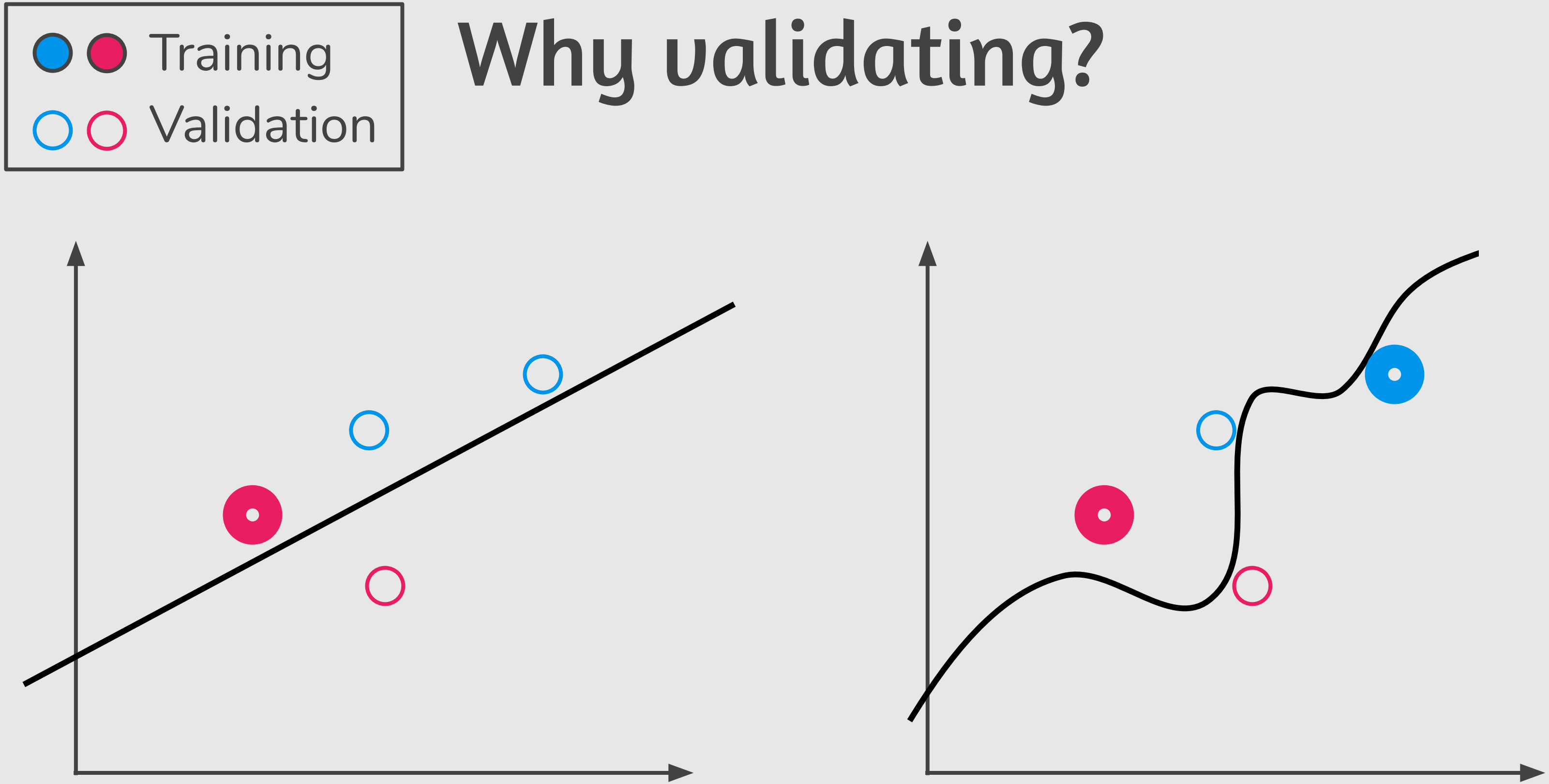
Why validating?



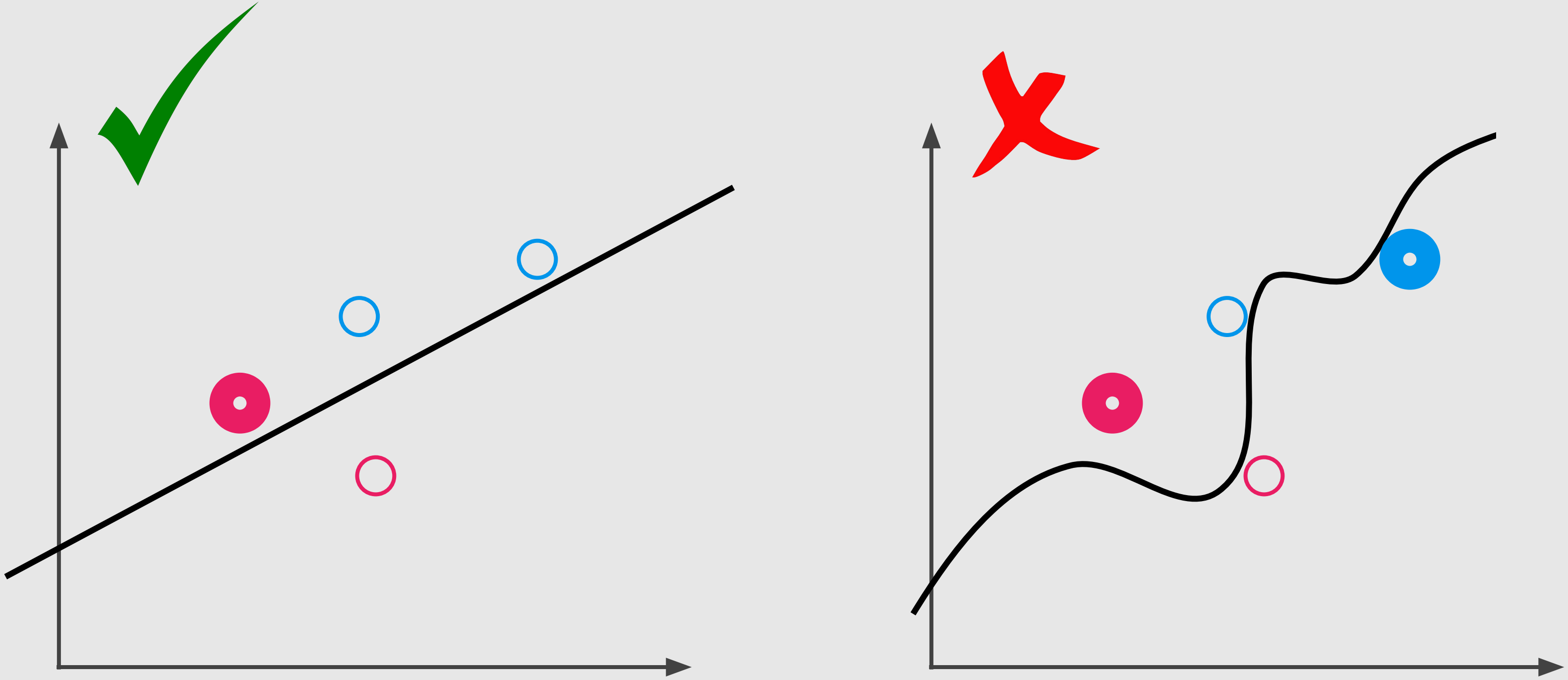
Why validating?



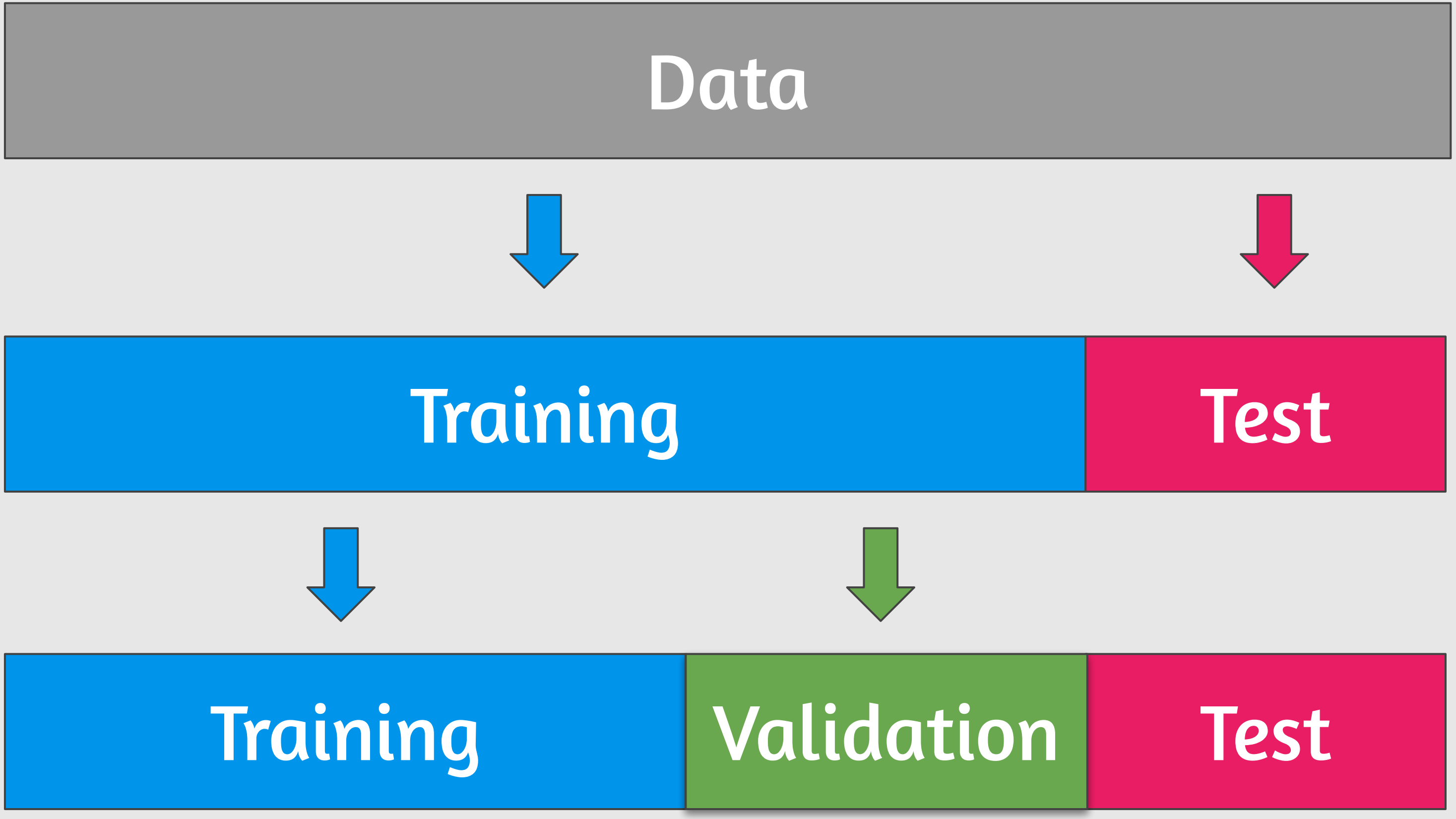
Why validating?



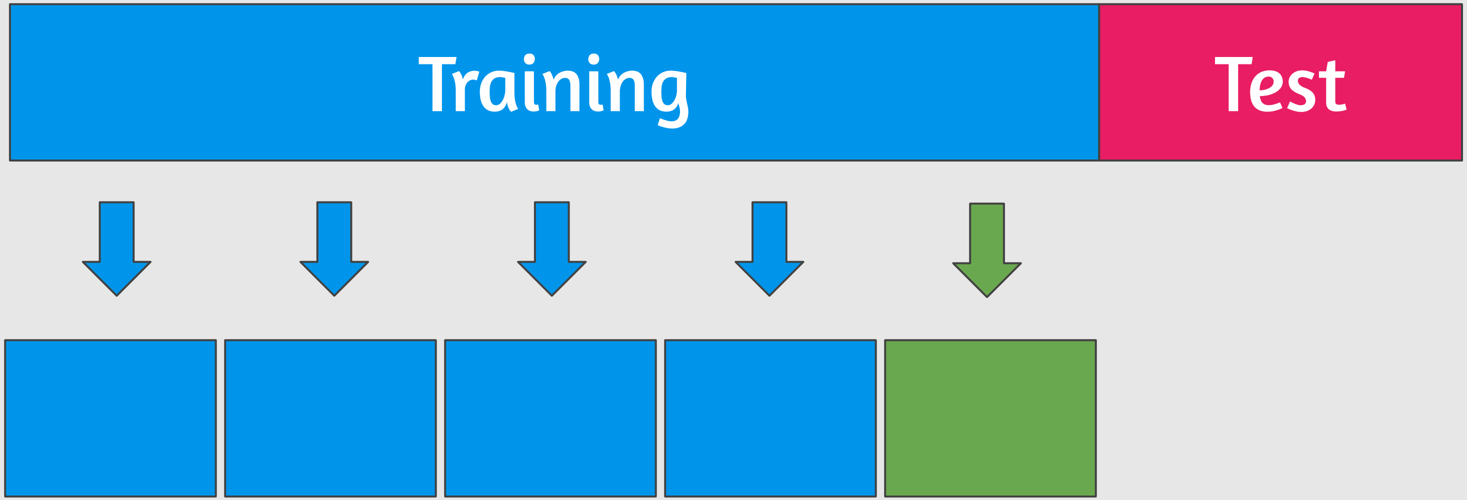
Why validating?



Friends don’t let friends use testing data for training


Data
Training
Test
Training
Validation
Test

k-fold Cross Validation



k-fold Cross Validation

Training

Validation

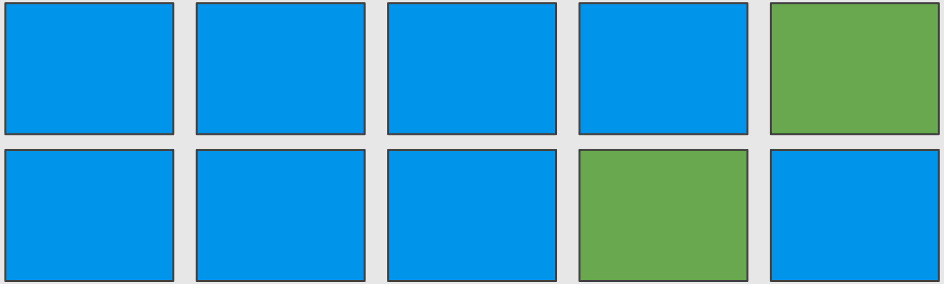
$k = 5$

k-fold Cross Validation

$k = 5$

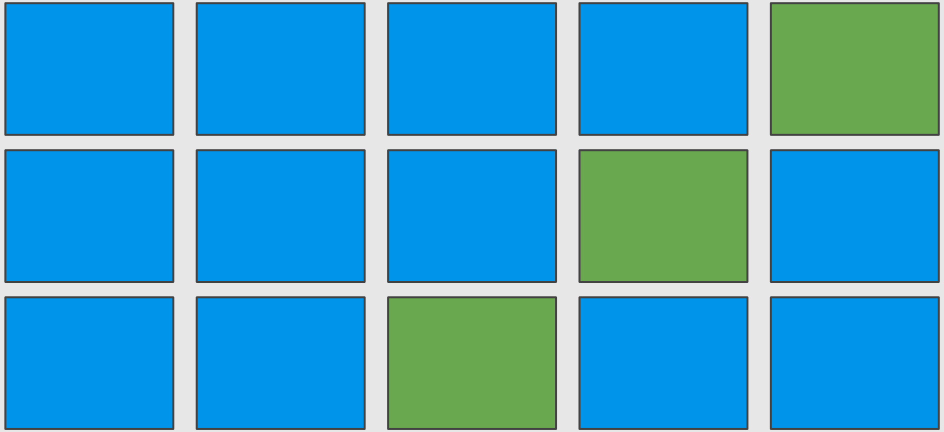
k-fold Cross Validation

k = 5



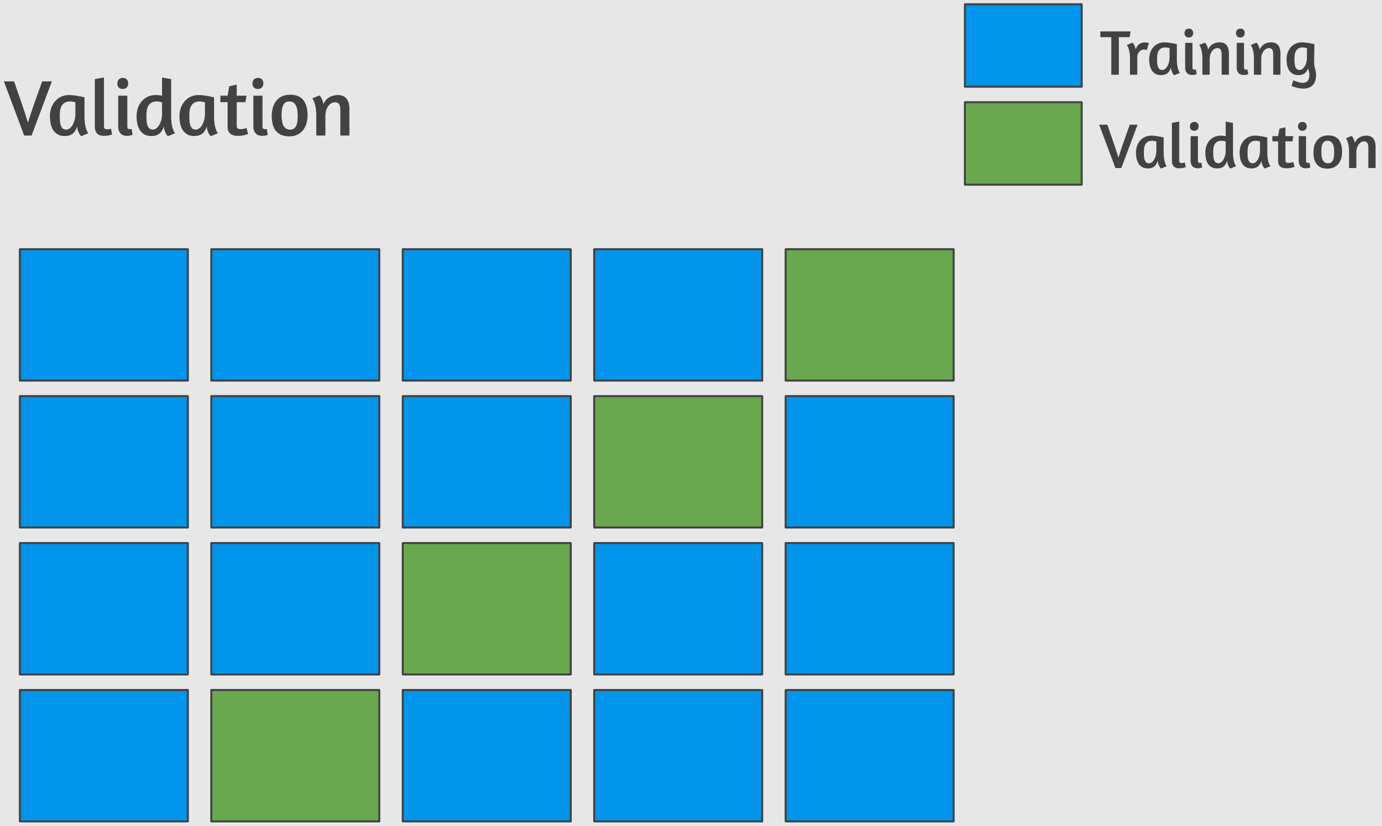
k-fold Cross Validation

k = 5



k-fold Cross Validation

$k = 5$



k-fold Cross Validation

k = 5

k×2-fold Cross Validation

Training

Validation

$k = 5$

k×2-fold Cross Validation

k = 5

k×2-fold Cross Validation

Training

Validation

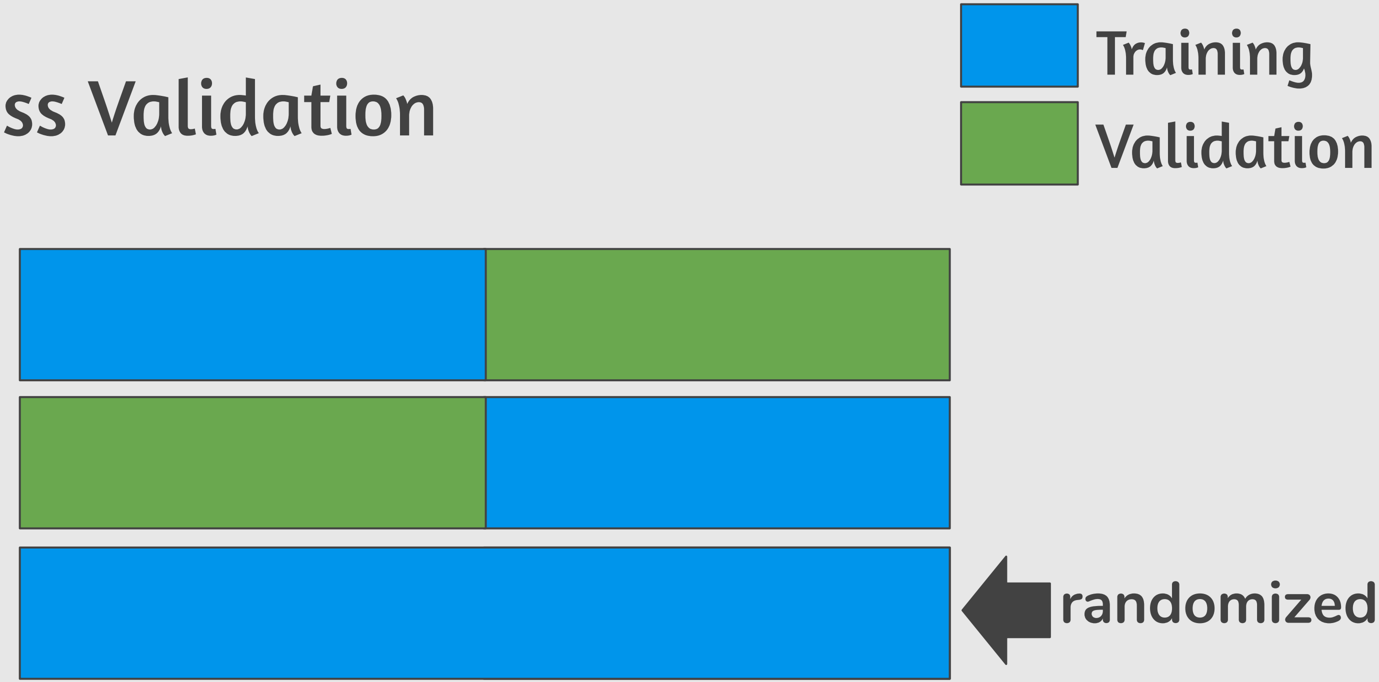
$k = 5$

k×2-fold Cross Validation

k = 5

k×2-fold Cross Validation

$k = 5$

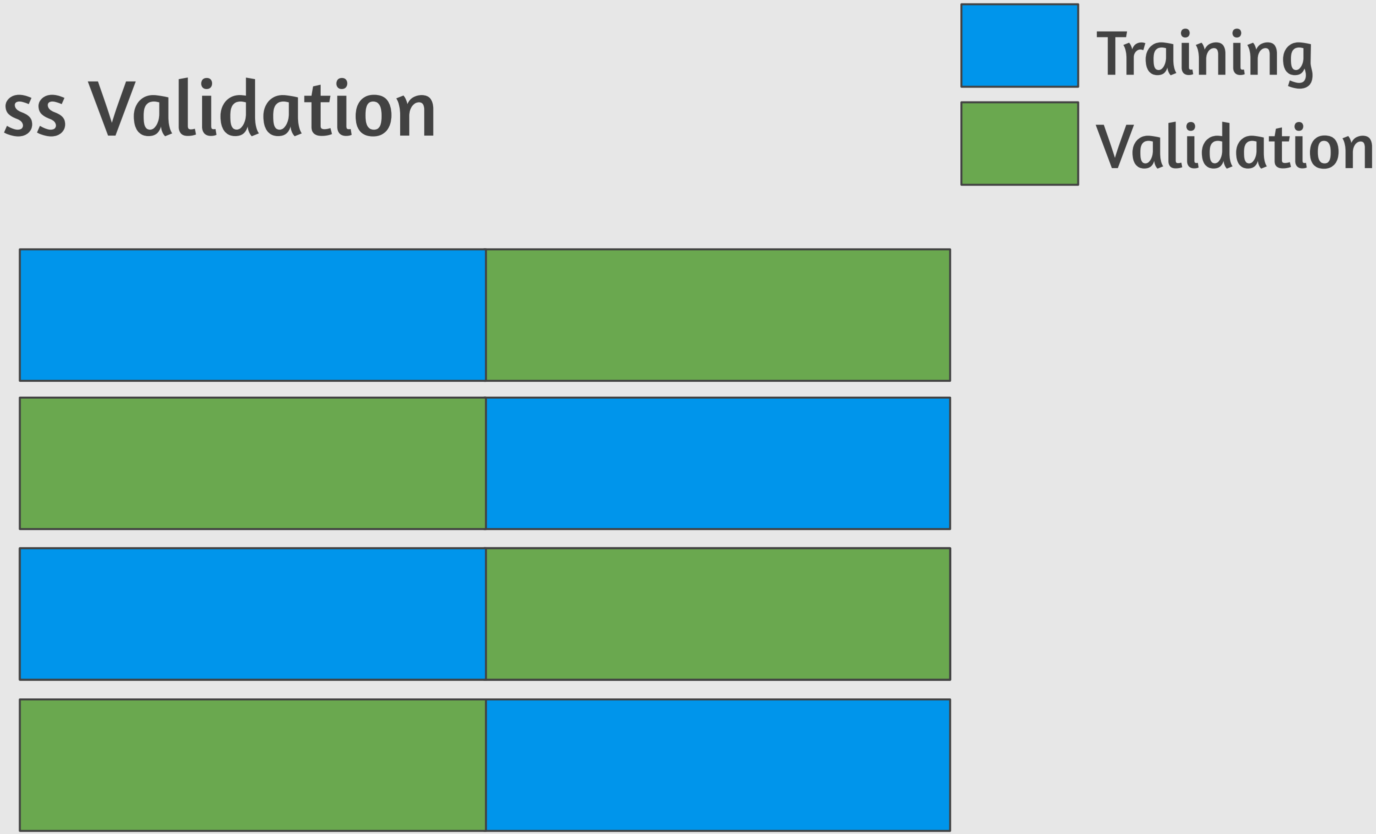


k×2-fold Cross Validation

k = 5

k×2-fold Cross Validation

$k = 5$



k×2-fold Cross Validation

Training
Validation

k = 5

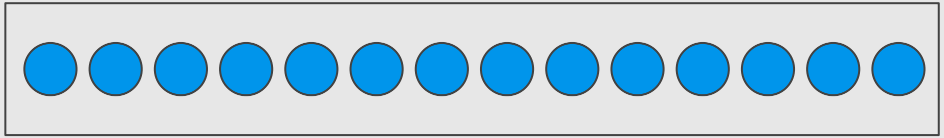
...

k times = k×2 folds

Randomizing in Cross Validation

Training

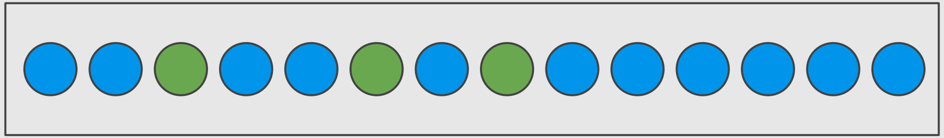
Validation



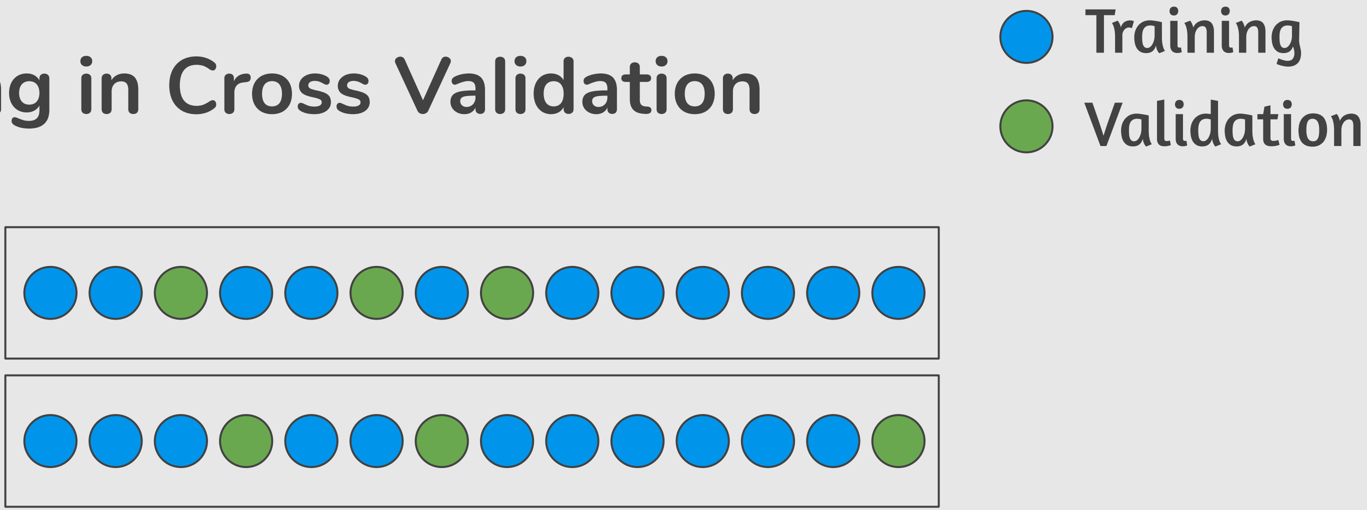
Randomizing in Cross Validation

Training

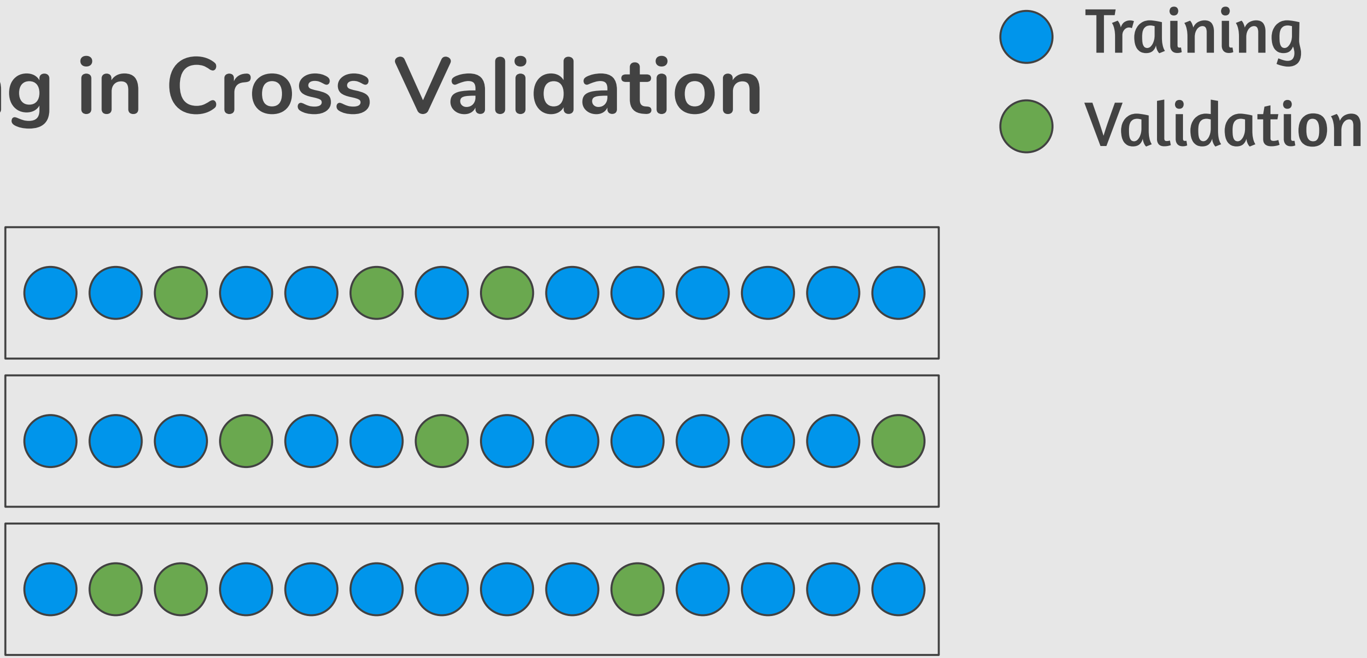
Validation



Randomizing in Cross Validation

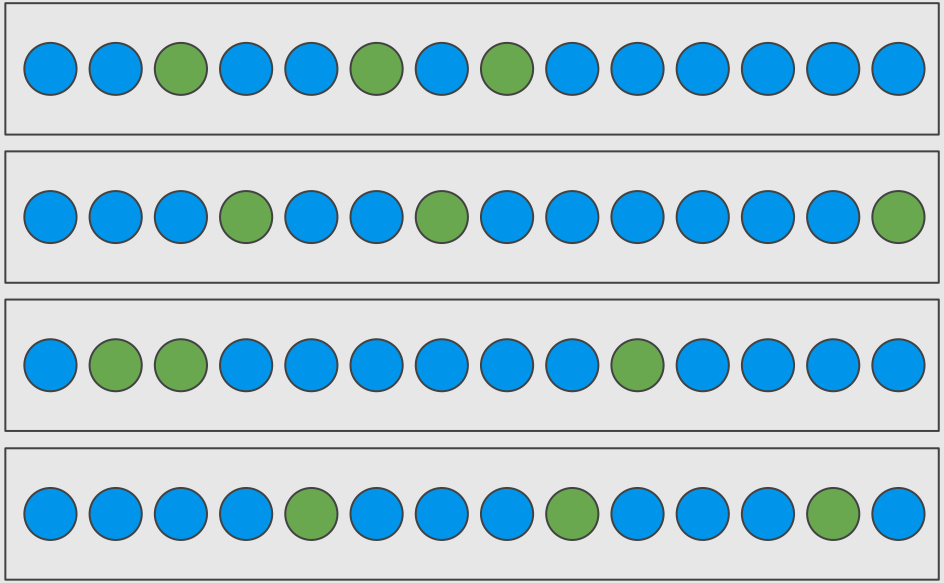


Randomizing in Cross Validation

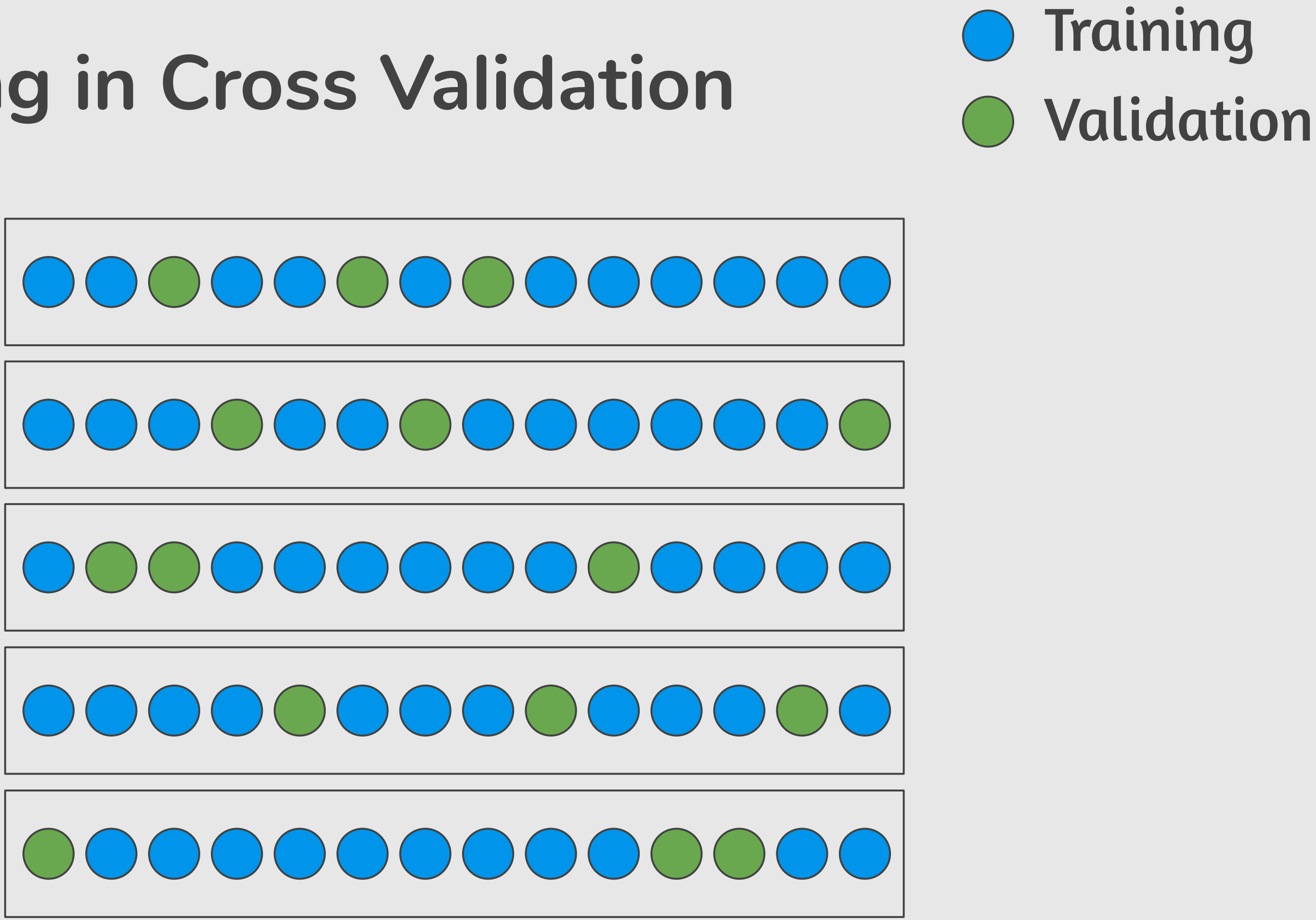


Randomizing in Cross Validation

Training
Validation



Randomizing in Cross Validation



MO850A: Tópicos Avançados em Ciência da Computação I — Scientific Methodology

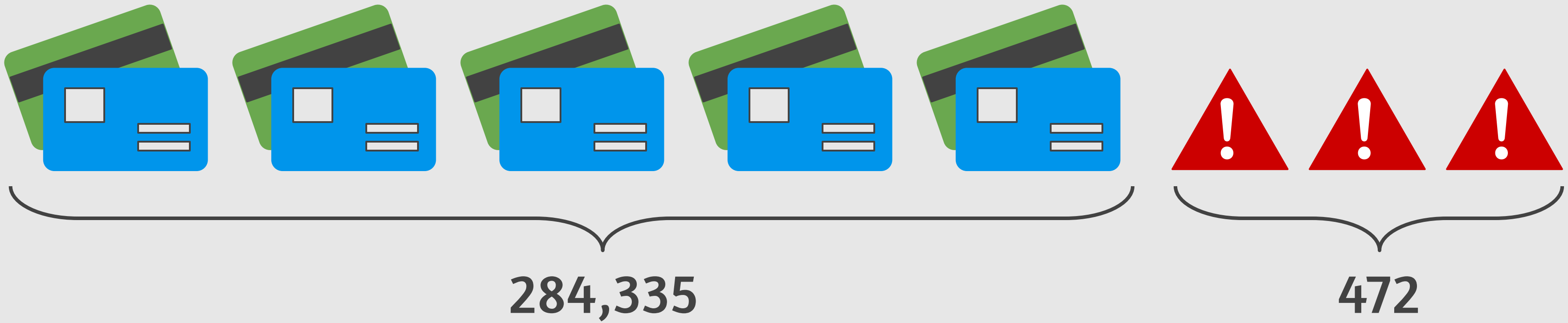
Prof. Jacques Wainer (IC/Unicamp)

Evaluation Metrics

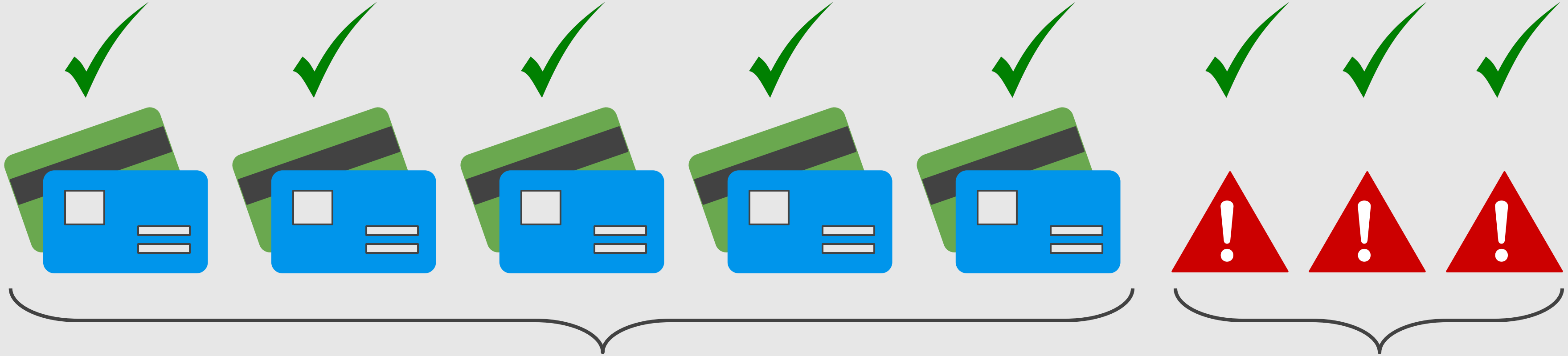
How well is my model doing?

Credit Card Fraud

Credit Card Fraud



Credit Card Fraud

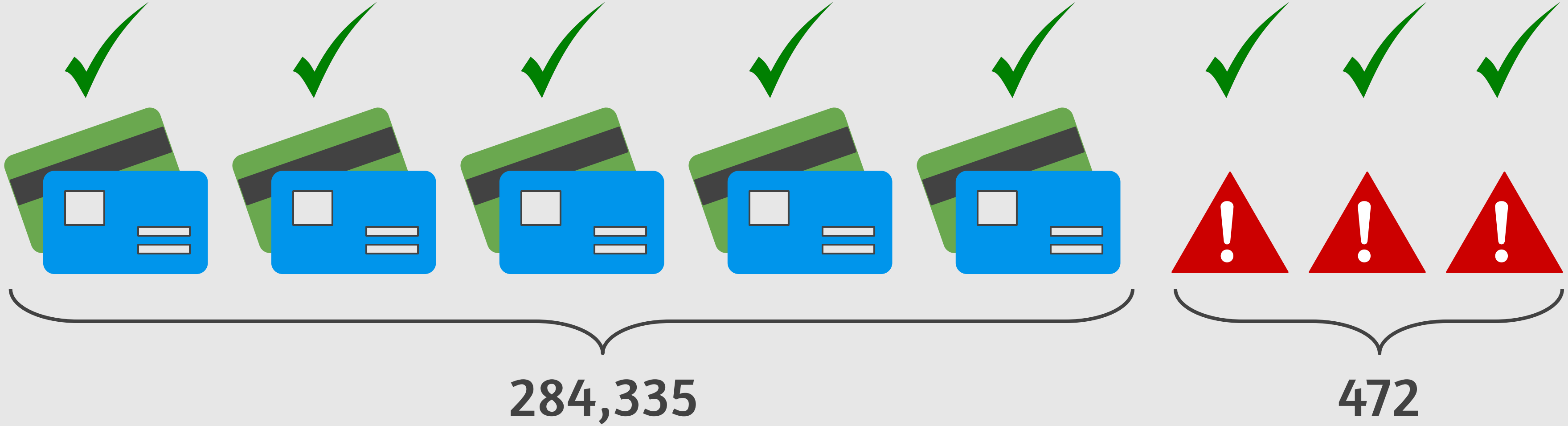


284,335

472

Model: All transactions are good.

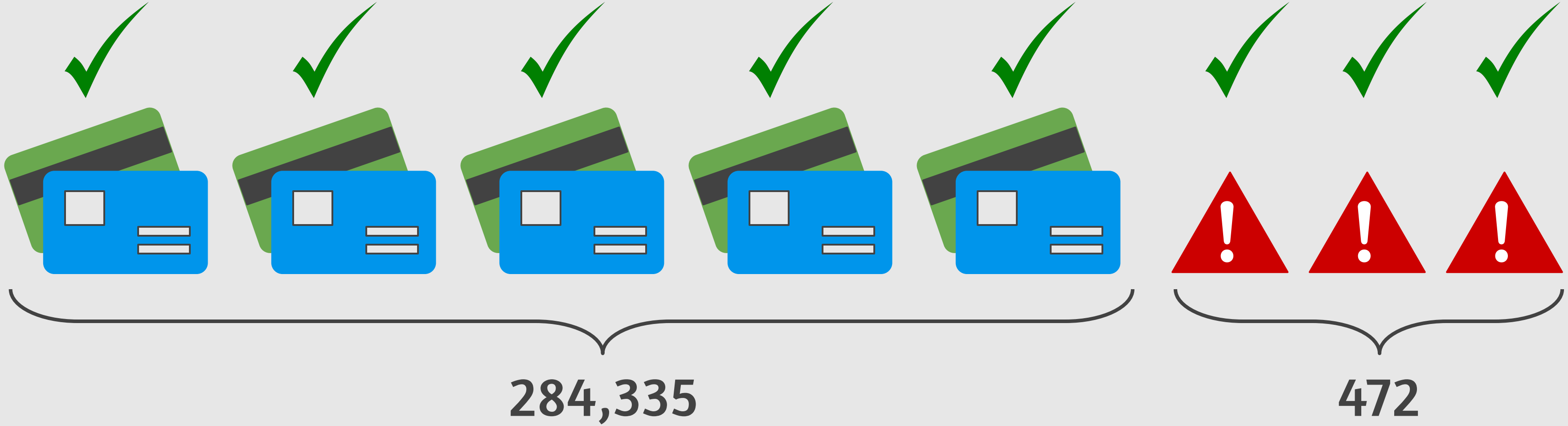
Credit Card Fraud



Model: All transactions are good.

$$\text{Correct} = \frac{284{,}335}{284{,}807} = 99.83\%$$

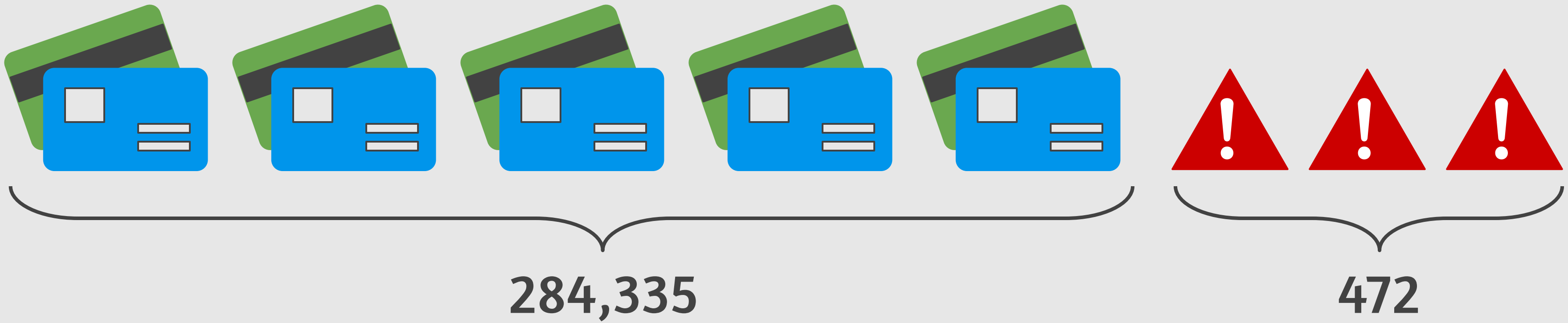
Credit Card Fraud



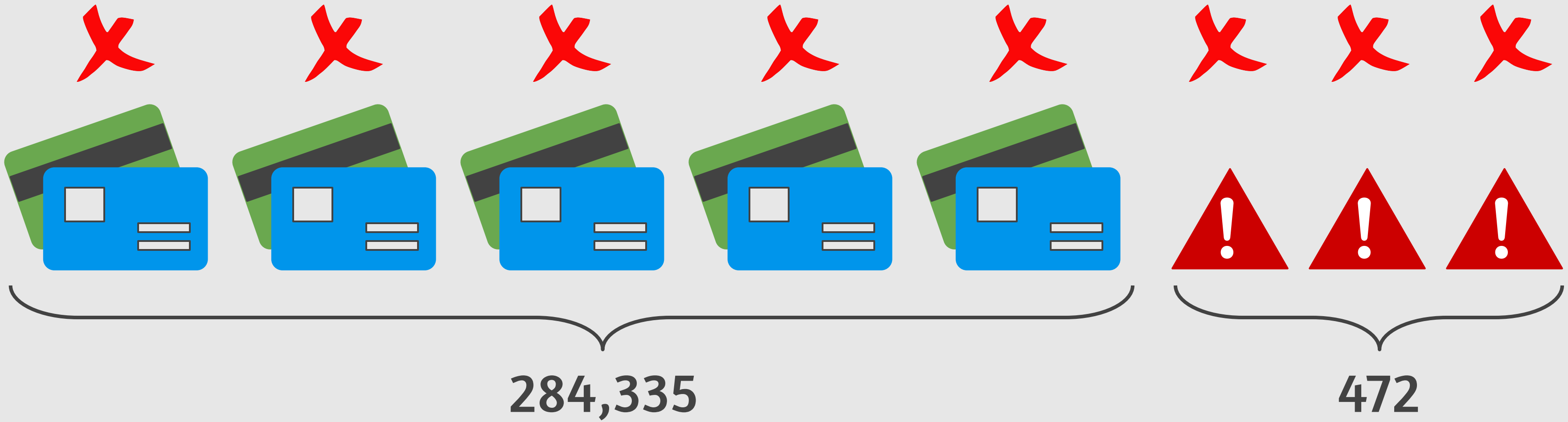
Model: All transactions are good.

Problem: I’m not catching any of the bad ones!

Credit Card Fraud

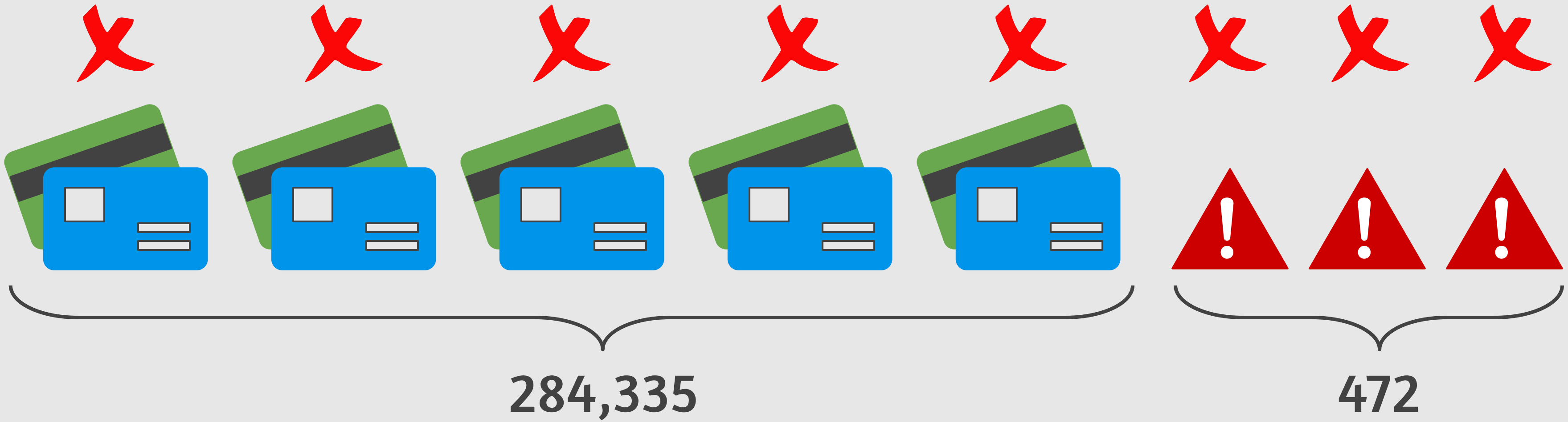


Credit Card Fraud



Model: All transactions are fraudulent.

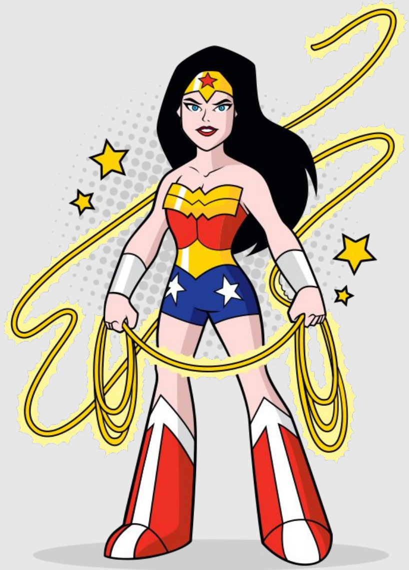
Credit Card Fraud



Model: All transactions are fraudulent.

Problem: I’m accidently catching all the good ones!

Medical Model



Health

Sick

Spam Classifier Model

Not Spam

Spam

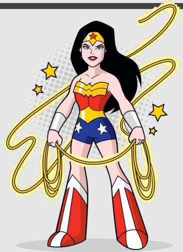
Confusion Matrix Table

	Diagnosed Sick	Diagnosed Healthy
Sick		
Healthy		

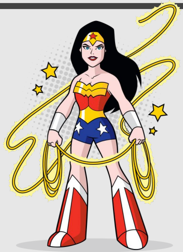
Confusion Matrix Table

	Diagnosed Sick	Diagnosed Healthy
Sick	True Positive 	
Healthy		

Confusion Matrix Table

	Diagnosed Sick	Diagnosed Healthy
Sick	True Positive 	
Healthy		True Negative 

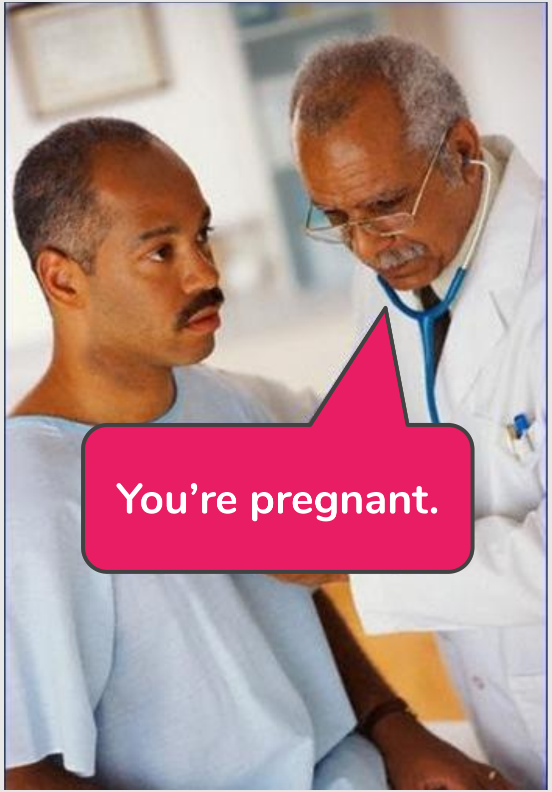
Confusion Matrix Table

	Diagnosed Sick	Diagnosed Healthy
Sick	True Positive 	False Negative 
Healthy		True Negative 

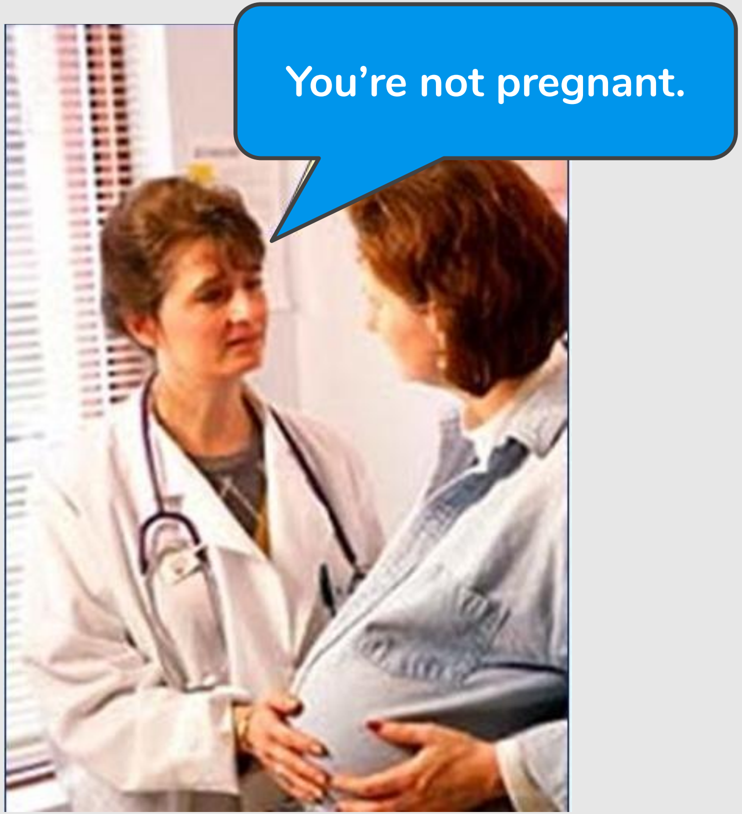
Confusion Matrix Table

	Diagnosed Sick	Diagnosed Healthy
Sick	True Positive 	False Negative 
Healthy	False Positive 	True Negative 

Type I Error
(False Positive)



Type II Error
(False Negative)



Confusion Matrix Table

10,000 patients

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1000	200
Healthy	800	8000

Confusion Matrix Table

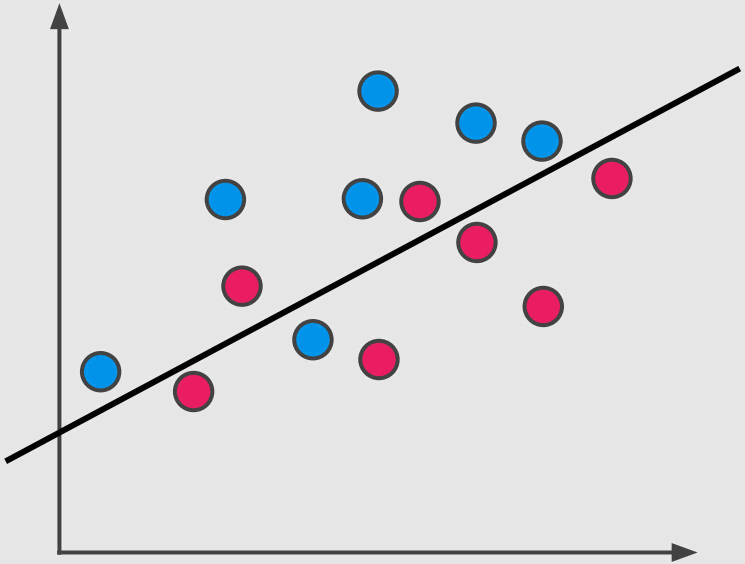
	Sent to Spam Folder	Sent to Inbox
Spam	True Positive	False Negative
Not Spam	False Positive	True Negative

Confusion Matrix Table

1,000 emails

Email \ Folder	Spam Folder	Inbox
Spam	100	170
Not Spam	30	700

Confusion Matrix Table

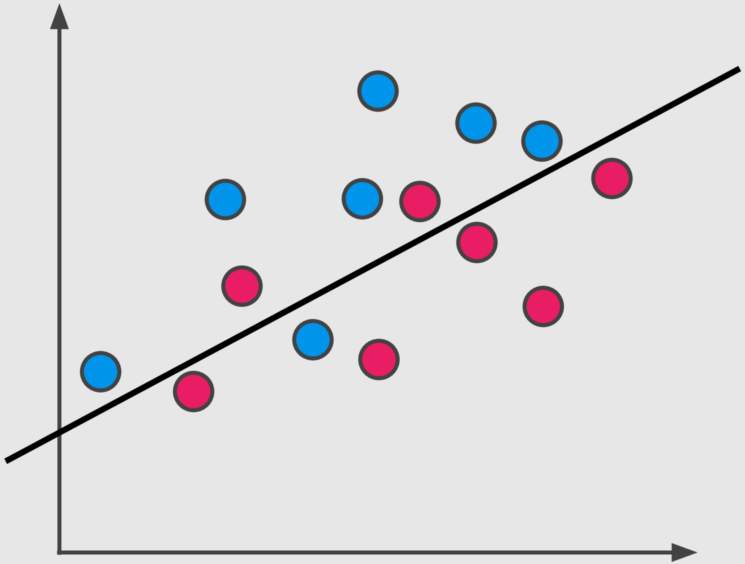


Prediction

Data

	Guessed Positive	Guessed Negative
Positive		
Negative		

Confusion Matrix Table

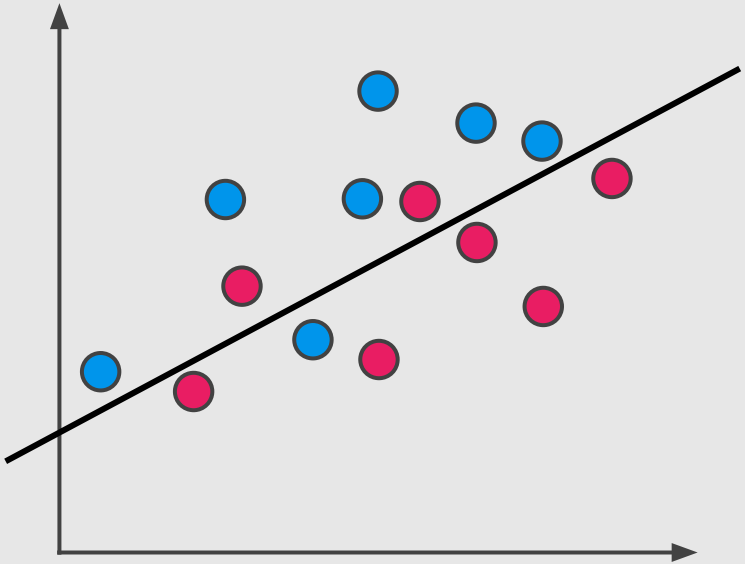


Prediction

Data

	Guessed Positive	Guessed Negative
Positive	6 True positives	
Negative		

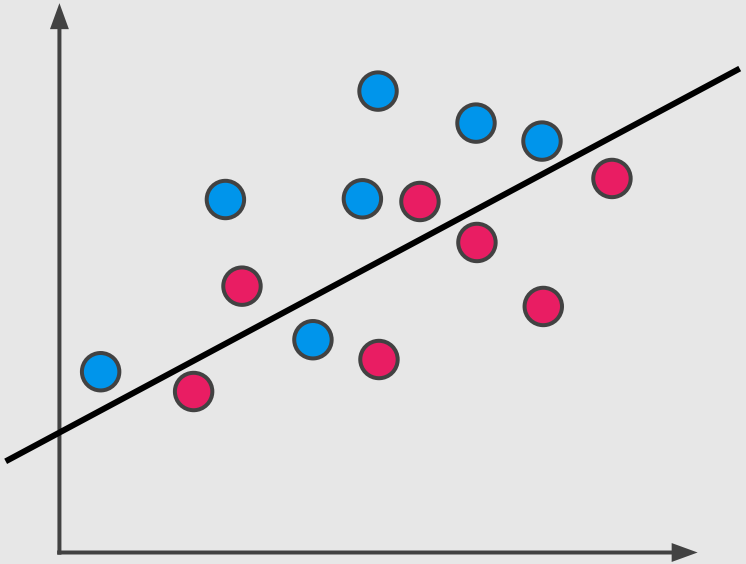
Confusion Matrix Table



Prediction

Data	Guessed Positive	Guessed Negative
Positive	6 True positives	
Negative		5 True negatives

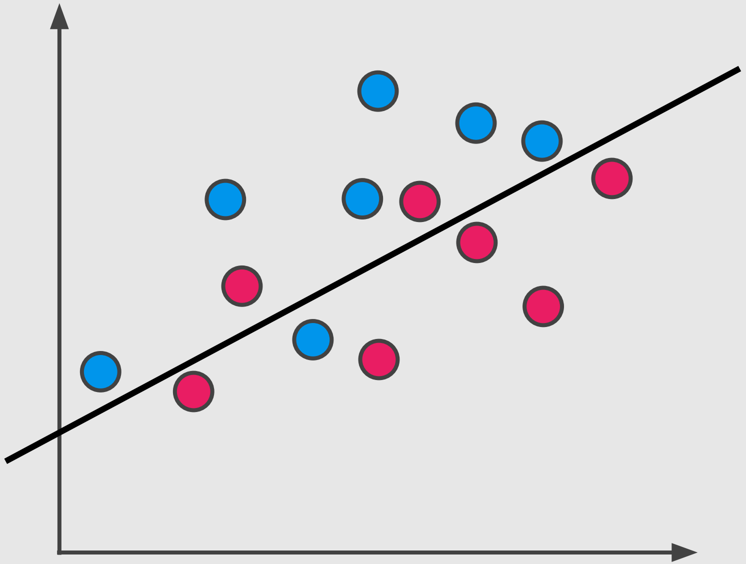
Confusion Matrix Table



Prediction

Data		Guessed Positive	Guessed Negative
	Positive	6 True positives	
	Negative	2 False positives	5 True negatives

Confusion Matrix Table

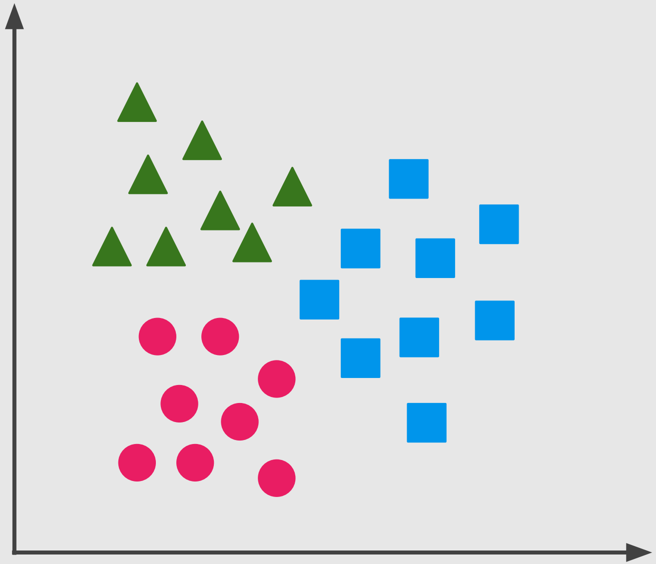


Prediction

Data		Guessed Positive	Guessed Negative
	Positive	6 True positives	1 False negative
	Negative	2 False positives	5 True negatives

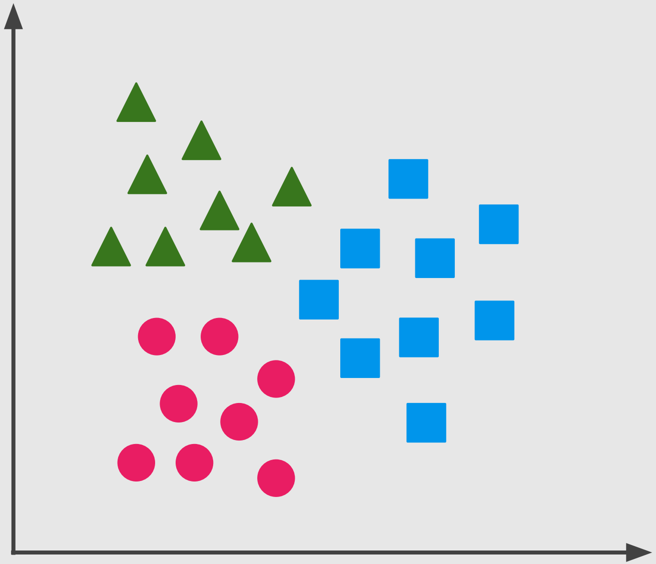
Confusion Matrix Table (n classes)

Class 1: ▲
Class 2: ■
Class 3: ●



Confusion Matrix Table (n classes)

Class 1: ▲
Class 2: ■
Class 3: ●

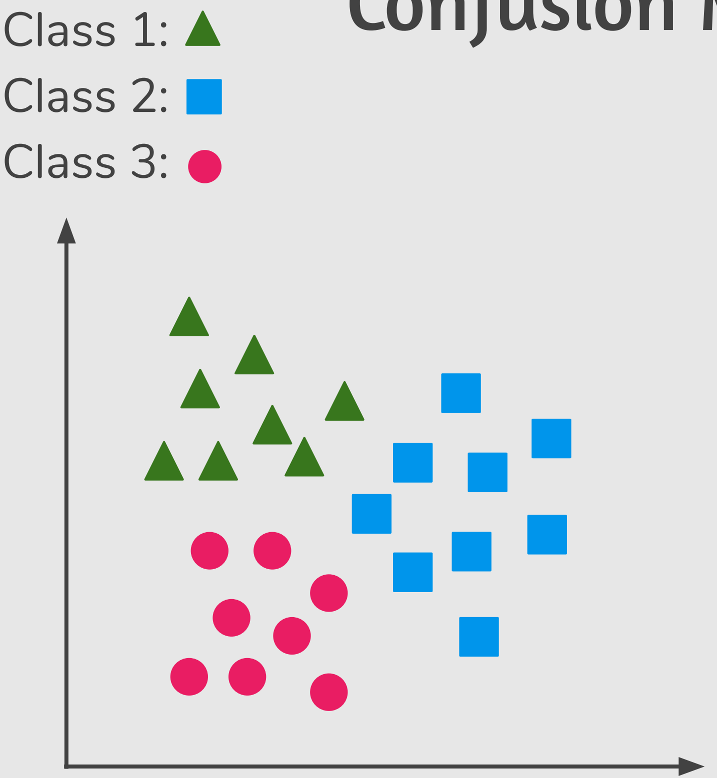


Predicted Class

True Class

	Guessed Class 1	Guessed Class 2	Guessed Class 3
Class 1			
Class 2			
Class 3			

Confusion Matrix Table (n classes)

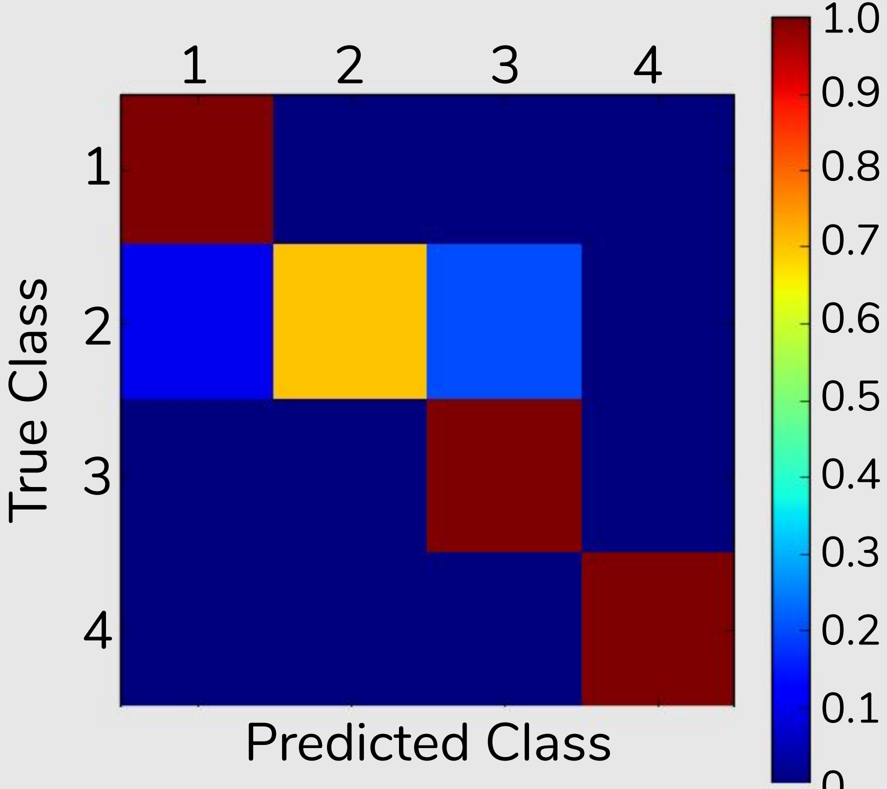


Predicted Class

True Class

	Guessed Class 1	Guessed Class 2	Guessed Class 3
Class 1	5	2	1
Class 2	3	6	0
Class 3	0	1	7

Confusion Matrix Table (n classes)



Accuracy

Patients	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Diagnosis

Accuracy

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Accuracy:
Out of all the **patients**, how many did we classify correctly?

Accuracy

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Accuracy:
Out of all the **patients**, how many did we classify correctly?

$$\text{Accuracy} = \frac{1{,}000 + 8{,}000}{}$$

Accuracy

Diagnosis

Patients	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Accuracy:
Out of all the **patients**, how many did we classify correctly?

Accuracy =

$$\frac{1{,}000 + 8{,}000}{10{,}000} = 90\%$$

Accuracy

Folder

Email	Spam Folder	Inbox
Spam	100	170
Not Spam	30	700

Accuracy:
Out of all the **emails**, how many did we classify correctly?

Accuracy

Folder

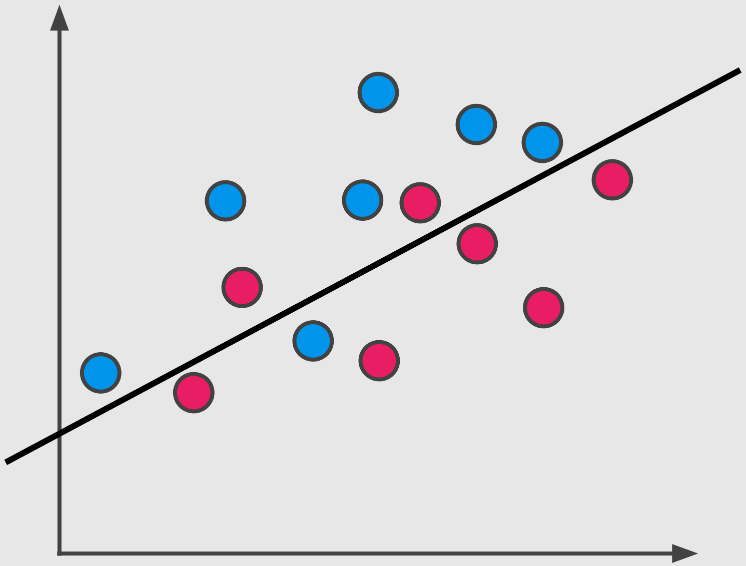
Email		Spam Folder	Inbox
	Spam	100	170
	Not Spam	30	700

Accuracy:
Out of all the **emails**, how many did we classify correctly?

Accuracy =

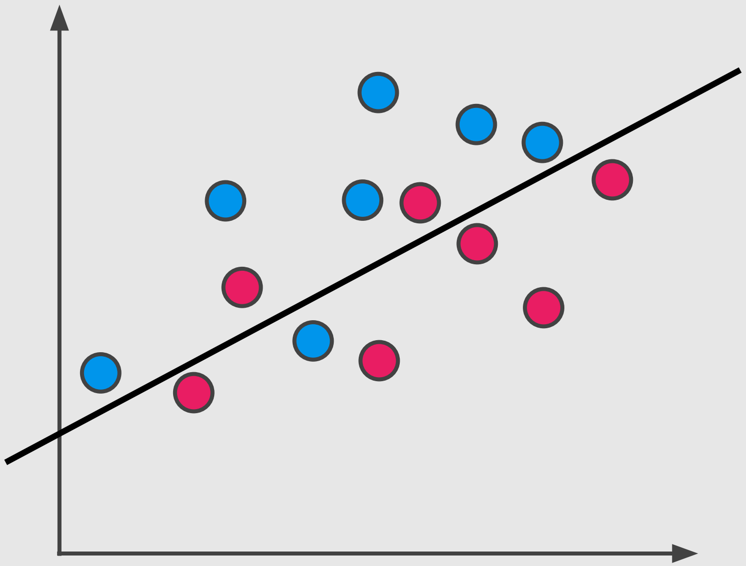
$$\frac{100 + 700}{1{,}000} = 80\%$$

Accuracy



Accuracy:
Out of all the **data**, how many points did we classify correctly?

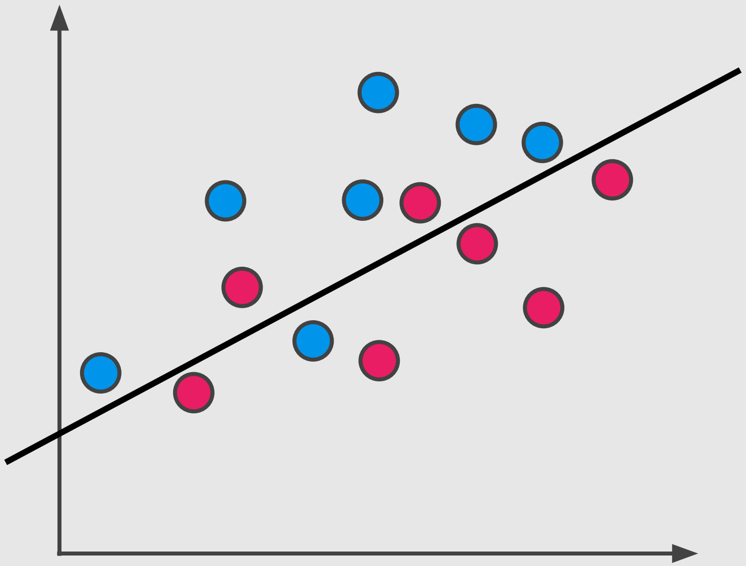
Accuracy



Accuracy:
Out of all the **data**, how many points did we classify correctly?

$$\text{Accuracy} = \frac{\text{Correctly Classified Points}}{\text{All points}}$$

Accuracy



Accuracy:
Out of all the **data**, how many points did we classify correctly?

Accuracy =

$$\frac{\text{Correctly Classified Points}}{\text{All points}}$$

$$\frac{11}{11 + 3} = 78.57\%$$

Accuracy

Prediction

Transactions		Fraudulent	Not Fraudulent
	Fraudulent	0	472
	Not Fraudulent	0	284,335

Accuracy:
Out of all the **transactions**, how many did we classify correctly?

Accuracy =

$$\frac{0 + 284{,}335}{284{,}807} = 99.83\%$$

Overall (Normalized) Accuracy

Transactions	Prediction: Fraudulent	Prediction: Not Fraudulent
Fraudulent	0	472
Not Fraudulent	0	284,335

Overall (Normalized) Accuracy

Transactions \ Prediction	Fraudulent	Not Fraudulent
Fraudulent	0	472
Not Fraudulent	0	284,335

Overall Accuracy =

$$\frac{\dfrac{TP}{TP + FN} + \dfrac{TN}{TN + FP}}{2} =$$

Overall (Normalized) Accuracy

Transactions	Prediction: Fraudulent	Prediction: Not Fraudulent
Fraudulent	0	472
Not Fraudulent	0	284,335

Overall Accuracy =

$$\frac{\frac{TP}{TP + FN} + \frac{TN}{TN + FP}}{2} =$$

$$\frac{\frac{0}{0 + 472} + \frac{284{,}335}{284{,}335 + 0}}{2} =$$

Overall (Normalized) Accuracy

Transactions \ Prediction	Fraudulent	Not Fraudulent
Fraudulent	0	472
Not Fraudulent	0	284,335

Overall Accuracy =

$$\frac{\frac{TP}{TP + FN} + \frac{TN}{TN + FP}}{2} =$$

$$\frac{\frac{0}{0 + 472} + \frac{284{,}335}{284{,}335 + 0}}{2} =$$

$$\frac{0 + 100}{2} = 50\%$$

Overall (Normalized) Accuracy

Accuracy = 80%

Folder

Email	Spam Folder	Inbox
Spam	100	170
Not Spam	30	700

Overall Accuracy =

$$\frac{\frac{TP}{TP + FN} + \frac{TN}{TN + FP}}{2} =$$

$$\frac{\frac{100}{100 + 170} + \frac{700}{700 + 30}}{2} =$$

$$\frac{37.0 + 95.9}{2} = 66.5\%$$

Overall (Normalized) Accuracy

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

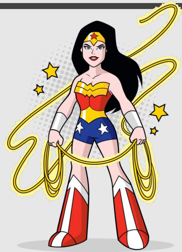
Accuracy = 90%

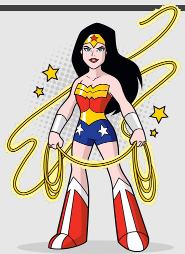
Overall Accuracy =

$$\frac{\frac{TP}{TP + FN} + \frac{TN}{TN + FP}}{2} =$$

$$\frac{\frac{1000}{1000 + 200} + \frac{8000}{8000 + 800}}{2} =$$

$$\frac{83.3 + 90.9}{2} = 87.1\%$$

	Diagnosed Sick	Diagnosed Healthy
Sick	True Positive 	False Negative 
Healthy	False Positive 	True Negative 

	Diagnosed Sick	Diagnosed Healthy
Sick		False Negative 
Healthy	False Positive 	

	Sent to Spam Folder	Sent to Inbox
Spam	True Positive 	False Negative 
Not Spam	False Positive 	True Negative 

	Sent to Spam Folder	Sent to Inbox
Spam		False Negative 
Not Spam	False Positive 	

Evaluation Metrics

Medical Model

False positives ok
False negatives **NOT** ok

Spam Detector

False positives **NOT** ok
False negatives ok

Evaluation Metrics

Medical Model

False positives ok
False negatives **NOT** ok

High Recall

Spam Detector

False positives **NOT** ok
False negatives ok

High Precision

Precision

		Diagnosis	
		Diagnosed Sick	Diagnosed Healthy
Patients	Sick	1,000	200
	Healthy	800	8,000

Precision

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Precision:
Out of all the patients we diagnosed with illness, how many were actually sick?

Precision

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Precision:
Out of all the patients we diagnosed with illness, how many were actually sick?

Precision

Diagnosis

Patients	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Precision:
Out of all the patients we diagnosed with illness, how many were actually sick?

Precision =

$$\frac{1{,}000}{1{,}000 + 800} = 55.7\%$$

Precision

		Folder	
		Spam Folder	Inbox
Email	Spam	100	170
	Not Spam	30	700

Precision:
Out of all the emails sent to the spam inbox, how many did were actually spam?

Precision

Folder

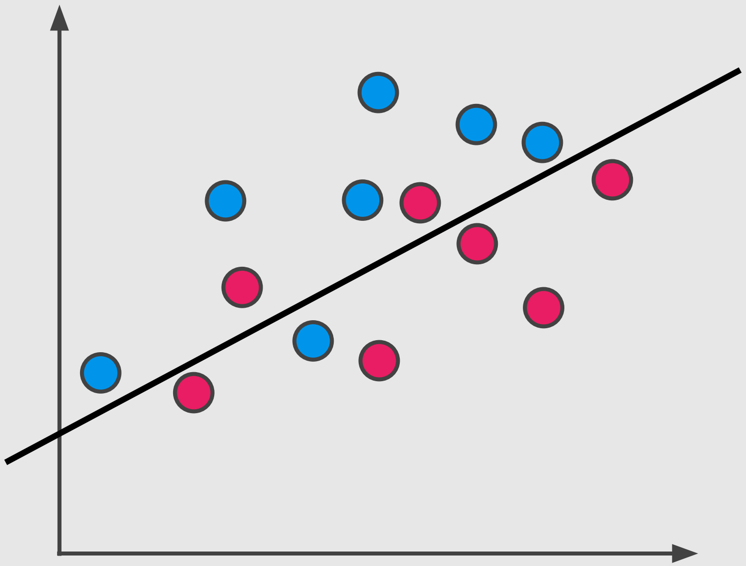
Email	Spam Folder	Inbox
Spam	100	170
Not Spam	30	700

Precision:
Out of all the emails sent to the spam inbox, how many did were actually spam?

Precision =

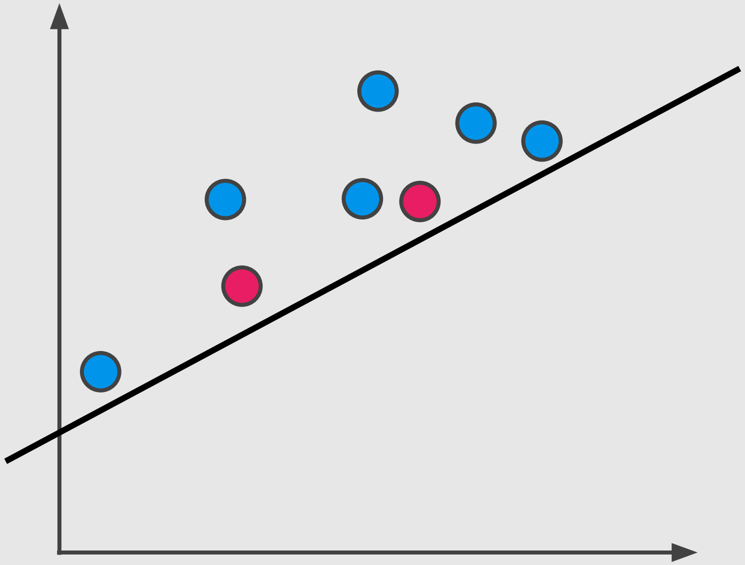
$$\frac{100}{100 + 300} = 76.9\%$$

Precision



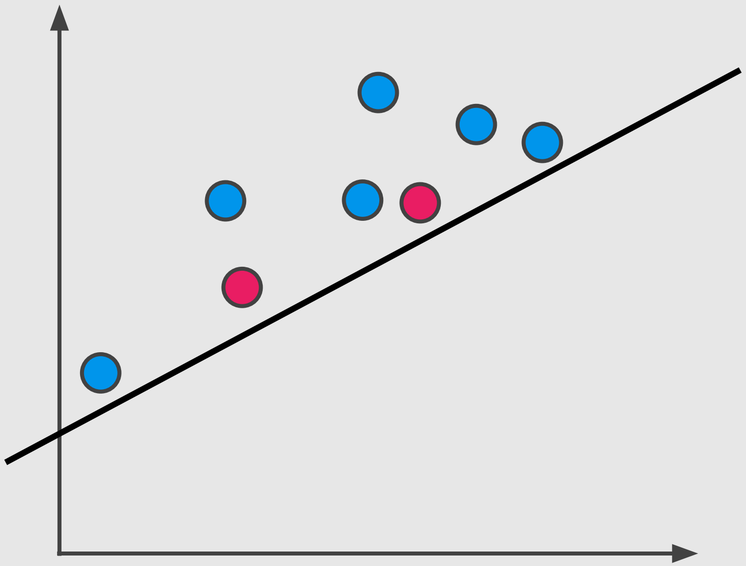
Precision:
Out of all the points we've predicted to be positive, how many are correct?

Precision



Precision:
Out of all the points we've predicted to be positive, how many are correct?

Precision



Precision:
Out of all the points we've predicted to be positive, how many are correct?

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$

Recall

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Recall

	Diagnosis: Diagnosed Sick	Diagnosis: Diagnosed Healthy
Patients: Sick	1,000	200
Patients: Healthy	800	8,000

Recall:
Out of all the sick patients, how many did we correctly diagnose as sick?

Recall

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Recall:
Out of all the sick patients, how many did we correctly diagnose as sick?

Recall

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

Recall:
Out of all the sick patients, how many did we correctly diagnose as sick?

Recall =

$$\frac{1{,}000}{1{,}000 + 200} = 83.3\%$$

Recall

Email		Folder	
		Spam Folder	Inbox
	Spam	100	170
	Not Spam	30	700

Recall:
Out of all the spam emails, how many were correctly sent to the spam folder?

Recall

Folder

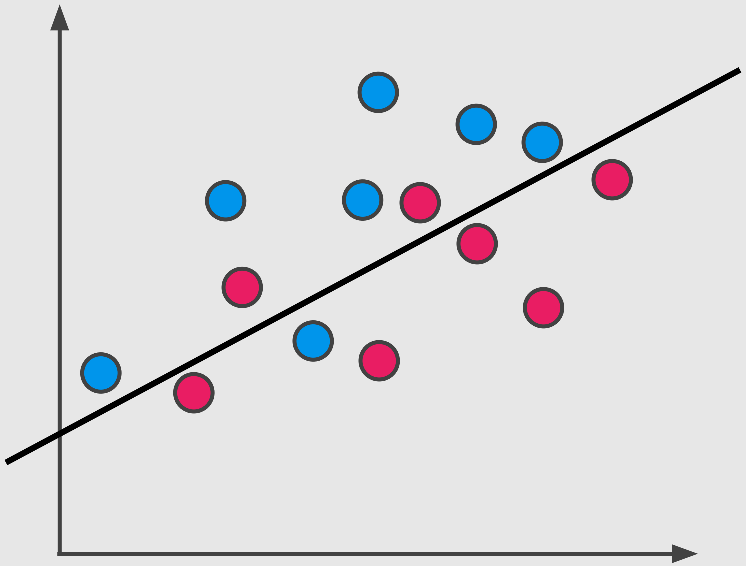
Email	Spam Folder	Inbox
Spam	100	170
Not Spam	30	700

Recall:
Out of all the spam emails, how many were correctly sent to the spam folder?

Recall =

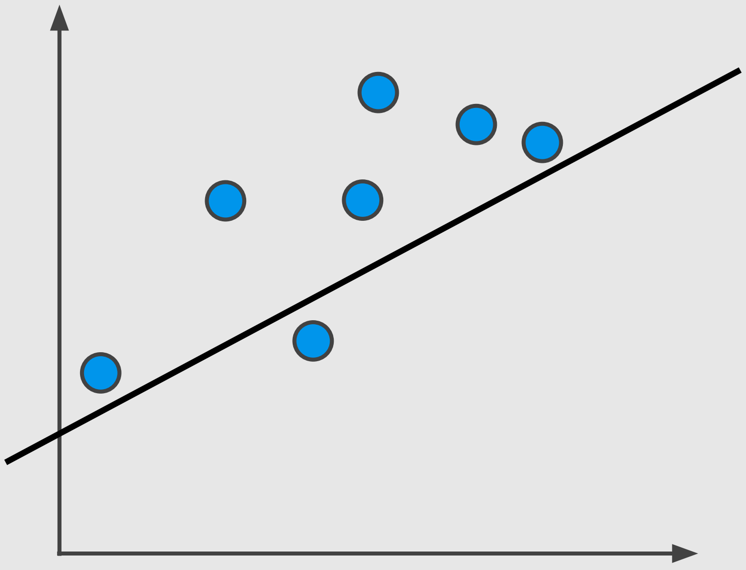
$$\frac{100}{100 + 170} = 37\%$$

Recall



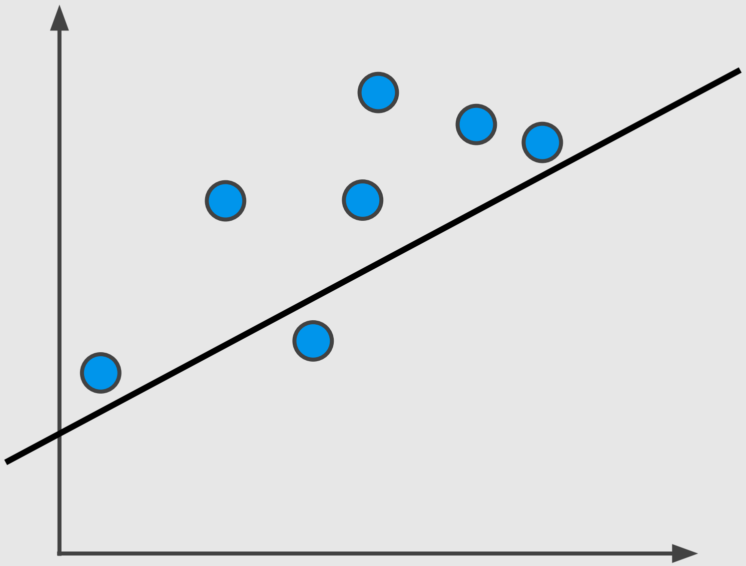
Recall:
Out of all the points labelled positive, how many did we correctly predict?

Recall



Recall:
Out of all the points labelled positive, how many did we correctly predict?

Recall

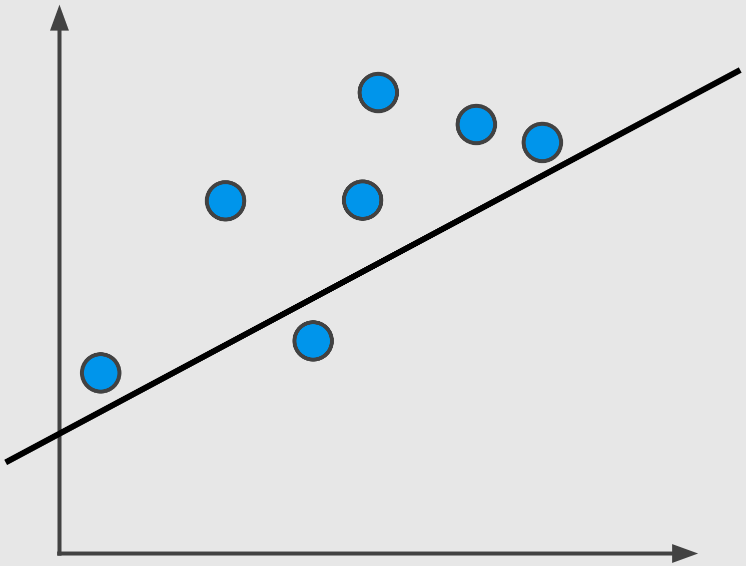


Recall:
Out of all the points labelled positive, how many did we correctly predict?

Recall =

$$\frac{\text{True Positives}}{\text{True Positives + False Negatives}}$$

Recall



Recall:
Out of all the points labelled positive, how many did we correctly predict?

$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

$$\frac{6}{6 + 1} = 85.7\%$$

Precision and Recall

Medical Model

Precision: 55.7%

Recall: 83.3%

Spam Detector

Precision: 76.9%

Recall: 37%

One Score?

Medical Model

Precision: 55.7%

Recall: 83.3%

Average = 69.5%

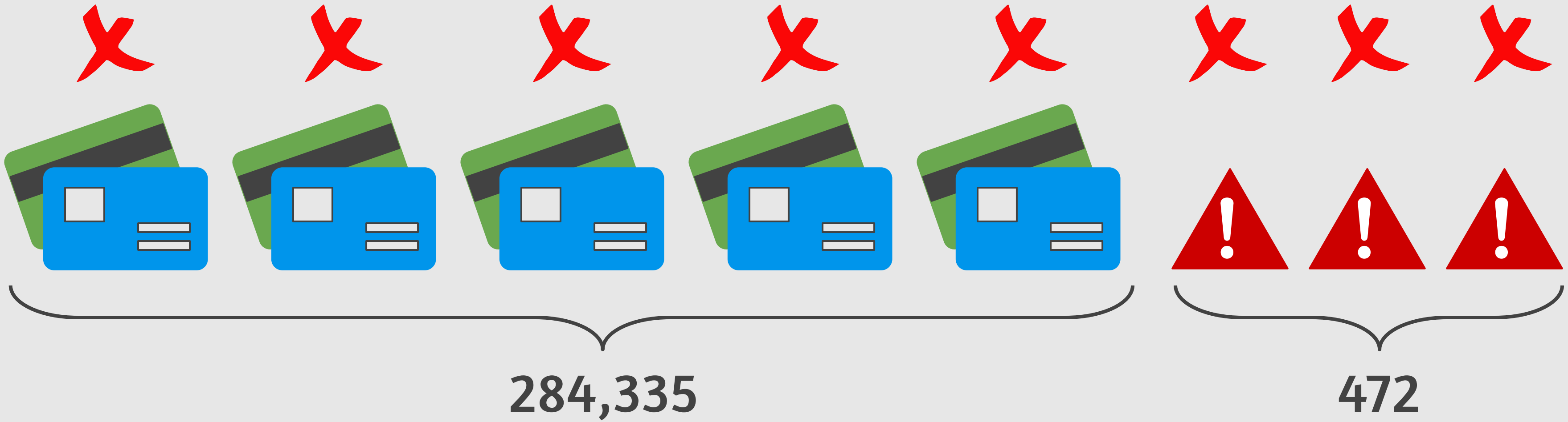
Spam Detector

Precision: 76.9%

Recall: 37%

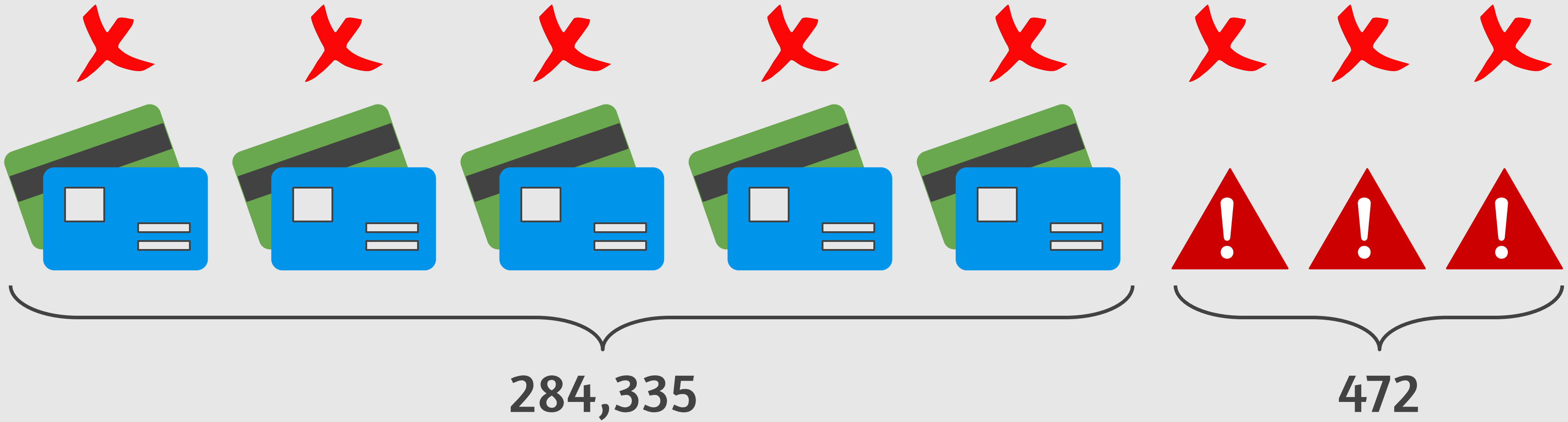
Average = 56.9%

Credit Card Fraud



Model: All transactions are fraudulent.

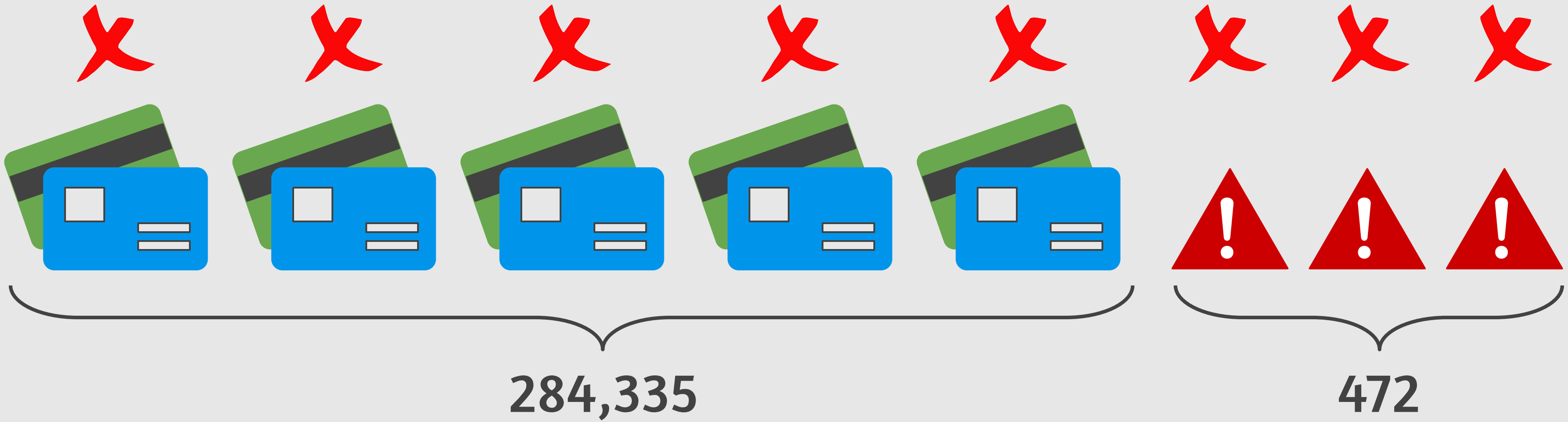
Credit Card Fraud



Model: All transactions are fraudulent.

$$\text{Precision} = \frac{472}{284{,}807} = 0.016\%$$

Credit Card Fraud



Model: All transactions are fraudulent.

$$\text{Precision} = \frac{472}{284{,}807} = 0.016\%$$

$$\text{Recall} = \frac{472}{472} = 100\%$$

Harmonic Mean

$$\text{Arithmetic Mean} = \frac{x + y}{2}$$

Harmonic Mean

$$\text{Arithmetic Mean} = \frac{x + y}{2}$$

$$\text{Harmonic Mean} = \frac{2xy}{x + y}$$

Harmonic Mean

$$\text{Arithmetic Mean} = \frac{x + y}{2}$$

$$\text{Harmonic Mean} = \frac{2xy}{x + y}$$

Precision: 1

Recall: 0

Average = 0.5

Harmonic Mean = 0

Harmonic Mean

$$\text{Arithmetic Mean} = \frac{x + y}{2}$$

$$\text{Harmonic Mean} = \frac{2xy}{x + y}$$

Precision: 1

Recall: 0

Average = 0.5

Harmonic Mean = 0

Precision: 0.2

Recall: 0.8

Average = 0.5

Harmonic Mean = 0.32

Harmonic Mean

$$\text{Arithmetic Mean} = \frac{x + y}{2}$$

$$\text{Harmonic Mean} = \frac{2xy}{x + y}$$

Precision: 1
Recall: 0
Average = 0.5
Harmonic Mean = 0

Precision: 0.2
Recall: 0.8
Average = 0.5
Harmonic Mean = 0.32

F1 Score = Harmonic Mean (Precision, Recall)

F1 Score

Medical Model

Precision: 55.7%

Recall: 83.3%

Average = 69.5%

F1 Score = 66.8%

F1 Score

Spam Detector

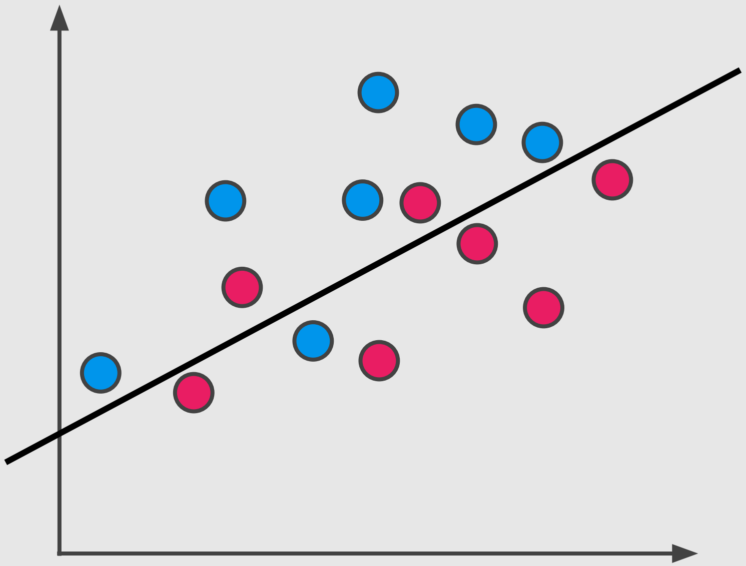
Precision: 76.9%

Recall: 37%

Average = 56.9%

F1 Score = 50.0%

F1 Score



Precision: 75%

Recall: 85.7%

Average = 80.3%

F1 Score = 80%

F_β Score

F_β Score

Precision

Recall

F_β Score

Precision F0.5 Score F1 Score F2 Score Recall

F_β Score

?

Precision F0.5 Score F1 Score F2 Score Recall

F_β Score

F10 Score

Precision F0.5 Score F1 Score F2 Score Recall

F_β Score

F10 Score

Precision

F0.5 Score

F1 Score

F2 Score

Recall

F_β Score

F1 Score = Harmonic Mean (Precision, Recall)

F_β Score

F1 Score = Harmonic Mean (Precision, Recall)

$$H = \frac{n}{\frac{1}{x_1} + \frac{1}{x_2} + \cdots + \frac{1}{x_n}}$$

F_β Score

F1 Score = Harmonic Mean (Precision, Recall)

$$H = \frac{n}{\frac{1}{x_1} + \frac{1}{x_2} + \cdots + \frac{1}{x_n}}$$

$$F_1 = 2\frac{1}{\frac{1}{\text{recall}} + \frac{1}{\text{precision}}} = 2\frac{\text{precison}\cdot\text{recall}}{\text{precision} + \text{recall}}$$

F_β Score

$$F_1 = 2\,\frac{\text{precison}\cdot\text{recall}}{\text{precision} + \text{recall}}$$

$$F_\beta = (1 + \beta^2)\,\frac{\text{precison}\cdot\text{recall}}{(\beta^2\cdot\text{precision}) + \text{recall}}$$

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- https://en.wikipedia.org/wiki/Binary_classification
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- https://www.quora.com/What-is-an-intuitive-explanation-of-F-score
- "Approximate Statistical Tests for Comparing Supervised Classification Learning Algorithms", Neural Computation, p. 1895-1923, 1998 https://www.mitpressjournals.org/doi/10.1162/089976698300017197

Machine Learning Courses

- Luis Serrano: https://www.youtube.com/watch?v=aDW44NPhNw0