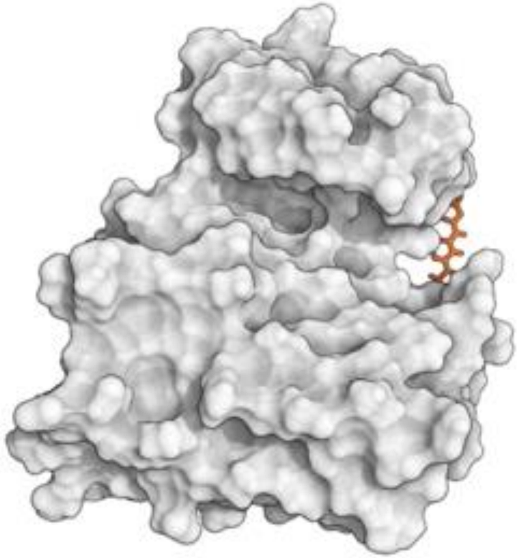
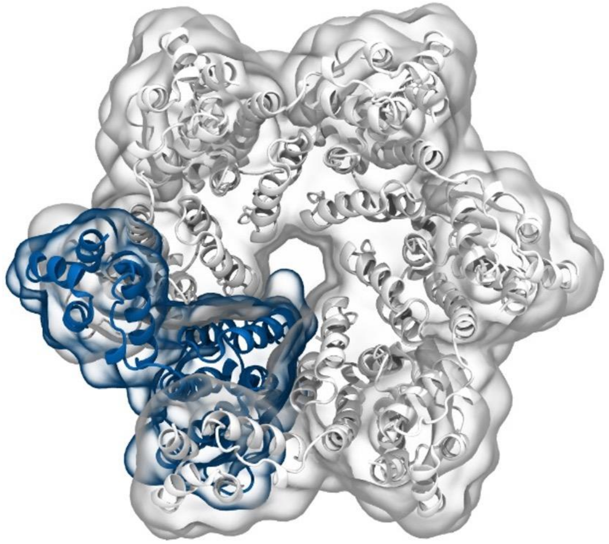
Simulation of Biomolecules



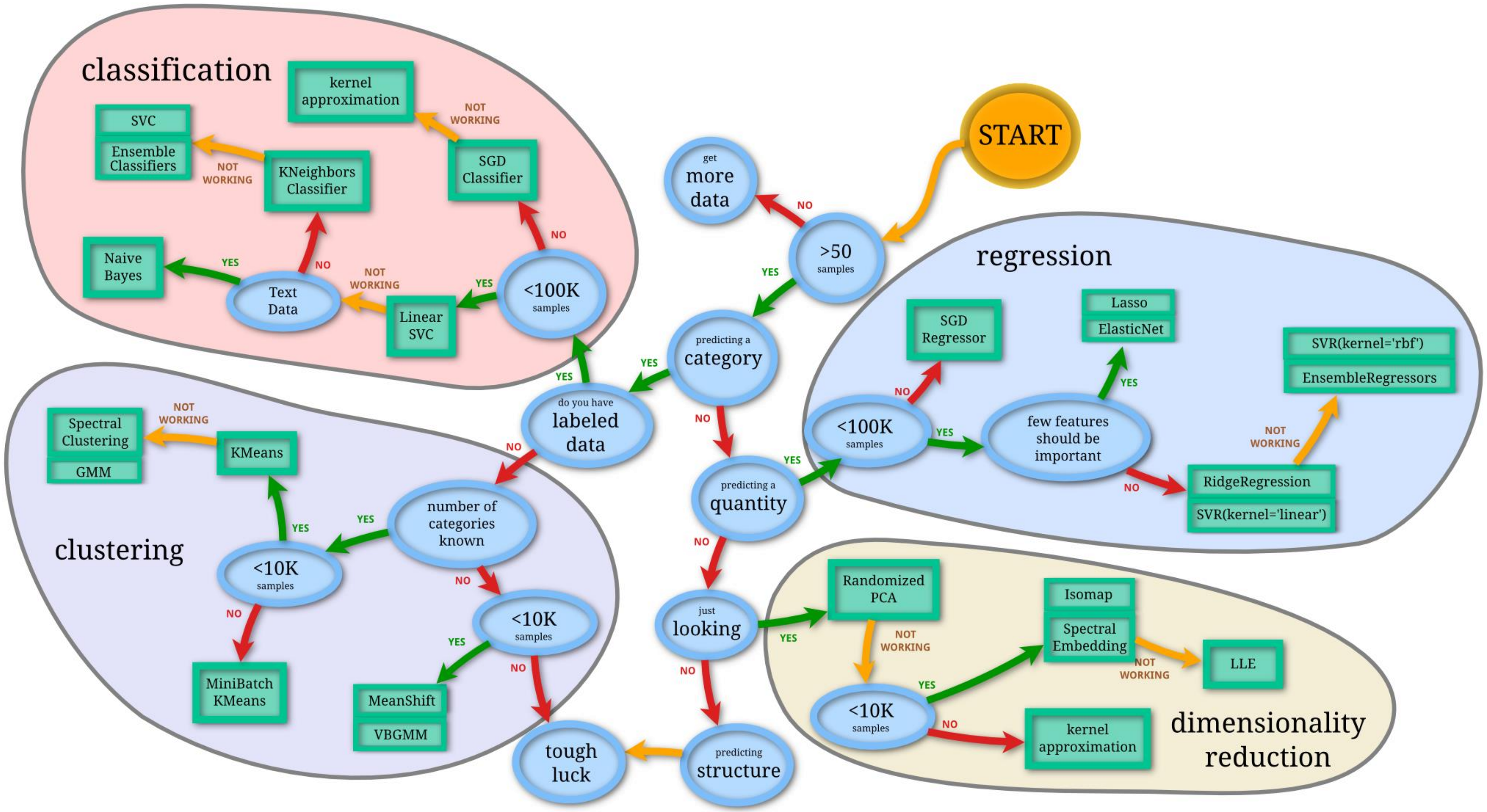
Classification



Dr Matteo Degiacomi
University of Edinburgh
matteo.degiacomi@ed.ac.uk

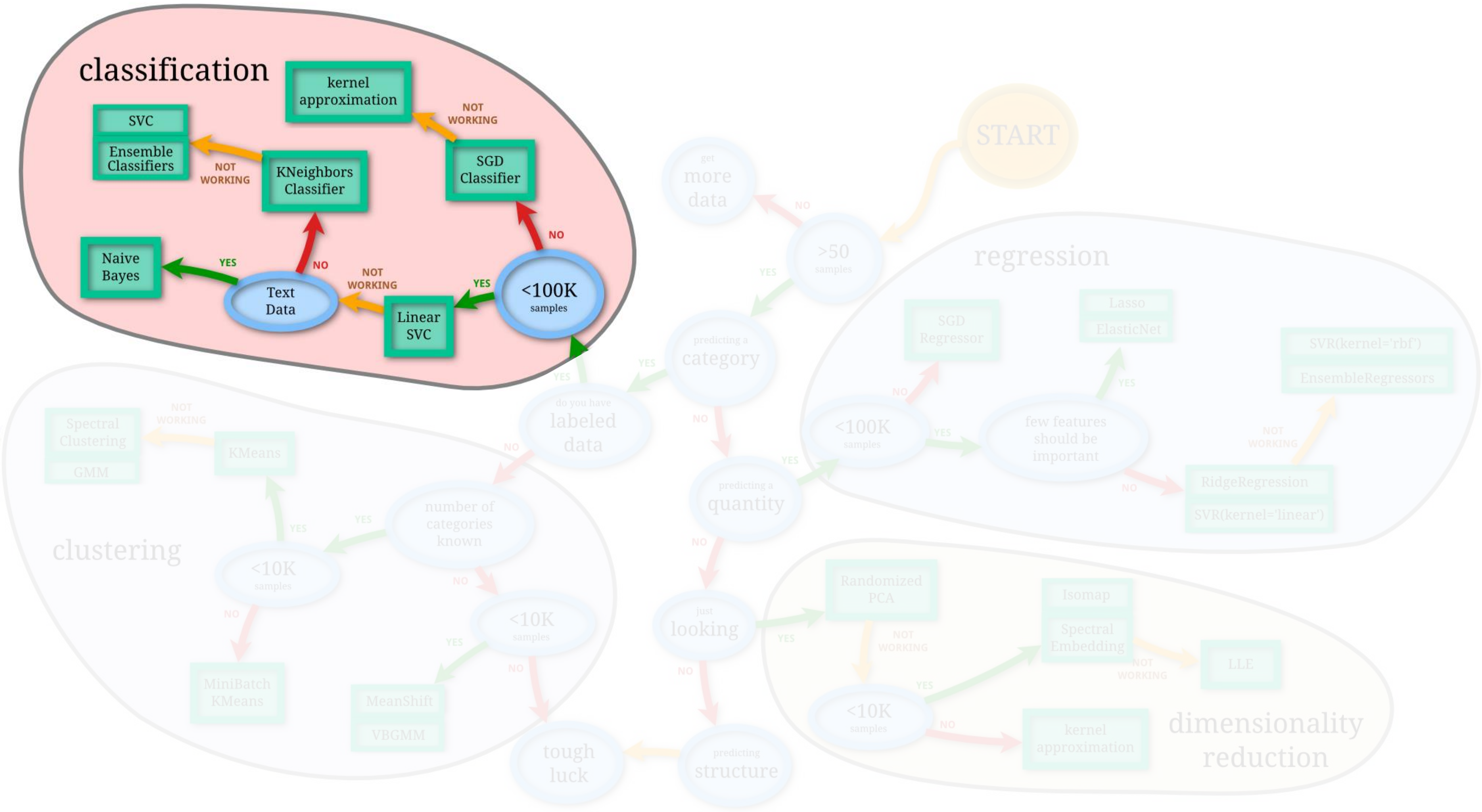
Dr Antonia Mey
University of Edinburgh
antonia.mey@ed.ac.uk

The Data Mining world



From **scikit-learn.org**

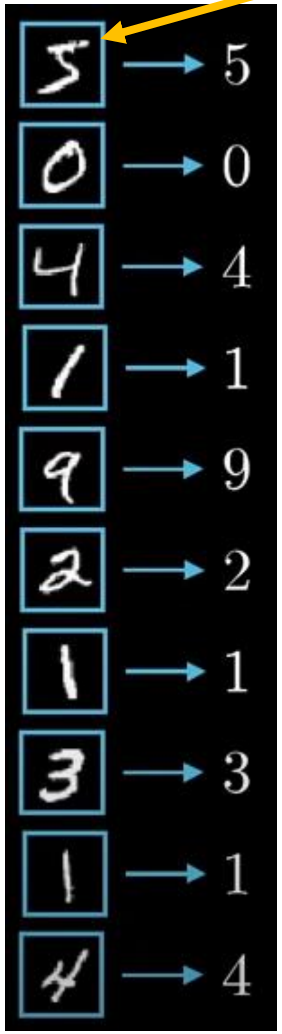
The Data Mining world

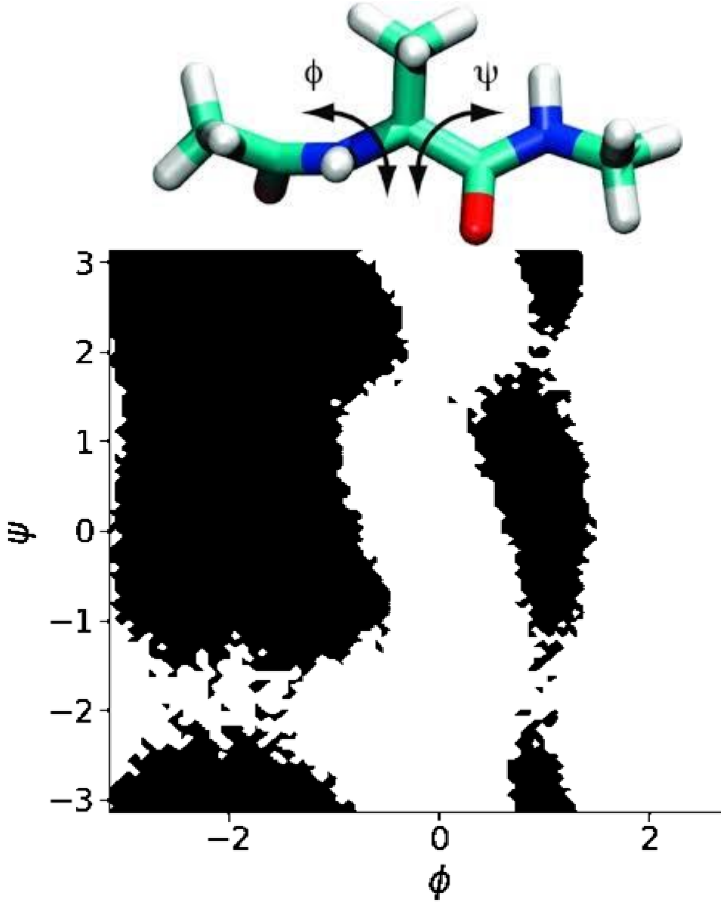


From **scikit-learn.org**

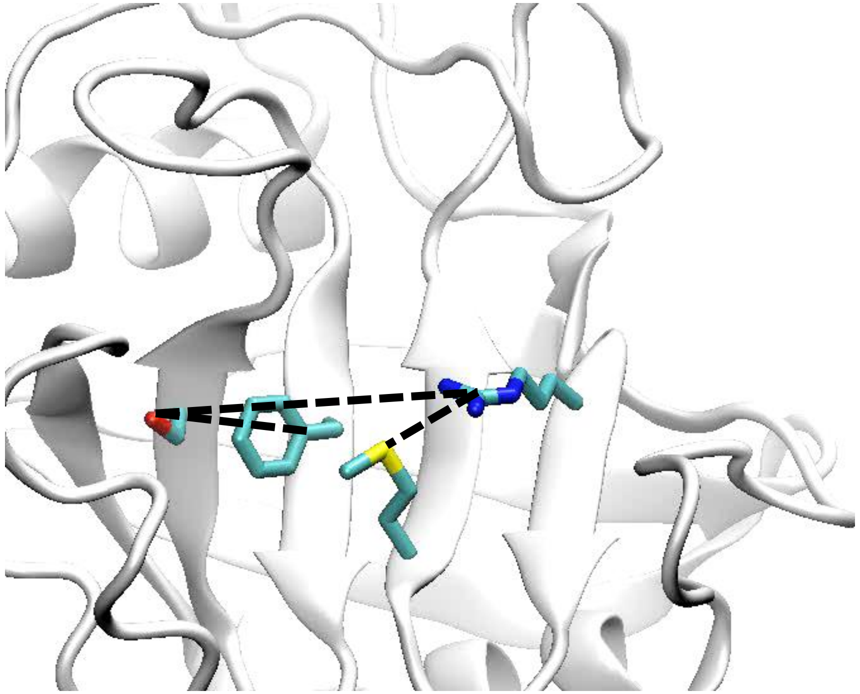
Features are possible ways to represent data

Pixels colour





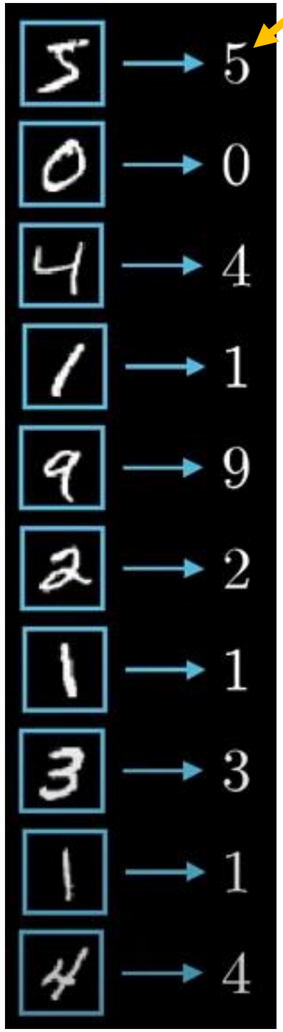
Torsional angles

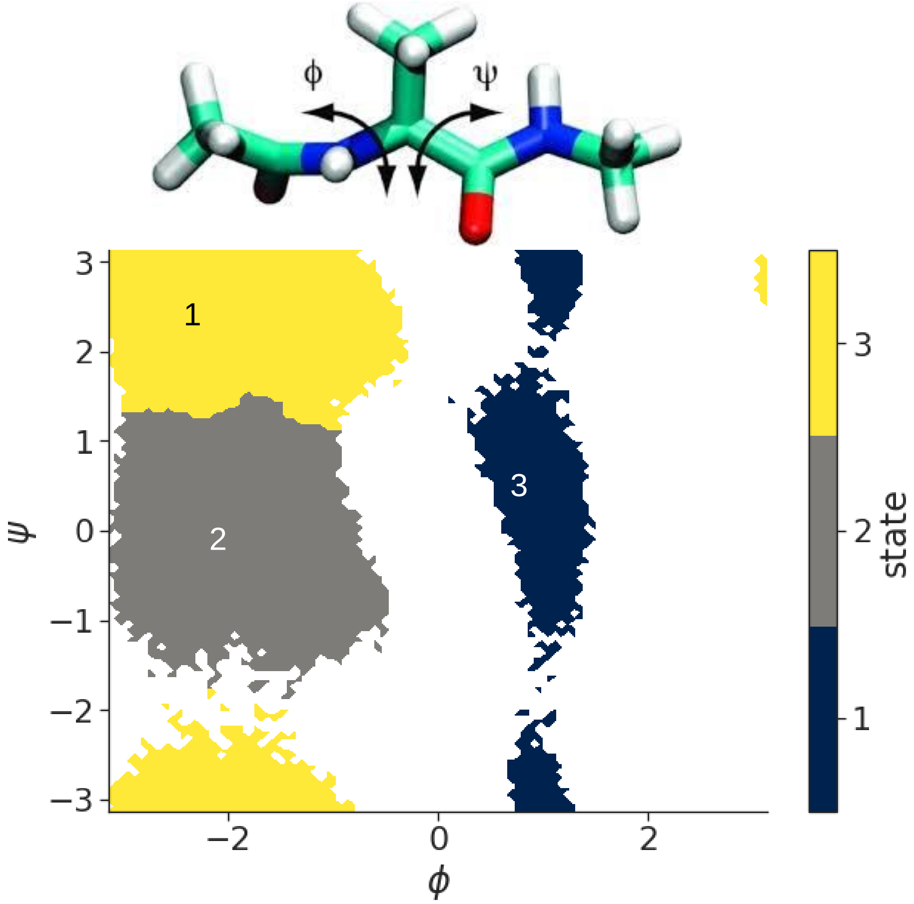


Interatomic distances

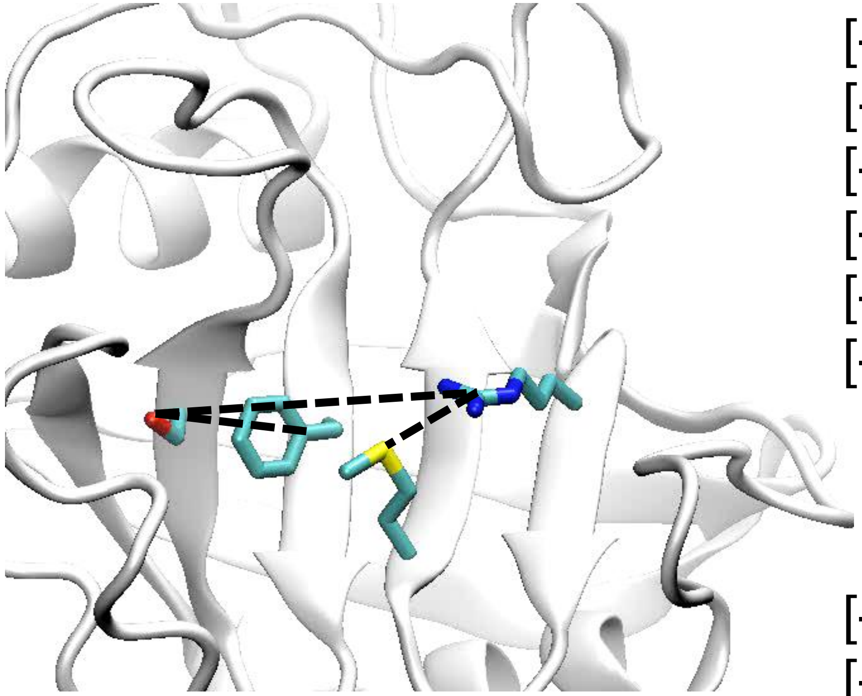
Labels assign featurised data into categories

Labelled digits





Labelled states

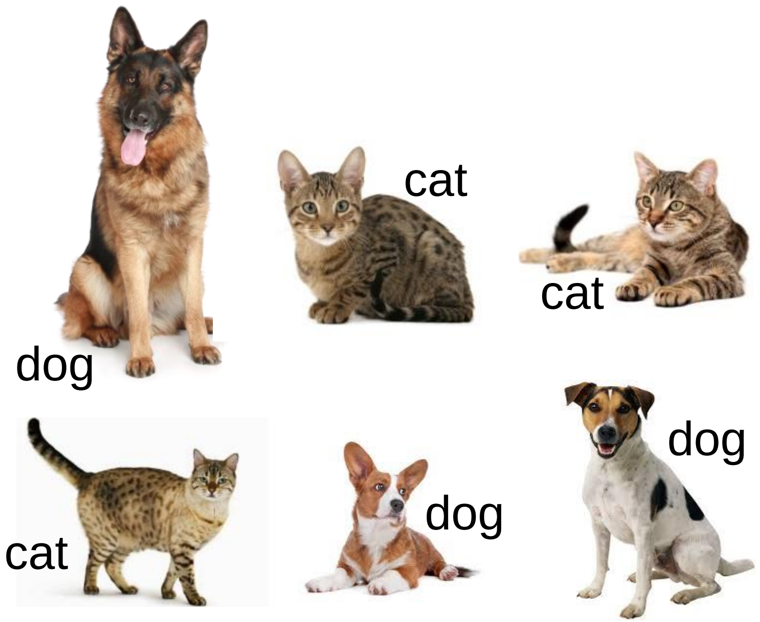


[-12008 kJ]
[-12078 kJ]
[-12045 kJ]
[-12083 kJ]
[-12062 kJ]
[-12058 kJ]
.
.
.
[-12099 kJ]
[-12093 kJ]

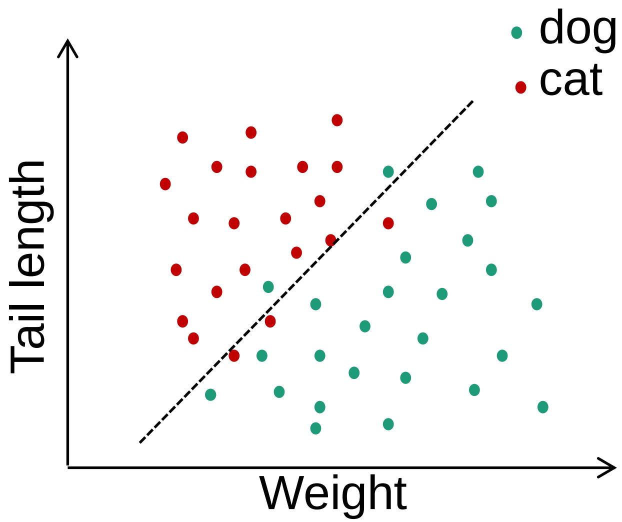
Labelled Energies

Data Classification via Supervised Learning

- take **labelled data**
- create an n-dimensional **feature vector** from data
- Separate «feature space» in different regions



Weight
Legs length
Tail length
Eye color
...



Data Classification via Supervised Learning

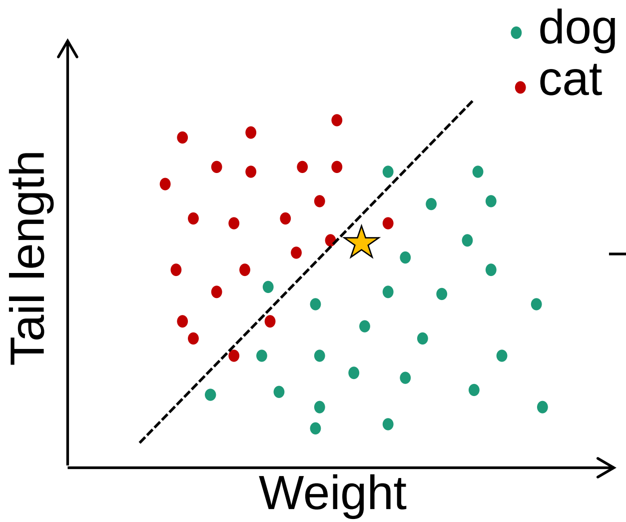
- take **labelled data**
- create an n-dimensional **feature vector** from data
- Separate «feature space» in different regions

?

→

Weight
Legs length
Tail length
Eye color
...

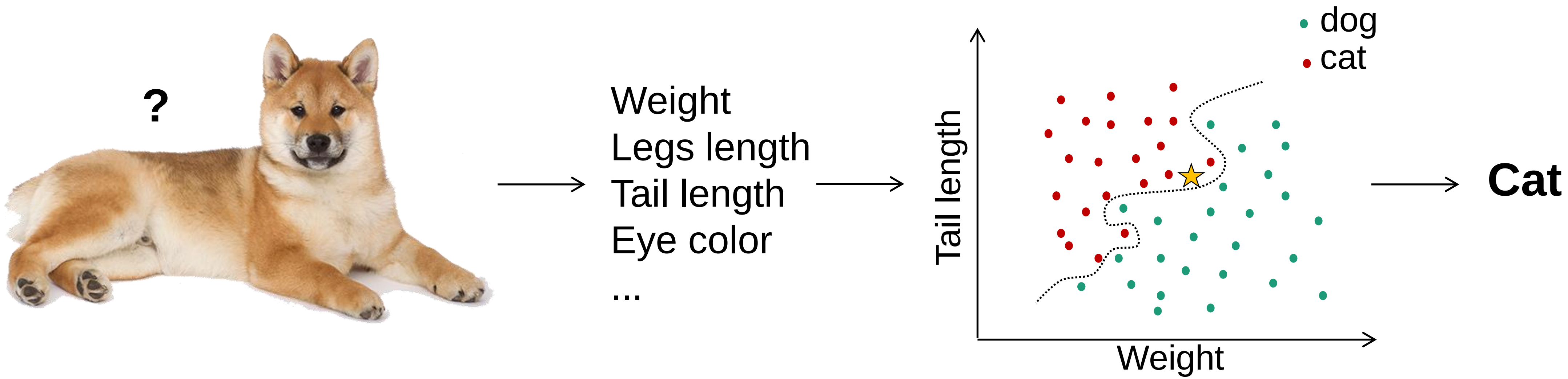
→



→ **Dog**

Data Classification via Supervised Learning

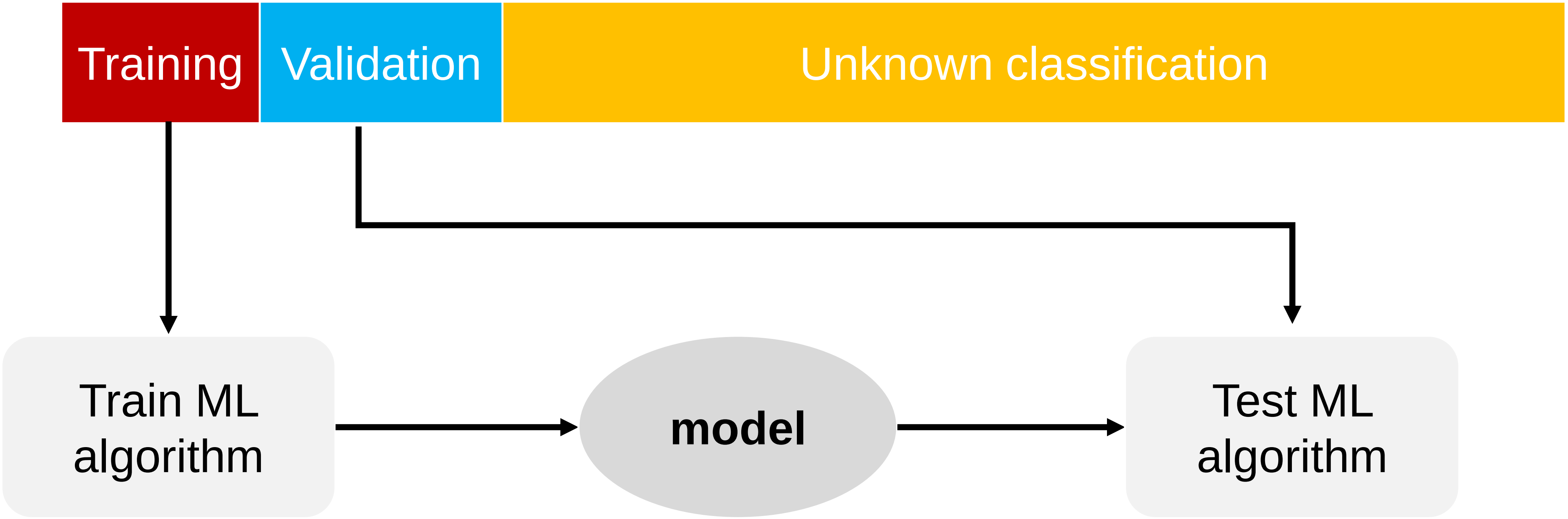
- take **labelled data**
- create an n-dimensional **feature vector** from data
- Separate «feature space» in different regions
- Warning: a too precise classification of examples might sacrifice generality (**overfitting**)



Data Classification via Supervised Learning

Data

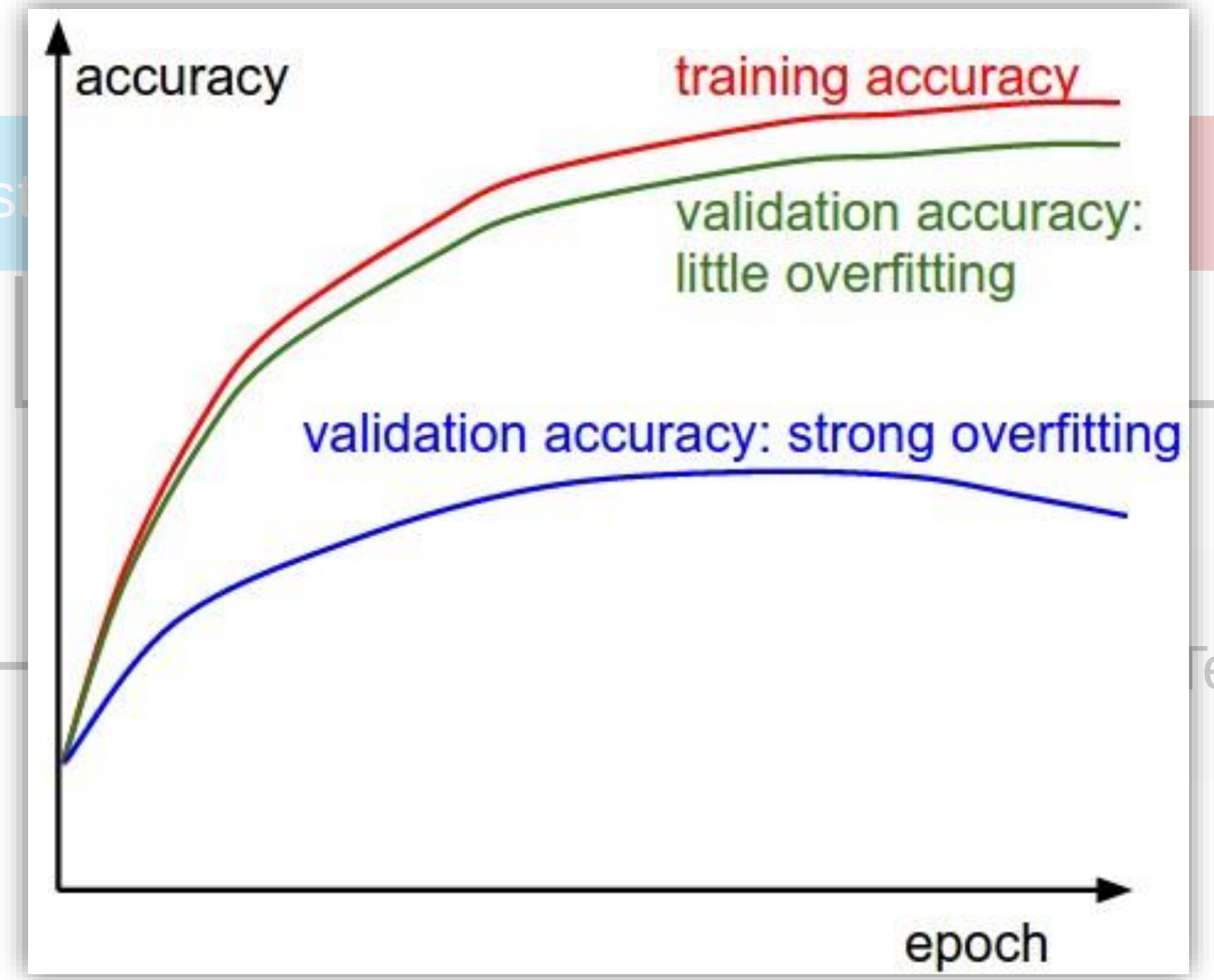
Data Classification via Supervised Learning



Data Classification via Supervised Learning

Trainin
g

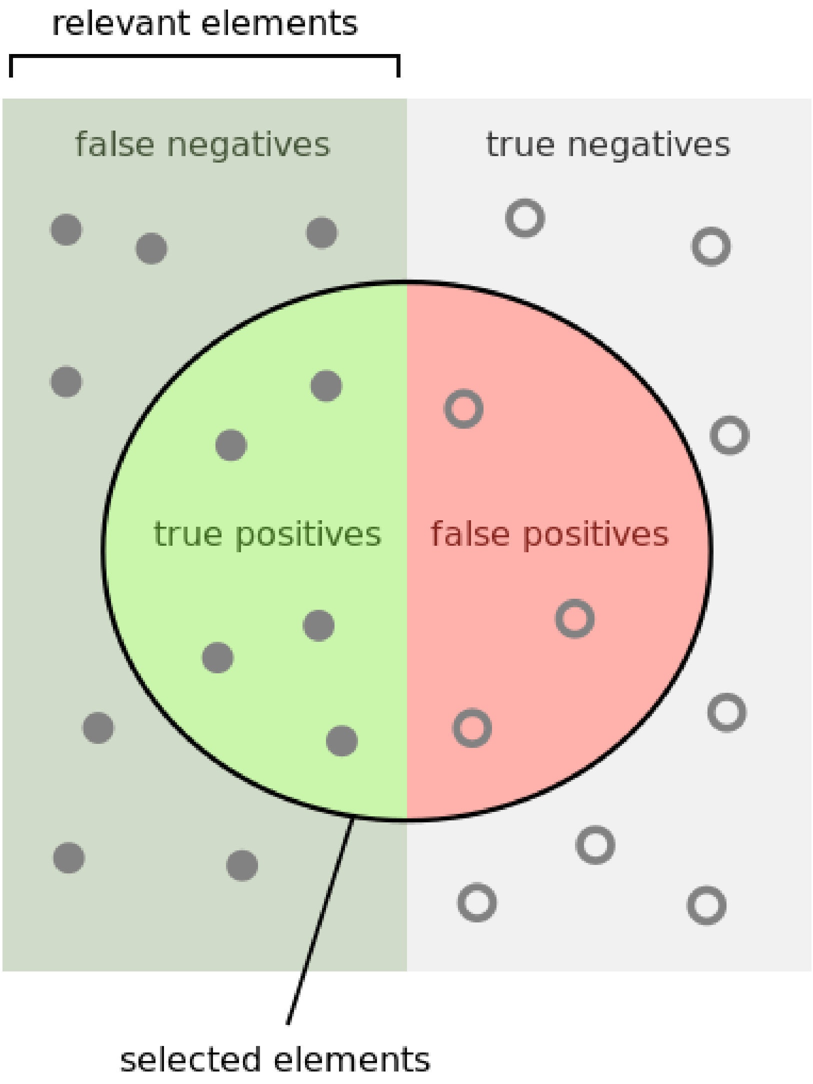
Tes



Train

Test

Some terminology



- **Confusion Matrix:**
  describes classification results
  can also describe n classes

result \ real	Dog	Cat
Dog	90	10
Cat	12	88

- $\textbf{precision} = \frac{\text{true positives}}{\text{selected elements}}$ =

- $\textbf{sensitivity} = \textbf{recall} = \frac{\text{true positives}}{\text{relevant elements}}$ =

- $\textbf{accuracy} = \frac{\text{true positives+true negatives}}{\text{total population}}$

en.wikipedia.org/wiki/Precision_and_recall

Learning Algorithms

- Artificial Neural Network (ANN)
- Decision Tree (DT)
- Random Forests (RF)
- Support Vector Machine (SVM)
- Logistic Regression (LOGRES)
- Naïve Bayes (NB)
- K Nearest Neighbor (KNN)
- ...

Learning Algorithms

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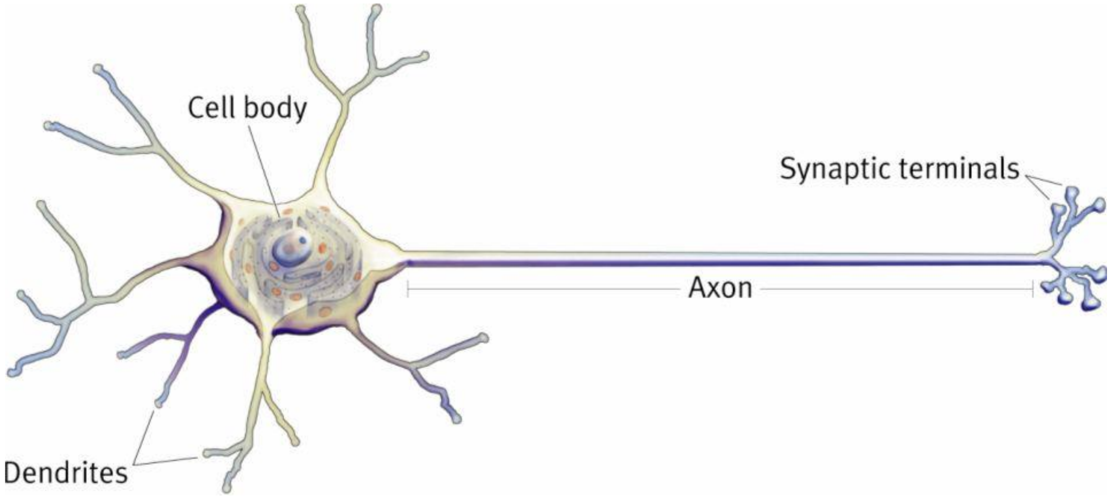
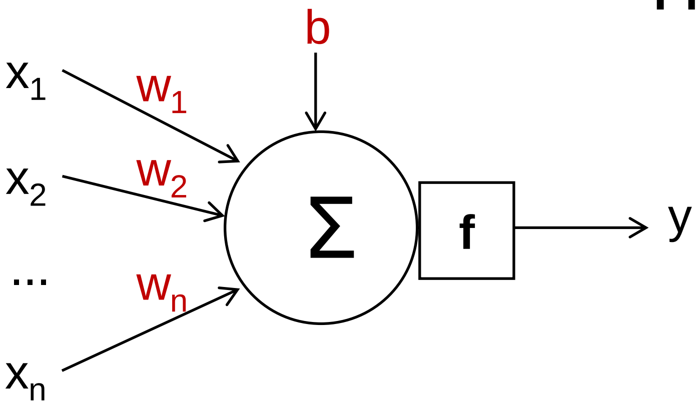
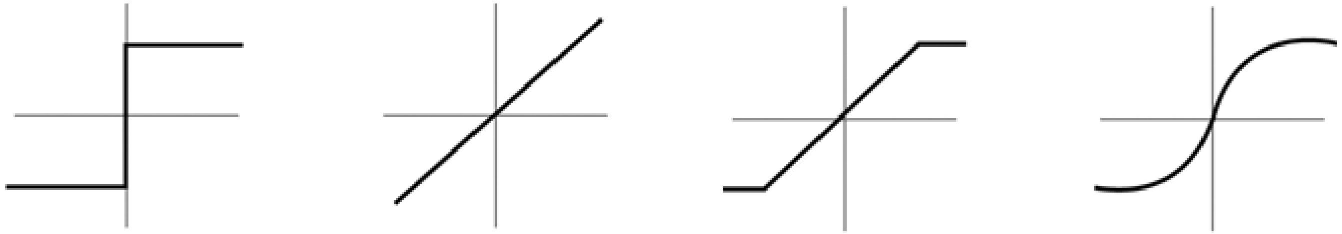
Artificial Neural Network (ANN)



A **neuron** fires if input signal is above a threshold

The activation function **f** can take several shapes



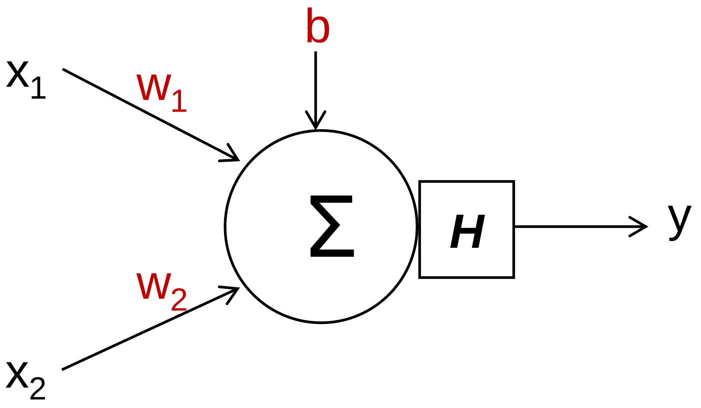


...

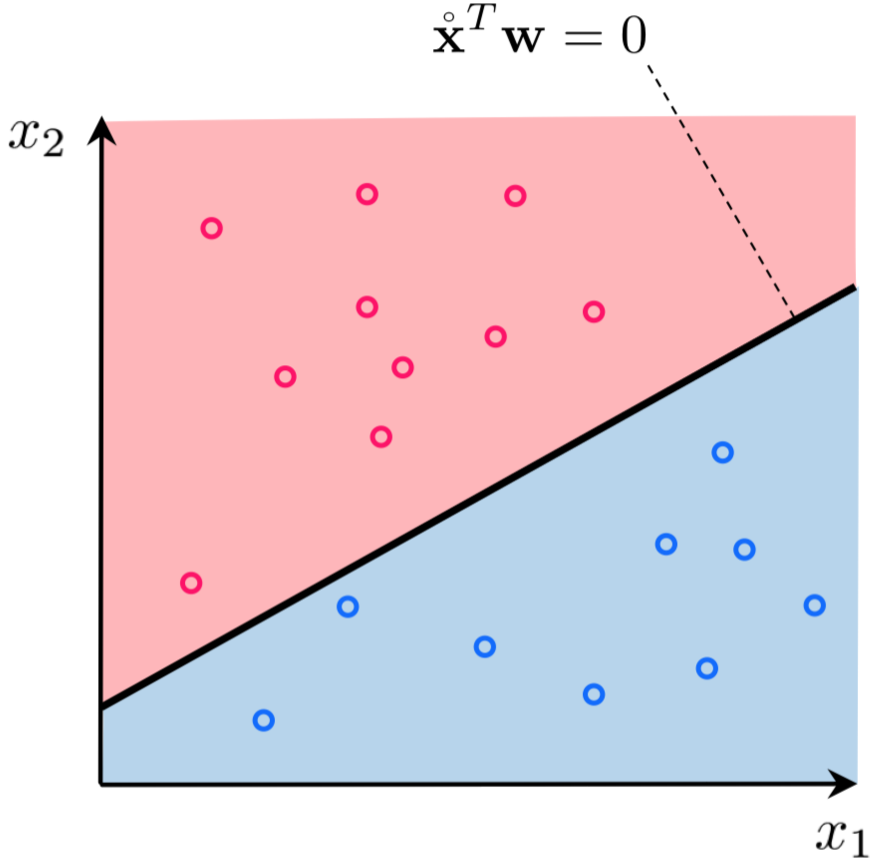
$$\mathbf{f}(w_1x_1 + w_2x_2 + \dots + w_nx_n + b) = y$$

Artificial Neural Network (ANN)

A single neuron can be used to take simple decisions

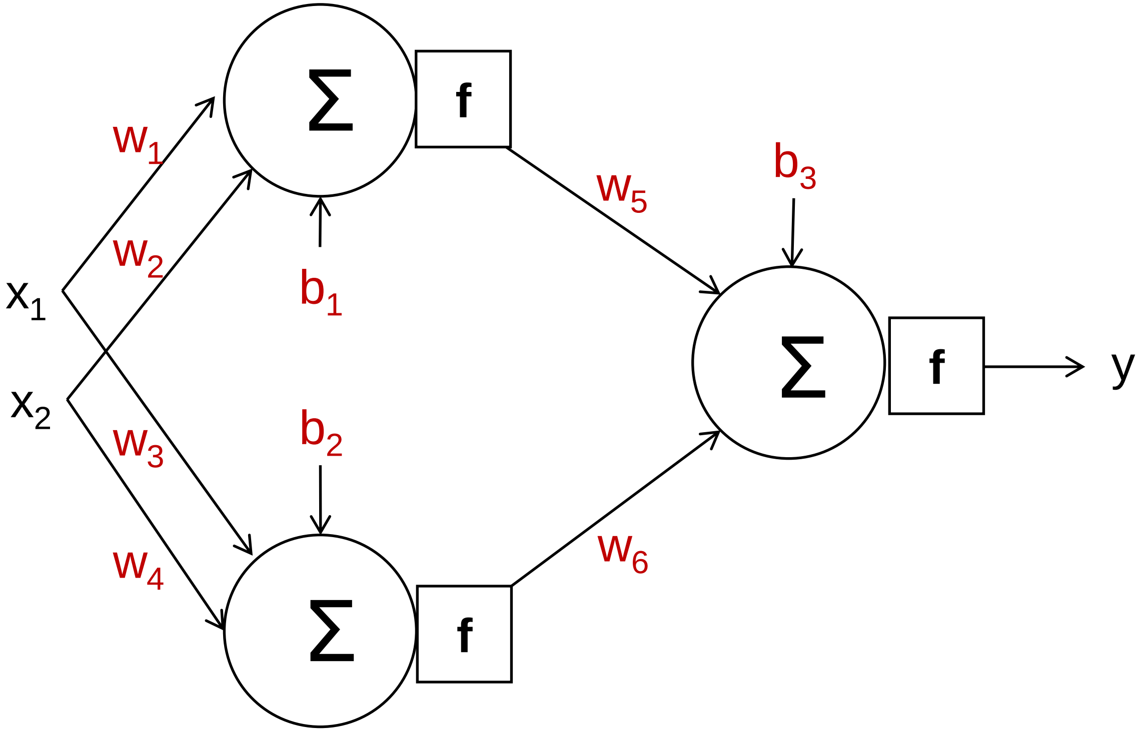


$$H(w_1x_1 + w_2x_2 + b) = y$$



Artificial Neural Network (ANN)

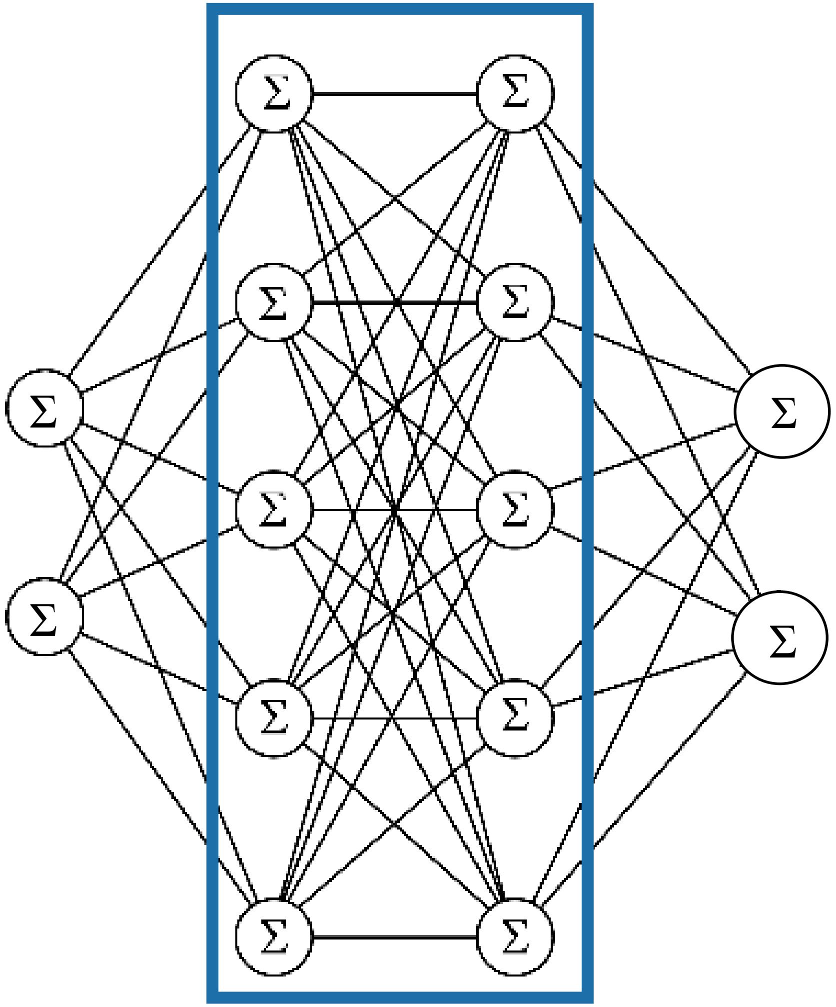
A single neuron can be used to take simple decisions



Complex decision making emerges when arranging neurons into **networks**

Artificial Neural Network (ANN)

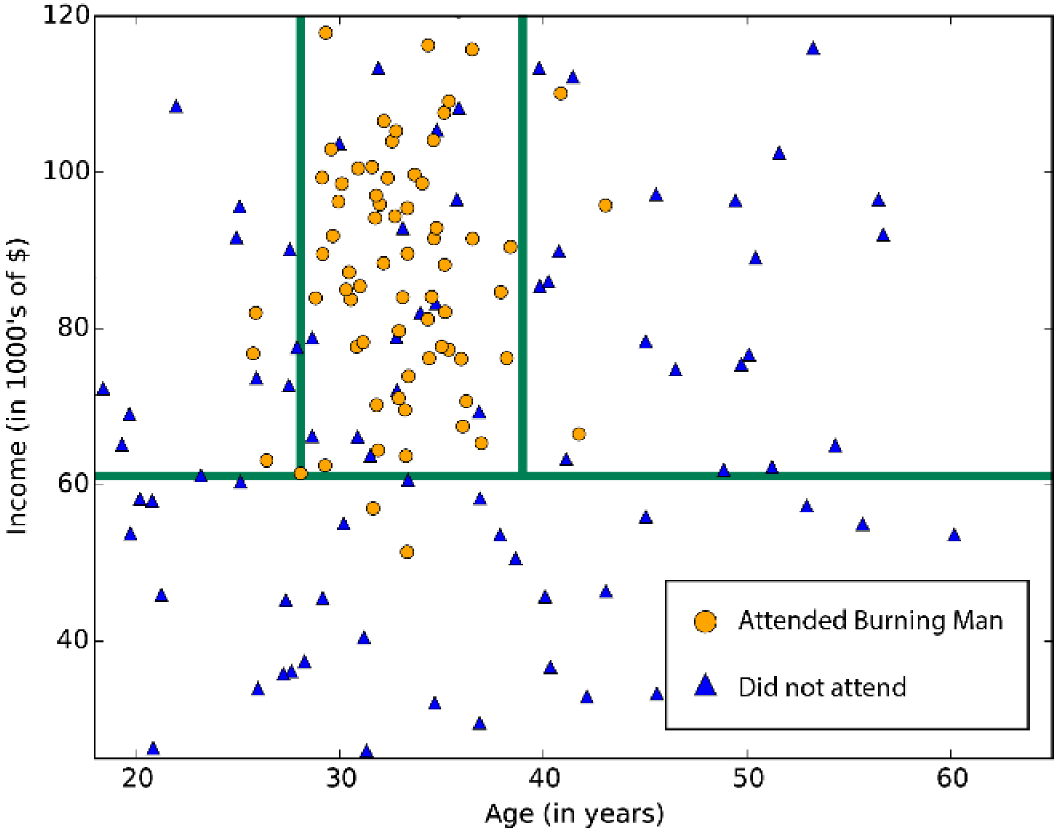
A single neuron can be used to take simple decisions

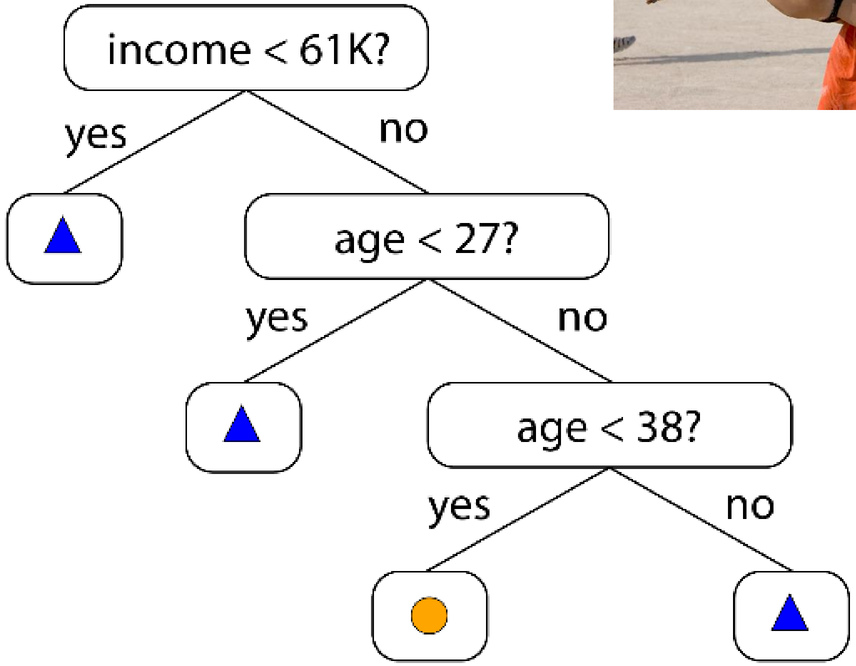


Complex decision making emerges when arranging neurons into **networks**

An ANN with one **hidden layer** can approximate any function

Decision Trees (DT)





- Subdivides features space in sectors
- Can overfit if space subdivision becomes too fine

azure.microsoft.com/en-us/documentation/articles/machine-learning-algorithm-choice

Bootstrap Aggregating (Bagging)

a weighted sum of weak classifiers creates a single strong classifier

Useful when a small change to training set causes large change in the output classifier (“learner is unstable”)

training set *D* with *m* examples

Create *N* bootstrap samples S drawing *m* random examples from *D with replacement*

D=	1	2	3	4	5	6	7	8	9	
S[0]=	5	1	7	2	7	9	2	6	5	→ C[0]
S[1]=	9	4	7	1	2	8	9	7	6	→ C[1]
S[2]=	0	8	2	0	9	7	7	0	1	→ C[2]
					…					
S[*N*]=	1	2	3	4	5	6	7	8	9	→ C[*N*]

Training: for every S, build a distinct classifier C using the same learning algorithm

L. Breiman, *Bagging Predictors,* in *Machine* Learning, Springer, 1996

[Extra] Boosting

- **a weighted sum of weak classifiers creates a single strong classifier**
- iteratively add classifiers to a pool, tweaked to give more importance to data misclassified by previous classifiers
- Weights based on learners accuracy

Random Forests (RF)

- **Data bagging**: creates *N* decision trees trained on bagged data
- **Feature bagging**: Given *M* features, every tree learns on $m \ll M$ randomly selected features
- Classification based on **voting** of resulting *forest*

Advantages:

- does *not* overfit easily
- Can handle thousands of features
- estimates what variables are important for classification

L. Breiman, *Random Forests*, Machine Learning, 2001

How do I pick the best learning algorithm?

Learning algorithms quality criteria:

- **accuracy**: percentage of correct classification
- **robustness**: handling noise and missing values
- efficiency: time to construct and use the model
- scalability: efficiency in memory requirements
- interpretability: how much the model is understandable

Conclusion

- Know what algorithms do, what their limitations are, and how their parameters may affect results
- Pick your algorithm depending on the nature of your data
- Better data often beats better algorithms
- Getting started: consider Python!