Lecture 23: Machine learning

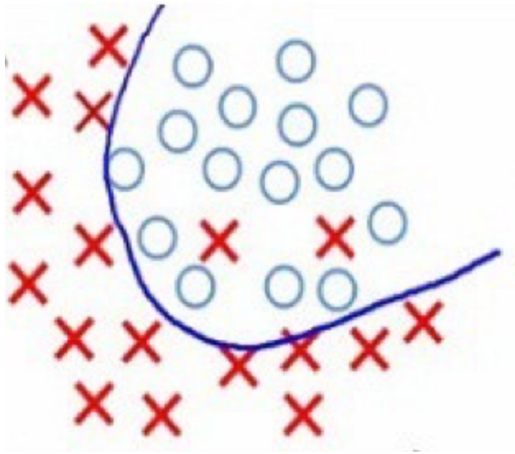
Instructor: Michael Szell
Nov 22, 2023

Today you will see an overview of machine learning

Difference to traditional programming

Fundamental definitions and techniques

Model evaluation



Machine learning is everywhere

Facial Recognition

Spam Detection

Recommendations

Medical Diagnosis

Smart Cars

Fraud Detection

Online Search

Speech

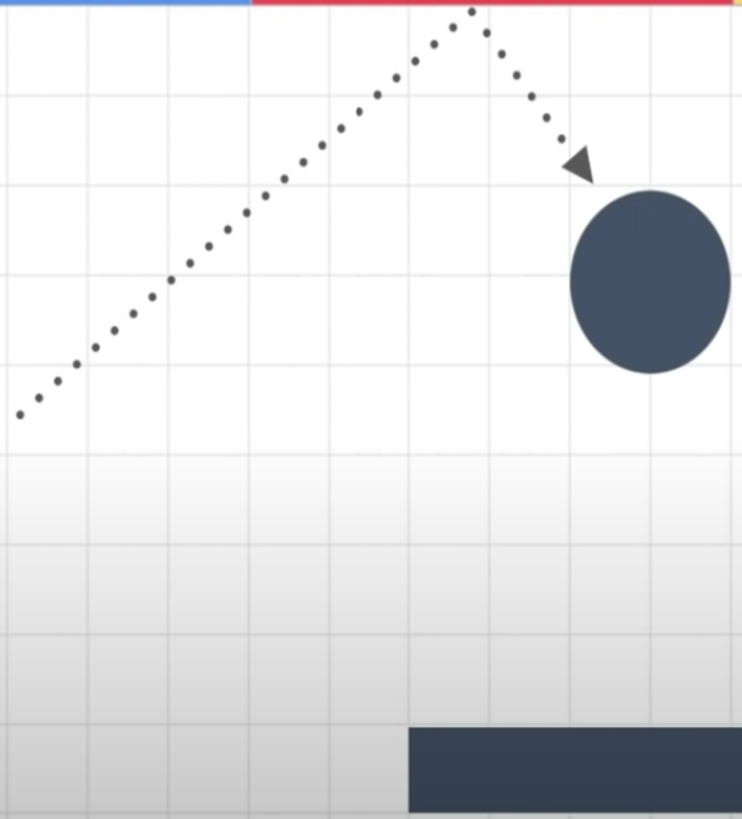
There is no common definition of machine learning

“Field of study that gives computers the ability to learn without being explicitly programmed”. Arthur Samuel (1959)

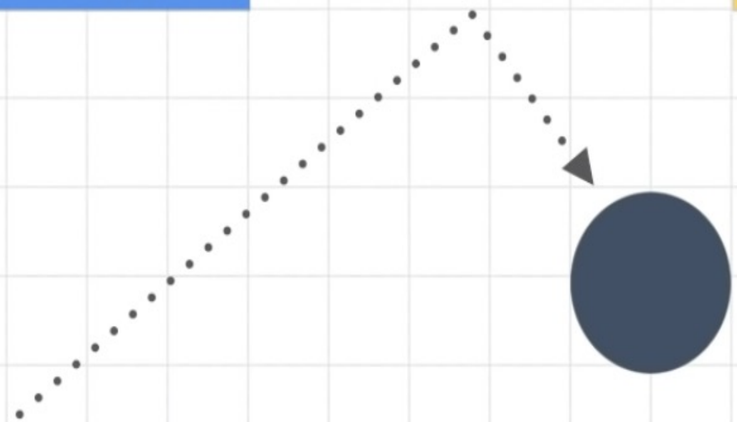
Creating and using models that are learned from data

Traditional programming
versus
Machine learning

Traditional programming



```
if (ball.collide(brick)){
    removeBrick();
    ball.dy=-1*(ball.dy);
}
```



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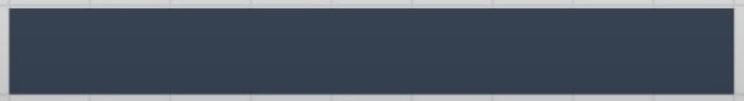
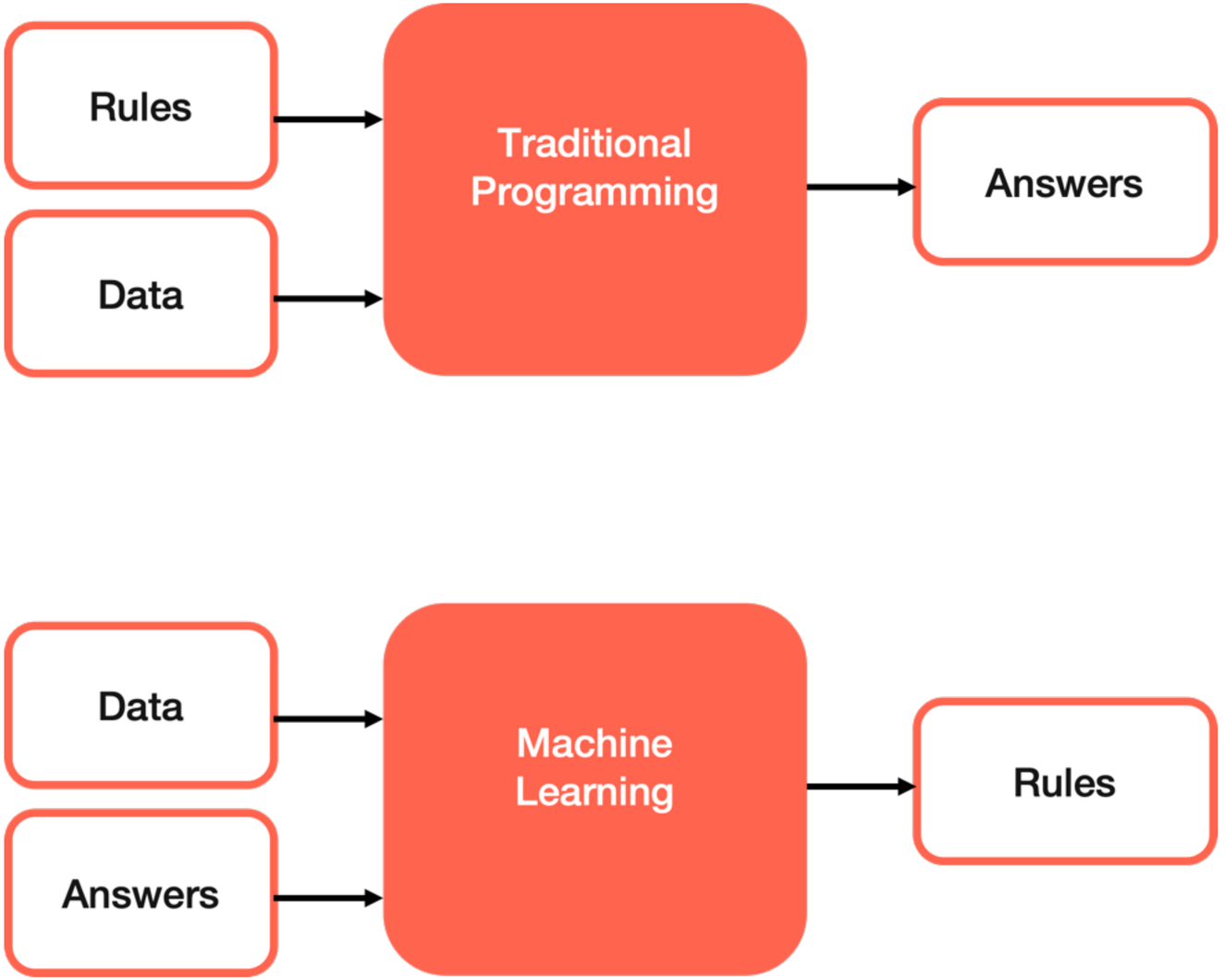


Traditional programming

Traditional programming vs Machine learning



Activity recognition in traditional programming

```
if(speed<4){
    status=WALKING;
}
```

Activity recognition in traditional programming

```
if(speed<4){
    status=WALKING;
}
```

```
if(speed<4){
    status=WALKING;
} else {
    status=RUNNING;
}
```

Activity recognition in traditional programming

```
if(speed<4){
    status=WALKING;
}
```

```
if(speed<4){
    status=WALKING;
} else {
    status=RUNNING;
}
```

```
if(speed<4){
    status=WALKING;
} else if(speed<12){
    status=RUNNING;
} else {
    status=BIKING;
}
```

Activity recognition in traditional programming

```
if(speed<4){
    status=WALKING;
}
```

```
if(speed<4){
    status=WALKING;
} else {
    status=RUNNING;
}
```

```
if(speed<4){
    status=WALKING;
} else if(speed<12){
    status=RUNNING;
} else {
    status=BIKING;
}
```

```
// Uh oh
```

Activity recognition in machine learning

```
0101001010100101
0101001010101001
0111010100101010
0101010010101001
010100101010
 Label =
 WALKING
```

```
1010100101001010
1010101010010010
0100010010011111
0101011111010100
100111101011
 Label =
 RUNNING
```

```
1001010011111010
1011101010111010
1011101010101111
0101010111111110
001111010101
 Label =
 BIKING
```

```
1111111111010011
1010011111010111
1101010101110101
0101011101010101
010100111110
 Label = GOLFING
 (Sort of)
```

Traditional programming of a data relation

X = -1, 0, 1, 2, 3, 4

Y = -2, 1, 4, 7, 10, 13

Traditional programming of a data relation

$$X = -1, 0, 1, 2, 3, 4$$

$$Y = -2, 1, 4, 7, 10, 13$$

$$Y = 3X + 1$$

Traditional programming of a data relation

```
getResult(x)
 {
   return (3 * x) + 1
 }


y = getResult(x);
```

Machine learning to learn a data relation

```
getResult(x)
 {
   p1, p2 = learn();
   return (p1*x)+p2;
 }

y = getResult(x);
```

How are things learned?

Supervised learning

Unsupervised learning

Reinforcement learning

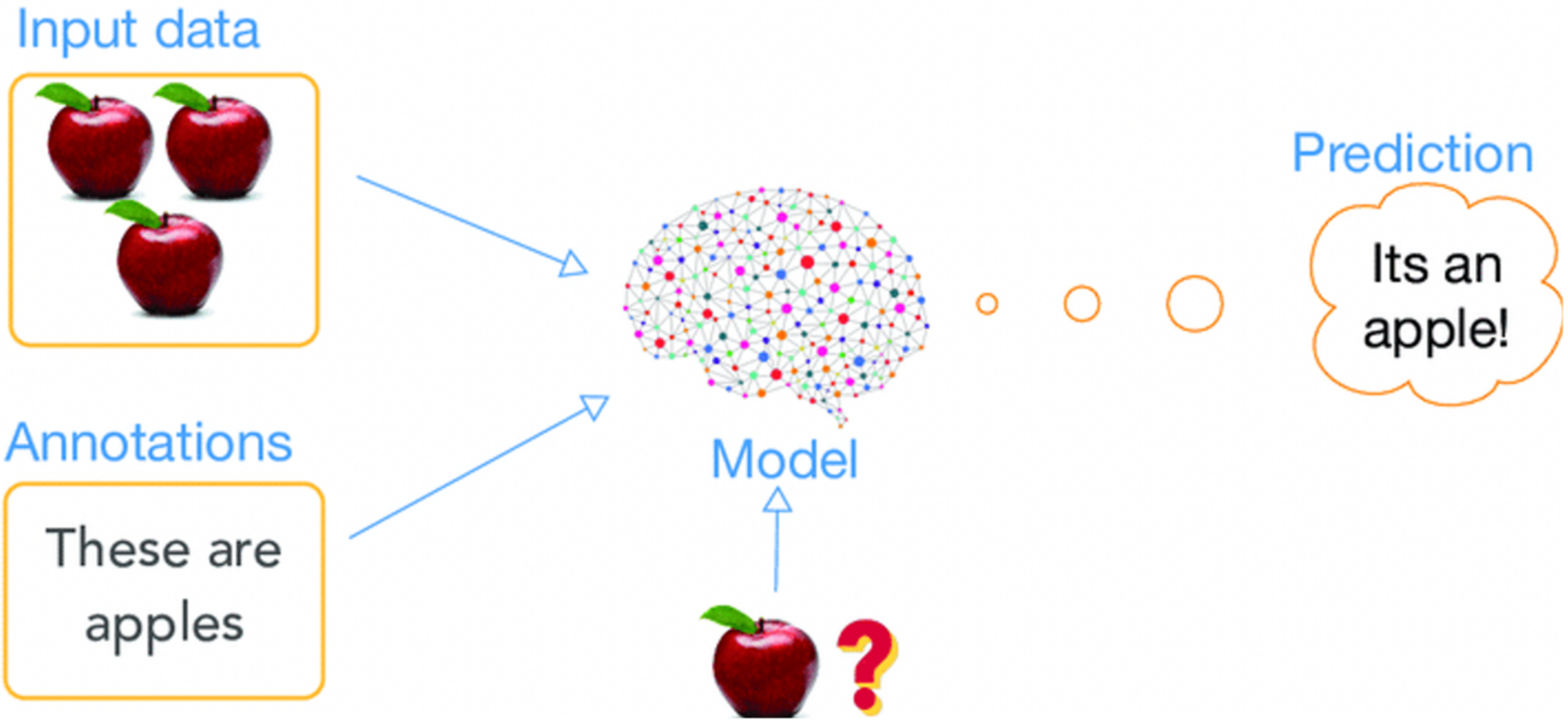
How are things learned?

Supervised learning

Unsupervised learning

Reinforcement learning

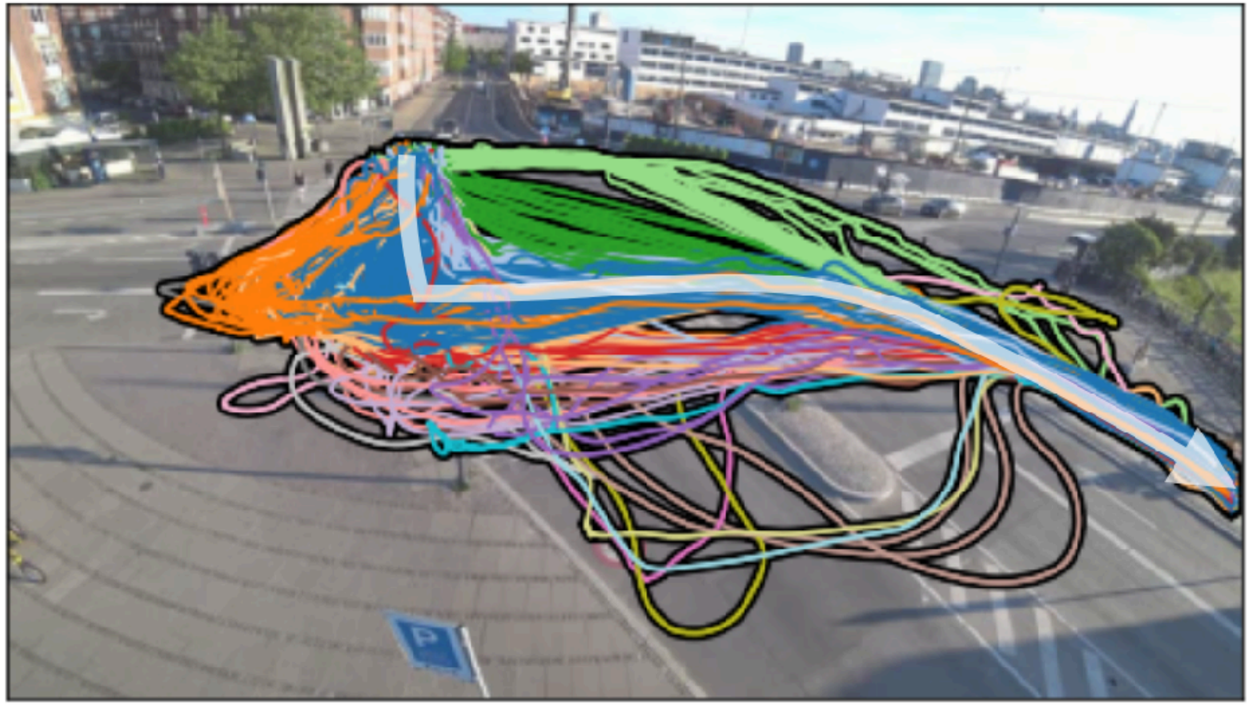
Supervised learning



Supervised learning

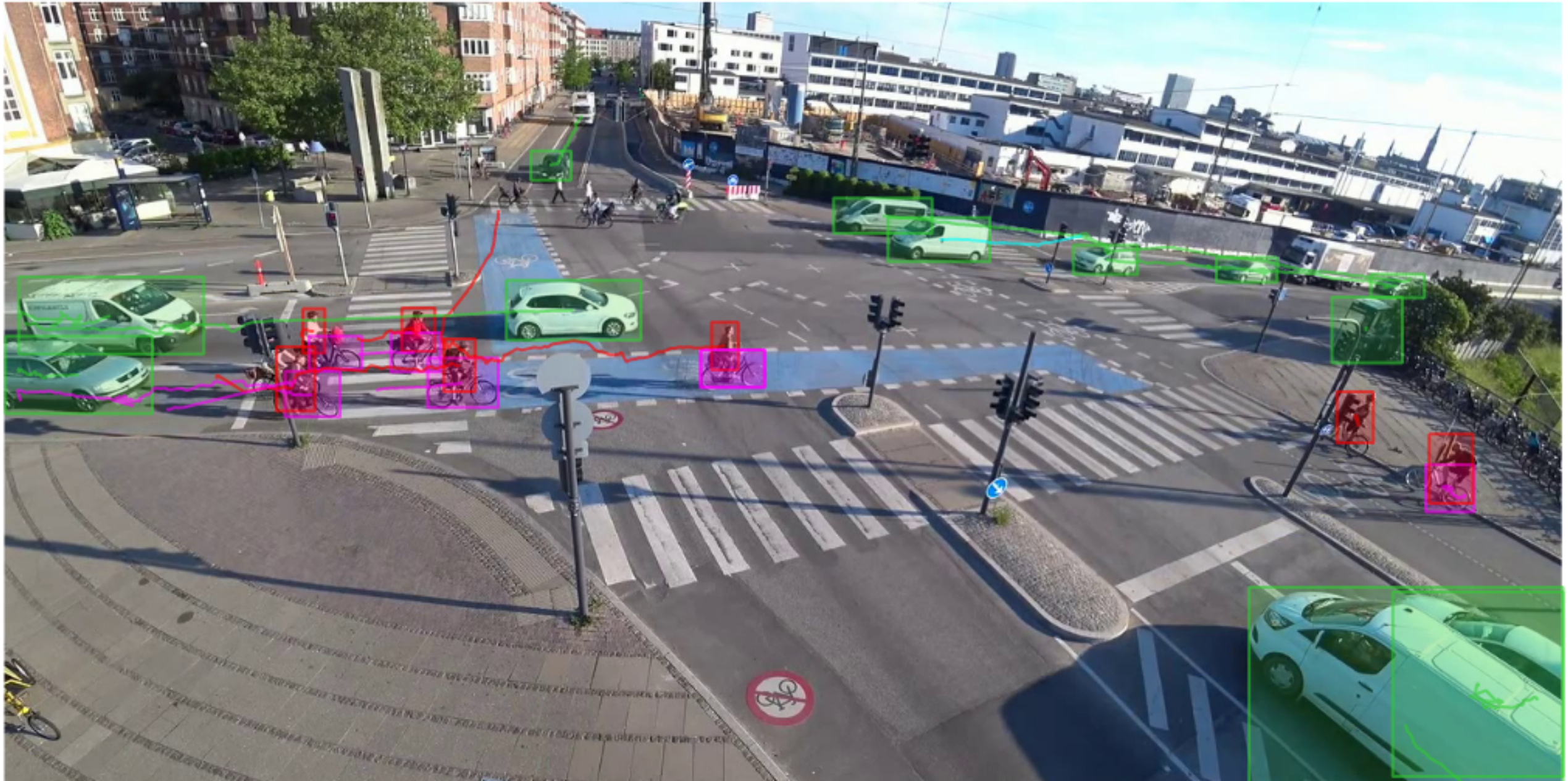
Design

Reality



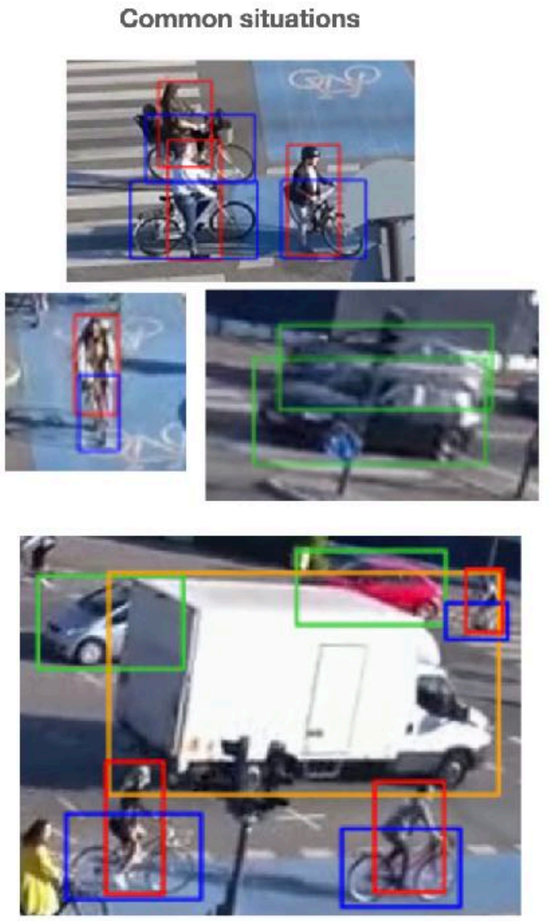
Breum, Kostic & Szell. Computational Desire Line Analysis of Cyclists on the Dybbølsbro Intersection in Copenhagen, Transport Findings 56683 (2022)

Supervised learning



Supervised learning

Instructions for a data annotation tool to label traffic participants



How are things learned?

Supervised learning

A model learns from a labeled dataset with guidance

Unsupervised learning

Reinforcement learning

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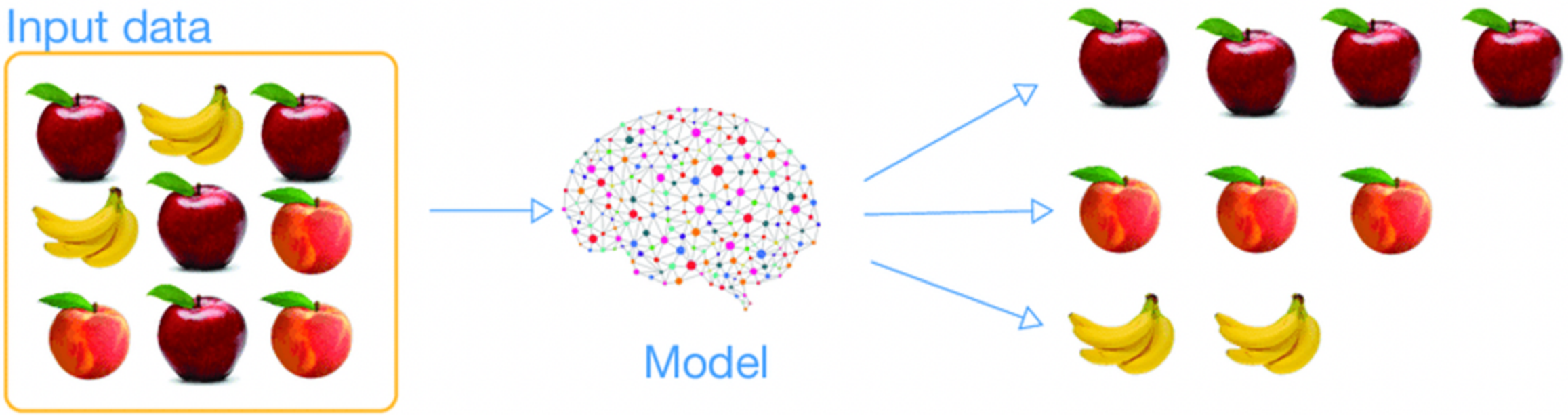

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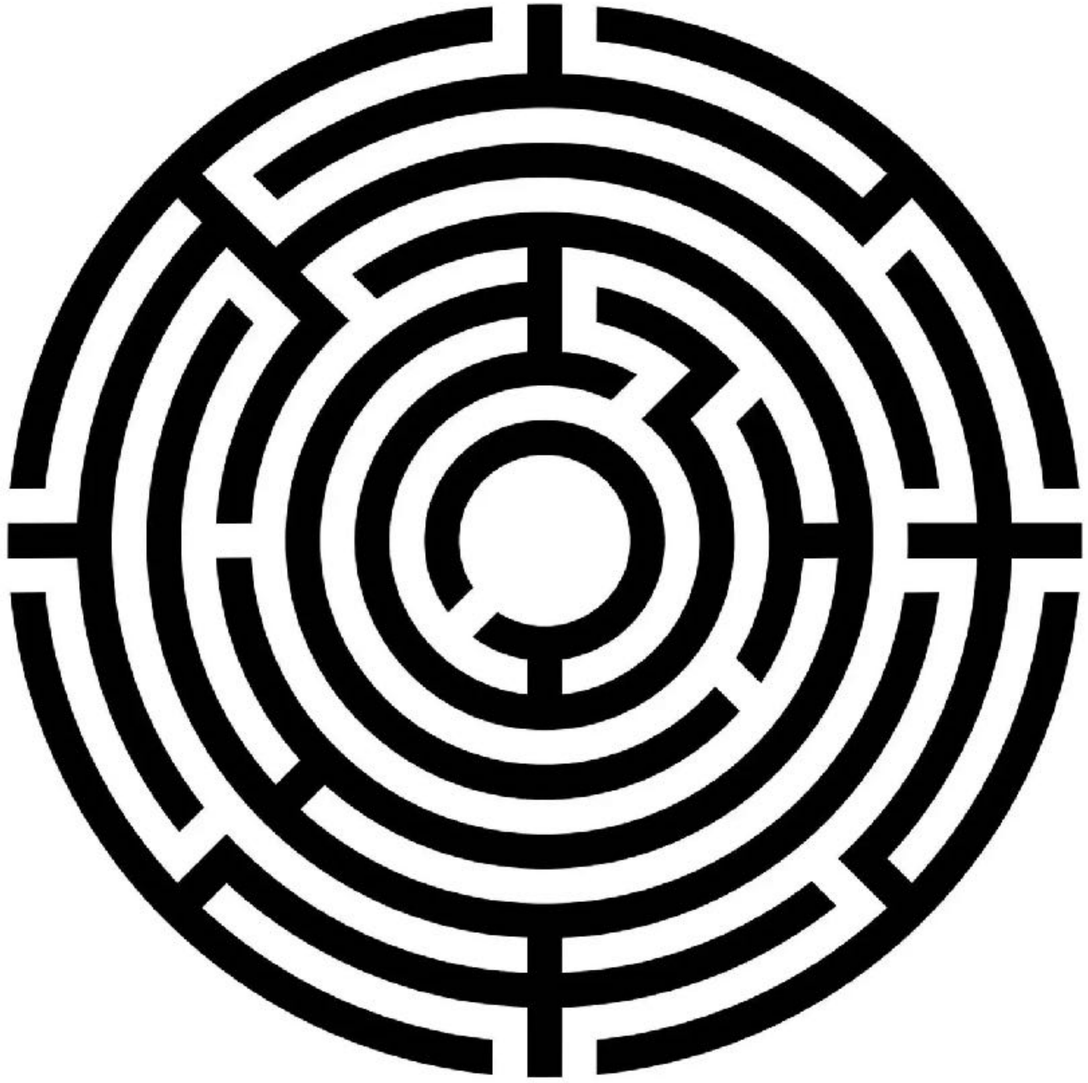
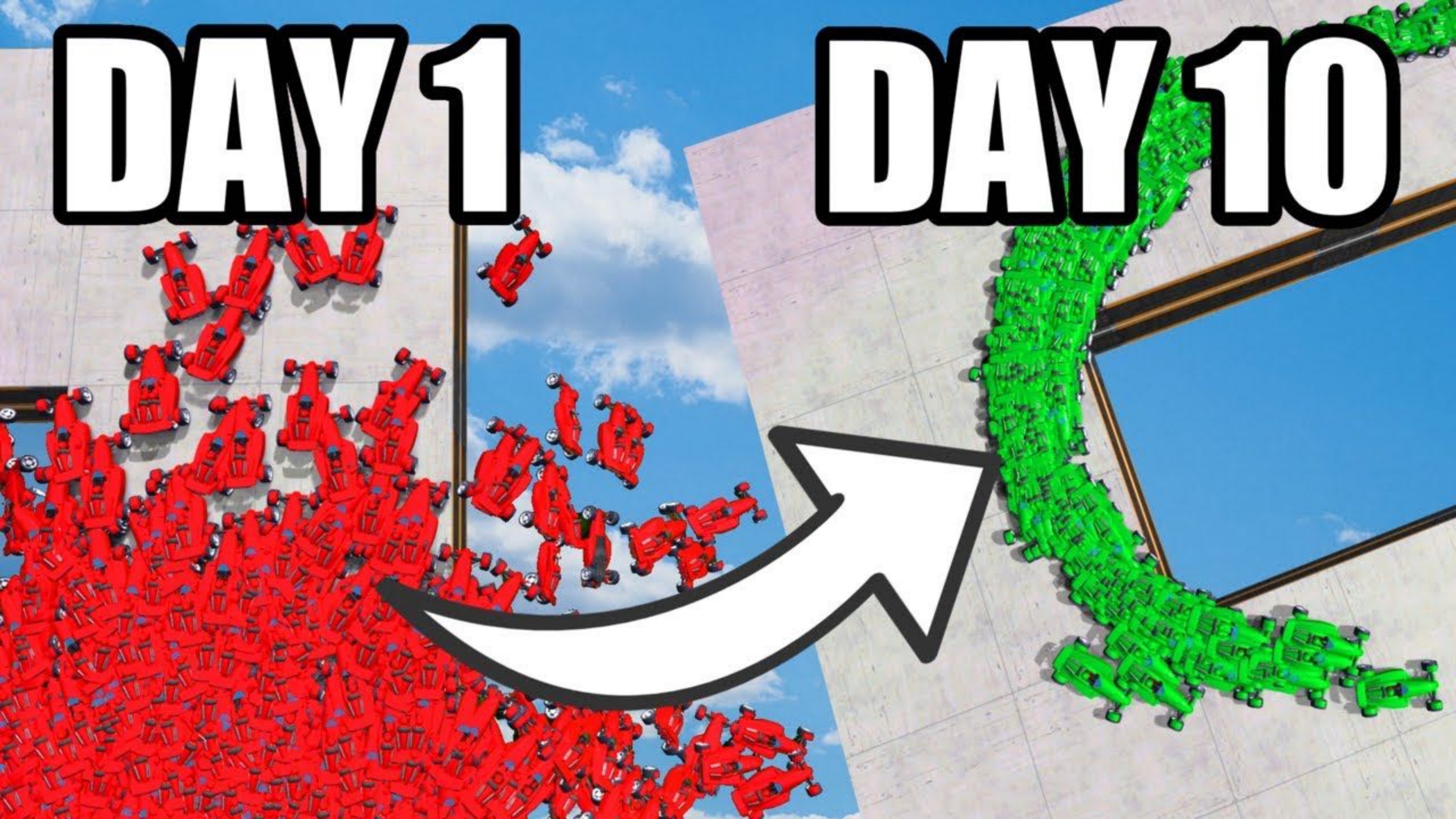
Reinforcement learning




DAY 1
DAY 10

How are things learned?

Supervised learning

A model learns from a labeled dataset with guidance

Unsupervised learning

A model learns from an unlabeled dataset without guidance

Reinforcement learning

A model interacts with an environment and learns by trial-and-error

What is a model?

In machine learning:

> A program that has been trained to recognize certain patterns in data or to make predictions

What is a model?

In machine learning:

A program that has been trained to recognize certain patterns in data or to make predictions

Outside of machine learning:

A specification of a mathematical or probabilistic relationship between different variables

Required choices for machine learning models

Training data and evaluation method

Feature representation / engineering

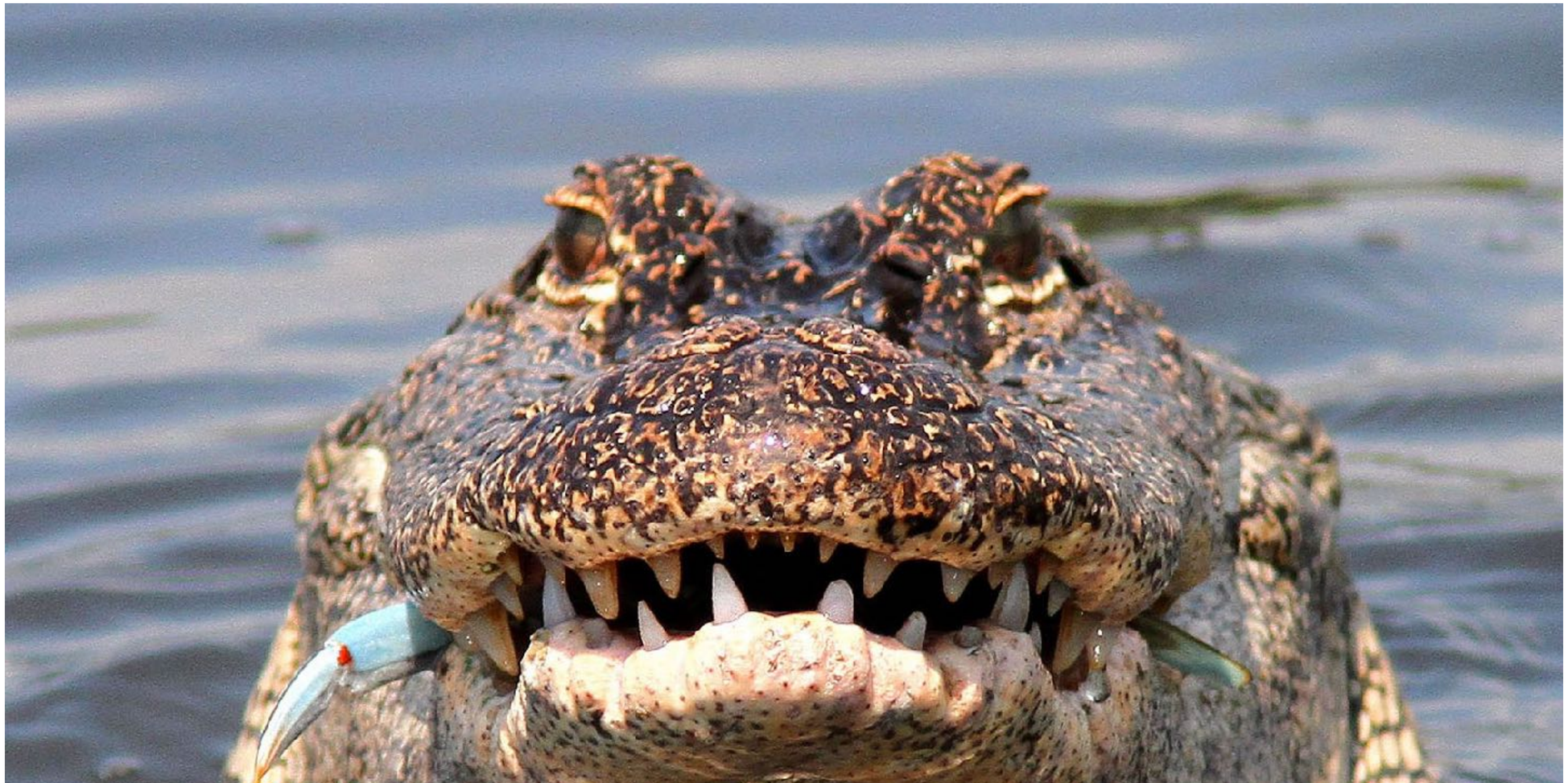
Distance metric for feature vectors

Today

Objective function and constraints

Optimisation method for learning the model

Labeling reptiles



Labeling reptiles

	Features					Label
Name	**Egg-laying**	**Scales**	**Poisonous**	**Cold-blooded**	**# Legs**	**Reptile**
Cobra	TRUE	TRUE	TRUE	TRUE	0	Yes

Model: not enough data to generalize

Labeling reptiles

	Features					Label
Name	**Egg-laying**	**Scales**	**Poisonous**	**Cold-blooded**	**# Legs**	**Reptile**
Cobra	TRUE	TRUE	TRUE	TRUE	0	Yes
Rattlensnake	TRUE	TRUE	TRUE	TRUE	0	Yes

Model: egg-laying & has scales & poisonous & cold-blooded & has no legs

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Rattlensnake	TRUE	TRUE	TRUE	TRUE	0	Yes
Boa Constrictor	FALSE	TRUE	FALSE	TRUE	0	Yes
Chicken	TRUE	TRUE	FALSE	FALSE	2	No

Model: has scales & cold-blooded & has no legs

Labeling reptiles

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Name	Egg-laying	Scales	Poisonous	Cold-blooded	# Legs	Reptile
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Chicken	TRUE	TRUE	FALSE	FALSE	2	No
Alligator	TRUE	TRUE	FALSE	TRUE	4	Yes

Model: has scales & cold-blooded & has no legs

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Chicken	TRUE	TRUE	FALSE	FALSE	2	No
Alligator	TRUE	TRUE	FALSE	TRUE	4	Yes

Model: has scales & cold-blooded & has 0 or 4 legs

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Chicken	TRUE	TRUE	FALSE	FALSE	2	No
Alligator	TRUE	TRUE	FALSE	TRUE	4	Yes
Dart frog	TRUE	FALSE	TRUE	FALSE	4	No

Model: has scales & cold-blooded & has 0 or 4 legs

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Salmon	TRUE	TRUE	FALSE	TRUE	0	No
Python	TRUE	TRUE	FALSE	TRUE	0	Yes

Model: has scales & cold-blooded & has 0 or 4 legs

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Model: has scales & cold-blooded & has 0 or 4 legs

Not enough data

Labeling reptiles

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Model: has scales & cold-blooded

What would be a machine learning approach?

Feature engineering: Turning raw data into feature vectors

A feature vector is a numeric representation of an object.

Feature engineering: Turning raw data into feature vectors

A feature vector is a numeric representation of an object.

- Which features to include?
- How to measure distance between training records?
- How to weight features?

Feature engineering: Turning raw data into feature vectors

A feature vector is a numeric representation of an object.

Name	Egg-laying	Scales	Poisonous	Cold-blooded	# Legs	Reptile
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Feature engineering: Turning raw data into feature vectors

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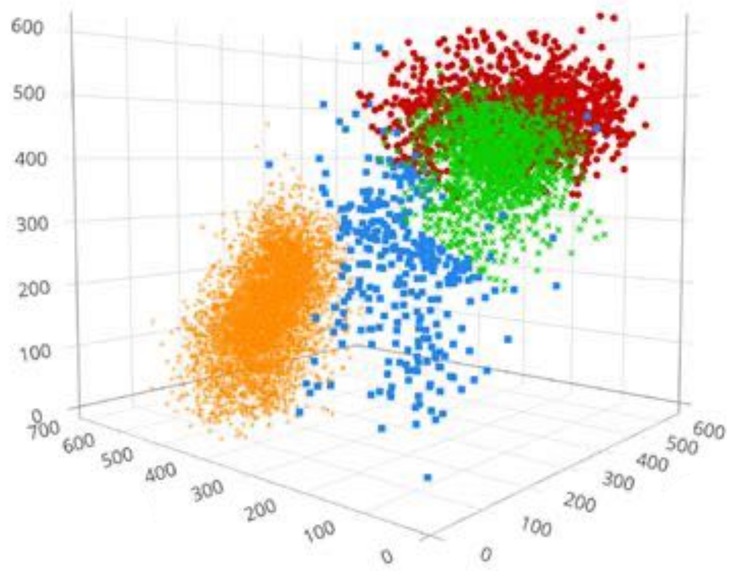
Boa Constrictor	FALSE	TRUE	FALSE	TRUE	0	Yes
Dart frog	TRUE	FALSE	TRUE	FALSE	4	No
	`bool`	`bool`	`bool`	`bool`	`int`	

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
```

Feature engineering: Turning raw data into feature vectors

The feature vectors represent points in a high-dimensional space.




```
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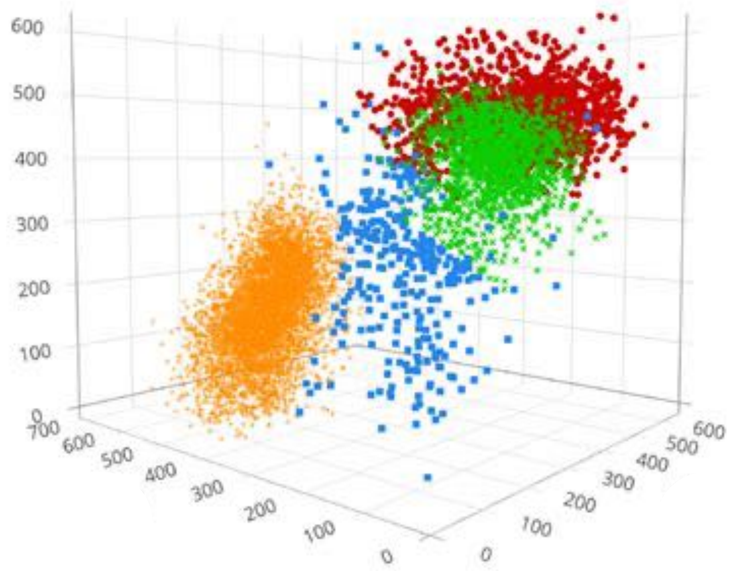

How distant are they to each other?

Do they cluster?

```
rattlesnake = [1,1,1,1,0]
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```

Feature engineering: Turning raw data into feature vectors

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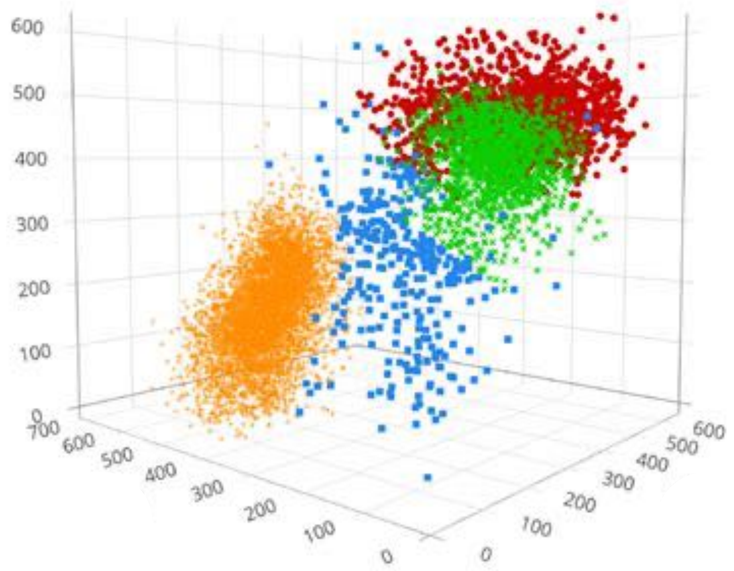


How distant are they to each other?

Do they cluster?

If so, find a classifier surface that optimally separates labeled clusters.

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
```

Defining distance

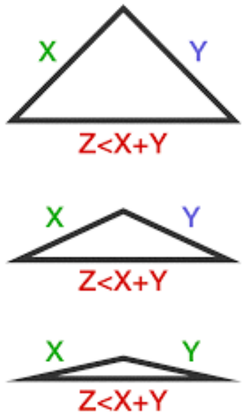
A distance measure $d(A, B)$ has the properties:

1) Symmetry: $d(A, B) = d(B, A)$

2) Identification: $d(A, B) = 0 \quad \text{only if} \quad A = B$

3) Non-negativity: $d(A, B) \geq 0$

4) Triangle inequality: $d(A, C) \leq d(A, B) + d(B, C)$



Euclidian distance

$$\mathbf{p} = (p_1, p_2, \ldots, p_n)$$

$$\mathbf{q} = (q_1, q_2, \ldots, q_n)$$

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

Euclidian distance

$$\mathbf{p} = (p_1, p_2, \ldots, p_n)$$
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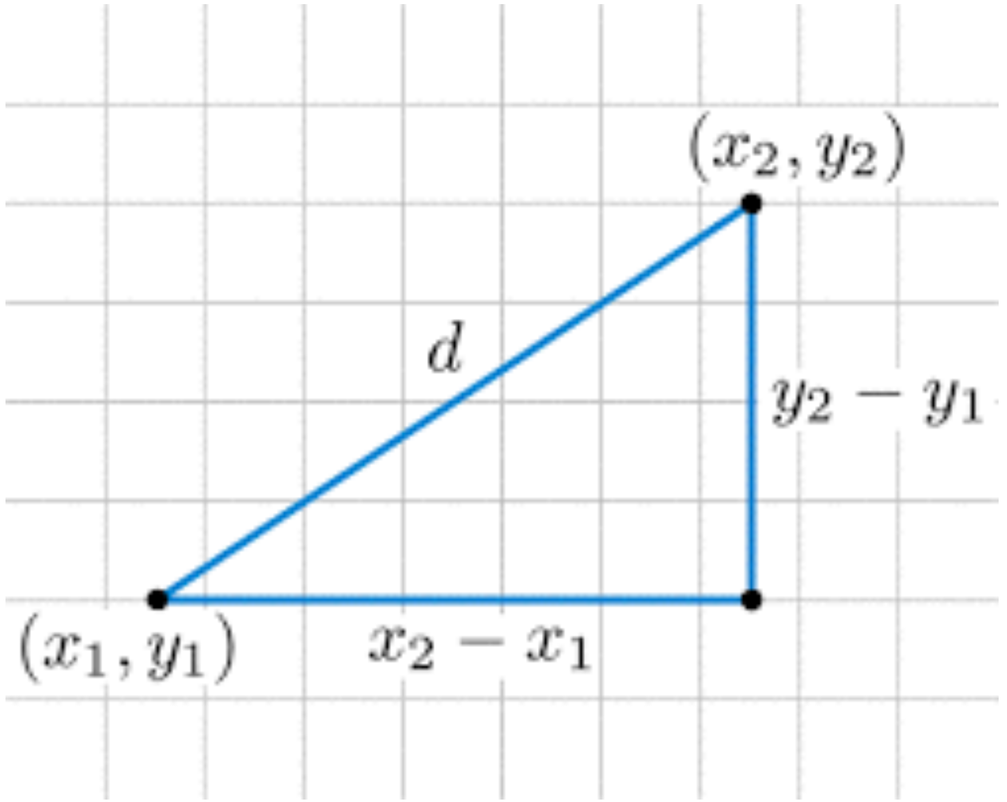
In 2 dimensions, a common notation is:

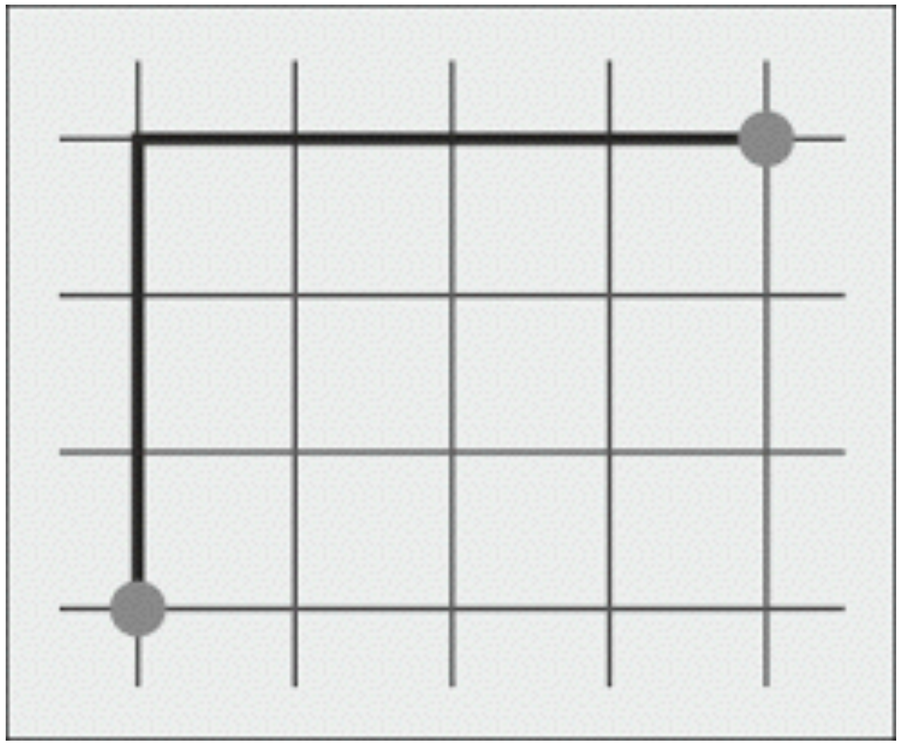
$$\mathbf{p} = (x_1, y_1)$$
$$\mathbf{q} = (x_2, y_2)$$

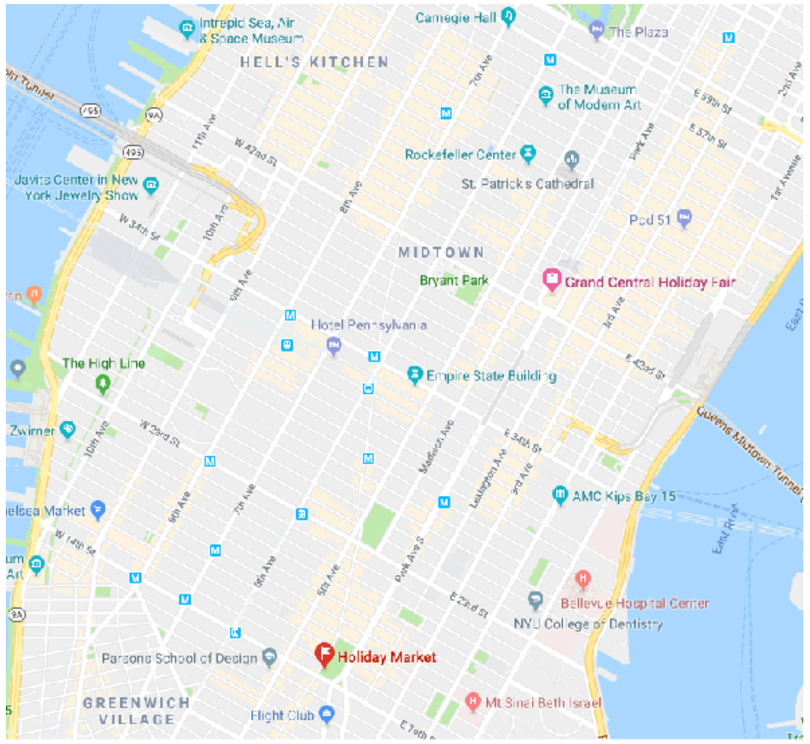


Manhattan distance

Also called: taxicab, L_1

$$d(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^{n} |p_i - q_i|$$

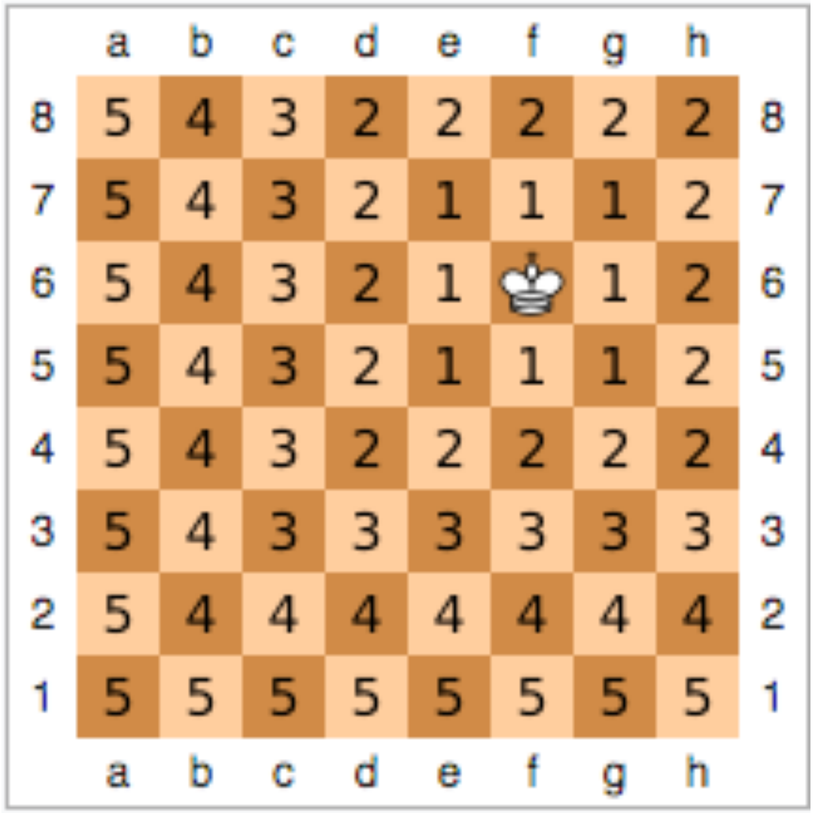




Chebyshev distance

Also called: maximum, chessboard, L_∞

$$d(\mathbf{p}, \mathbf{q}) = \max_i(|p_i - q_i|)$$

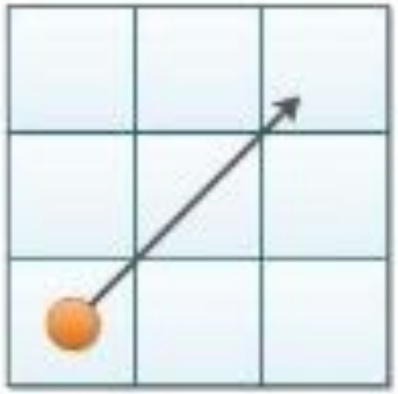


The Minkowski distance generalises these distances

$$d(\mathbf{p}, \mathbf{q}) = \left(\sum_{i=1}^{n} |p_i - q_i|^r \right)^{1/r}$$

$r = 2$

Euclidean Distance



$$\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

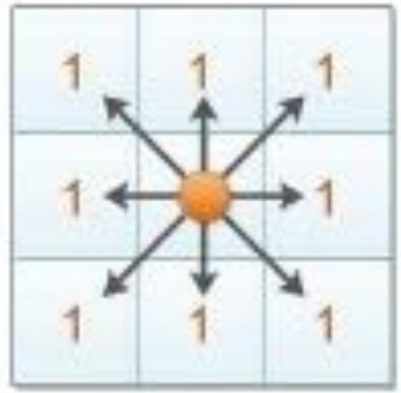
$r = 1$

Manhattan Distance

$$|x_1 - x_2| + |y_1 - y_2|$$

$r = \infty$

Chebyshev Distance



$$\max(|x_1 - x_2|, |y_1 - y_2|)$$

Hamming distance

Also called: edit

$$d(\texttt{karolin},\texttt{kerstin}) =$$

Hamming distance

Also called: edit

$$d(\texttt{karolin},\texttt{kerstin}) = 3$$

Hamming distance

Also called: edit

$$d(\texttt{karolin},\texttt{kerstin}) = 3$$

$$\mathbf{x} = (1, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$
$$\mathbf{y} = (0, 0, 0, 0, 0, 0, 1, 0, 0, 1)$$

$$d(\mathbf{x}, \mathbf{y}) = 3$$

Hamming distance

Also called: edit

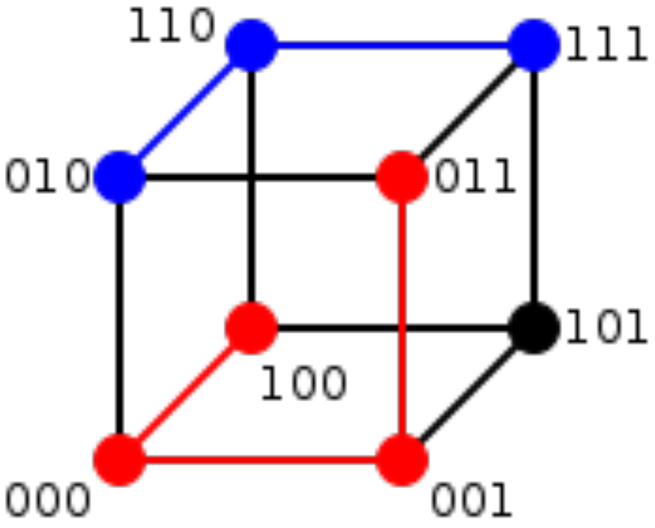
$$d(\texttt{karolin},\texttt{kerstin}) = 3$$

$$\mathbf{x} = (1, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$
$$\mathbf{y} = (0, 0, 0, 0, 0, 0, 1, 0, 0, 1)$$

$$d(\mathbf{x}, \mathbf{y}) = 3$$

For binary vectors this is the Manhattan distance:

$$d(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^{n} |p_i - q_i|$$



Euclidian distance between animals

Blackboard

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
```

$$d(\mathbf{p},\mathbf{q}) = \sqrt{\sum_{i=1}^{n}(p_i - q_i)^2}$$

	rattle snake	boa	frog
rattle snake	0	?	
boa	?	0	
frog			0

Euclidian distance between animals

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
      frog  = [1,0,1,0,4]
```

$$d(\mathbf{p},\mathbf{q}) = \sqrt{\sum_{i=1}^{n}(p_i - q_i)^2}$$

	rattle snake	boa	frog
rattle snake	0	1.41	
boa	1.41	0	
frog			0

Euclidian distance between animals

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
```

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

	rattle snake	boa	frog
rattle snake	0	1.41	4.24
boa	1.41	0	4.47
frog	4.24	4.47	0

Euclidian distance between animals

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
```

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

	rattle snake	boa	frog
rattle snake	0	1.41	4.24
boa	1.41	0	4.47
frog	4.24	4.47	0

Rattlesnake and boa are closer to each other than to the frog. Nice.

Euclidian distance between animals

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
  alligator = [1,1,0,1,4]
```

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

	rattle snake	boa	frog	alligator
rattle snake	0	1.41	4.24	4.12
boa	1.41	0	4.47	4.12
frog	4.24	4.47	0	1.73
alligator	4.12	4.12	1.73	0

Euclidian distance between animals

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
  alligator = [1,1,0,1,4]
```

$$d(\mathbf{p},\mathbf{q}) = \sqrt{\sum_{i=1}^{n}(p_i - q_i)^2}$$

The alligator is closer to frog than to the snakes. Why?

	rattle snake	boa	frog	alligator
rattle snake	0	1.41	4.24	4.12
boa	1.41	0	4.47	4.12
frog	4.24	4.47	0	1.73
alligator	4.12	4.12	1.73	0

Euclidian distance between animals

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,4]
  alligator = [1,1,0,1,4]
```

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

The alligator is closer to frog than to the snakes. Why?

Number of legs dominate instead of matching features!

	rattle snake	boa	frog	alligator
rattle snake	0	1.41	4.24	4.12
boa	1.41	0	4.47	4.12
frog	4.24	4.47	0	1.73
alligator	4.12	4.12	1.73	0

Euclidian distance between animals

```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,1]
  alligator = [1,1,0,1,1]
```

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

Solution: Binarize legs

	rattle snake	boa	frog	alligator
rattle snake	0	1.41	1.73	1.41
boa	1.41	0	2.24	1.41
frog	1.73	2.24	0	1.73
alligator	1.41	1.41	1.73	0

Euclidian distance between animals

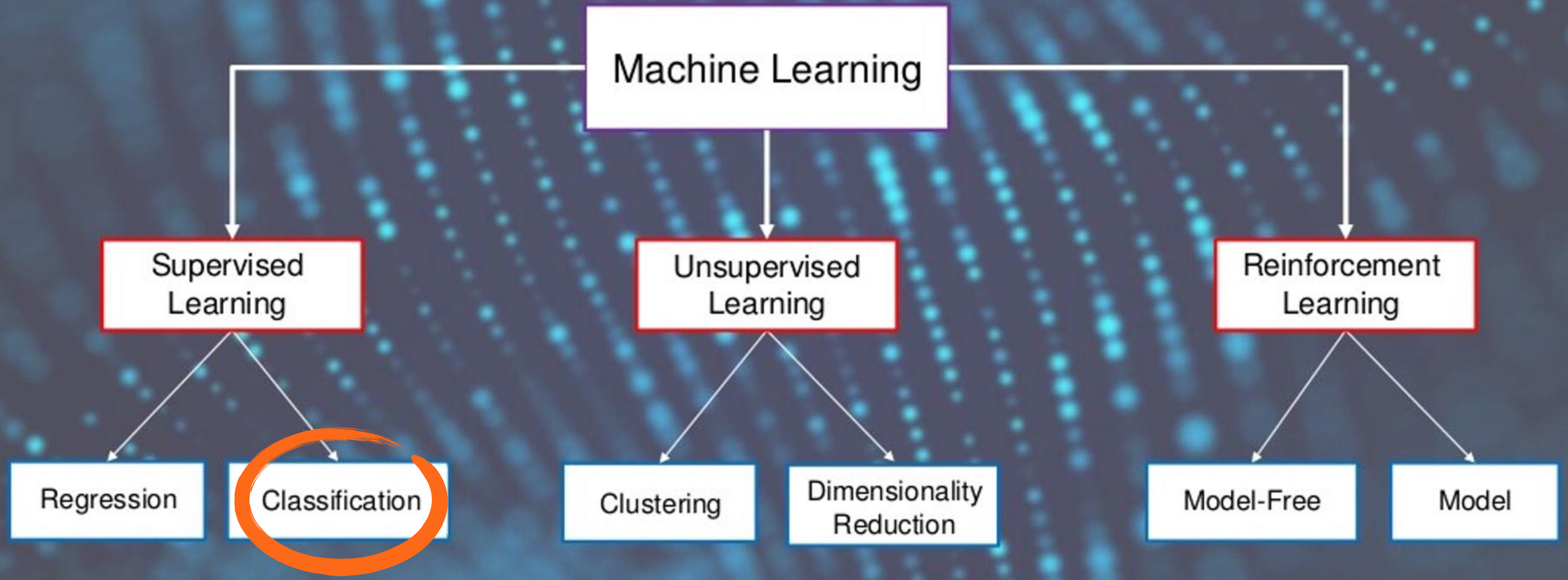
```
rattlesnake = [1,1,1,1,0]
        boa = [0,1,0,1,0]
       frog = [1,0,1,0,1]
  alligator = [1,1,0,1,1]
```

$$d(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

	rattle snake	boa	frog	alligator
rattle snake	0	1.41	1.73	1.41
boa	1.41	0	2.24	1.41
frog	1.73	2.24	0	1.73
alligator	1.41	1.41	1.73	0

The alligator is now closer to the snakes than to the frog. Nice.

Type of Machine Learning



What is Classification?

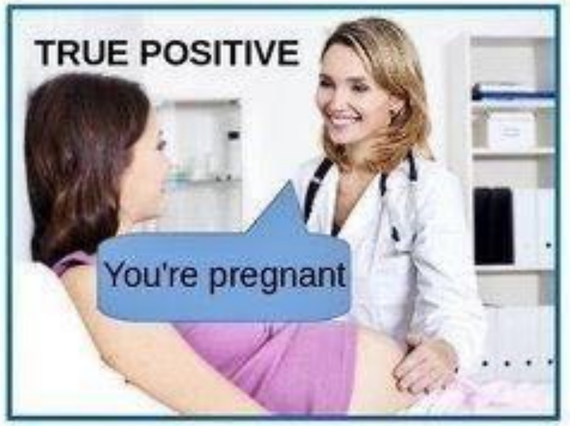
Classification is the process of classifying data into different categories based on some of their common characteristics

Example: A system to **classify spam emails**

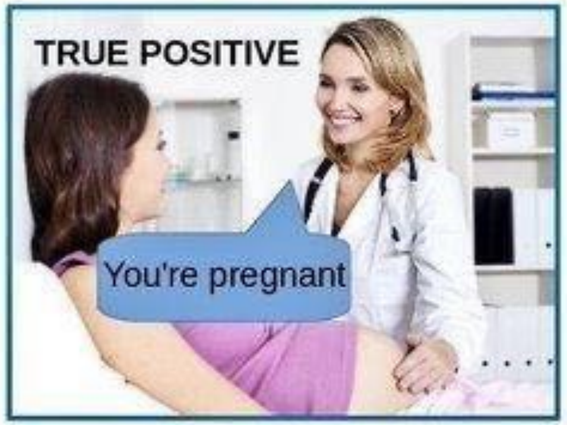
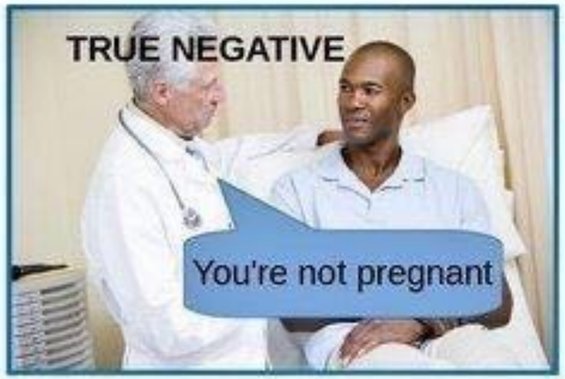
Need for Confusion Matrices

During classification, we also have to overcome the limitations of accuracy. Accuracy can be misleading for classification problems. If there is a significant class imbalance, a model might predict the majority class for all cases and have a high accuracy score

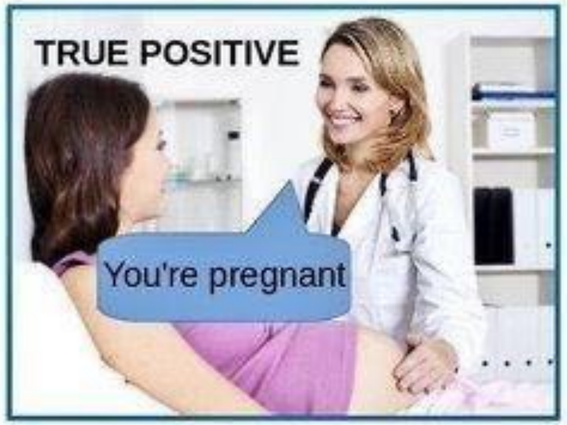
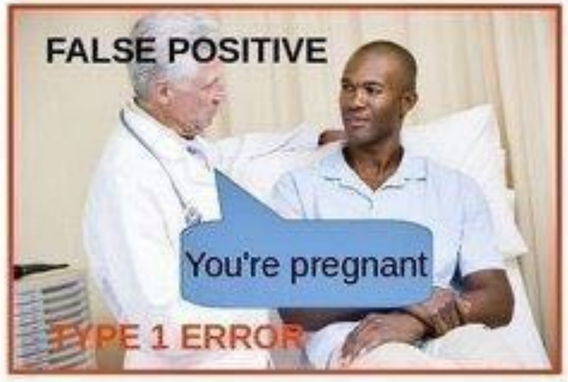
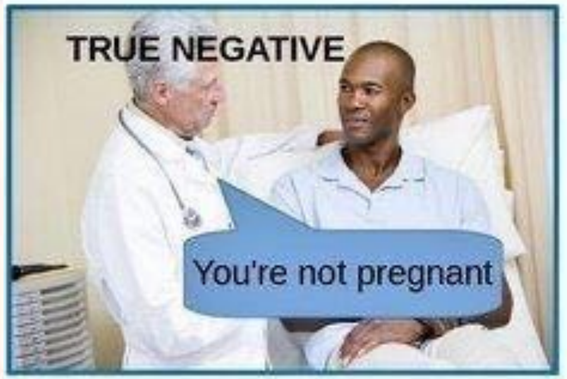
The confusion matrix shows results from binary classification

		Predicted	
		Positive	Negative
Actual	Positive		
	Negative		

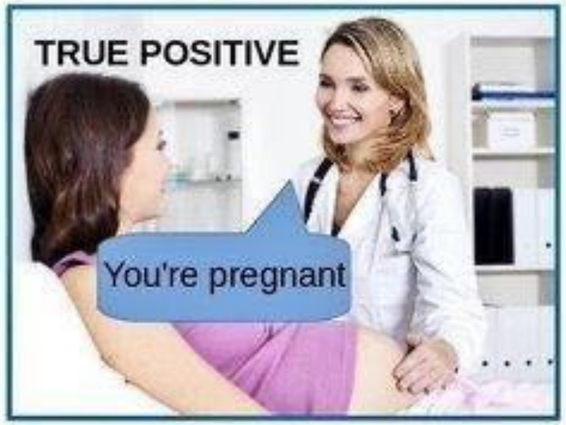
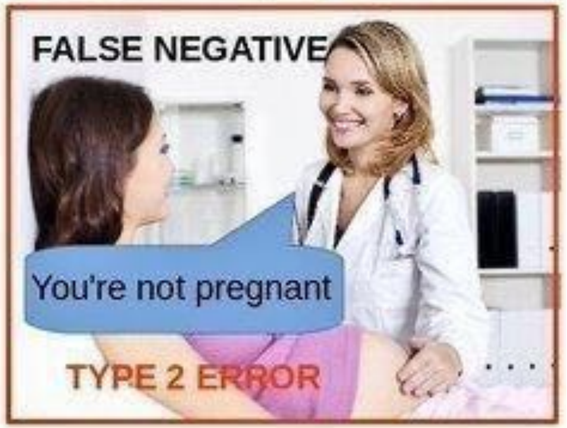
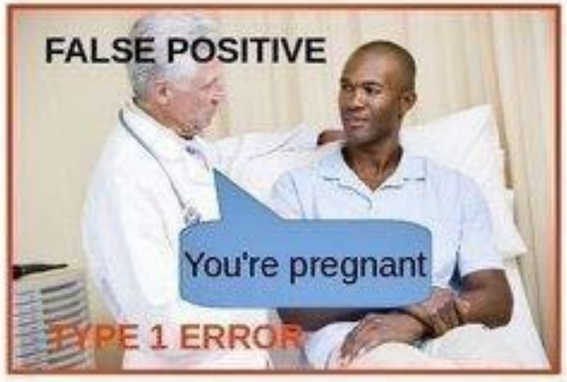
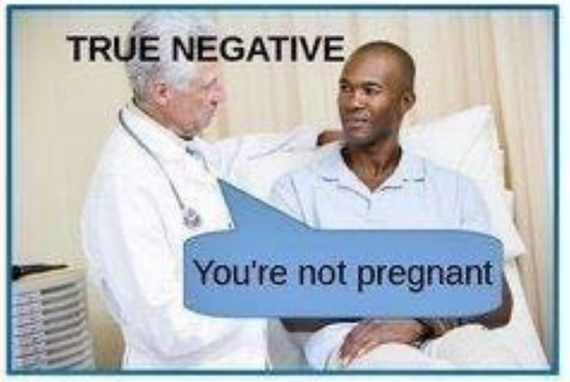
The confusion matrix shows results from binary classification

		Predicted	
		Positive	Negative
Actual	Positive		
	Negative		

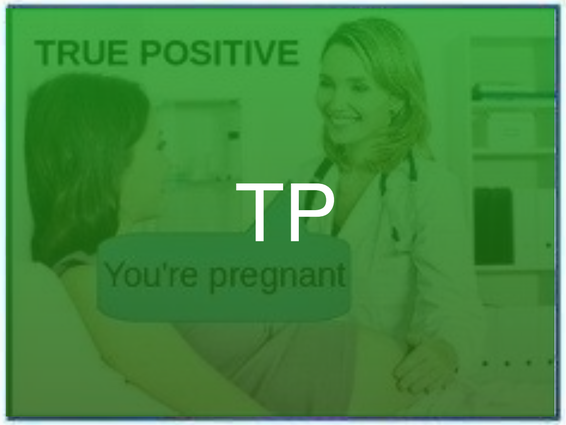
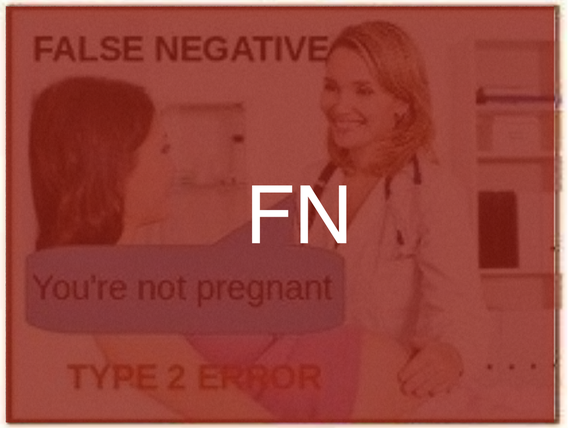
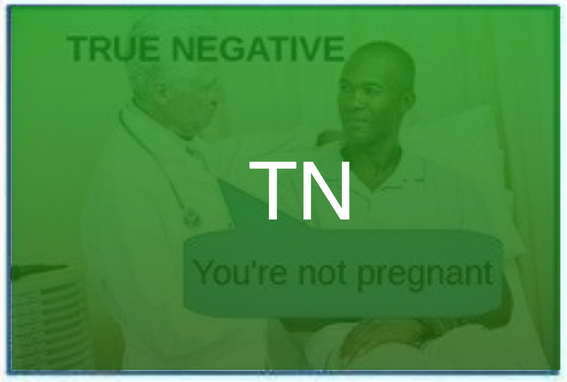
The confusion matrix shows results from binary classification

		Predicted	
		Positive	Negative
Actual	Positive		
	Negative		

The confusion matrix shows results from binary classification

		Predicted	
		Positive	Negative
Actual	Positive		
	Negative		

The confusion matrix shows results from binary classification

		Predicted	
		Positive	Negative
Actual	Positive		
	Negative		

Performance metrics help judge model performance

- Accuracy
- Precision — Positive predictive value (PPV)
- Sensitivity — Recall, true positive rate (TPR)
- Specificity — Selectivity, true negative rate (TNR)

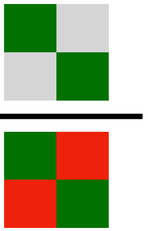
- and many more...

Accuracy: How often is it right?

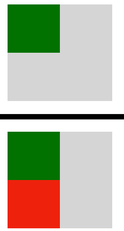
$$\text{Accuracy} = \frac{\text{Correct predictions}}{\text{All predictions}} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} = \frac{}{}$$

Precision: How often is it right when predicting positive?

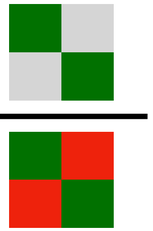
$$\text{Accuracy} = \frac{\text{Correct predictions}}{\text{All predictions}} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} = \frac{}{}$$

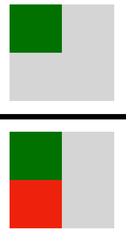


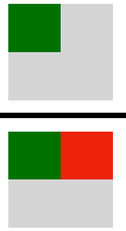
$$\text{Precision} = \frac{\text{True positives}}{\text{Predicted positives}} = \frac{\text{TP}}{\text{TP} + \text{FP}} = \frac{}{}$$



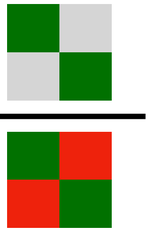
Sensitivity: How often is it right when actually positive?

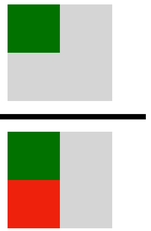
$$\text{Accuracy} = \frac{\text{Correct predictions}}{\text{All predictions}} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} =$$ 

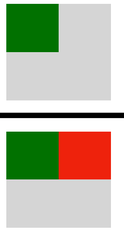
$$\text{Precision} = \frac{\text{True positives}}{\text{Predicted positives}} = \frac{\text{TP}}{\text{TP} + \text{FP}} =$$ 

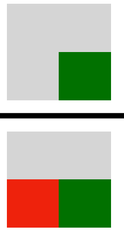
$$\text{Sensitivity} = \frac{\text{True positives}}{\text{Actual positives}} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$ 

Specificity: How often is it right when actually negative?

$$\text{Accuracy} = \frac{\text{Correct predictions}}{\text{All predictions}} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} =$$ 

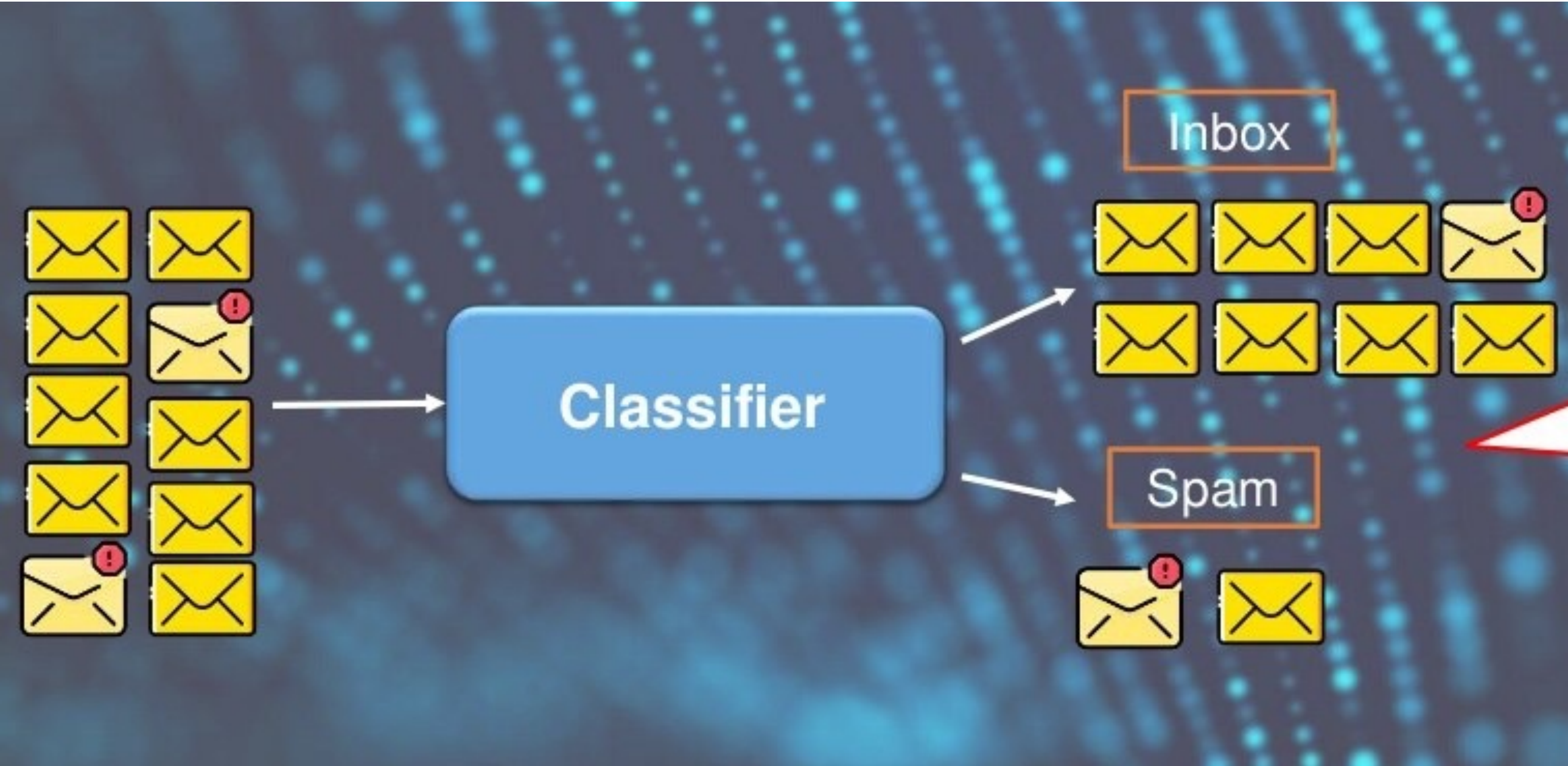
$$\text{Precision} = \frac{\text{True positives}}{\text{Predicted positives}} = \frac{\text{TP}}{\text{TP} + \text{FP}} =$$ 

$$\text{Sensitivity} = \frac{\text{True positives}}{\text{Actual positives}} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$ 

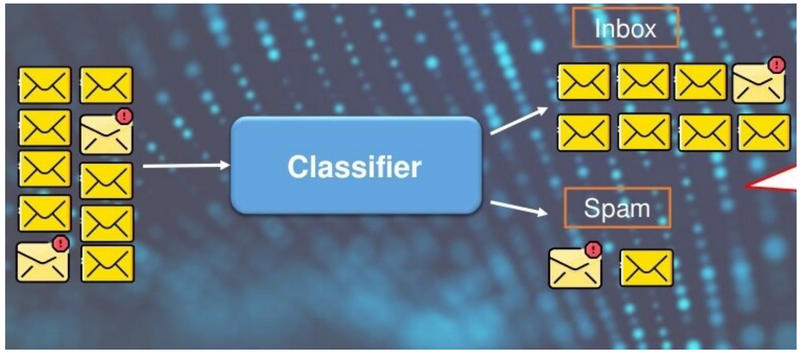
$$\text{Specificity} = \frac{\text{True negatives}}{\text{Actual negatives}} = \frac{\text{TN}}{\text{TN} + \text{FP}} =$$ 

Example: Spam filter

Blackboard



Example: Spam filter



$$\text{Accuracy} = \frac{8}{10} = 80\,\%$$

		Predicted: Positive	Predicted: Negative
Actual	Positive	1	1
Actual	Negative	1	7

$$\text{Sensitivity} = \frac{1}{2} = 50\,\%$$

$$\text{Specificity} = \frac{7}{8} = 87.5\,\%$$

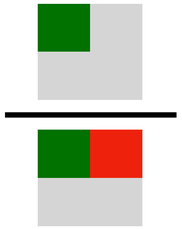
$$\text{Precision} = \frac{1}{2} = 50\,\%$$

There is a trade-off between Sensitivity and Specificity

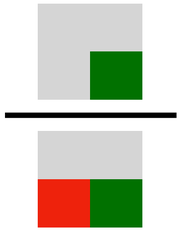
Example: Spam filter

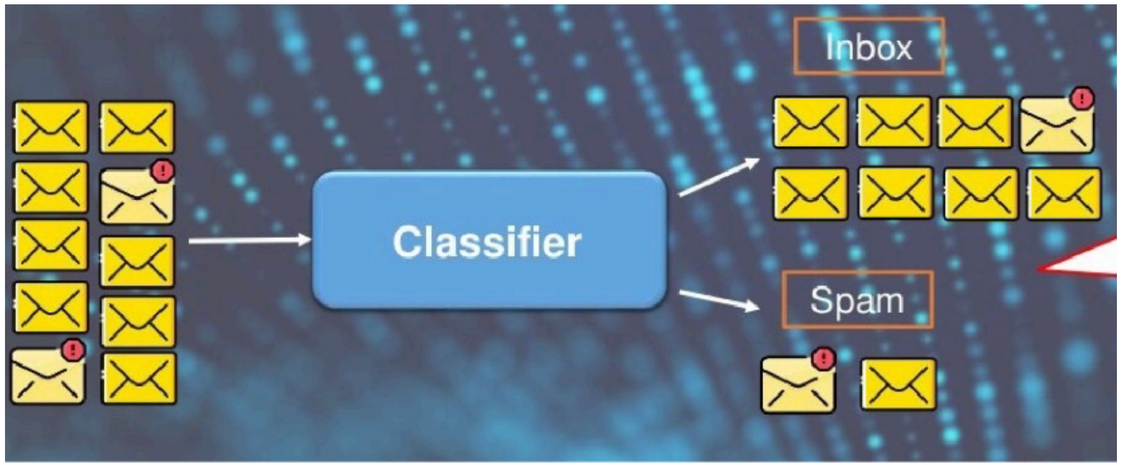
What do we want?

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$



$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}} =$$

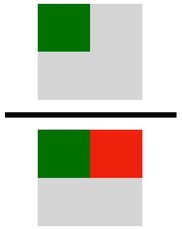




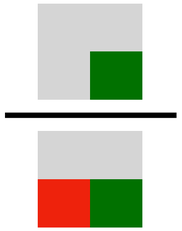
There is a trade-off between Sensitivity and Specificity

Example: Spam filter

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$



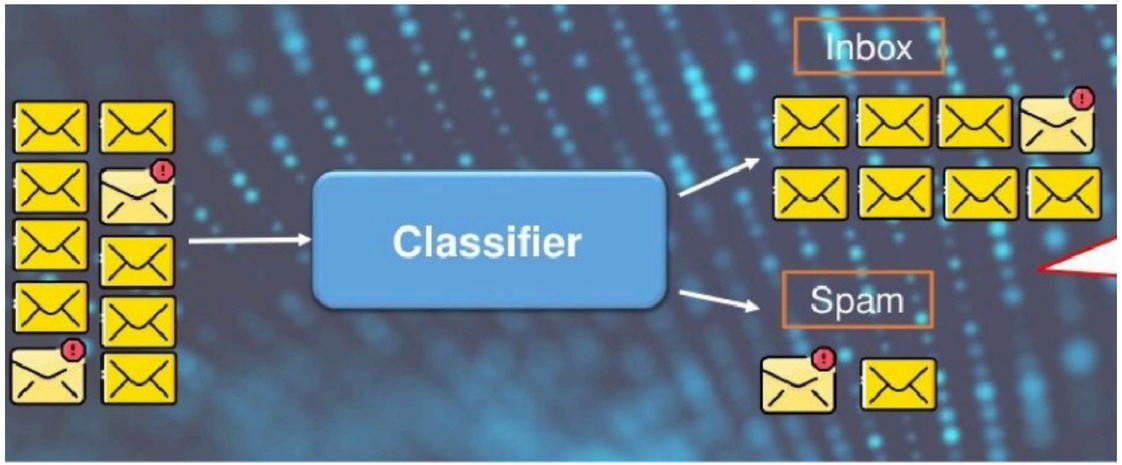
$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}} =$$



What do we want?

Low: It's OK if some spam slips into our inbox

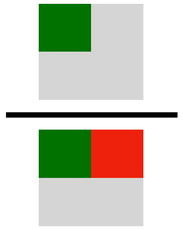
High: Legitimate email should never land in spam



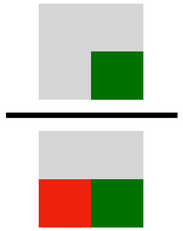
There is a trade-off between Sensitivity and Specificity

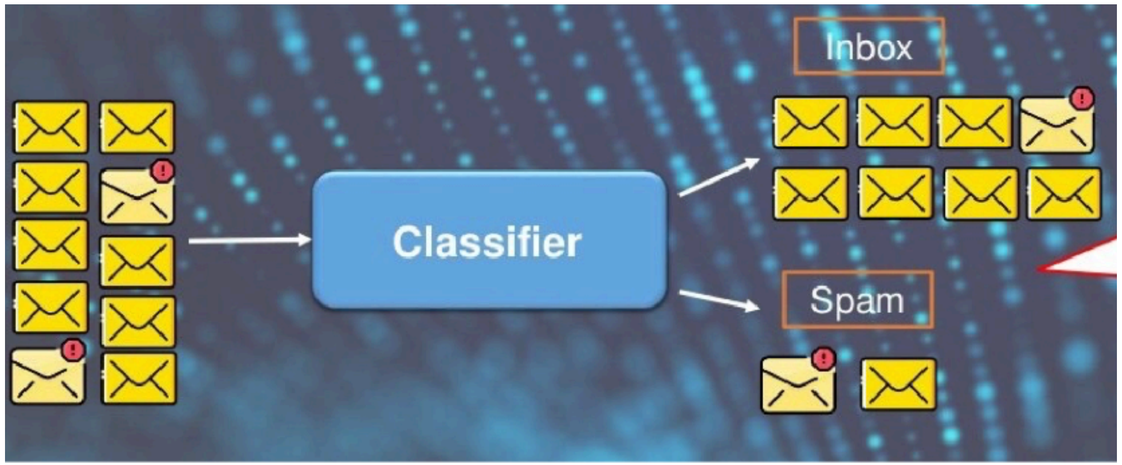
Example: Spam filter

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$



$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}} =$$





What do we want?

Low: It's OK if some spam slips into our inbox

High: Legitimate email should never land in spam

Here important: Precision

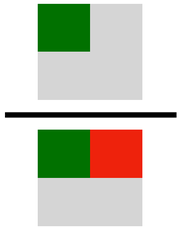
If we predict spam, it should be spam!

There is a trade-off between Sensitivity and Specificity

Example: Security scanner

What do we want?

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$



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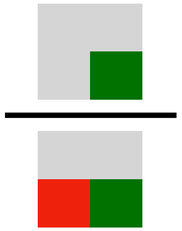
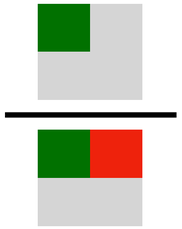


There is a trade-off between Sensitivity and Specificity

Example: Security scanner

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$



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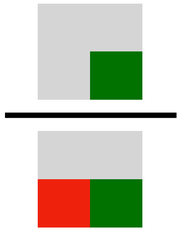


What do we want?

High: Want to catch all terrorists

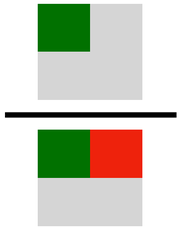
Low: OK if some false alarms
(but not too many..)

There is a trade-off between Sensitivity and Specificity

Example: Pregnancy test

What do we want?

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}} =$$



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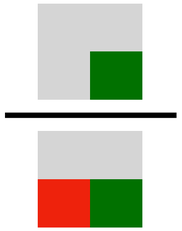

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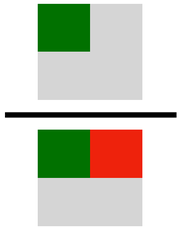

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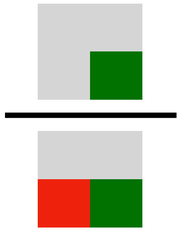


What do we want?

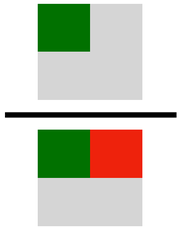
High: Do not want to miss a pregnancy

High: Do not want to make non-pregnant women go to doctor

There is a trade-off between Sensitivity and Specificity

Example: Pregnancy test

$$\text{Sensitivity} = \frac{TP}{TP + FN} =$$



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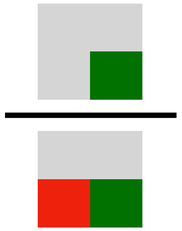


What do we want?

High: Do not want to miss a pregnancy

High: Do not want to make non-pregnant women go to doctor

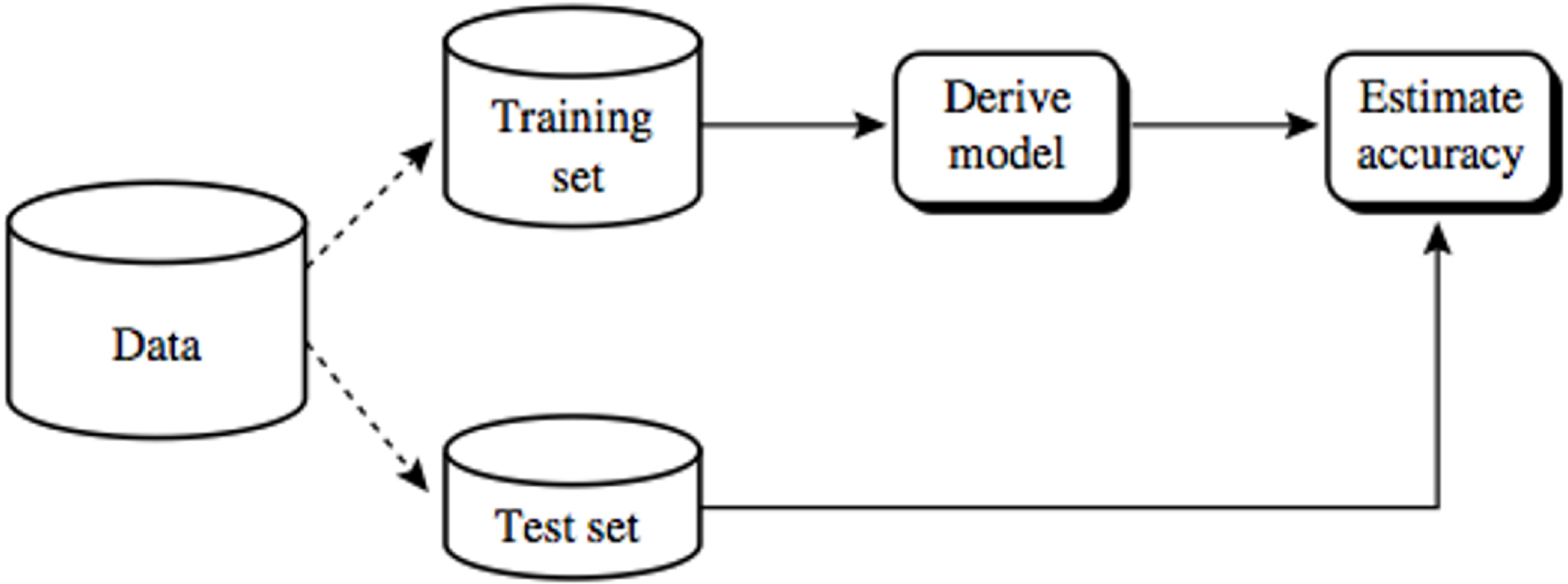
Difficult in practice:

Clinical performance of hCG pregnancy test kits with 99 urine and 99 serum samples

Test	Sensitivity	Specificity	False +	False -	True +	True -	Accuracy
Urine tests							
Tandem	90.6	100	0	8	77	14	91.9
NovoClone	70.6	92.9	1	25	60	13	73.7
Abbott	84.7	100	0	13	72	14	86.9
Serum tests							
Tandem	89.4	85.7	2	9	76	12	88.9
NovoClone	67.1	100	0	28	57	14	71.7
Abbott	94.1	78.6	3	5	80	11	91.9

Alfthan, Bjorses, Tiitinen, Stenman. Specificity and detection limit of ten pregnancy tests, Scan J clin lab inv 216: 105-13 (1993)

To train and check a model we split up data into training and test



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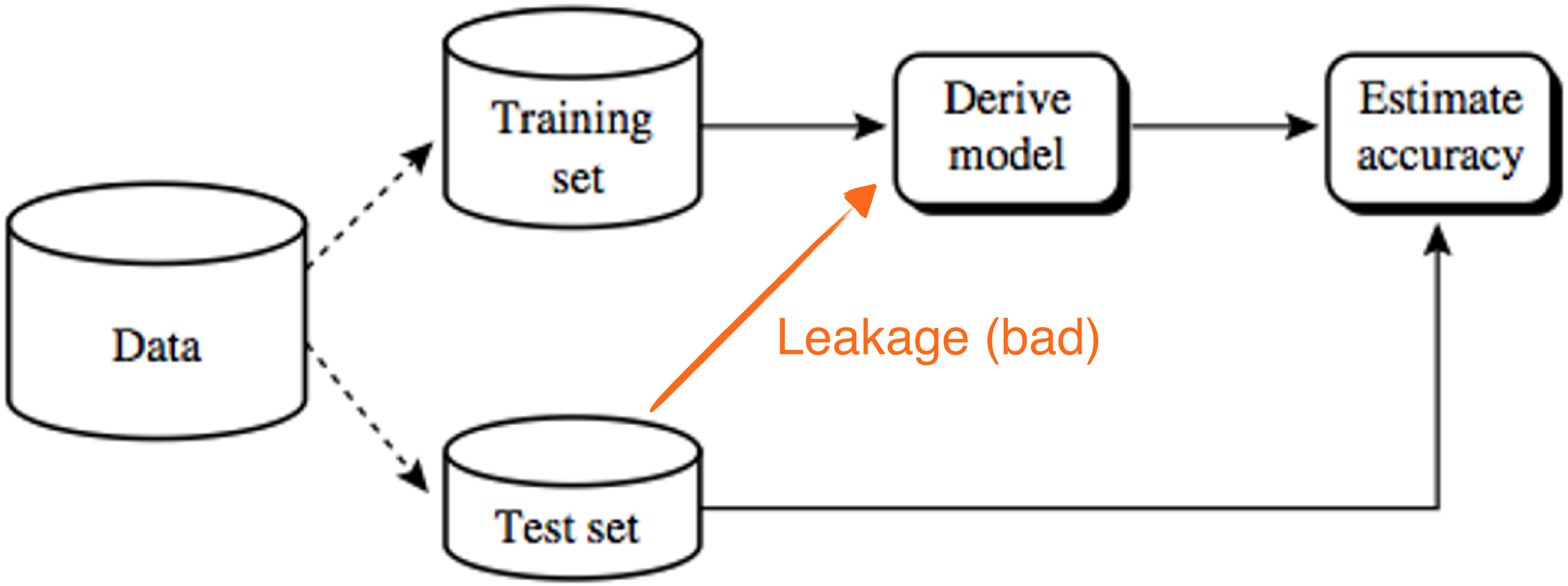
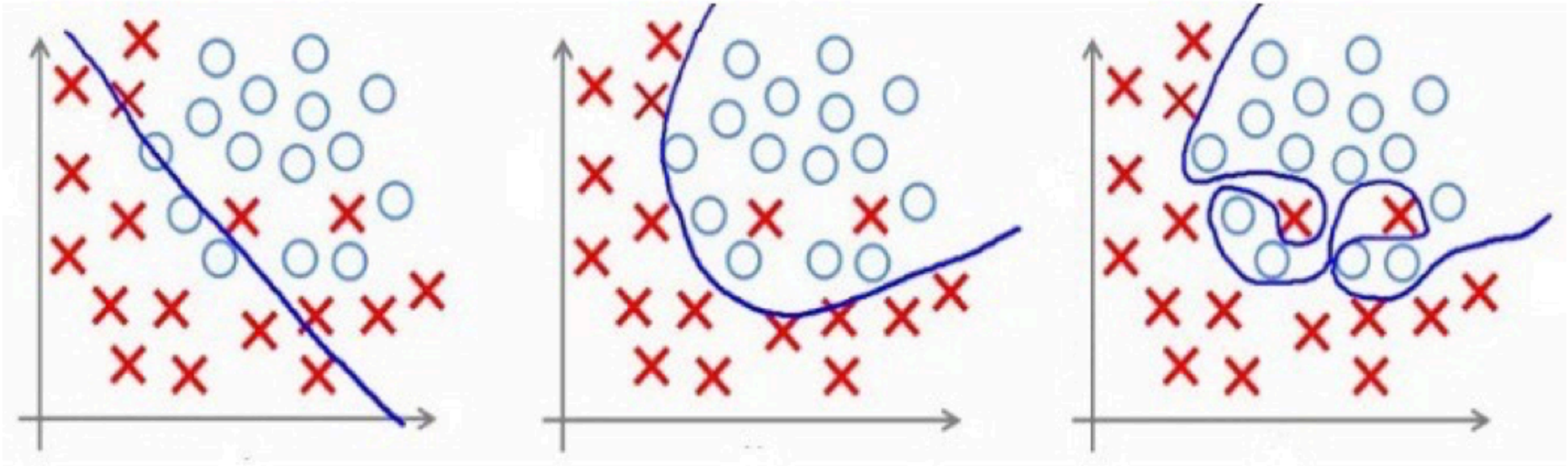


There is a trade-off between underfitting and overfitting

Underfitting: The model does not perform well for both training and testing data

Overfitting: The model performs well for training, but not for testing data

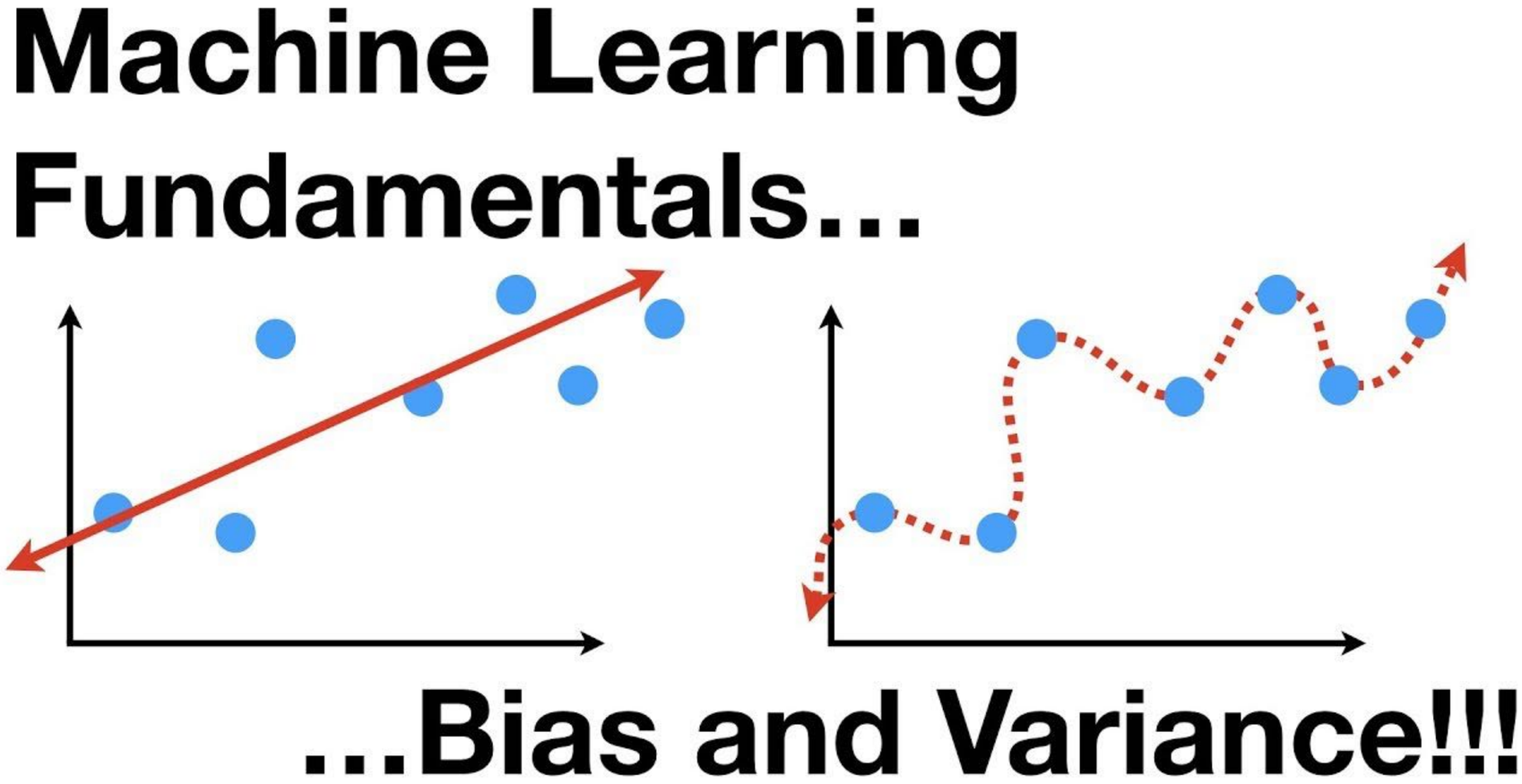


Underfitting

Overfitting

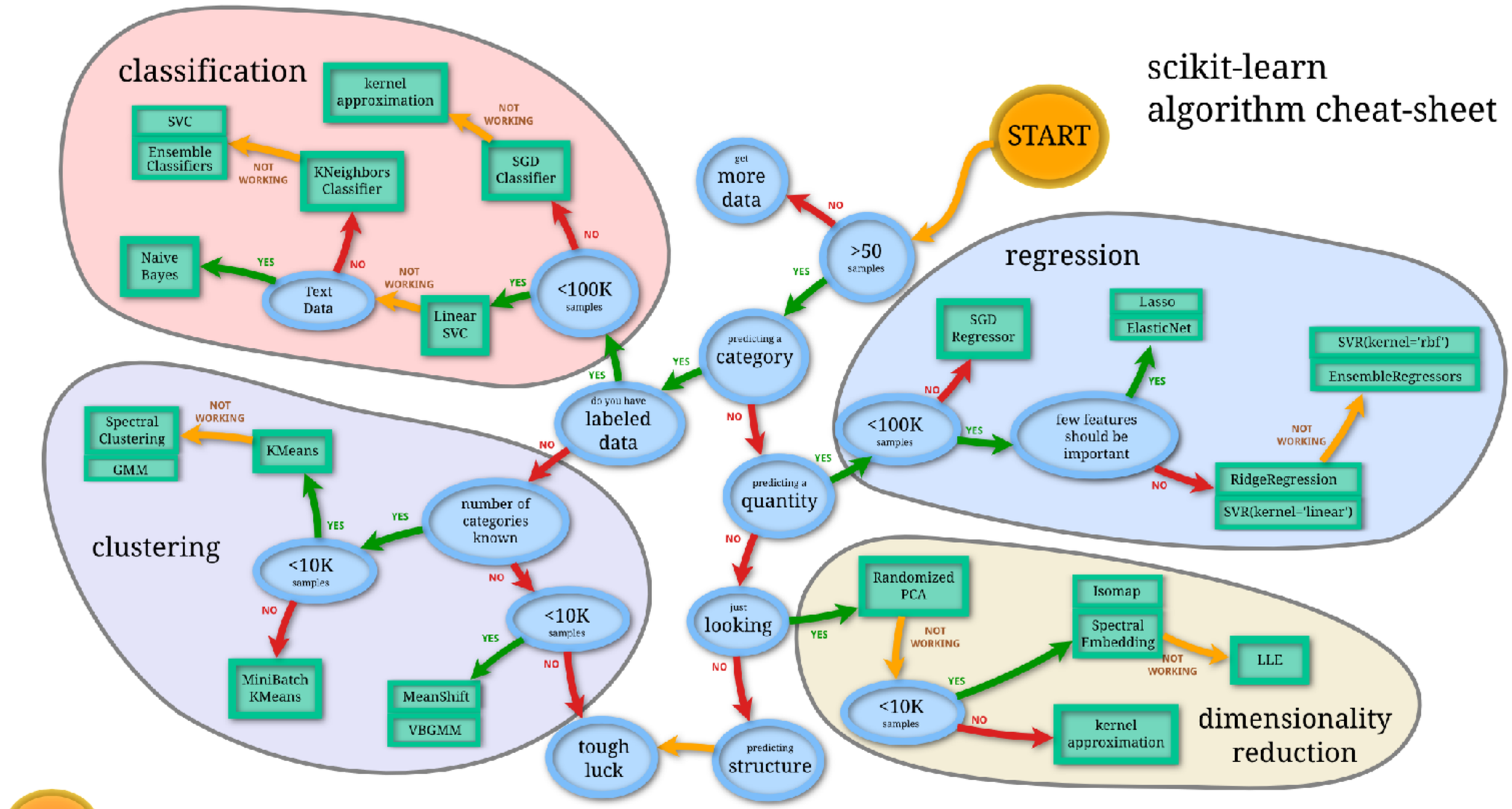
Jupyter

The bias-variance trade-off



https://www.youtube.com/watch?v=EuBBz3bI-aA&feature=youtu.be&t=21

scikit-learn is the standard Python library for ML



http://scikit-learn.org/stable/tutorial/machine_learning_map/

Take home messages

Machine learning tries to find patterns or rules in data

Choice of features and distance measure influences results

Performance metrics, like the confusion matrix, help evaluate models