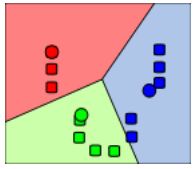
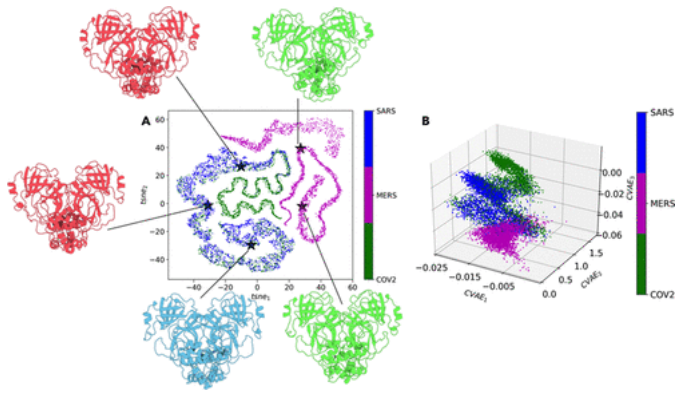
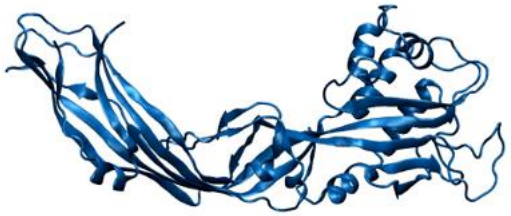
From biomolecular data to information

Antonia Mey

Matteo Degiacomi







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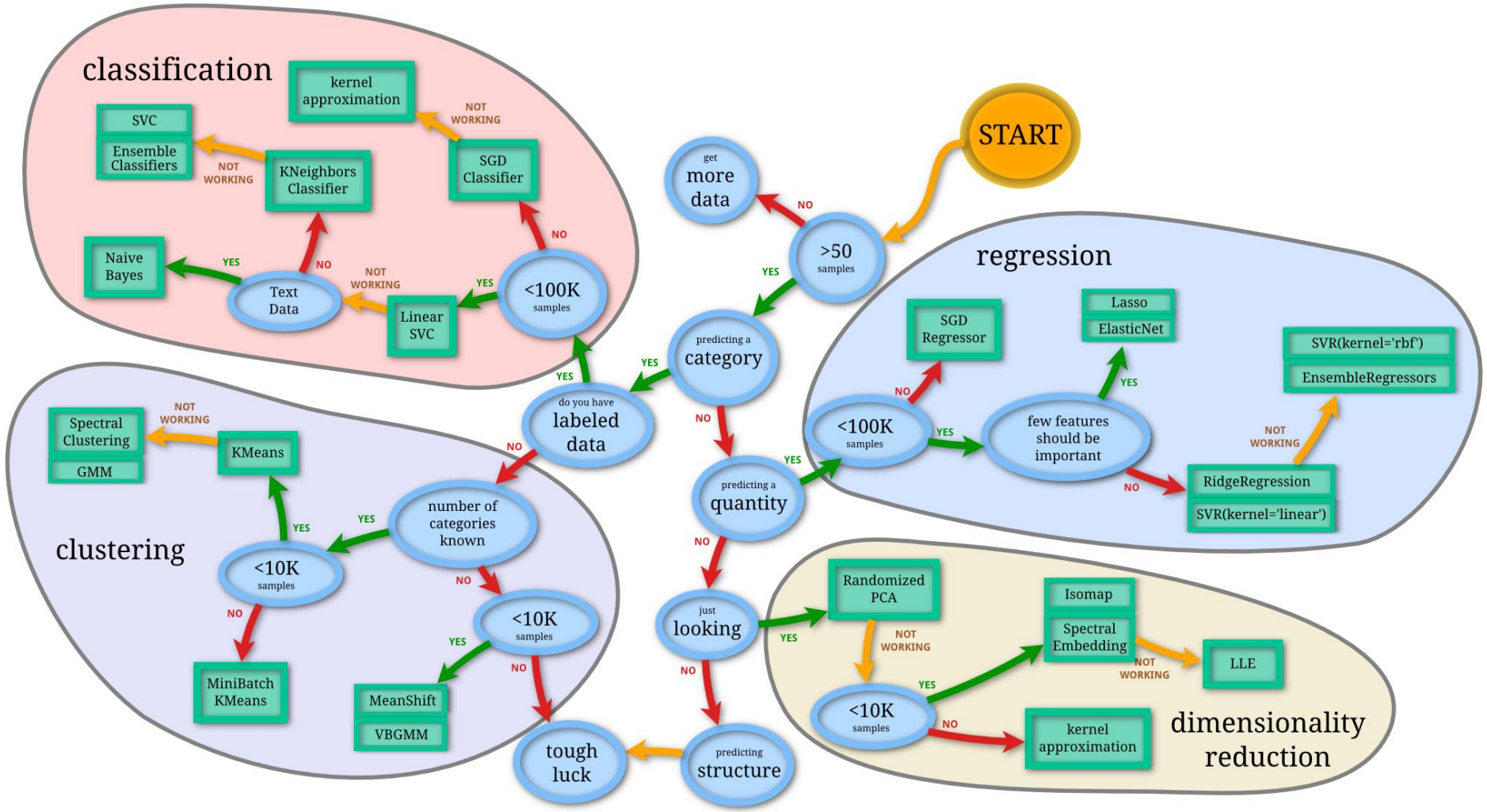
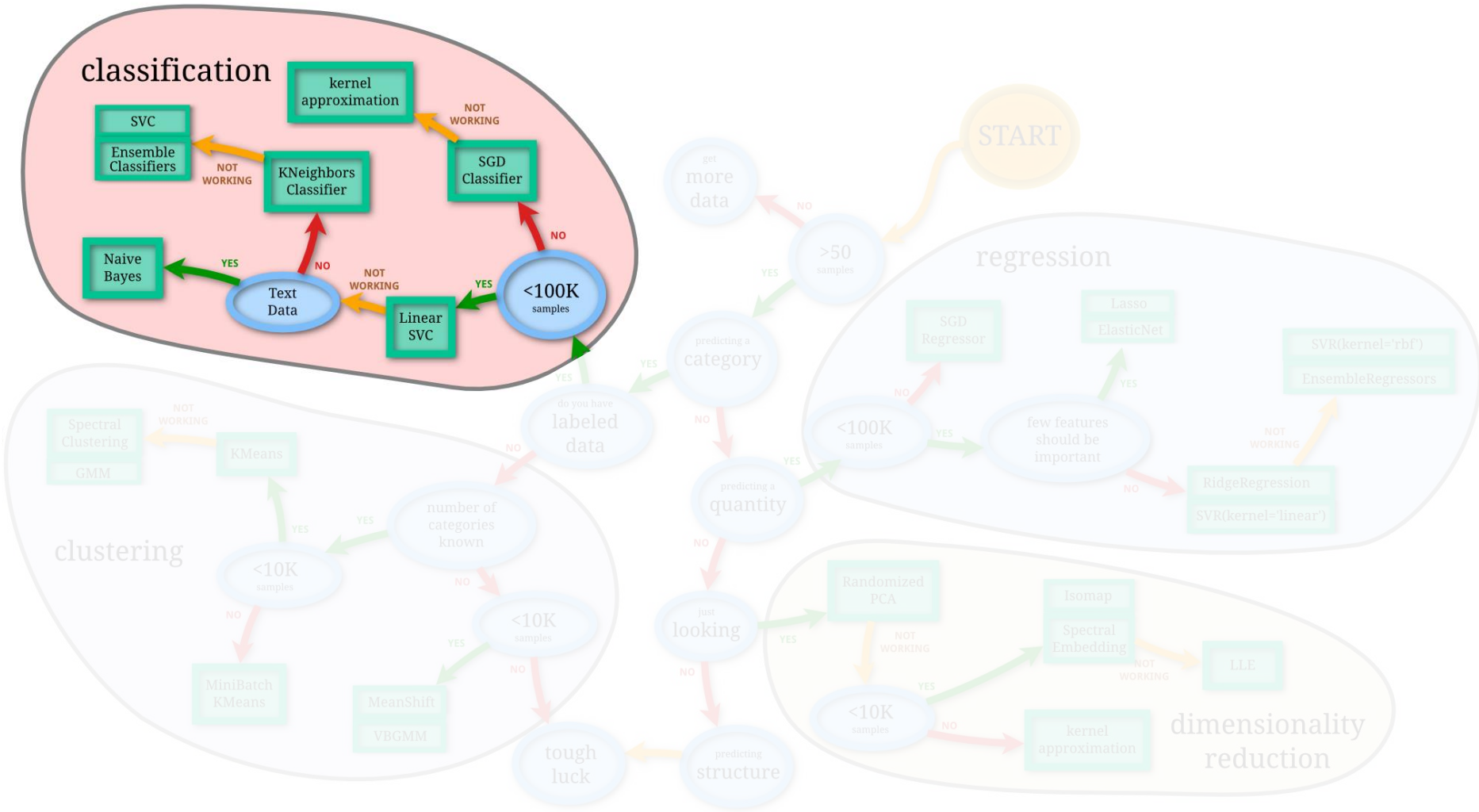
THE UNIVERSITY of EDINBURGH

The Data Mining world



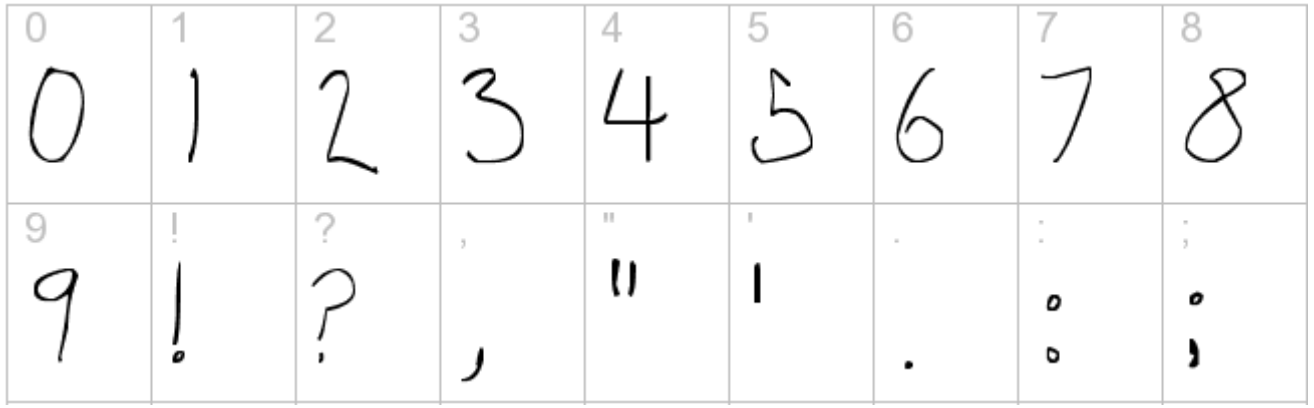
From **scikit-learn.org**

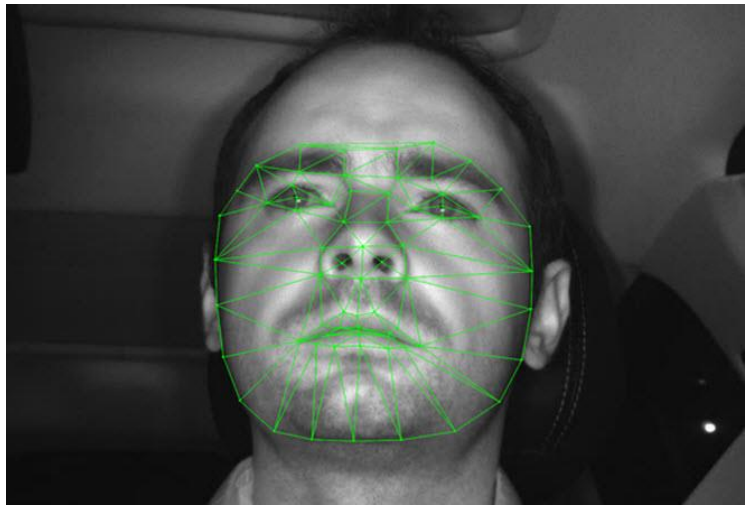
The Data Mining world

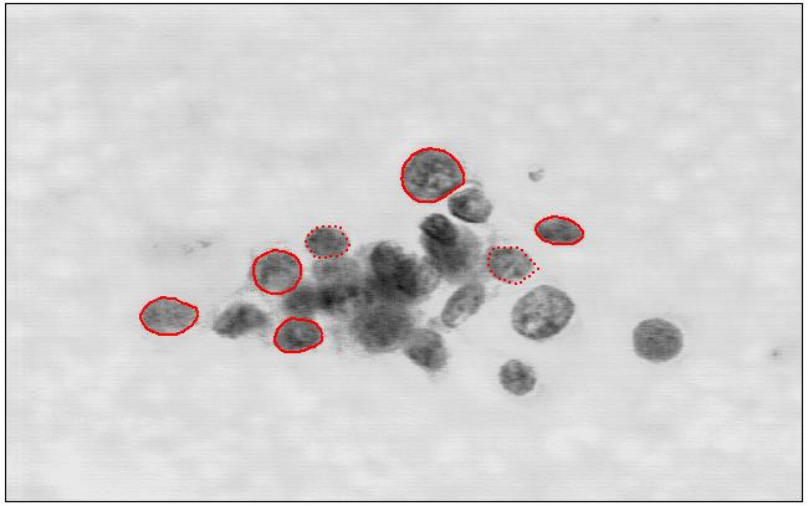


From **scikit-learn.org**

Classification problems are ubibiquitous

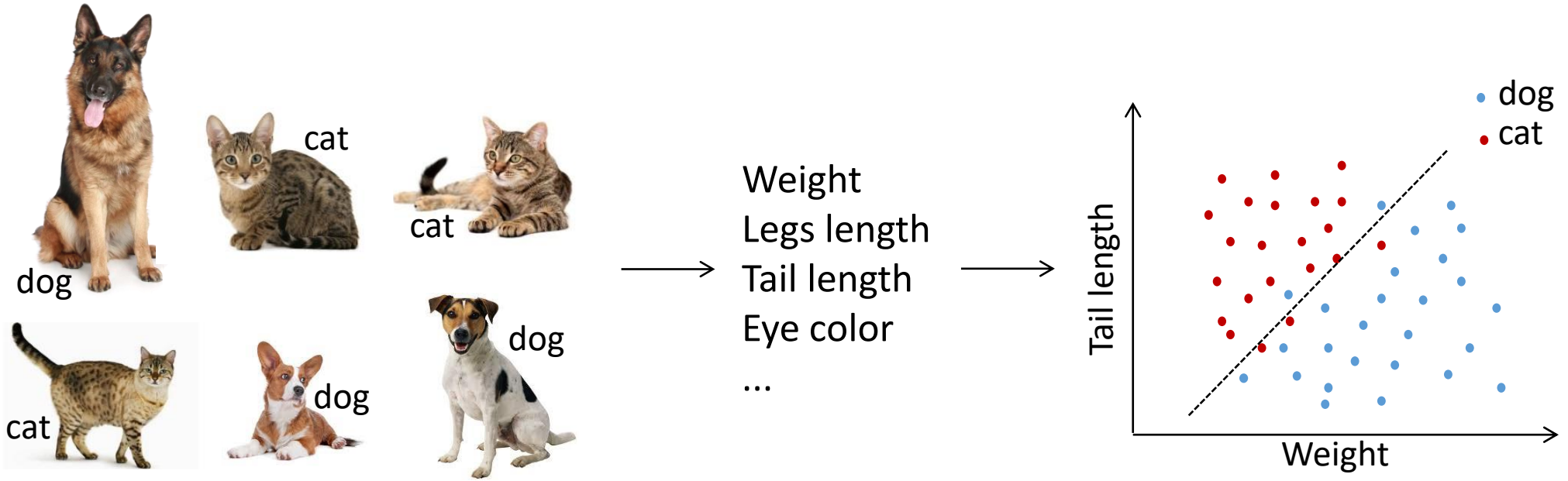






Data Classification via Supervised Learning

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



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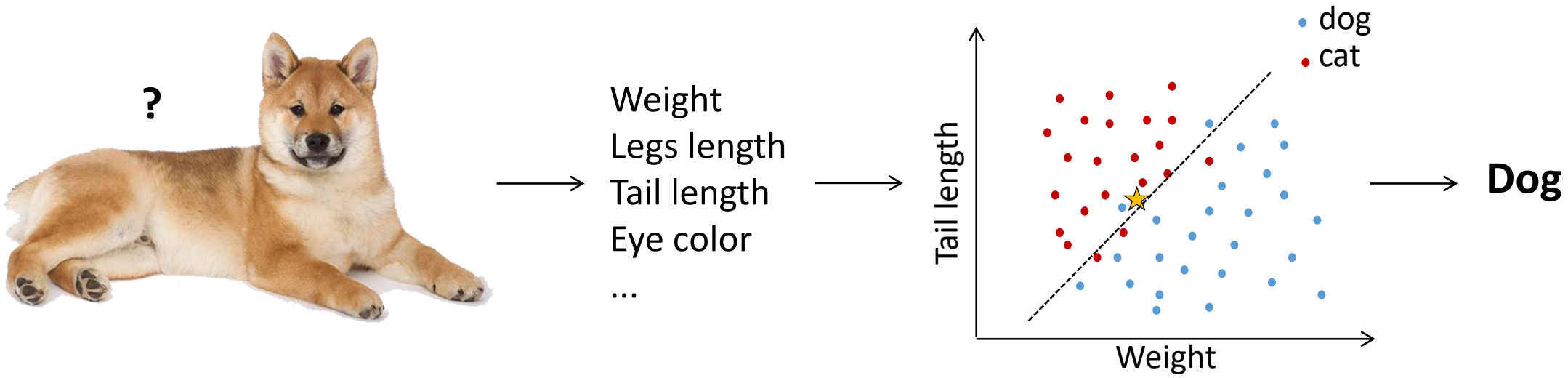
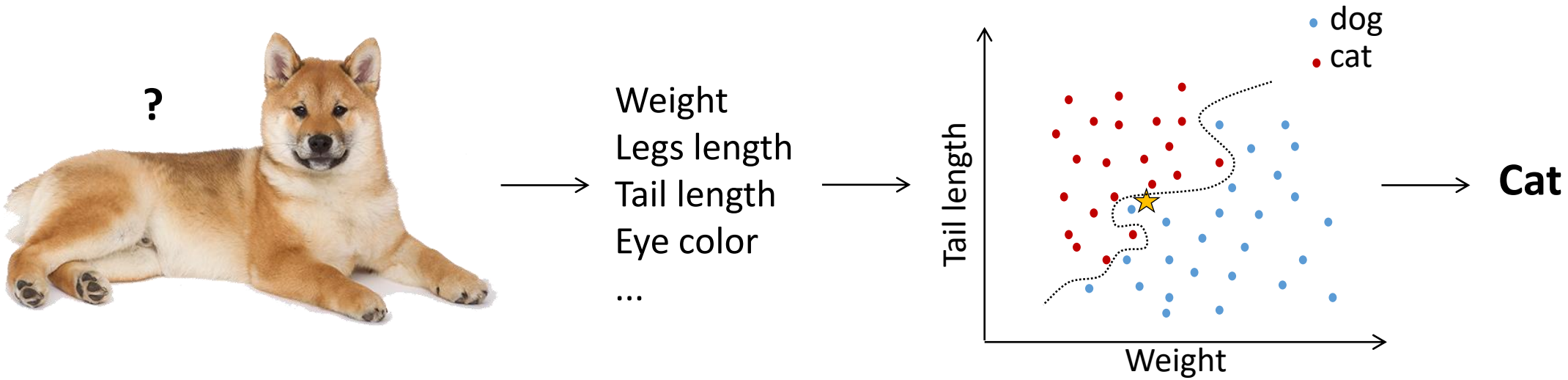


Data Classification via Supervised Learning

- 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 using supervised learning

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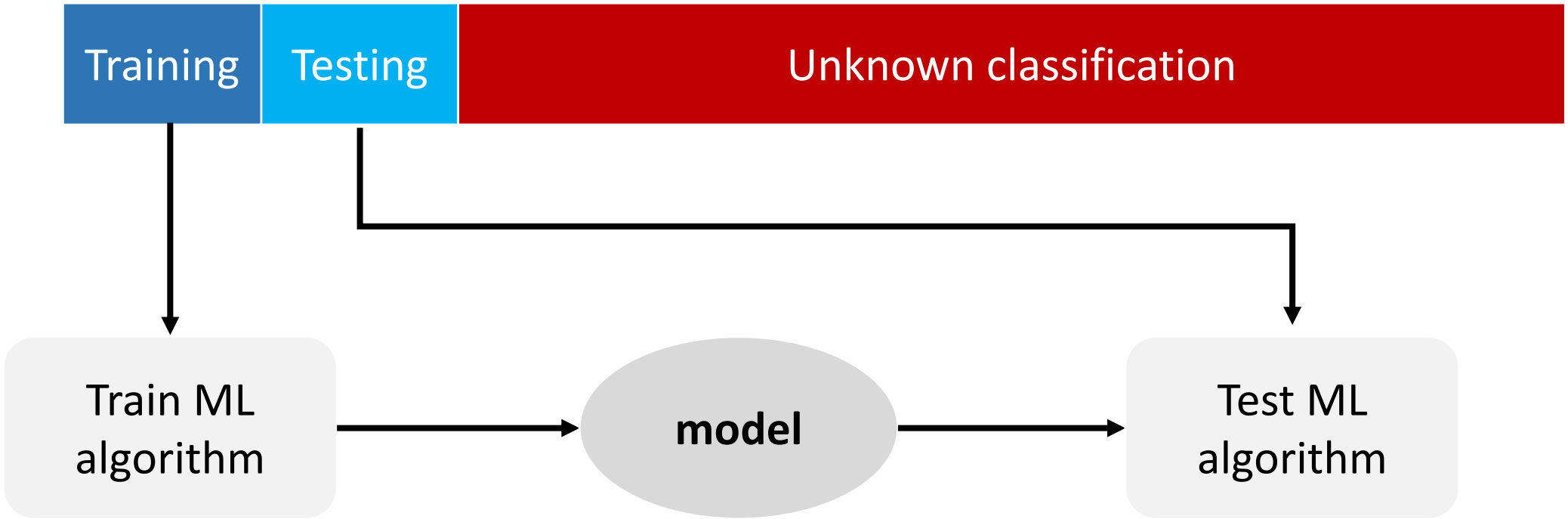

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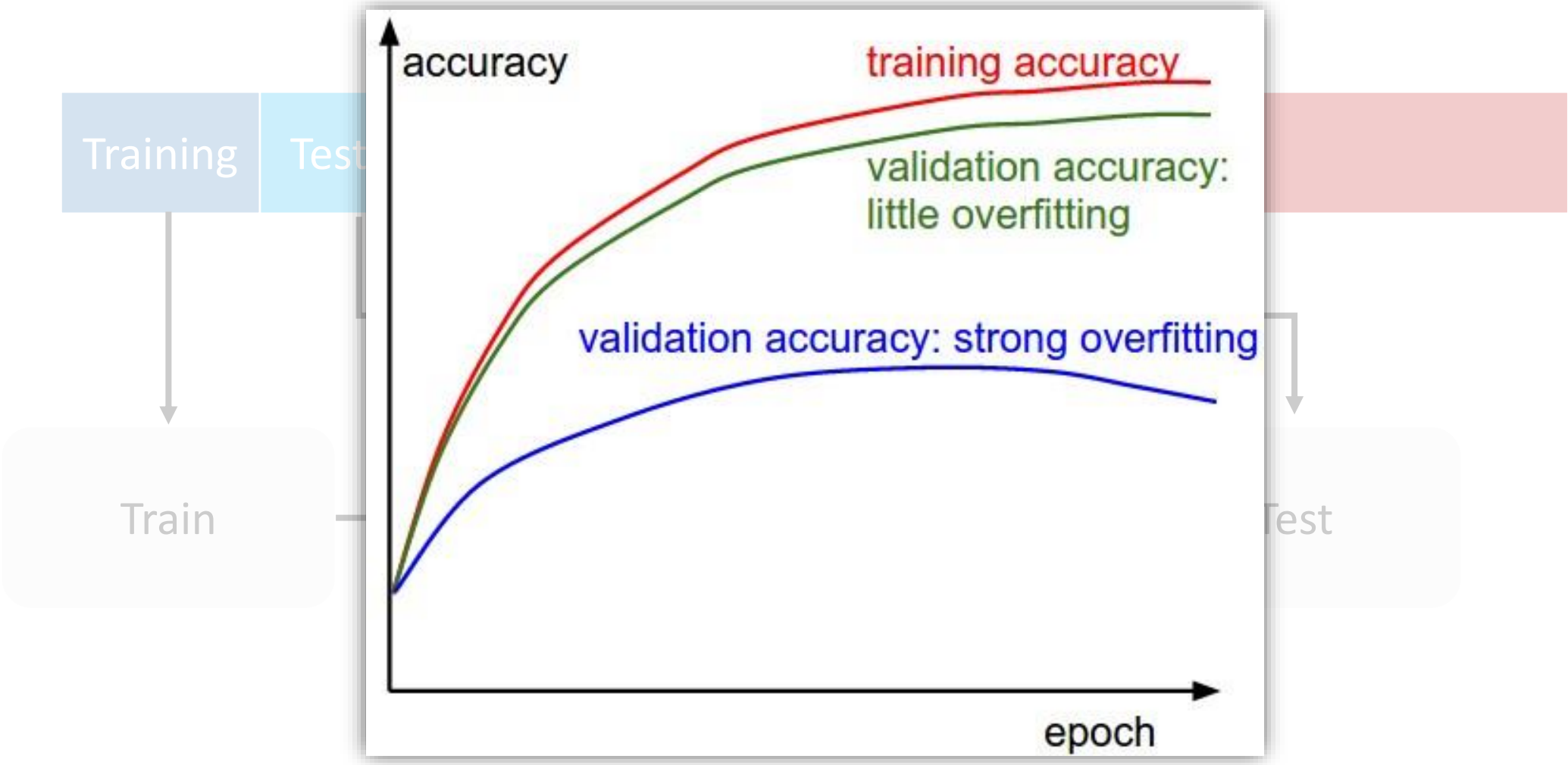
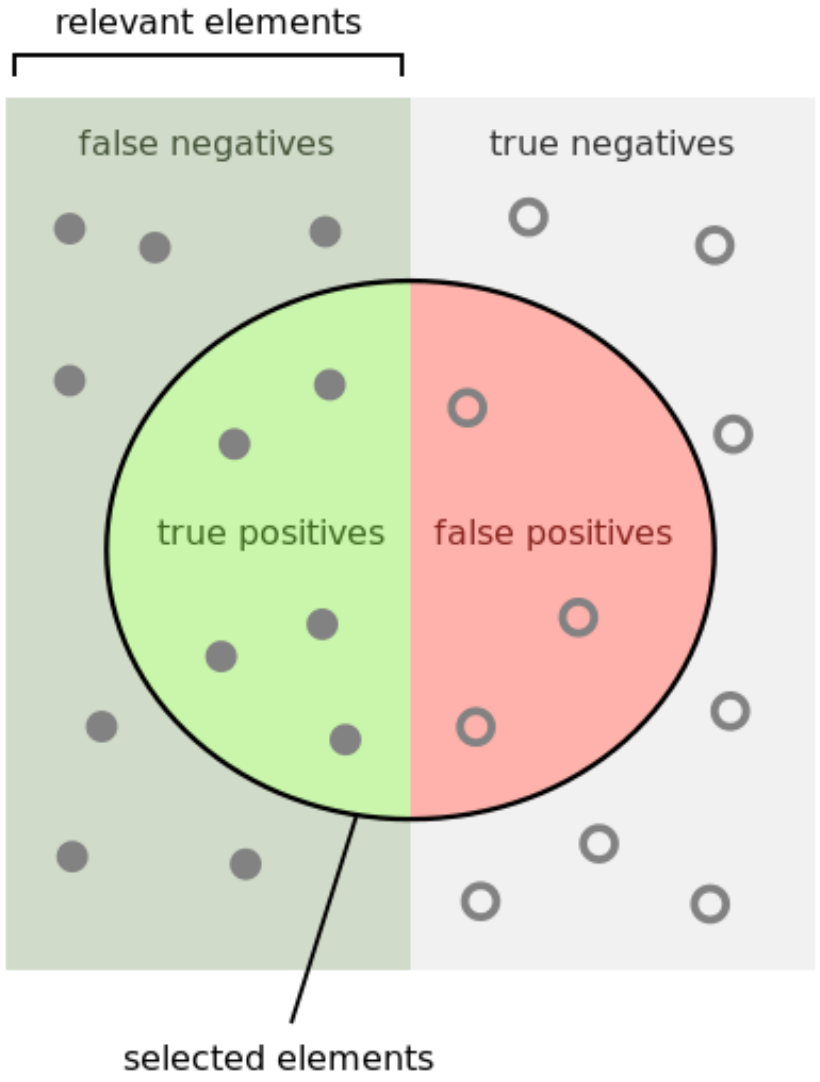


Some terminology



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

result \ real	Dog	Cat
Dog	90	10
Cat	12	88

- **precision** $= \frac{\text{true positives}}{\text{selected elements}} =$ 
- **sensitivity** $=$ **recall** $= \frac{\text{true positives}}{\text{relevant elements}} =$ 
- **accuracy** $= \frac{\text{true positives+true negatives}}{\text{total population}}$

en.wikipedia.org/wiki/Precision_and_recall

Learning Algorithms

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

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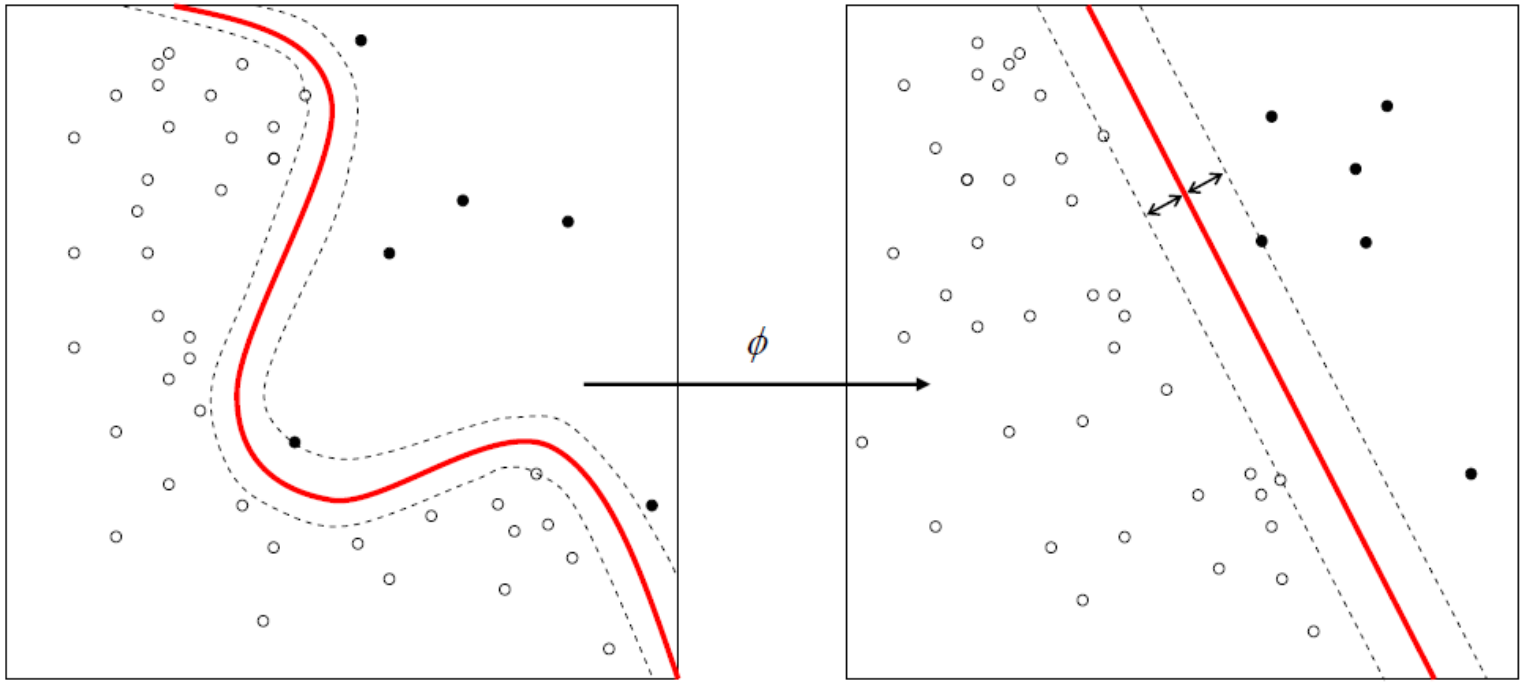
How do I pick the best learning algorithm?

Learning algorithms quality criteria:

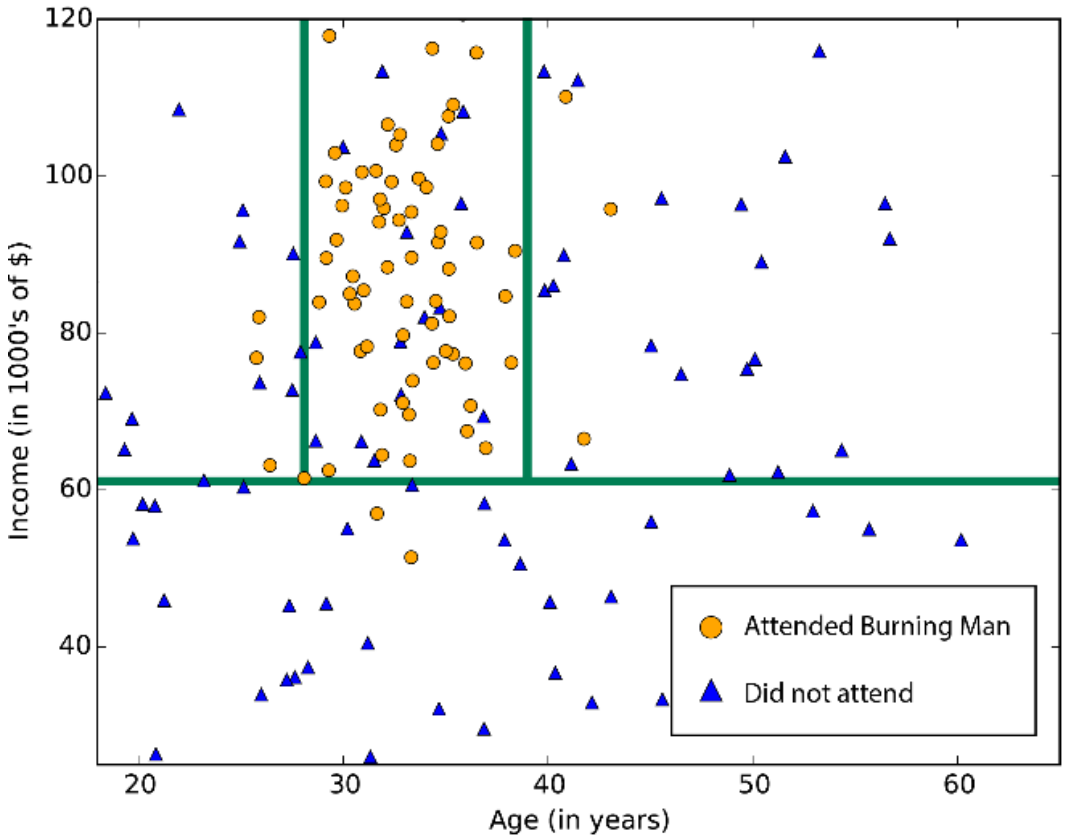
- **accuracy**: percentage of correct classification
- **robustness**: handling noise and missing values
- **efficiency**: time to construct and use the model
- **scalability**: efficiency in memory requirements
- **interpretability**: how much the model is understandable

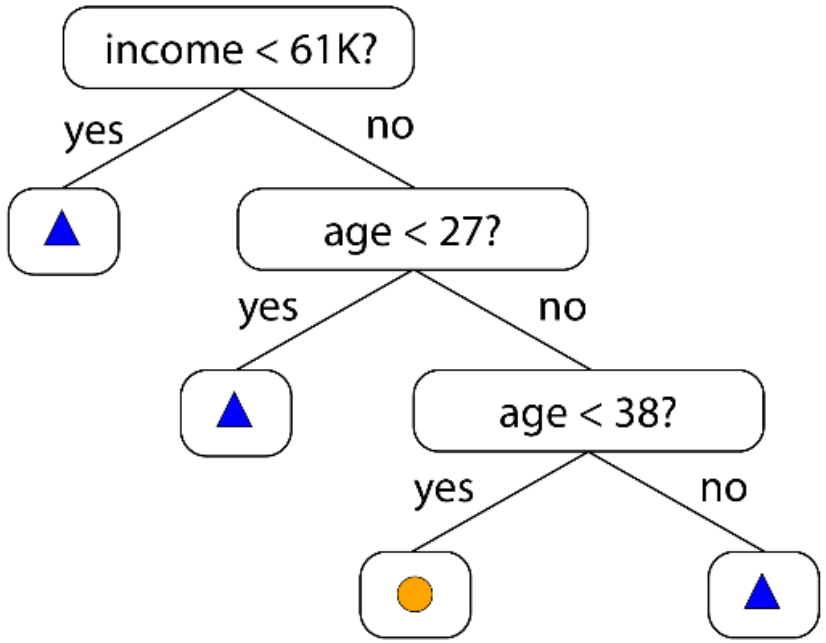
[Extra] Support Vector Machine (SVM)

- invented by V. Vapnik *et al.* in the 1970s in Russia, but only known to the West in 1992
- **linear classifier** finding a hyperplane to separate **two class** of data
- **Kernel functions** (Φ) used for nonlinear separation



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

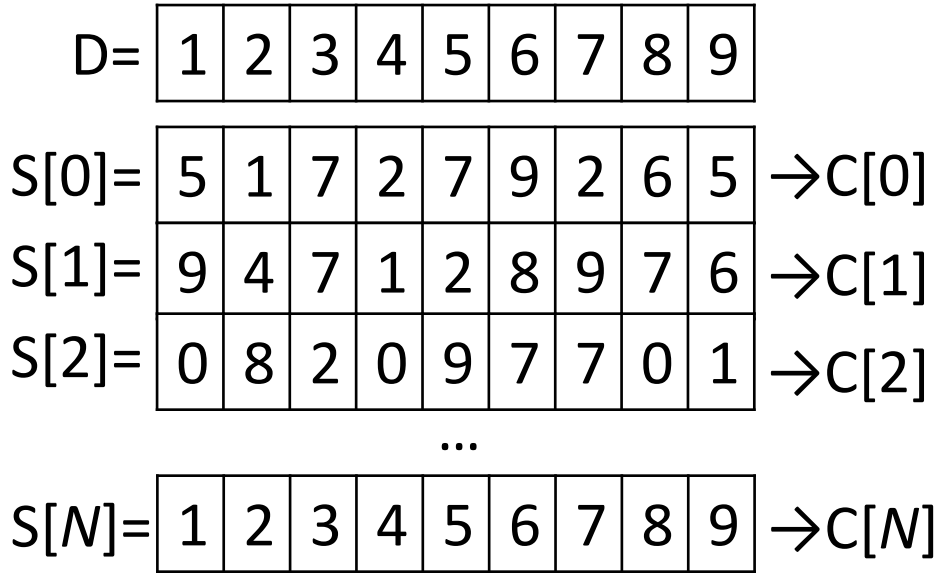
Bootstrap Aggregating (Bagging)

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*



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:

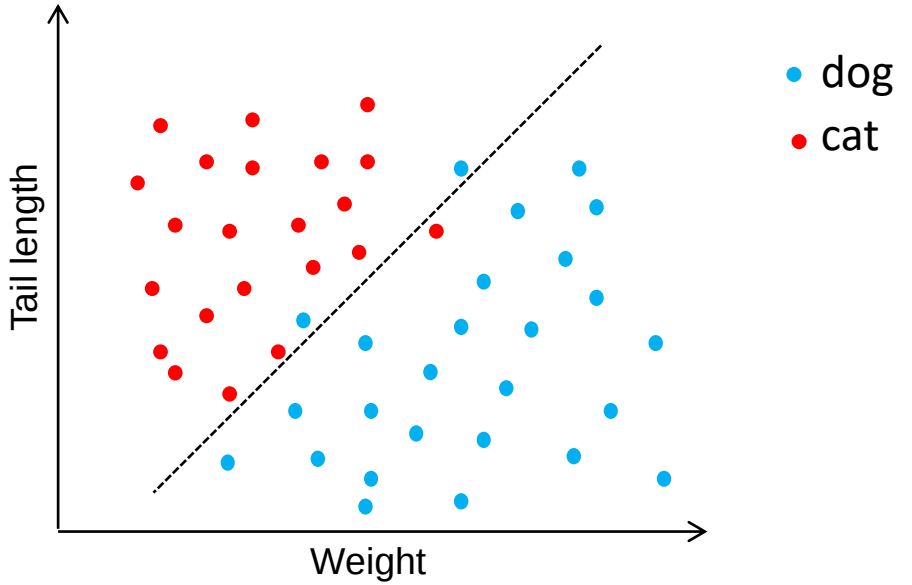
- does *not* overfit
- Can handle thousands of features
- estimates what variables are important for classification

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

[Extra] Example: Finding Protein Assembly Symmetry

Can we use experimental data to identify the topology of a protein assembly?

Random Forests



G.K.A. Hochberg, D.A. Shepherd, E.G. Marklund, I. Santhanagoplan, M.T. Degiacomi *et al.*, ***Science***, 2018

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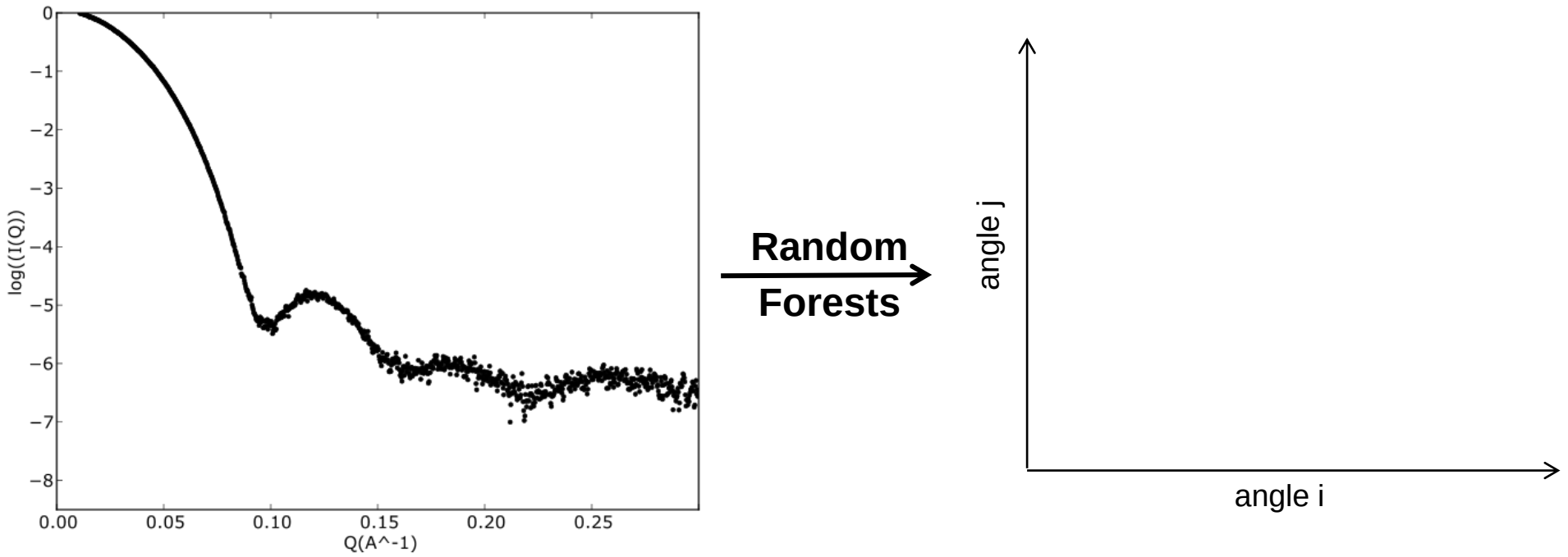

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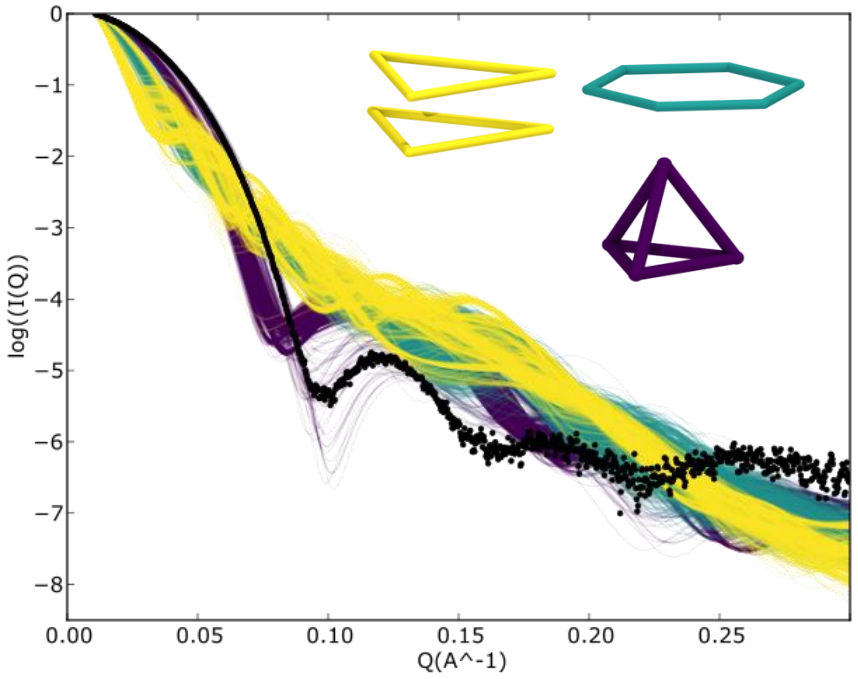
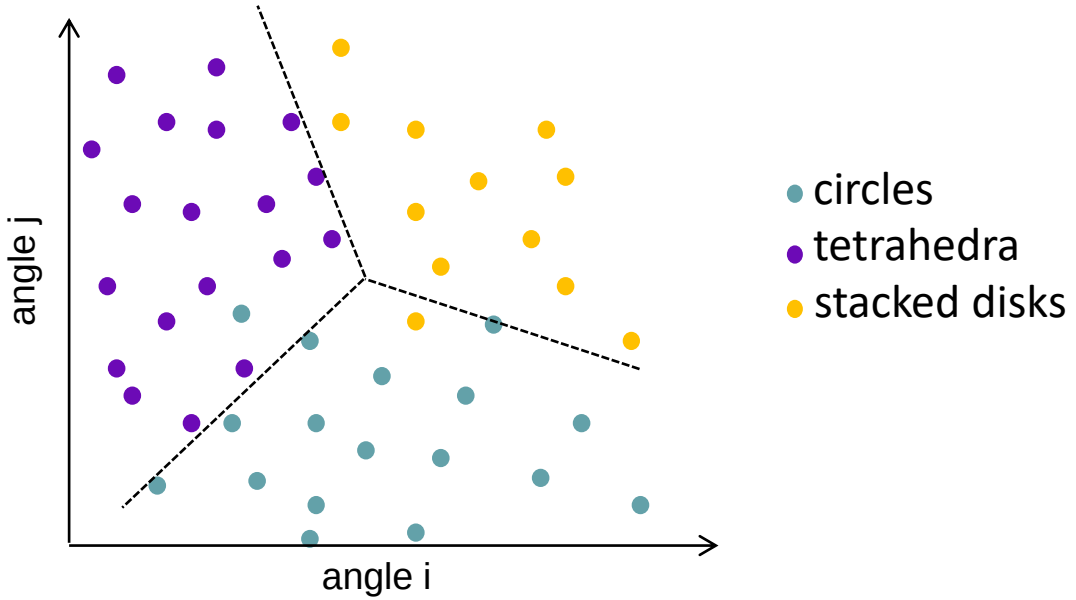


Random Forests



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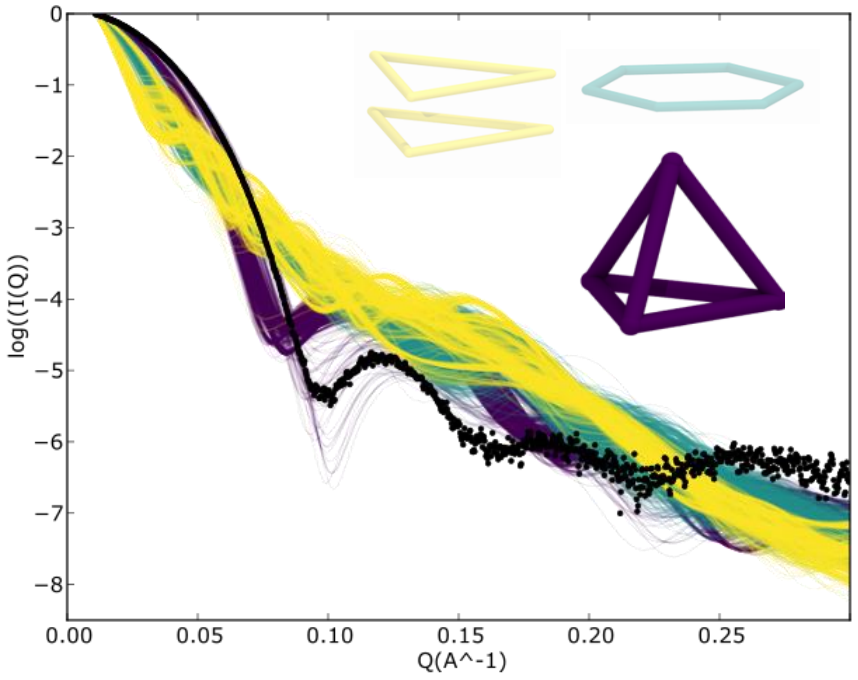

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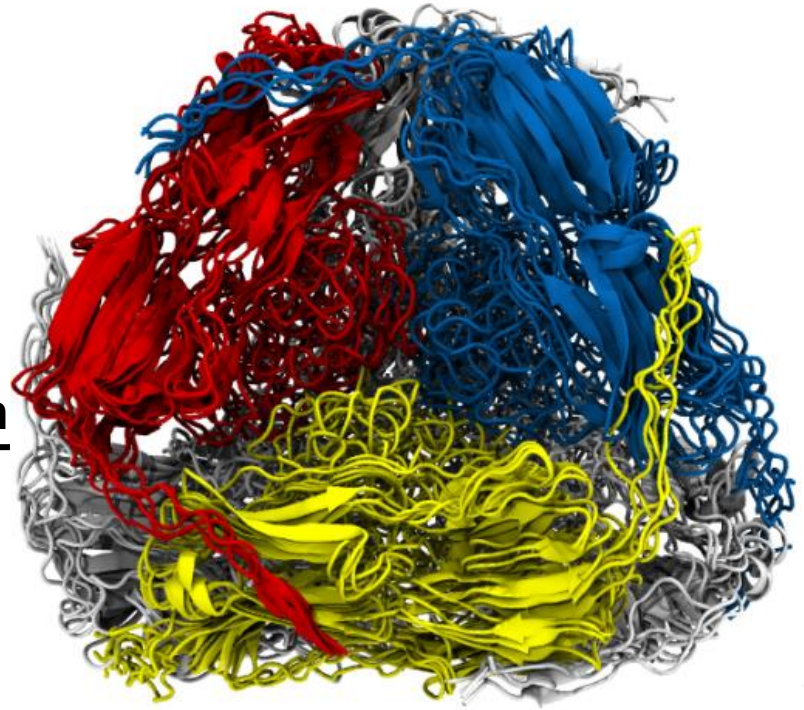

- circles
- tetrahedra
- stacked disks

G.K.A. Hochberg, D.A. Shepherd, E.G. Marklund, I. Santhanagoplan, M.T. Degiacomi *et al.*, ***Science***, 2018

[Extra] Accuracy and robustness benchmark (1)

R. Caruana *et al.* systematically tested learning algorithms against different datasets

PROBLEM	#ATTR	TRAIN SIZE	TEST SIZE	%POZ
ADULT	14/104	5000	35222	25%
BACT	11/170	5000	34262	69%
COD	15/60	5000	14000	50%
CALHOUS	9	5000	14640	52%
COV_TYPE	54	5000	25000	36%
HS	200	5000	4366	24%
LETTER.P1	16	5000	14000	3%
LETTER.P2	16	5000	14000	53%
MEDIS	63	5000	8199	11%
MG	124	5000	12807	17%
SLAC	59	5000	25000	50%

Problem	Attr	Train	Valid	Test	%Pos
Sturn	761	10K	2K	9K	33.65
Calam	761	10K	2K	9K	34.32
Digits	780	48K	12K	10K	49.01
Tis	927	5.2K	1.3K	6.9K	25.13
Cryst	1344	2.2K	1.1K	2.2K	45.61
KDD98	3848	76.3K	19K	96.3K	5.02
R-S	20958	35K	7K	30.3K	30.82
Cite	105354	81.5K	18.4K	81.5K	0.17
Dse	195203	120K	43.2K	107K	5.46
Spam	405333	36K	9K	42.7K	44.84
Imdb	685569	84K	18.4K	84K	0.44

R. Caruana and A. Niculescu-Mizil, *An Empirical Comparison of Supervised Learning Algorithm*, Proceedings of the 23rd International Conference on Machine Learning, 2006

R. Caruana et al., *An Empirical Evaluation of Supervised Learning in High Dimensions*, Proceedings of the 25rd International Conference on Machine Learning, 2008

[Extra] Accuracy and robustness benchmark (2)

Bootstrap analysis: all methods learn from of a random training subset, and get ranked by accuracy

Not high dimensional

MODEL	1ST	2ND	3RD	4TH	5TH	6TH	7TH	8TH	9TH	10TH
BST-DT	0.580	0.228	0.160	0.023	0.009	0.000	0.000	0.000	0.000	0.000
RF	0.390	0.525	0.084	0.001	0.000	0.000	0.000	0.000	0.000	0.000
BAG-DT	0.030	0.232	0.571	0.150	0.017	0.000	0.000	0.000	0.000	0.000
SVM	0.000	0.008	0.148	0.574	0.240	0.029	0.001	0.000	0.000	0.000
ANN	0.000	0.007	0.035	0.230	0.606	0.122	0.000	0.000	0.000	0.000
KNN	0.000	0.000	0.000	0.009	0.114	0.592	0.245	0.038	0.002	0.000
BST-STMP	0.000	0.000	0.002	0.013	0.014	0.257	0.710	0.004	0.000	0.000
DT	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.616	0.291	0.089
LOGREG	0.000	0.000	0.000	0.000	0.000	0.000	0.040	0.312	0.423	0.225
NB	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.030	0.284	0.686

High dimensional

AVG	1ST	2ND	3RD	4TH	5TH	6TH	7TH	8TH	9TH	10TH
RF	0.727	0.207	0.054	0.011	0.001	0	0	0	0	0
ANN	0.053	0.172	0.299	0.256	0.119	0.072	0.019	0.011	0	0
BSTDT	0.059	0.228	0.18	0.222	0.18	0.075	0.044	0.012	0.001	0
SVM	0.043	0.195	0.213	0.193	0.156	0.088	0.08	0.031	0.001	0
LR	0.089	0.132	0.073	0.075	0.108	0.177	0.263	0.081	0	0
BAGDT	0.002	0.012	0.109	0.123	0.251	0.284	0.123	0.078	0.016	0
KNN	0.023	0.045	0.051	0.057	0.085	0.172	0.122	0.177	0.258	0.01
BSTST	0.004	0.009	0.021	0.063	0.086	0.109	0.3	0.387	0.02	0
PRC	0	0	0	0	0.013	0.024	0.047	0.222	0.695	0
NB	0	0	0	0	0	0	0	0	0.01	0.99

Post-its

Schedule

Thursday — Antonia Mey

13:30-14:45	ML Clustering
14:45-15:00	☕ break ☕
15:00-16:20	ML Dimensionality Reduction
16:20-16:30	Closing remarks
18:00-onwards	Informal social event

Friday — Matteo Degiacomi

09:30-10:45	ML Classification
10:45-11:00	☕ break ☕
11:00-12:30	ML Regressions and Neural Networks
12:30-13:30	Lunch
13:30-onwards	Bring your own problem