Recall from last time …

The Problem of Overfitting

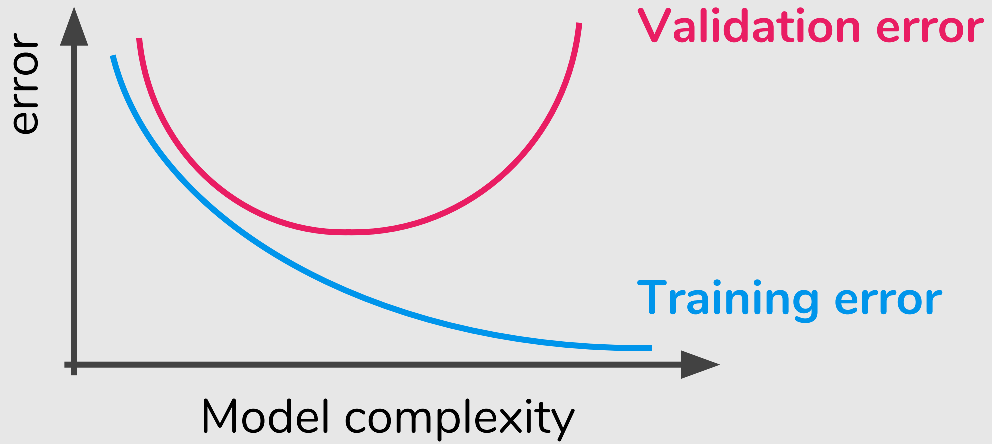

THE BEST WAY TO EXPLAIN OVERFITTING
imgflip.com
ADDTEXT.COM

Underfitting (High Bias)

Overfitting (High Variance)

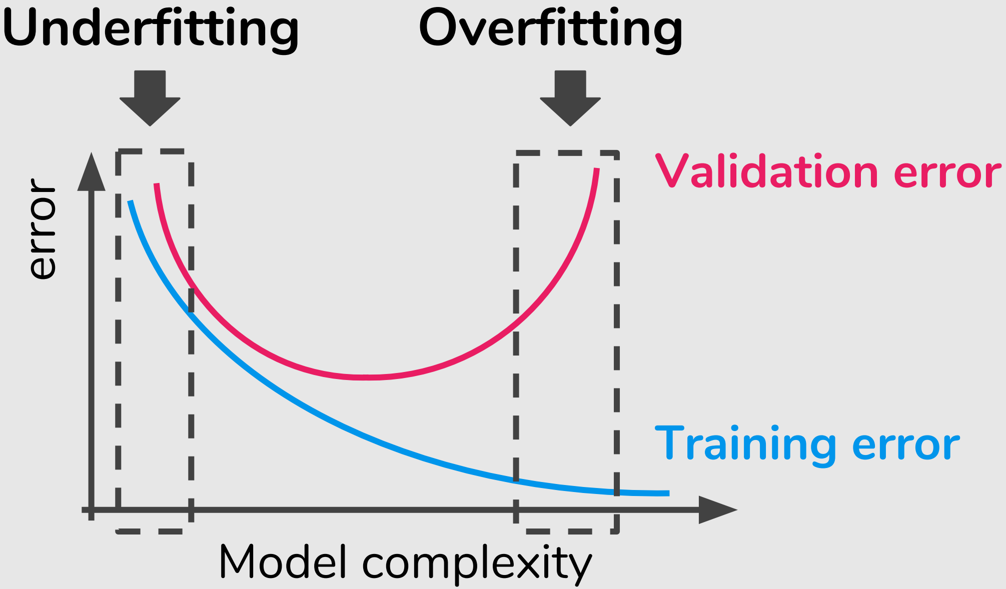
Diagnosing
Bias vs. Variance

Diagnosing Bias vs. Variance



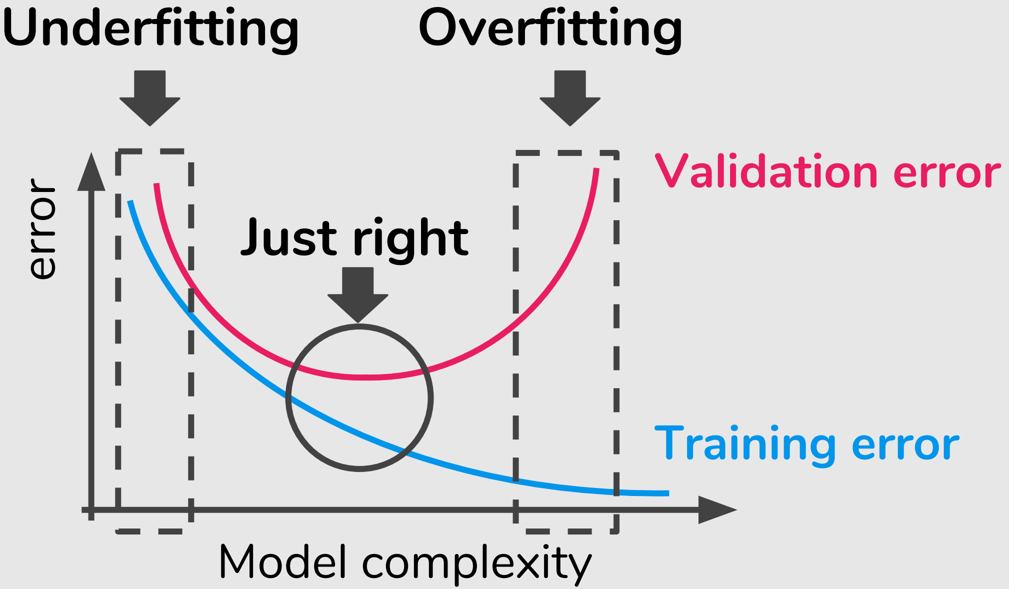
Understanding the Bias-Variance Tradeoff: http://scott.fortmann-roe.com/docs/BiasVariance.html

Diagnosing Bias vs. Variance



Understanding the Bias-Variance Tradeoff: http://scott.fortmann-roe.com/docs/BiasVariance.html

Diagnosing Bias vs. Variance



Understanding the Bias-Variance Tradeoff: http://scott.fortmann-roe.com/docs/BiasVariance.html

Cost Function

Regularization

$$J(\theta) = \frac{1}{2m}\left[\underbrace{\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2}_{\text{to fit the training data well}} + \overset{\text{Regularization parameter}}{\overset{\Uparrow}{\boxed{\lambda}}}\underbrace{\sum_{j=1}^{n}\theta_j^2}_{\text{to keep the parameters small}}\right]$$

Regularized Linear Function

Gradient Descent

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update θ_j for $j =$ ✖ $1, \ldots, n$)

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

Gradient Descent

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update θ_j for $j = \cancel{0} \ 1, \ldots, n$)

$$\theta_j := \theta_j \boxed{(1 - \alpha \frac{\lambda}{m})} - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

Gradient Descent

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

repeat {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update θ_j for $j = \xcancel{0,}\ 1, \ldots, n$)

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

References

Machine Learning Books

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 4
- Pattern Recognition and Machine Learning, Chap. 3
- Understanding the Bias-Variance Tradeoff:
  http://scott.fortmann-roe.com/docs/BiasVariance.html

Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 3 & 6

Testing and Error Metrics

Machine Learning and Pattern Recognition

(Largely based on slides from Luis Serrano)

Prof. Sandra Avila
Institute of Computing (IC/Unicamp)

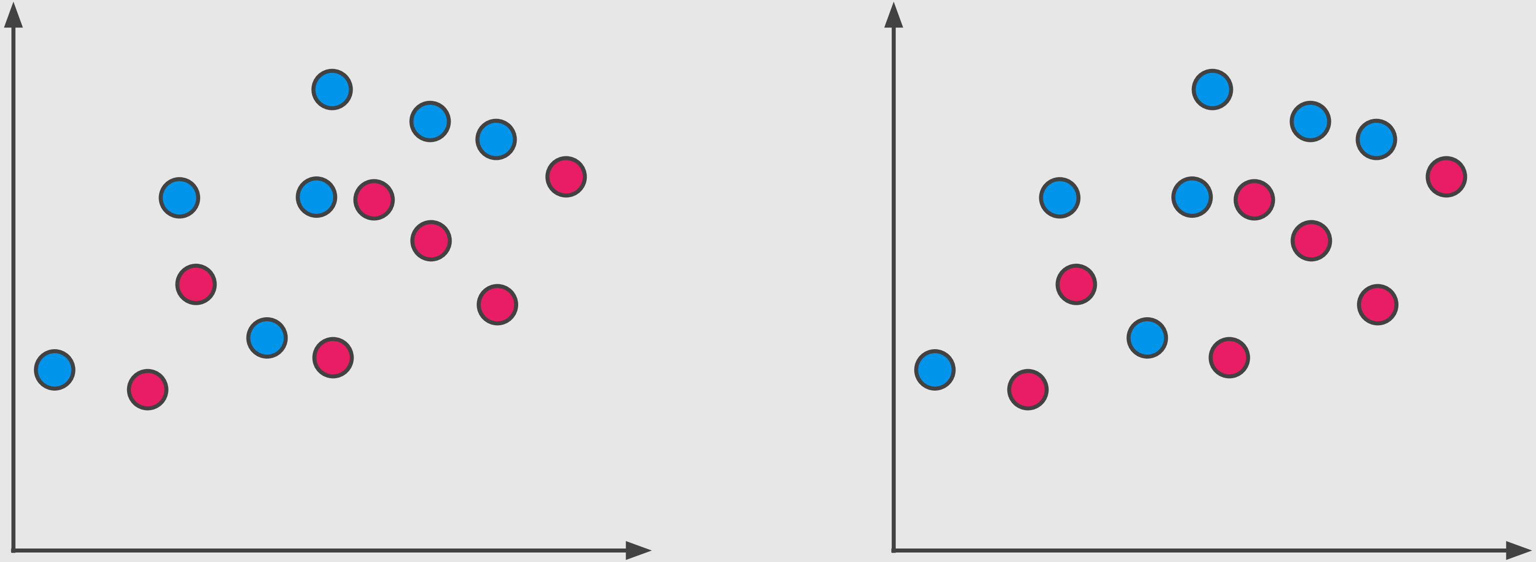
MC886/MO444, August 30, 2018

How well is my model doing?

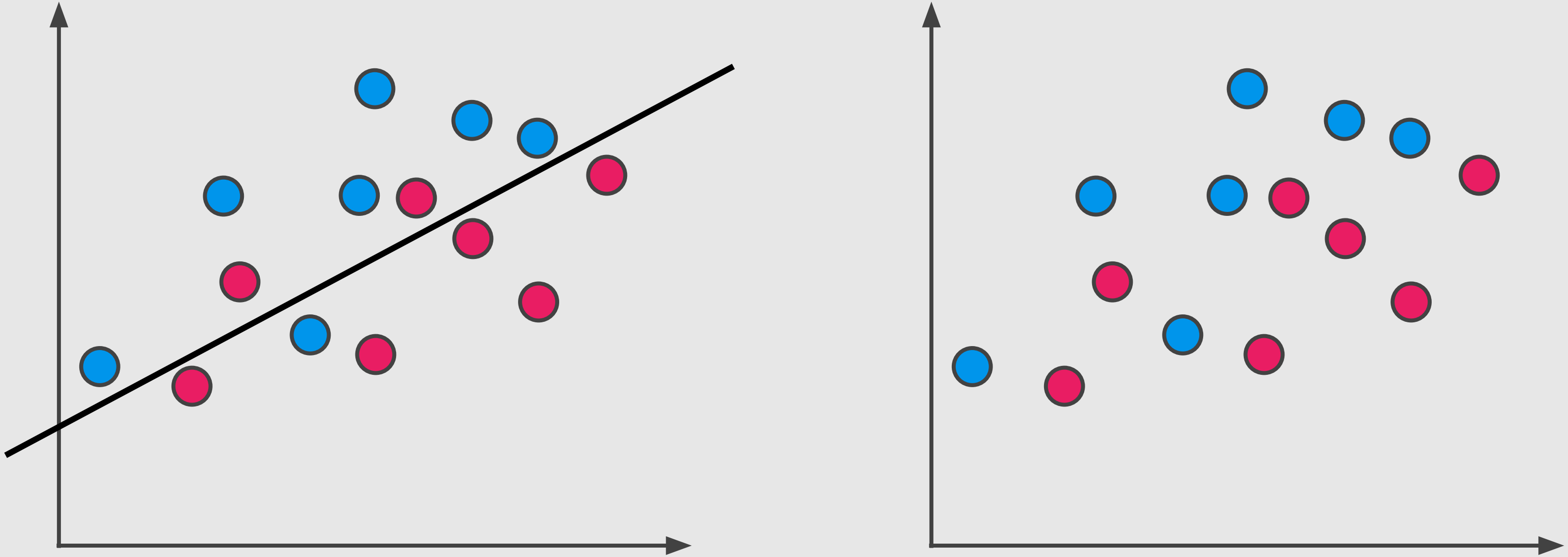
Today's Agenda

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

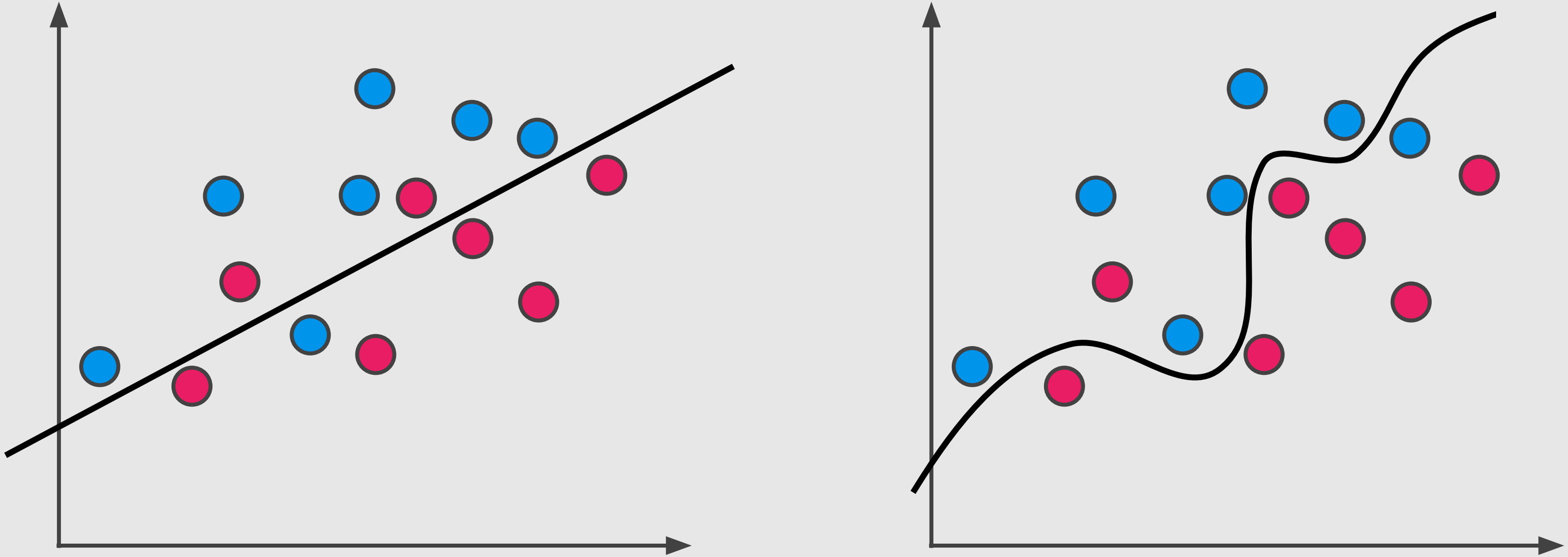
Which model is better?



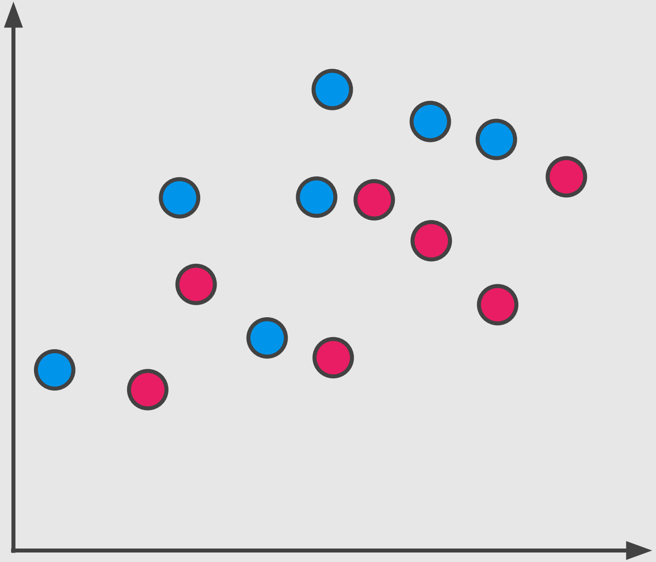
Which model is better?



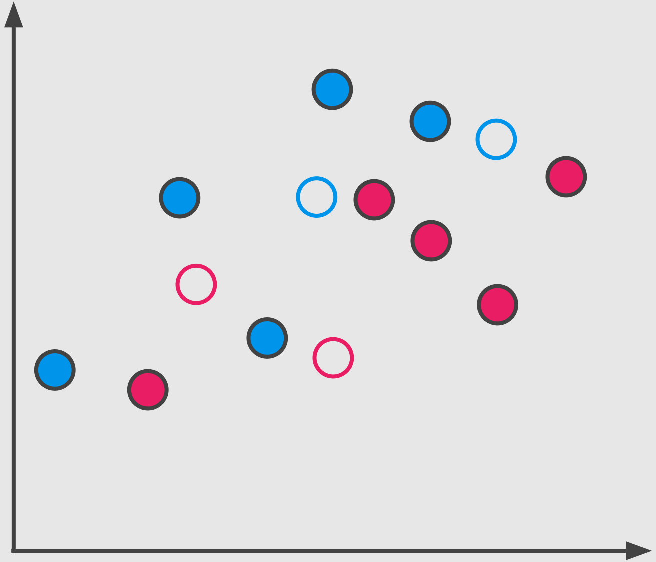
Which model is better?



Why testing?



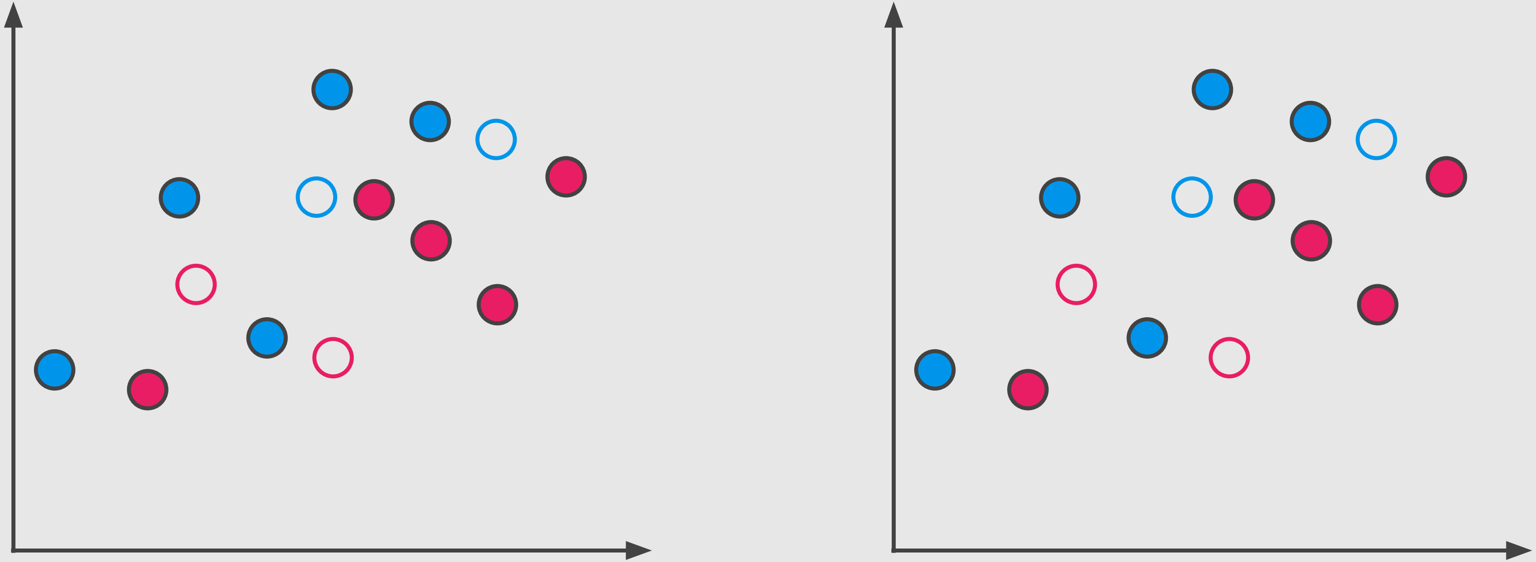
Why testing?



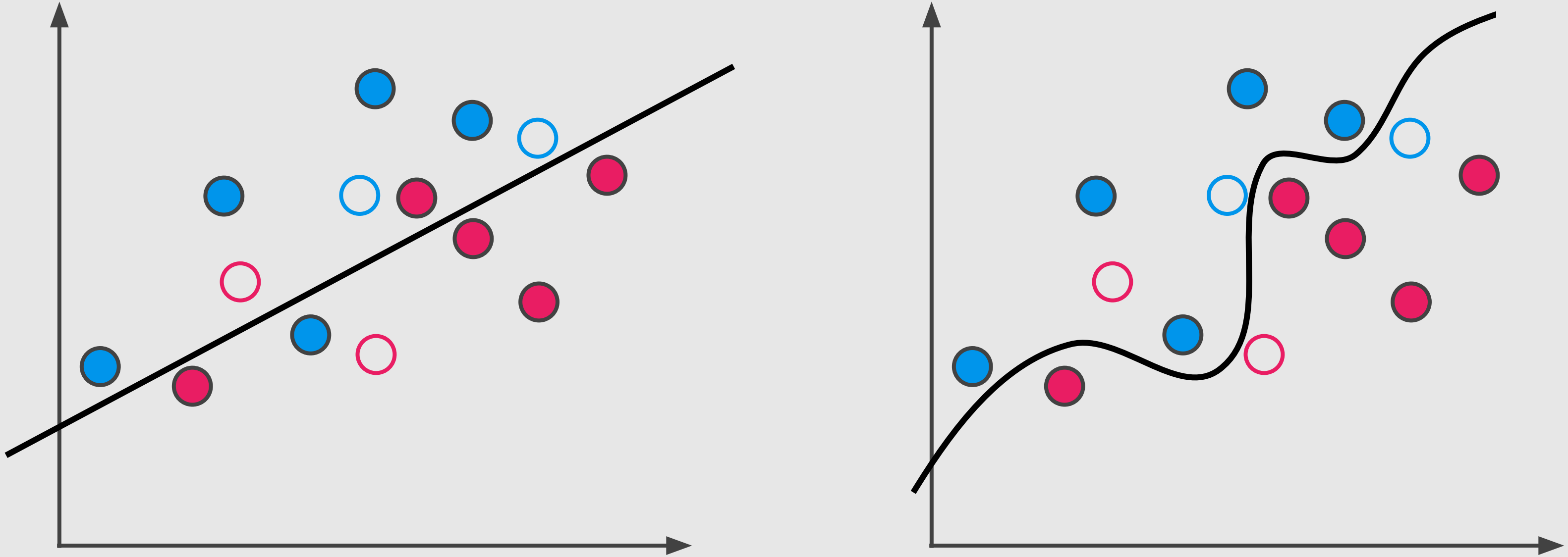
● ● Train

○ ○ Test

Why testing?



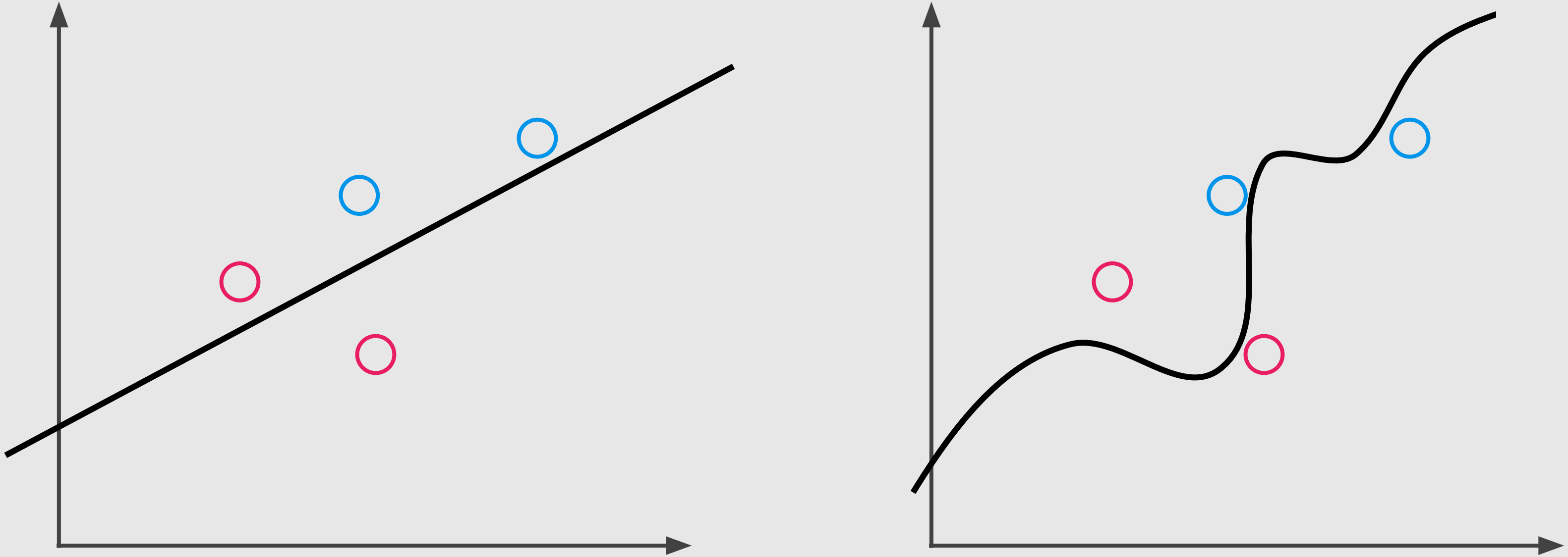
Why testing?



Why testing?

● ● Train

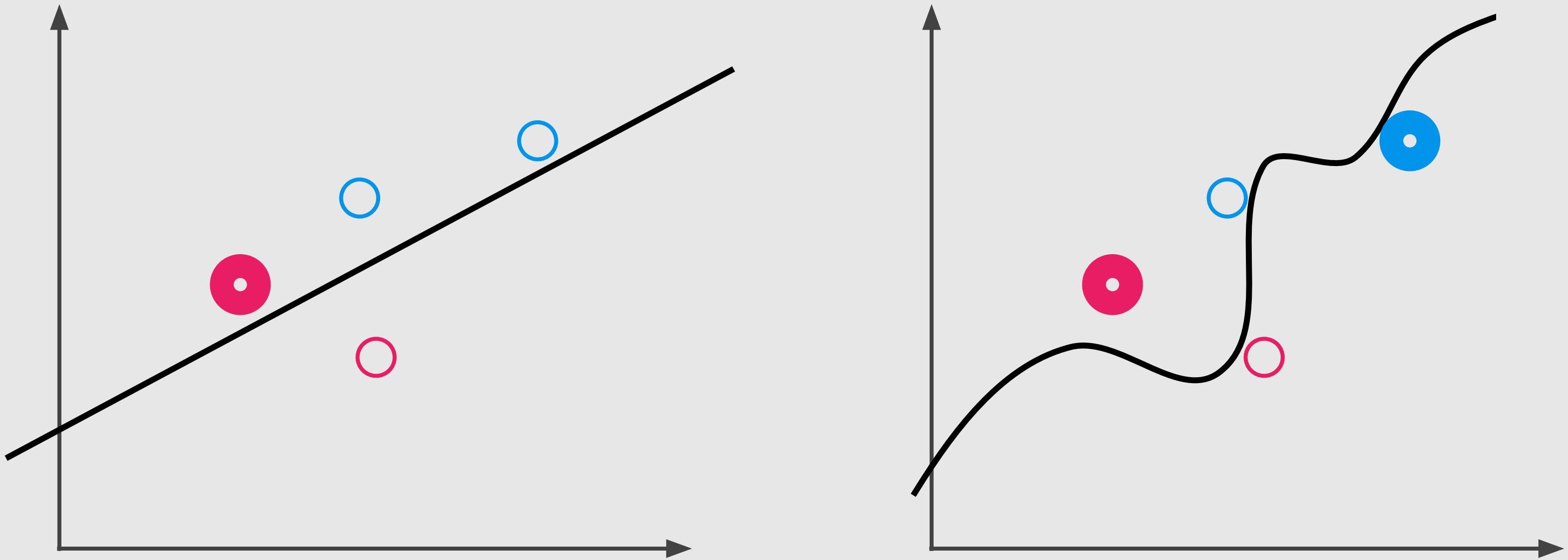
○ ○ Test



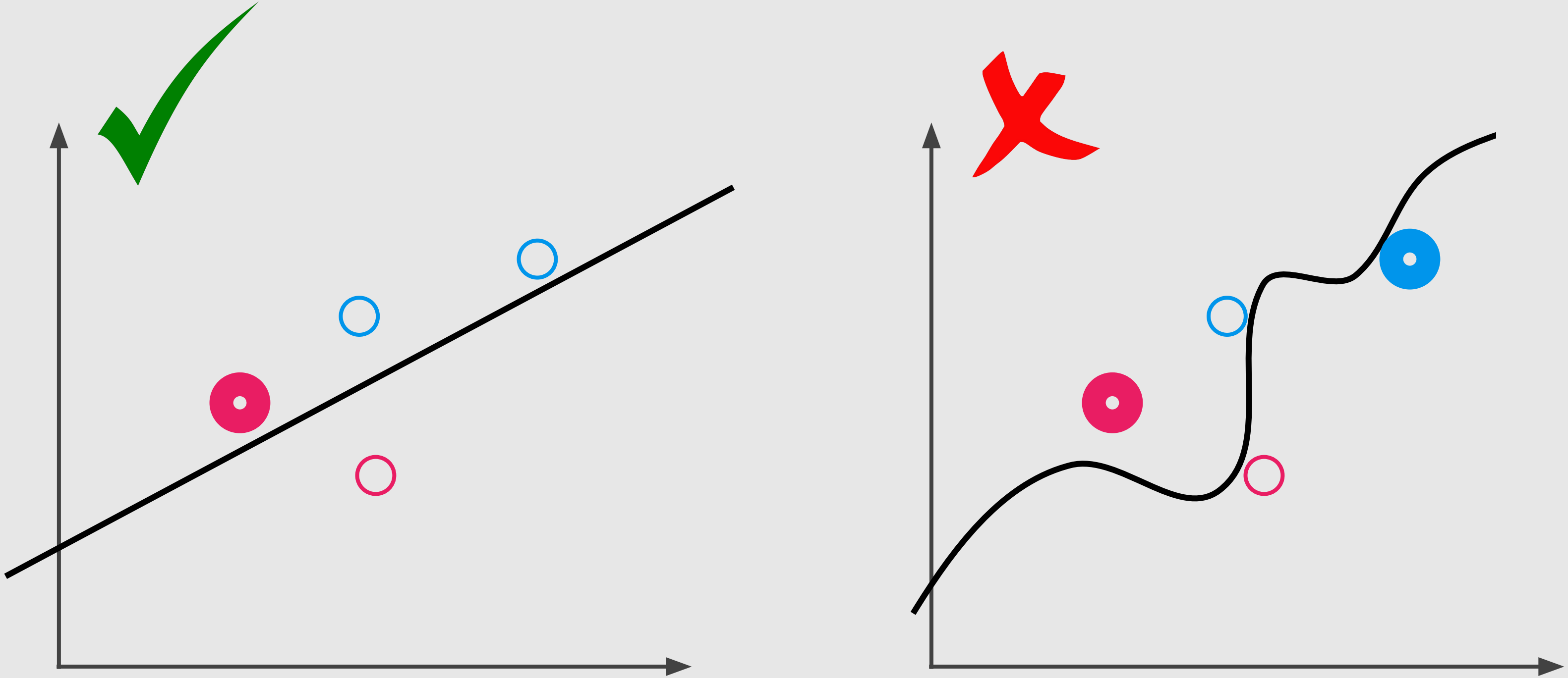
Why testing?

● ● Train

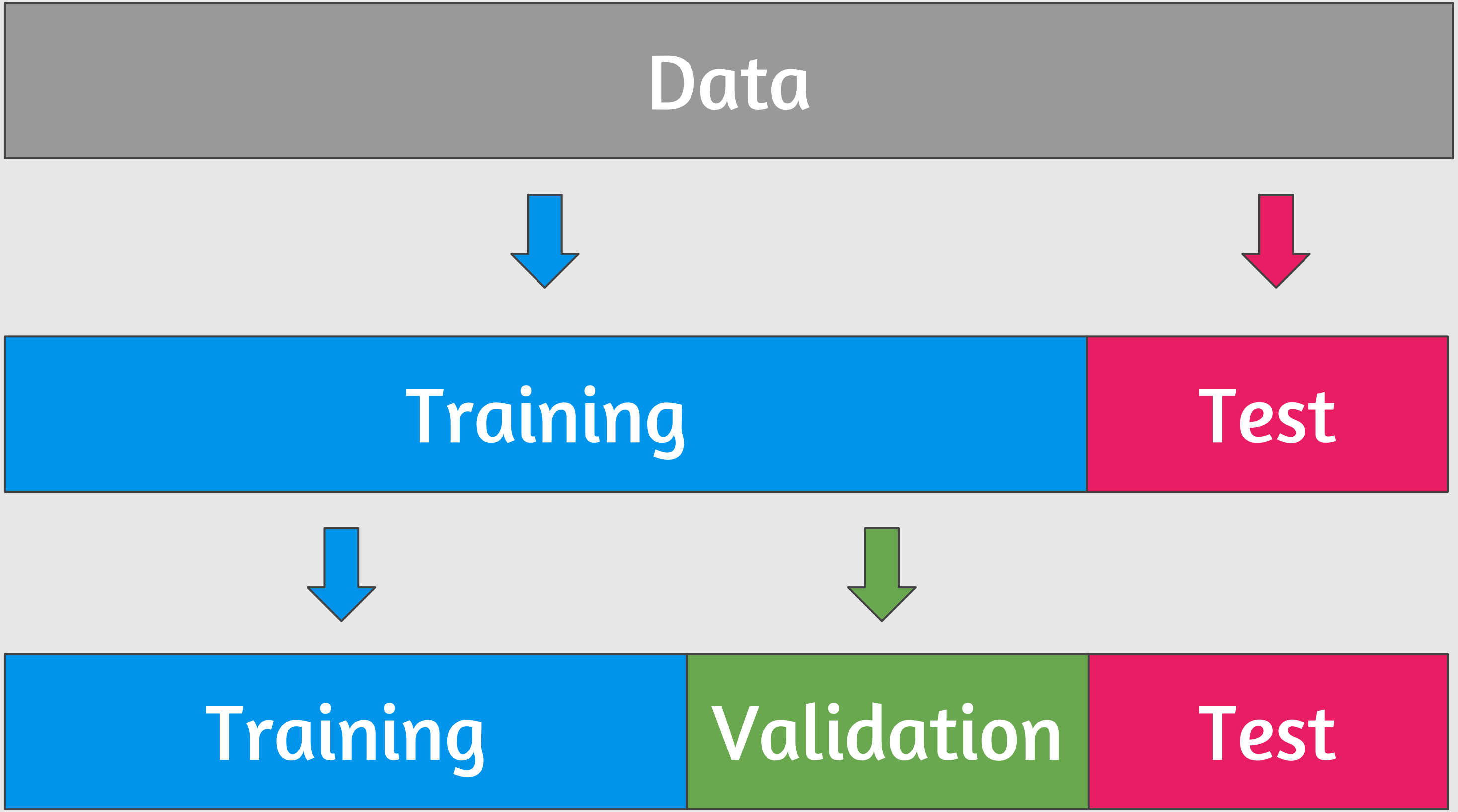
○ ○ Test



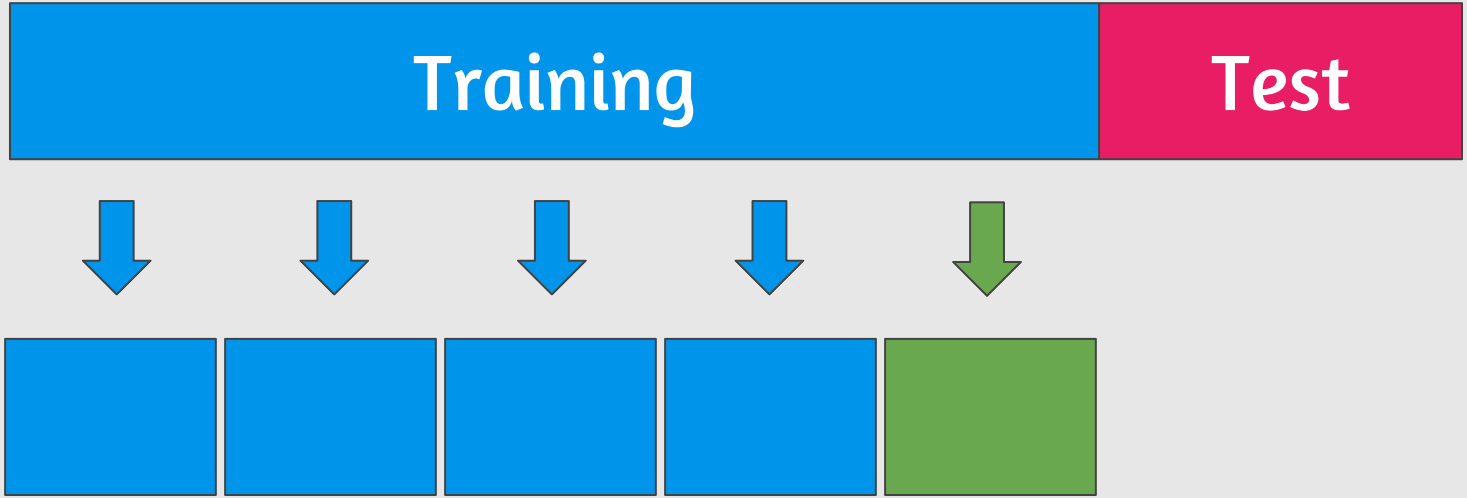
Why testing?



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

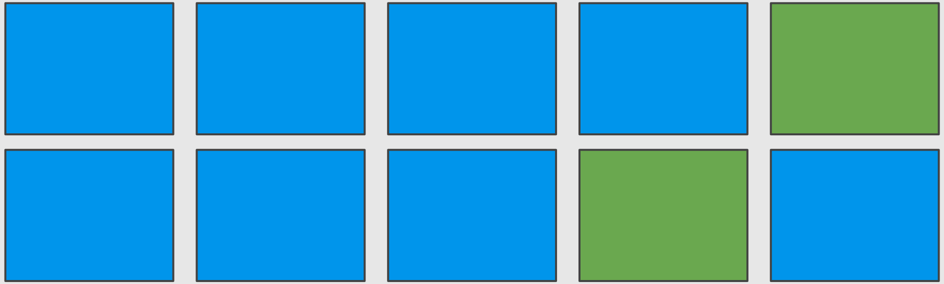
🟦 Training
🟩 Validation

$k = 5$

k-fold Cross Validation

🟦 Training
🟩 Validation

k = 5

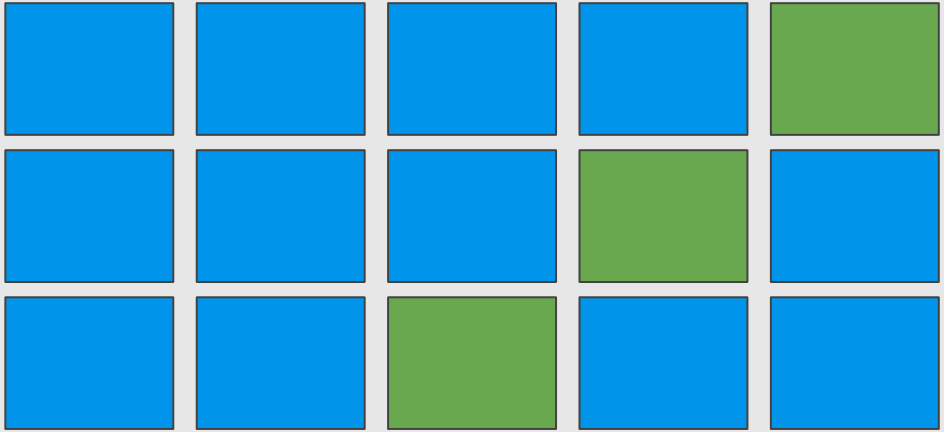


k-fold Cross Validation

🟦 Training

🟩 Validation

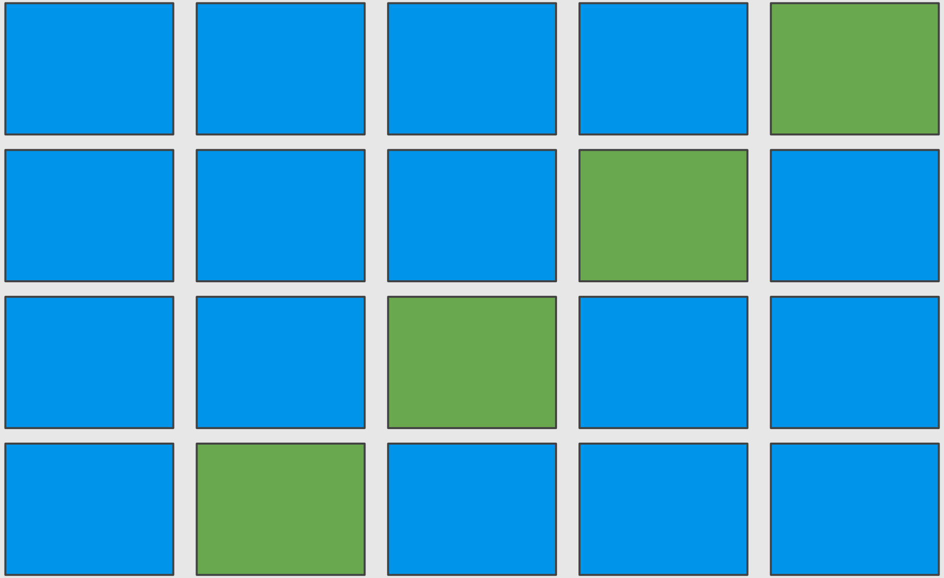
k = 5



k-fold Cross Validation

🟦 Training
🟩 Validation

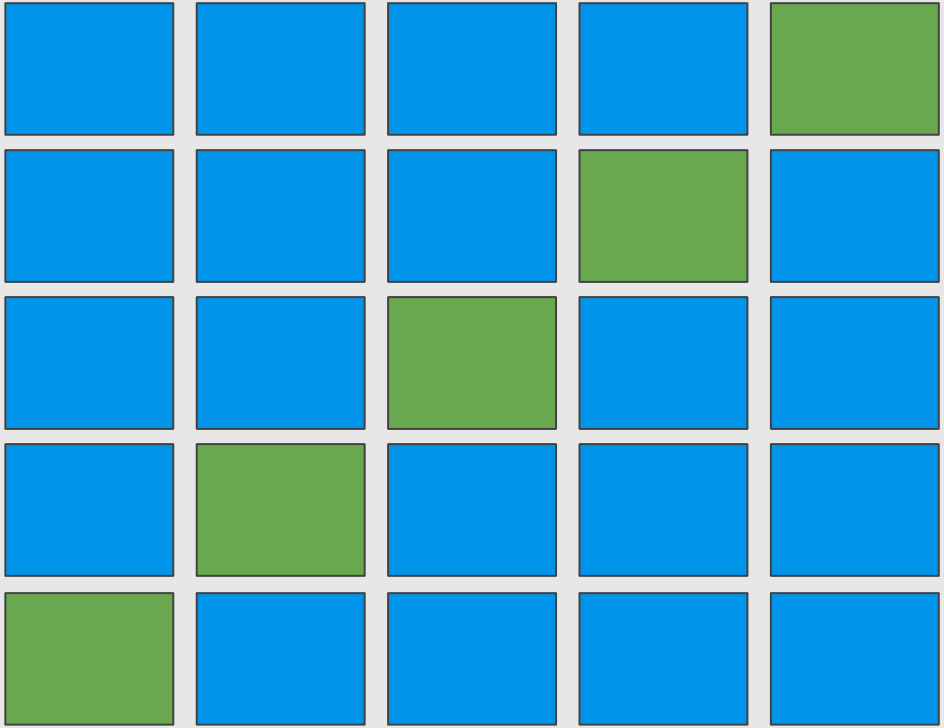
k = 5



k-fold Cross Validation

🟦 Training
🟩 Validation

k = 5



k×2-fold Cross Validation

🟦 Training

🟩 Validation

k = 5

k×2-fold Cross Validation

🟦 Training

🟩 Validation

$k = 5$

randomized

k×2-fold Cross Validation

🟦 Training

🟩 Validation

k = 5

k×2-fold Cross Validation

🟦 Training

🟩 Validation

k = 5

k×2-fold Cross Validation

🟦 Training

🟩 Validation

k = 5

randomized

k×2-fold Cross Validation

🟦 Training

🟩 Validation

$k = 5$

k×2-fold Cross Validation

🟦 Training

🟩 Validation

k = 5

k×2-fold Cross Validation

🟦 Training
🟩 Validation

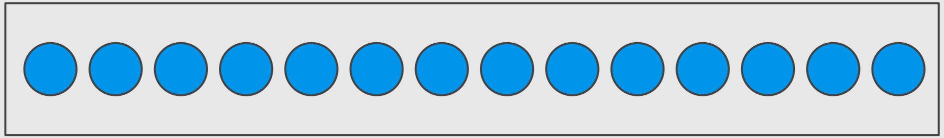
k = 5

k times = k×2 folds

Randomizing in Cross Validation

🔵 Training

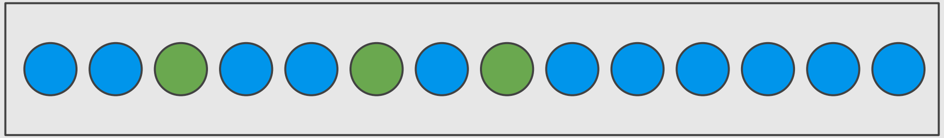
🟢 Validation



Randomizing in Cross Validation

🔵 Training

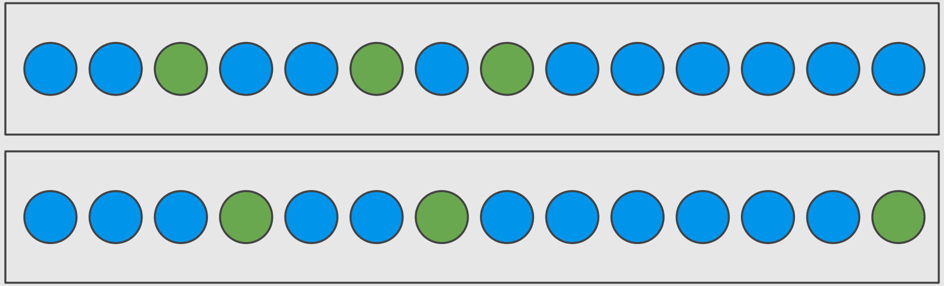
🟢 Validation



Randomizing in Cross Validation

🔵 Training

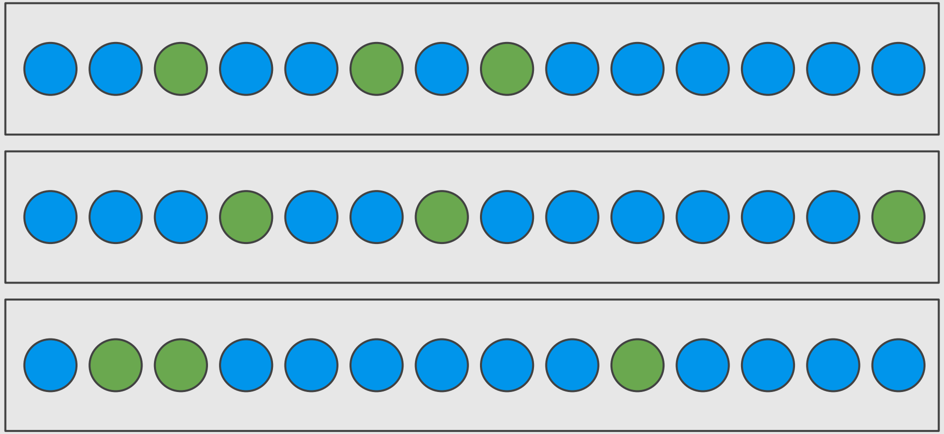
🟢 Validation



Randomizing in Cross Validation

● Training

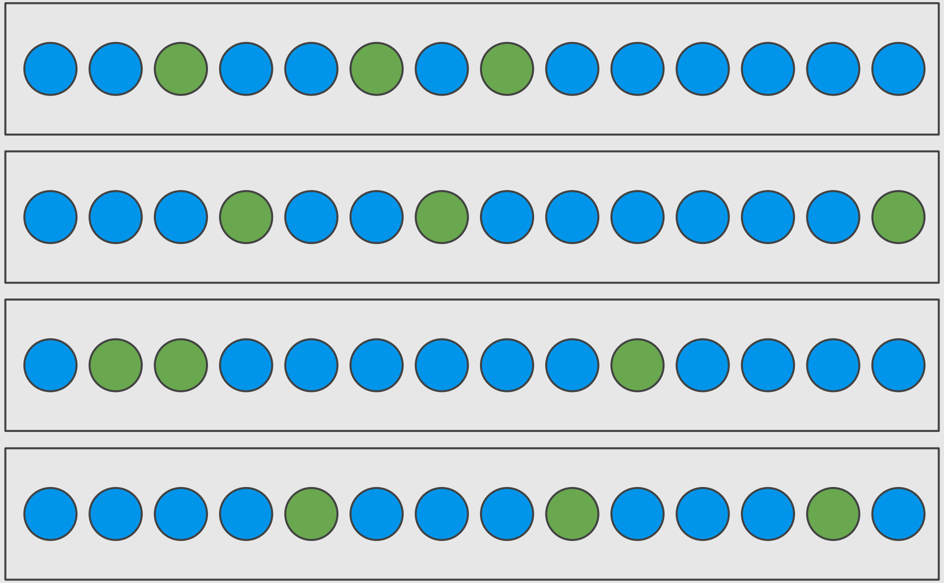
● Validation



Randomizing in Cross Validation

🔵 Training

🟢 Validation



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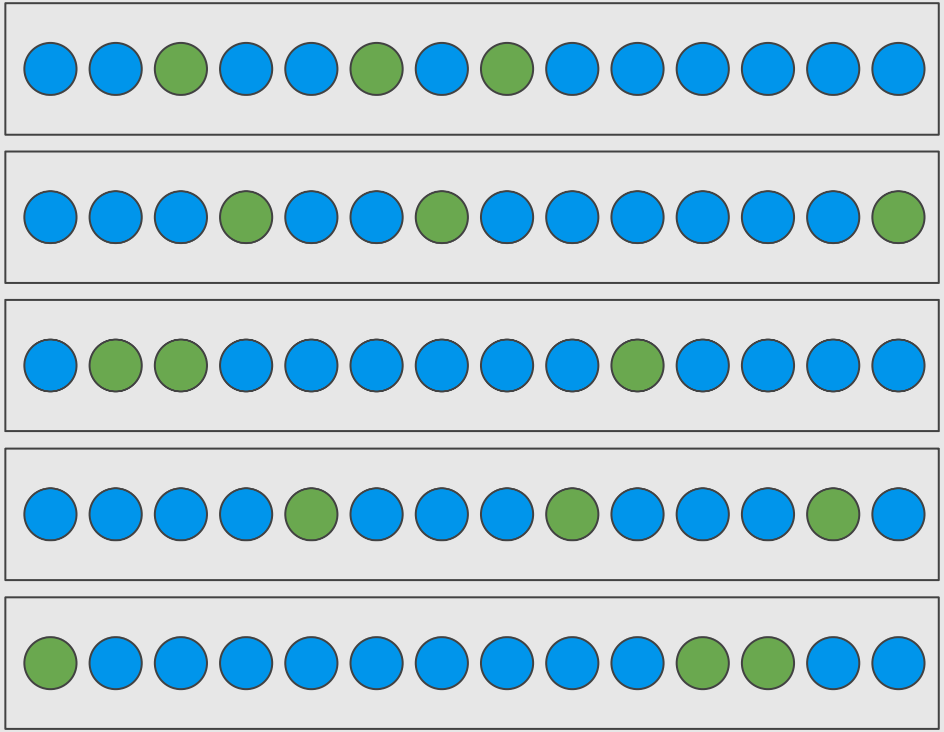
Randomizing in Cross Validation

🔵 Training

🟢 Validation



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

Prof. Jacques Wainer (IC/Unicamp)

Evaluation Metrics

How well is my model doing?

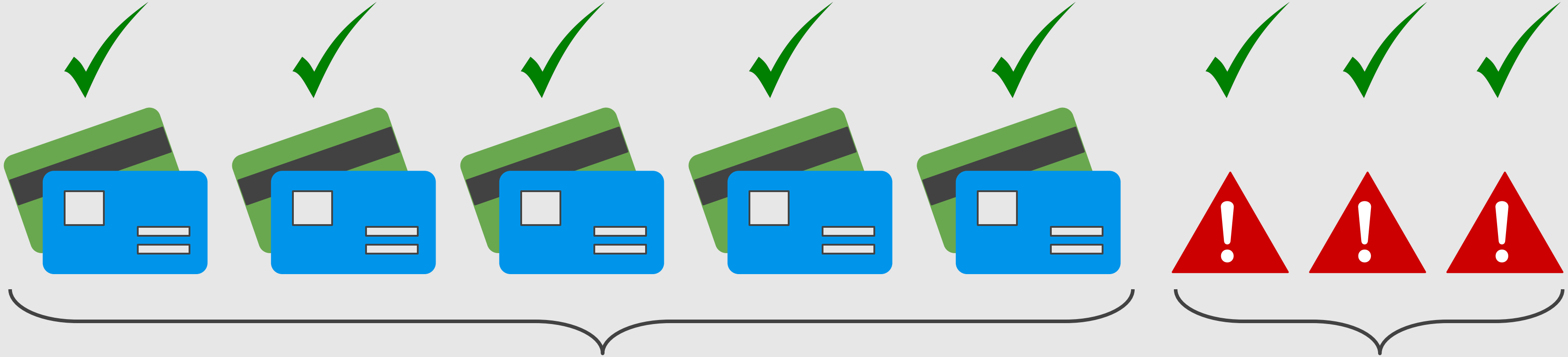
Credit Card Fraud

Credit Card Fraud

284,335

472

Credit Card Fraud

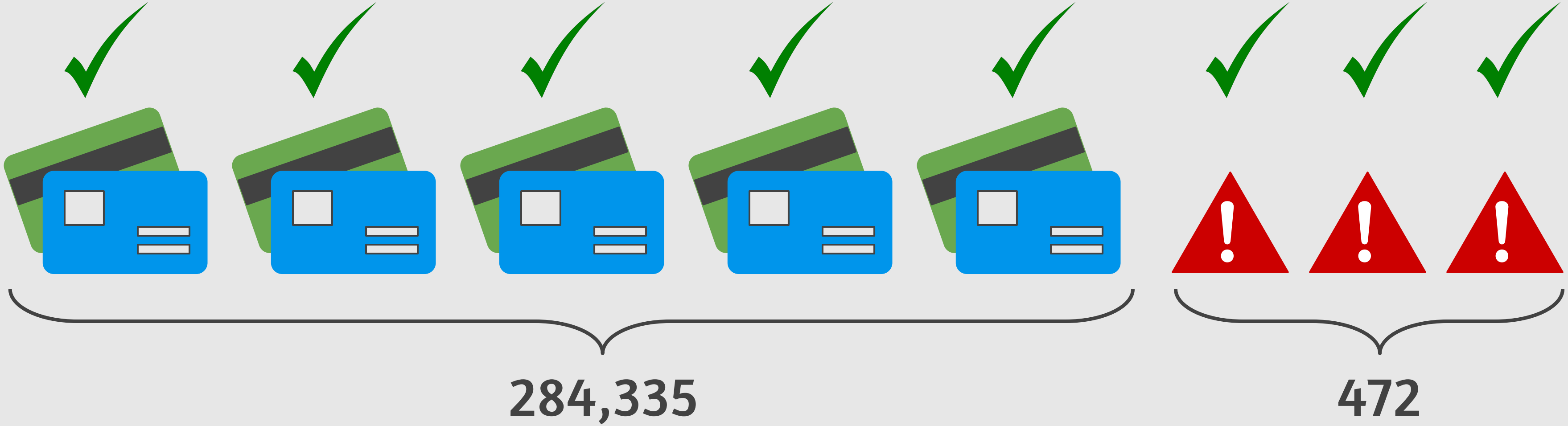


284,335

472

Model: All transactions are good.

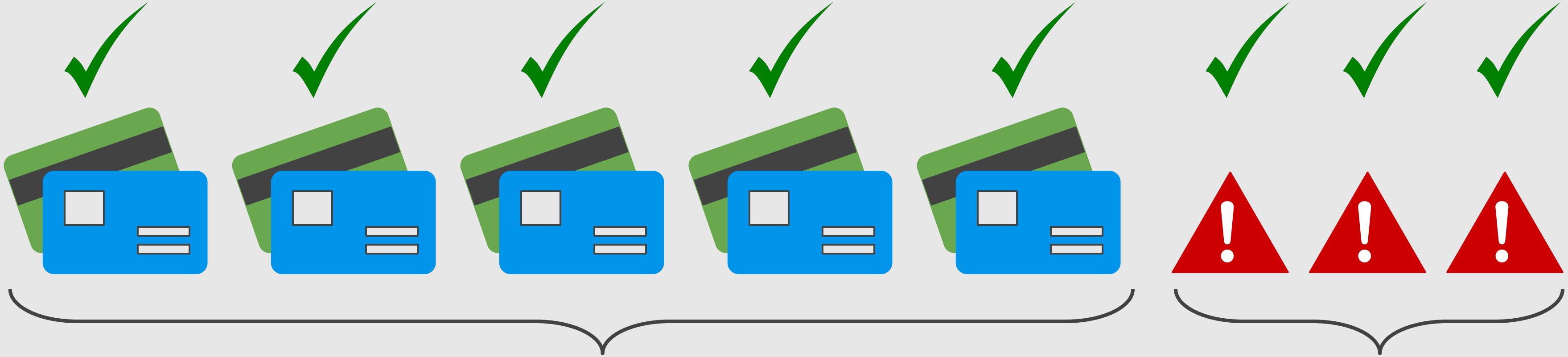
Credit Card Fraud



Model: All transactions are good.

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

Credit Card Fraud



284,335

472

Model: All transactions are good.

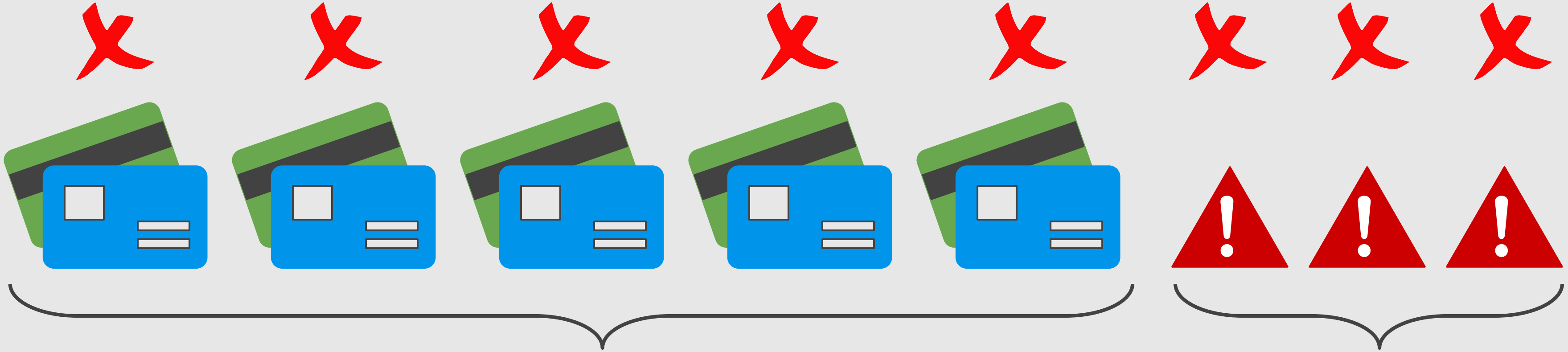
Problem: I’m not catching any of the bad ones!

Credit Card Fraud

284,335

472

Credit Card Fraud

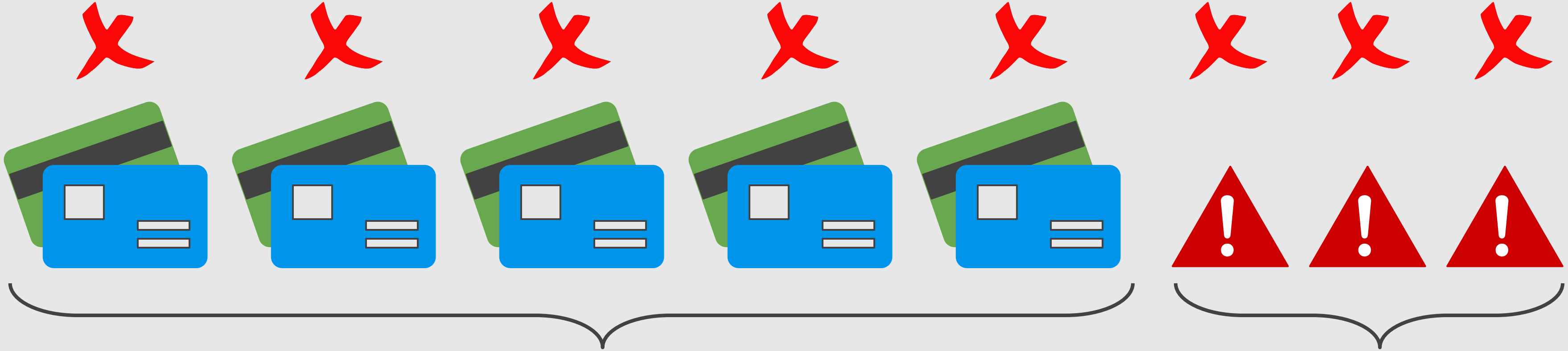


284,335

472

Model: All transactions are fraudulent.

Credit Card Fraud

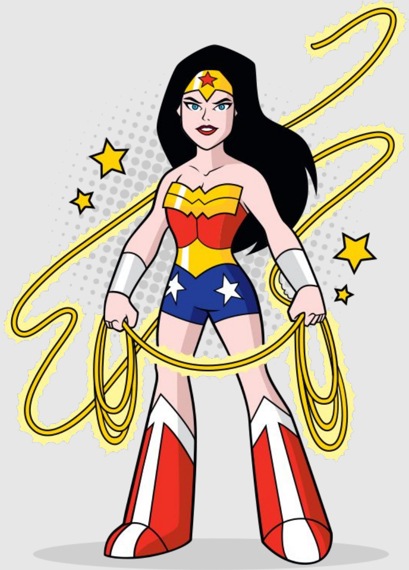


284,335

472

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		

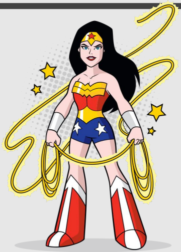
Confusion Matrix Table

	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 

Confusion Matrix Table

10,000
patients

		Diagnosis	
		Diagnosed Sick	Diagnosed Healthy
Patients	Sick	1000	200
	Healthy	800	8000

Confusion Matrix Table

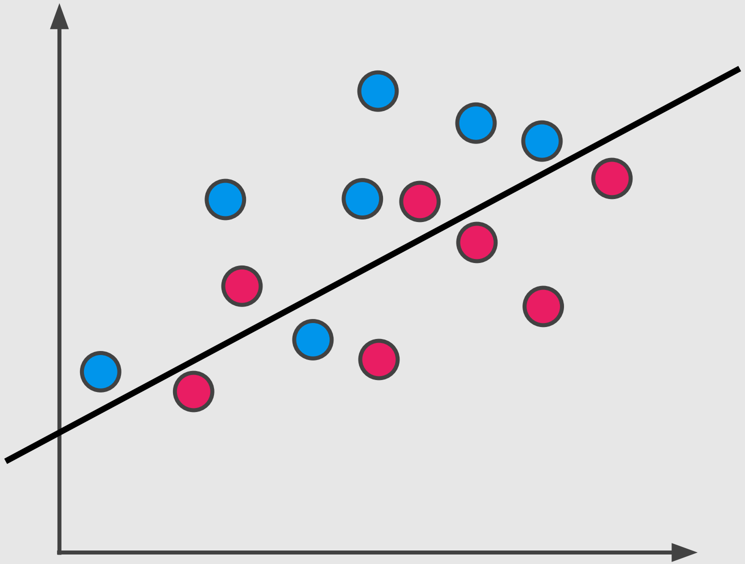
	Sent to Spam Folder	Sent to Inbox
Spam	True Positive 	False Negative 
Not Spam	False Positive 	True Negative 

Confusion Matrix Table

1,000
emails

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

Confusion Matrix Table

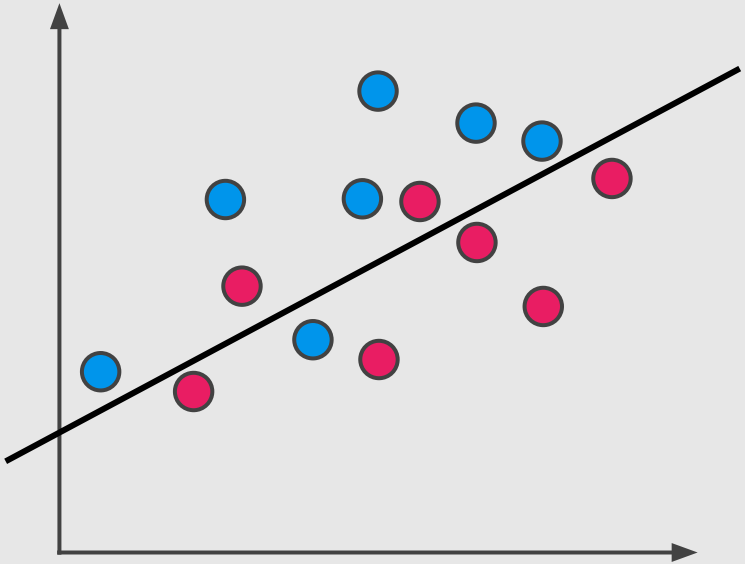


Prediction

Data

	Guessed Positive	Guessed Negative
Positive		
Negative		

Confusion Matrix Table

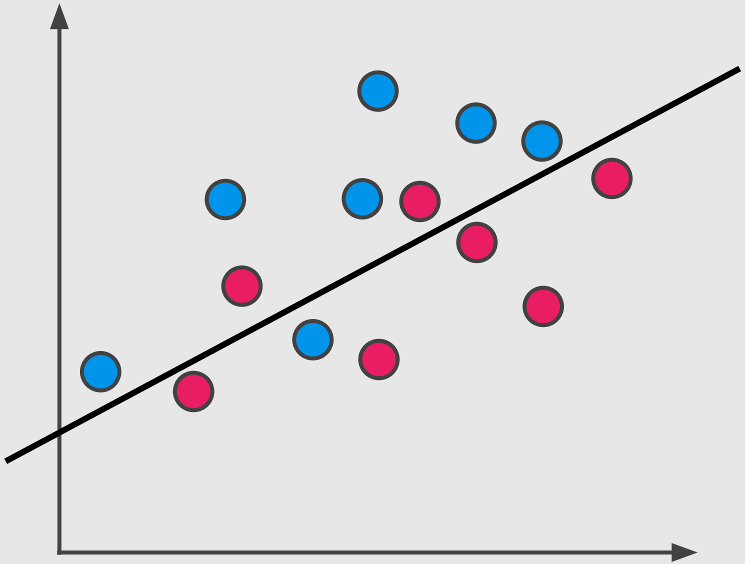


Prediction

Data

	Guessed Positive	Guessed Negative
Positive	6 True positives	
Negative		

Confusion Matrix Table

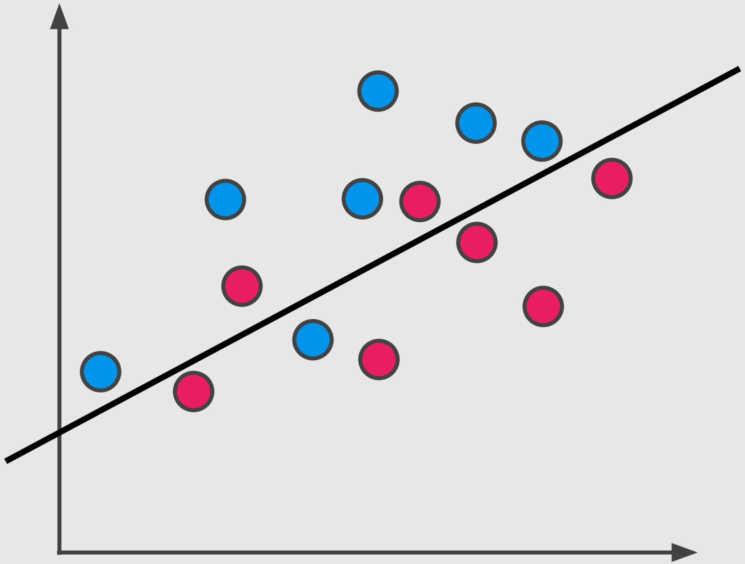


Prediction

Data

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

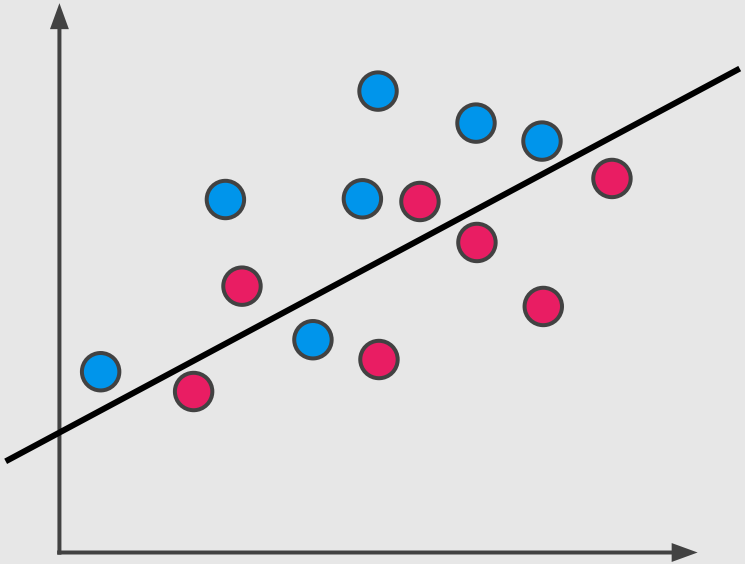
Confusion Matrix Table



Prediction

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

Confusion Matrix Table



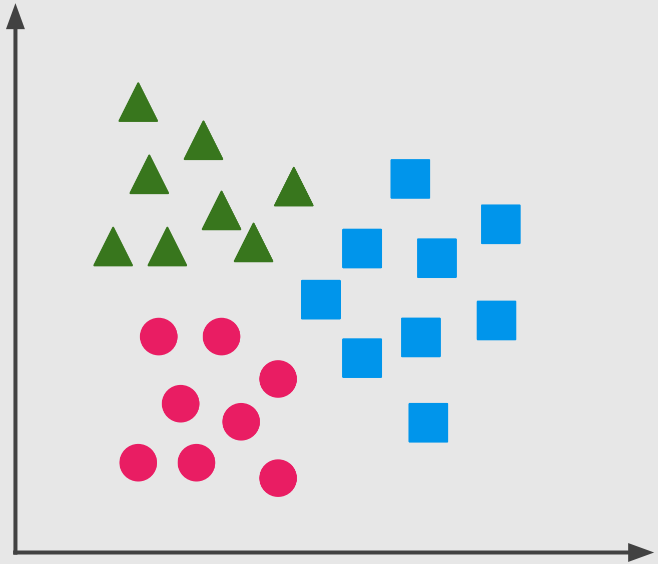
Prediction

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: ●

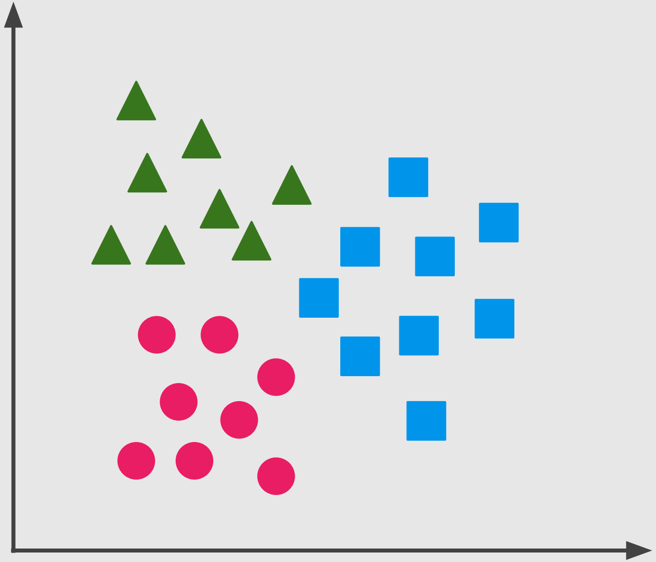


Confusion Matrix Table (n classes)

Class 1: ▲

Class 2: ■

Class 3: ●



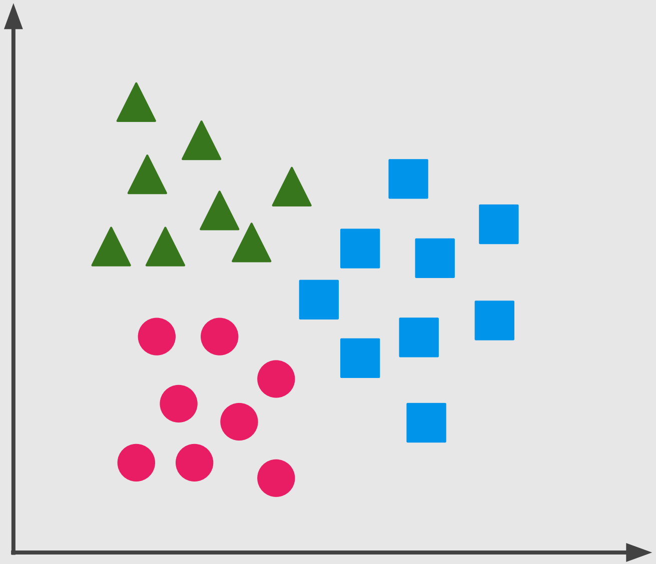
Predicted Class

True Class

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

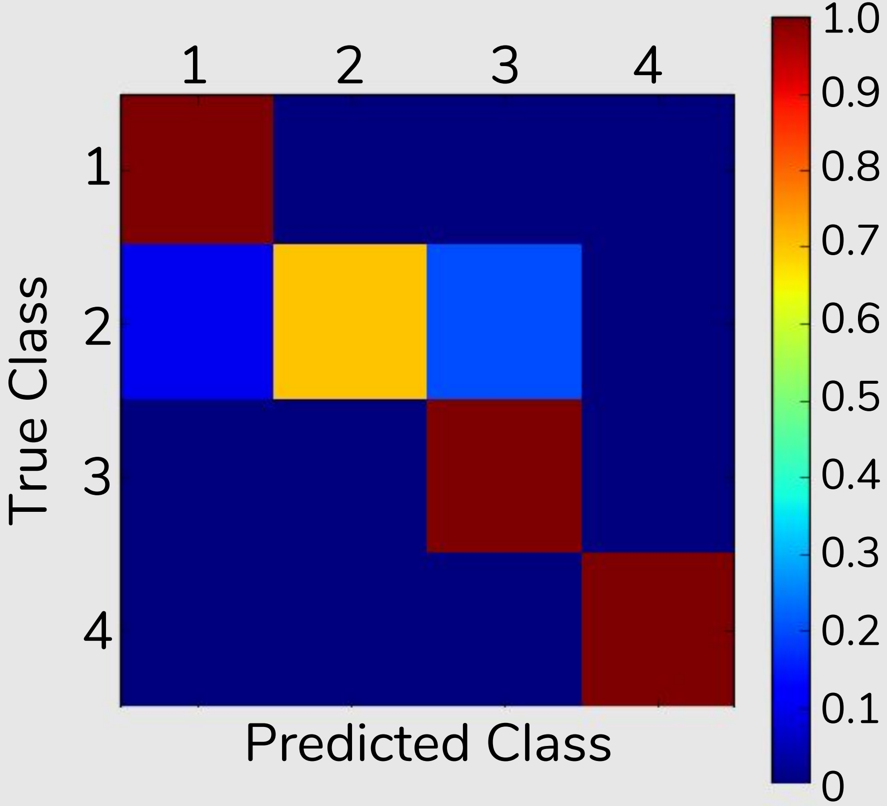
Confusion Matrix Table (n classes)

Class 1: ▲
Class 2: ■
Class 3: ●



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

Confusion Matrix Table (n classes)



Accuracy

Diagnosis

Patients

	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	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

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?

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

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	
		Spam Folder	Inbox
Email	Spam	100	170
	Not Spam	30	700

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

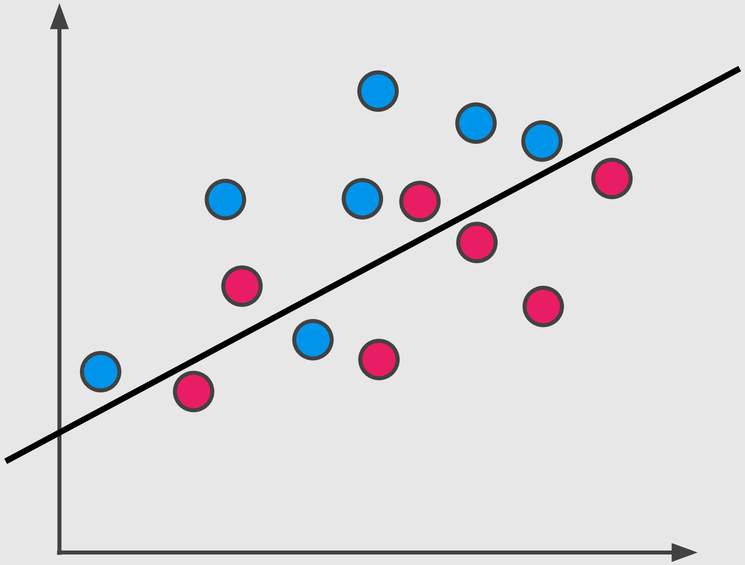
Accuracy

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

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

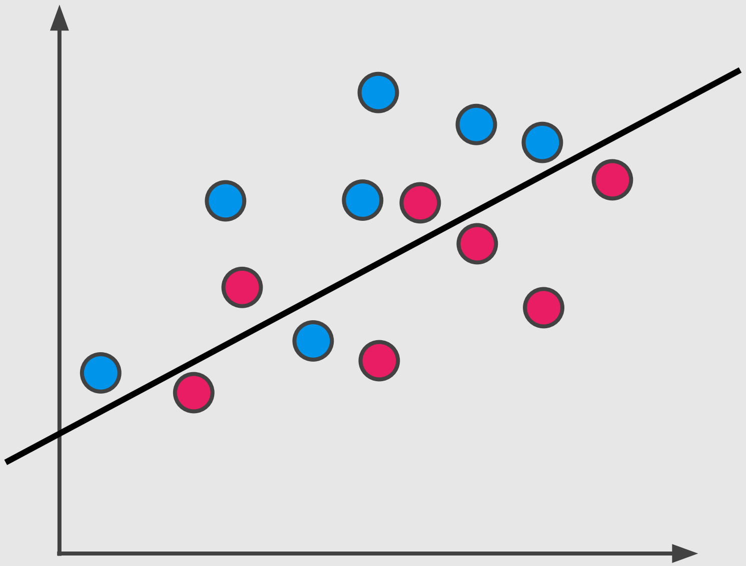
$$\text{Accuracy} = \frac{100 + 700}{1{,}000} = 80\%$$

Accuracy



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

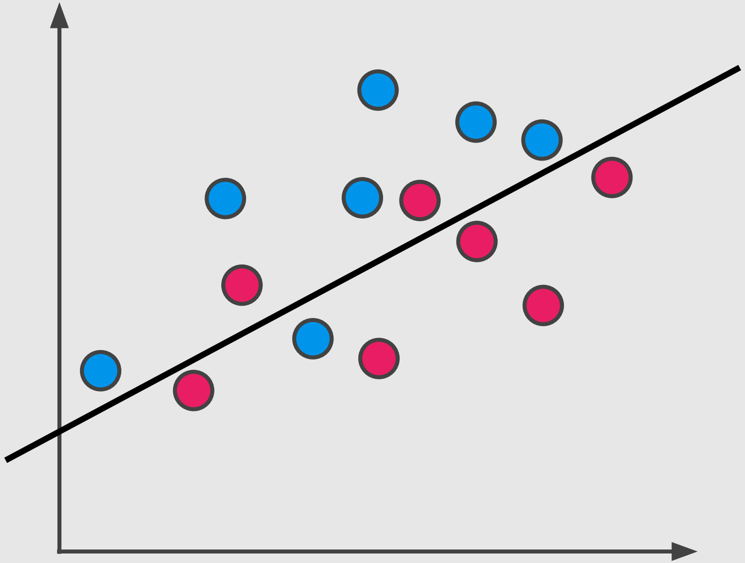
Accuracy



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?

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

Normalized Accuracy

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

Normalized Accuracy

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

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

Normalized Accuracy

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

Normalized Accuracy =

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

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

Normalized Accuracy

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

Normalized Accuracy =

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

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

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

Normalized Accuracy

Accuracy = 80%

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

Normalized Accuracy =

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

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

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

Normalized Accuracy

Accuracy = 90%

Diagnosis

Patients

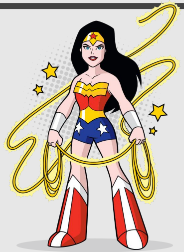
	Diagnosed Sick	Diagnosed Healthy
Sick	1,000	200
Healthy	800	8,000

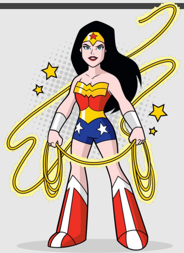
Normalized Accuracy =

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

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

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

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

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

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

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

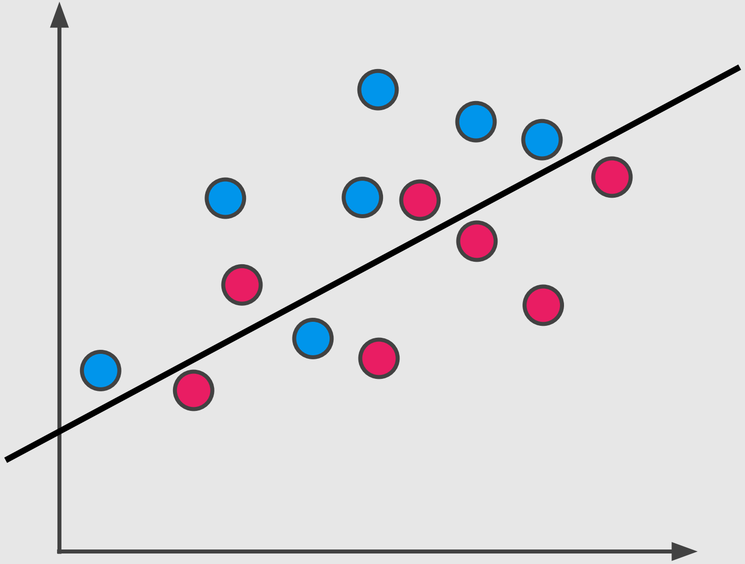
	Spam Folder	Inbox
Spam	100	170
Not Spam	30	700

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

Precision =

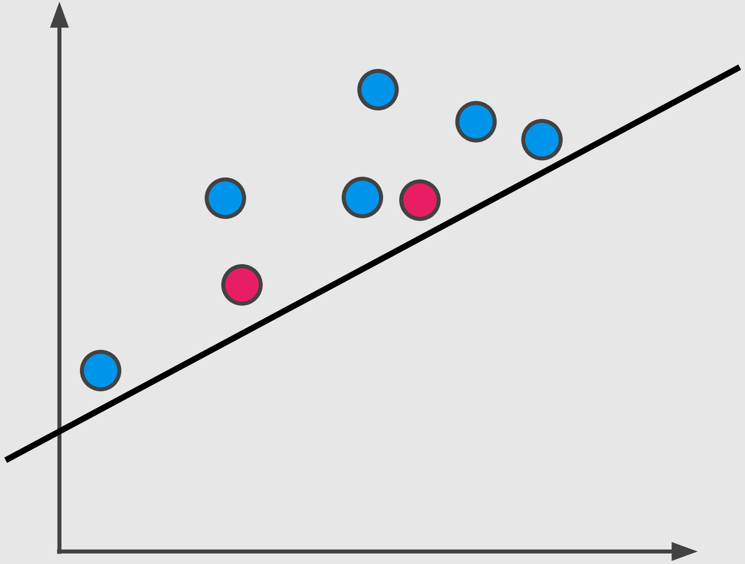
$$\frac{100}{100 + 300} = 76.9\%$$

Precision



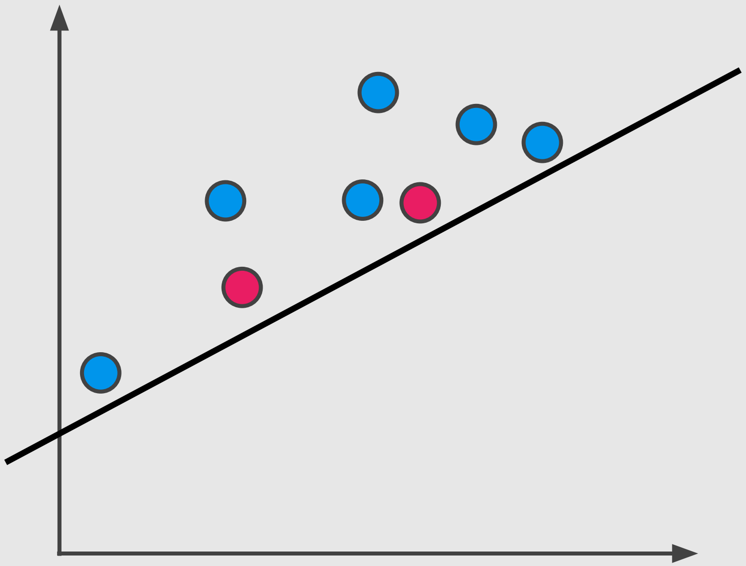
Precision:
Out of all the points we've predicted to be positive, how many are correct?

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?

Precision =

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

Recall

Diagnosis

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

Recall

		Diagnosis	
		Diagnosed Sick	**Diagnosed Healthy**
Patients	**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

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?

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

Recall

		Folder	
		Spam Folder	Inbox
Email	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

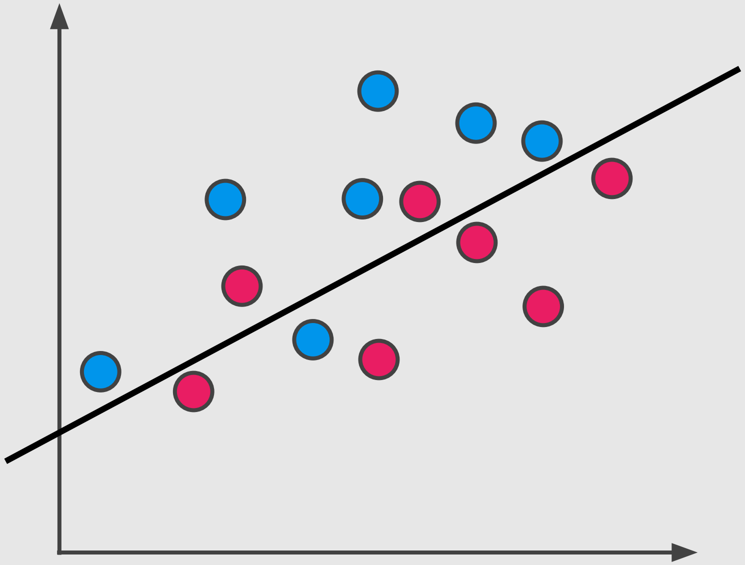
	Spam Folder	Inbox
Spam	100	170
Not Spam	30	700

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

Recall =

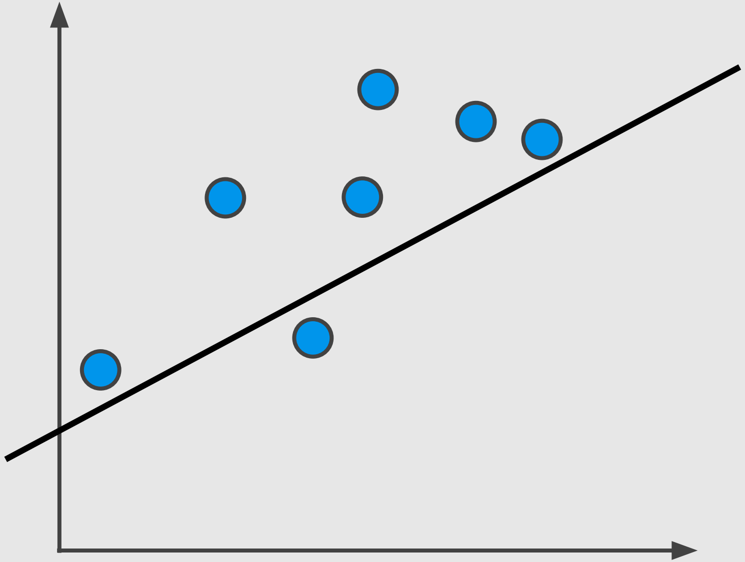
$$\frac{100}{100 + 170} = 37\%$$

Recall



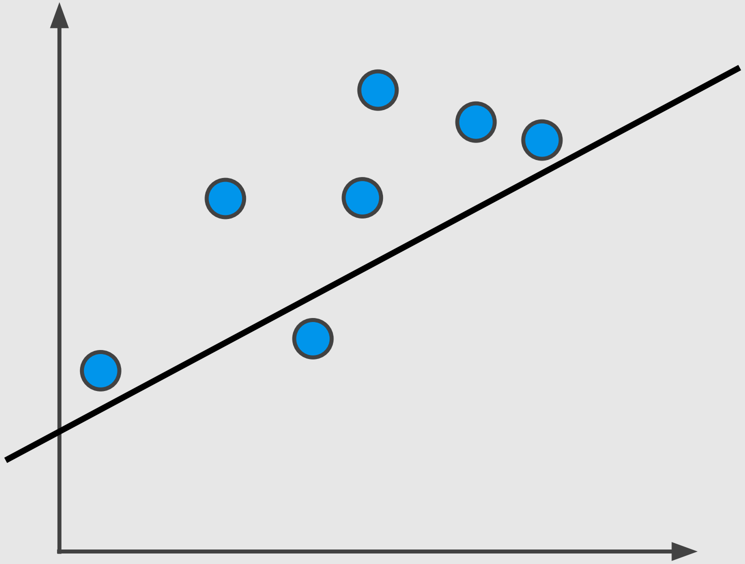
Recall:
Out of all the points labelled positive,
how many did we correctly predict?

Recall



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

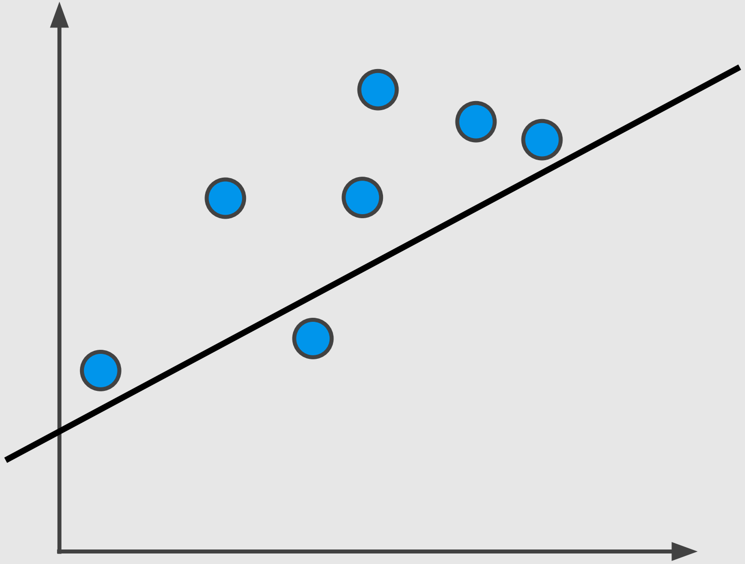
Recall



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

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

Recall



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

Recall =

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

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

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%

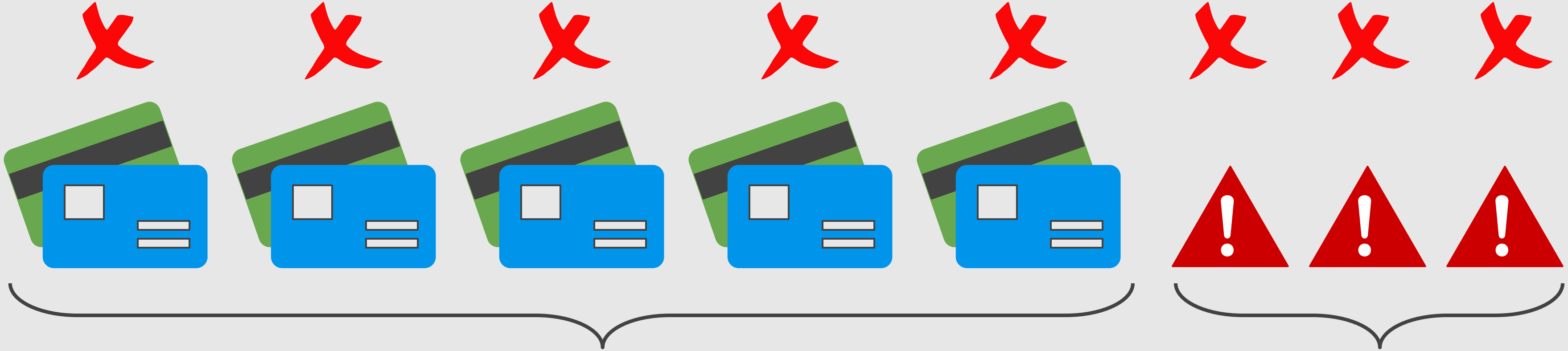
Spam Detector

Precision: 76.9%

Recall: 37%

Average = 56.9%

Credit Card Fraud

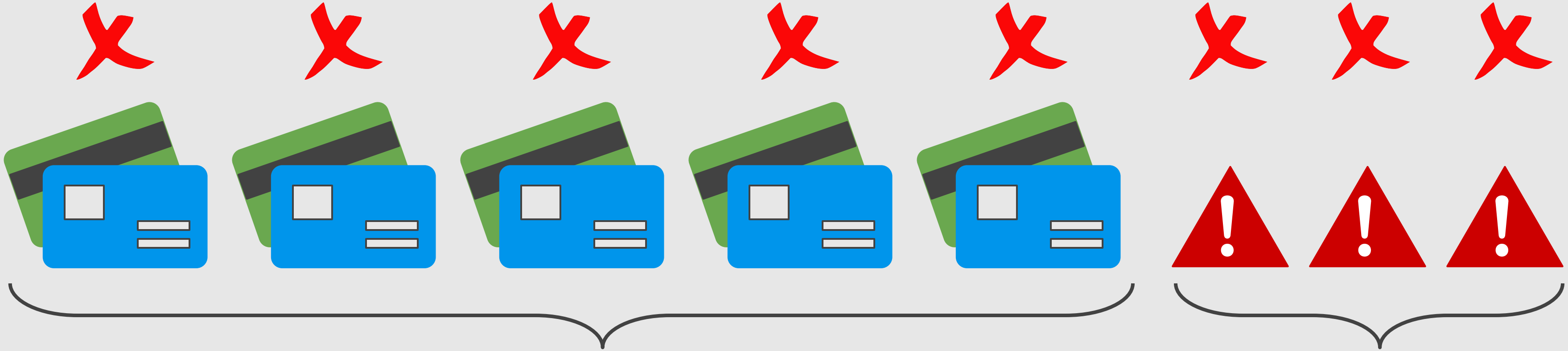


284,335

472

Model: All transactions are fraudulent.

Credit Card Fraud



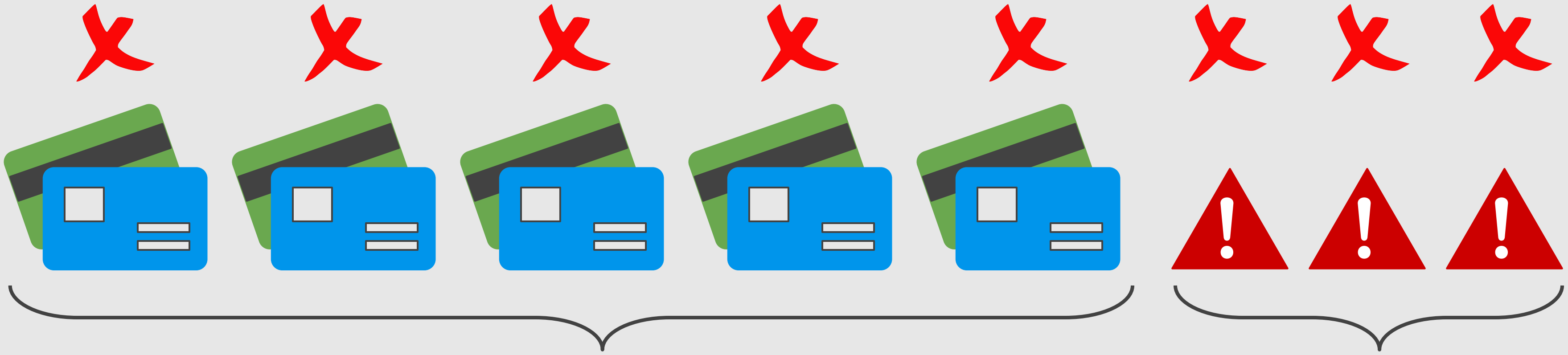
284,335

472

Model: All transactions are fraudulent.

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

Credit Card Fraud



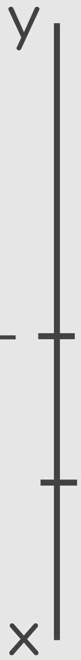
284,335

472

Model: All transactions are fraudulent.

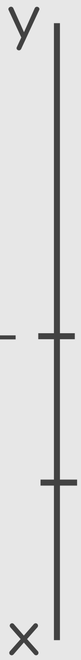
$$\text{Precision} = \frac{472}{284{,}807} = 0.016\% \qquad \text{Recall} = \frac{472}{472} = 100\%$$

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

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

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

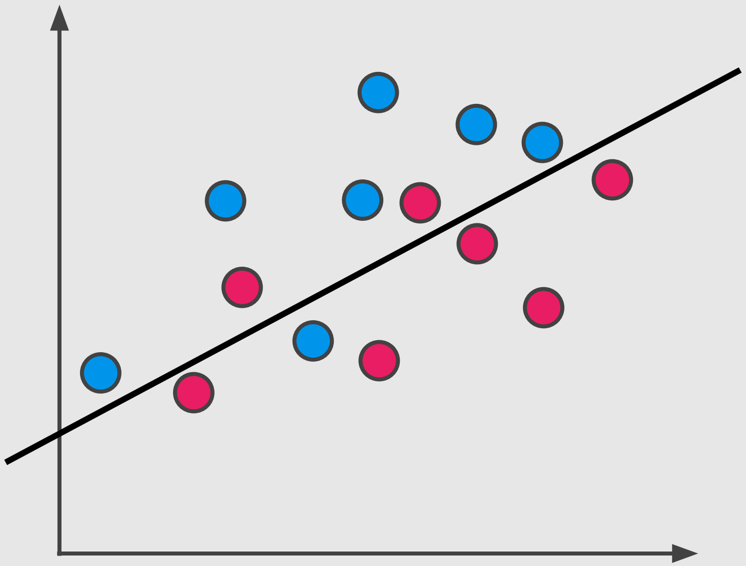
Precision: 76.9%

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)

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

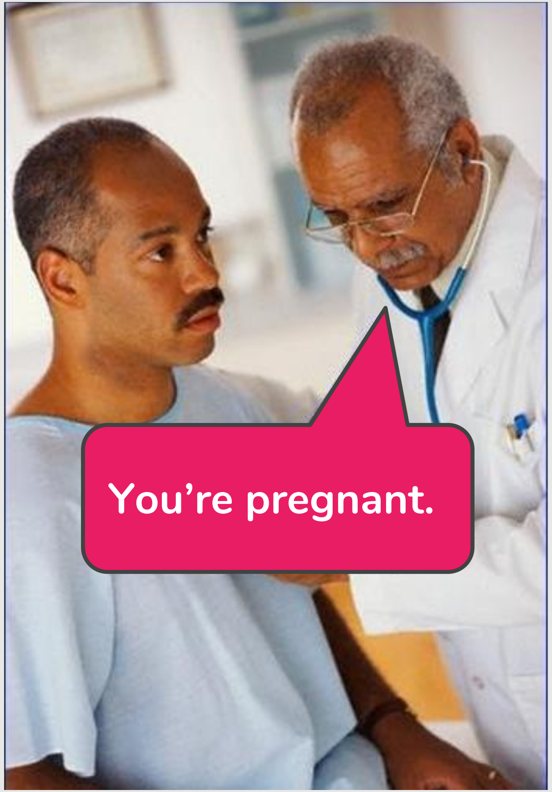
$$F_1 = 2\frac{1}{\frac{1}{\mathrm{recall}} + \frac{1}{\mathrm{precision}}} = 2\frac{\mathrm{precison}\cdot\mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}$$

F_β Score

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

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

Type I Error
(false positive)



Type II Error
(false negative)

References

- https://en.wikipedia.org/wiki/Precision_and_recall
- https://en.wikipedia.org/wiki/Binary_classification
- https://en.wikipedia.org/wiki/F1_score
- 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