A short introduction to Machine Learning

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Slides also by: Maria Astefanoaei

Acknowledgements

- Workshop design: Benson Muite, Claudia Beleites, Martino Sorbaro

- Previously existing materials:
  - introductory slides partly by Maria Astefanoei (ITU Copenhagen)
  - machine learning and statistics class by David Kirkby (UC Irvine)
    https://github.com/dkirkby/MachineLearningStatistics

Outline

- Morning
  - Introduction (this lesson)
  - Clustering tutorial
  - Coffee break
  - Dimensionality reduction and supervised classification tutorial

- Afternoon
  - Model validation
  - Regression methods

- ~~Tomorrow~~
  - ~~Deep learning~~

What is machine learning?

How has computing changed?

Data: terabytes, petabytes, exabytes

Speed: gigahertz, teraflops, megabits/second

Algorithms: new methods that enable us to find new ways to create, manipulate and analyse data

All three aspects were needed for the current boom of machine learning usage.

Data center (cybrain; iStock by Getty Images)

Machine learning

Arthur Samuel: "the field of study that gives computers the ability to learn without being explicitly programmed."

Tom Mitchell: "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."

Example: object recognition in images

Input is a photograph, as a bitmap

Challenges:

- position, orientation, scale, color

Using pixels would not work

Example: object recognition in images

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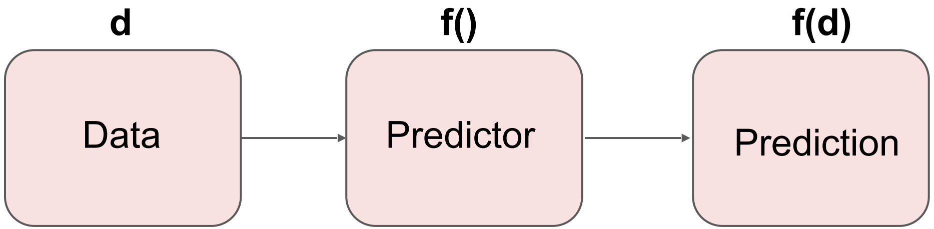
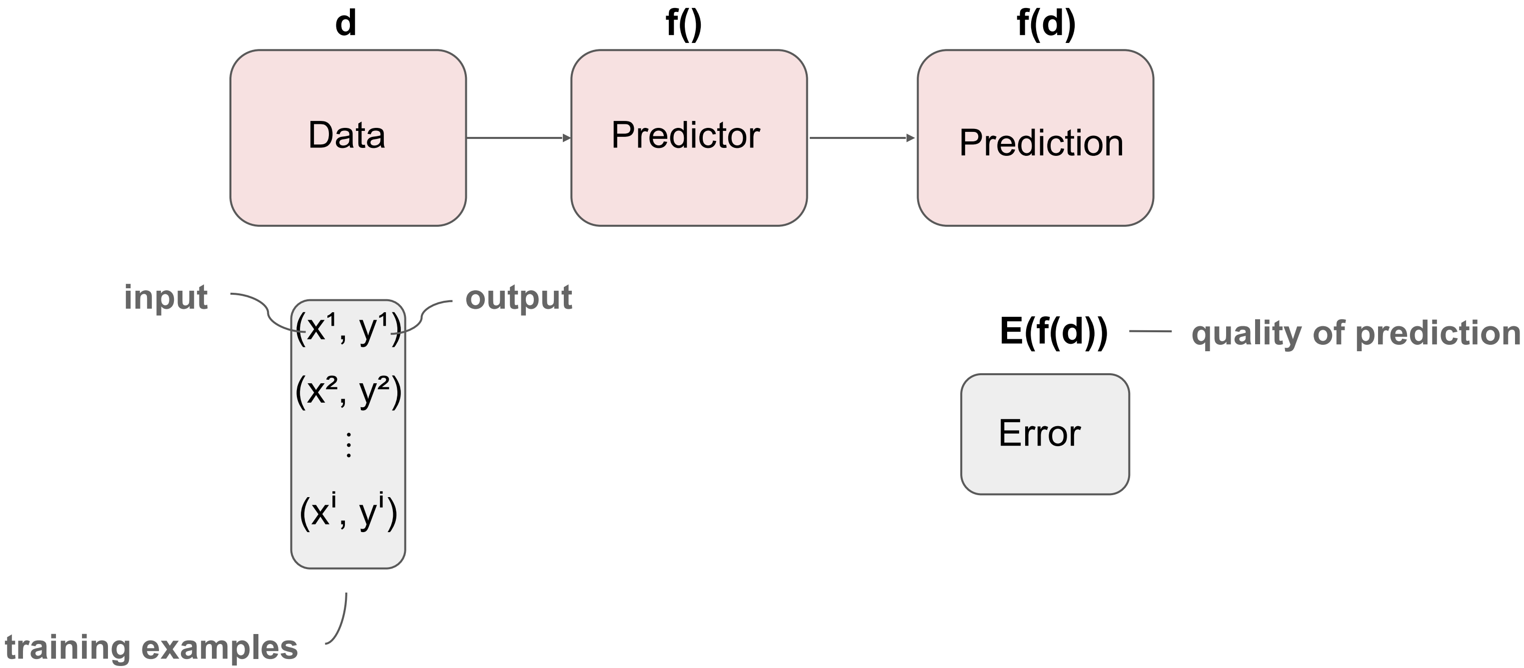
Using pixels would not work

we want to automatically find the relevant features in the data

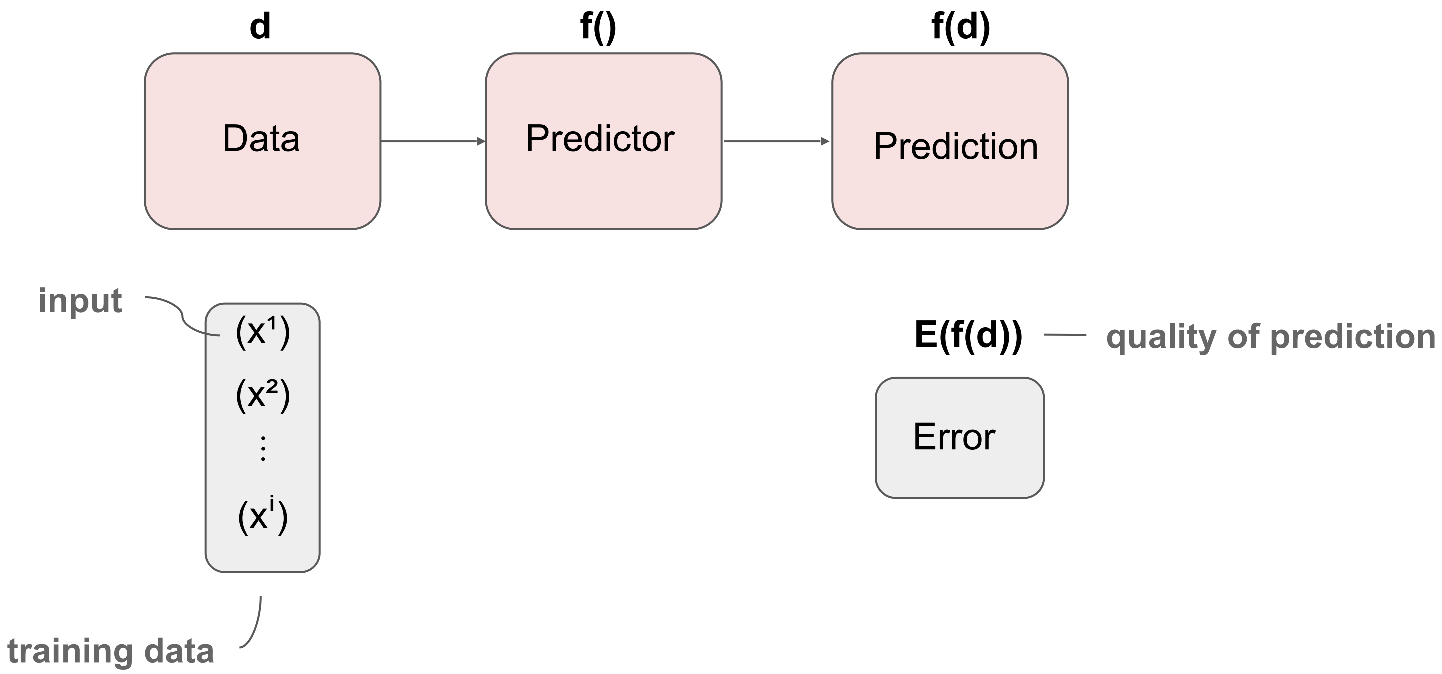
Machine learning



Machine learning

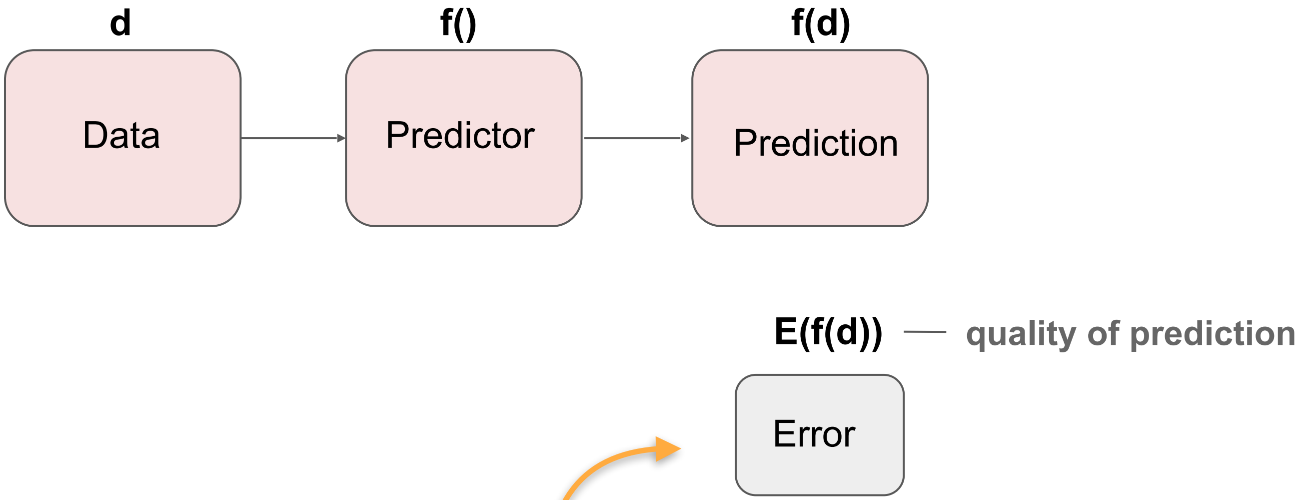


Machine learning



Machine learning

This function depends on parameters...



...which we choose by optimizing a metric ("loss", "error", "fitness")

Types of learning

Types of learning

- Supervised learning
  - explicit examples of output, (input, desired output) pairs
  - accuracy computed directly
  - classification, regression
- Unsupervised learning
  - letting the computer learn by itself
  - model the underlying structure; does not require labeled data
  - evaluation is indirect or qualitative
  - clustering

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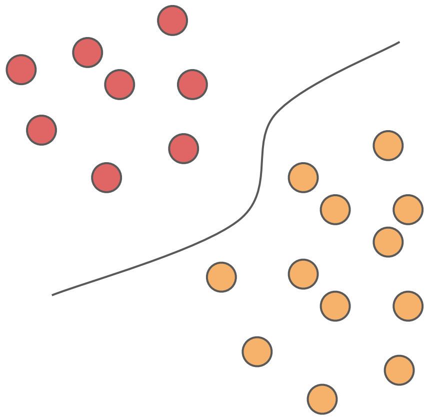

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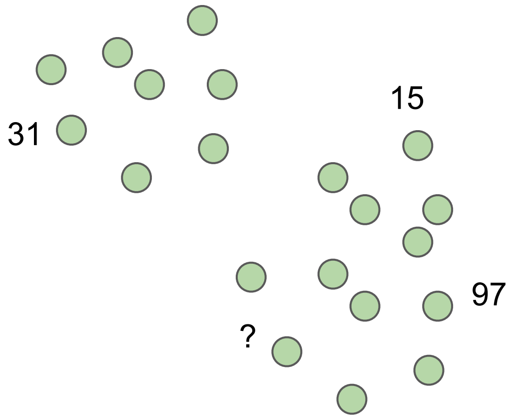

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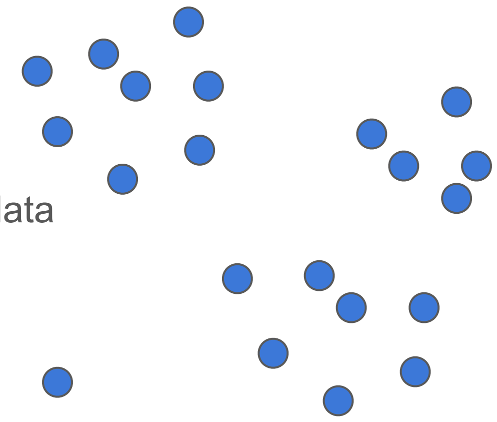

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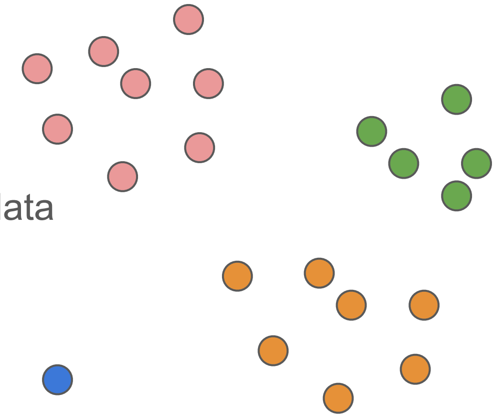
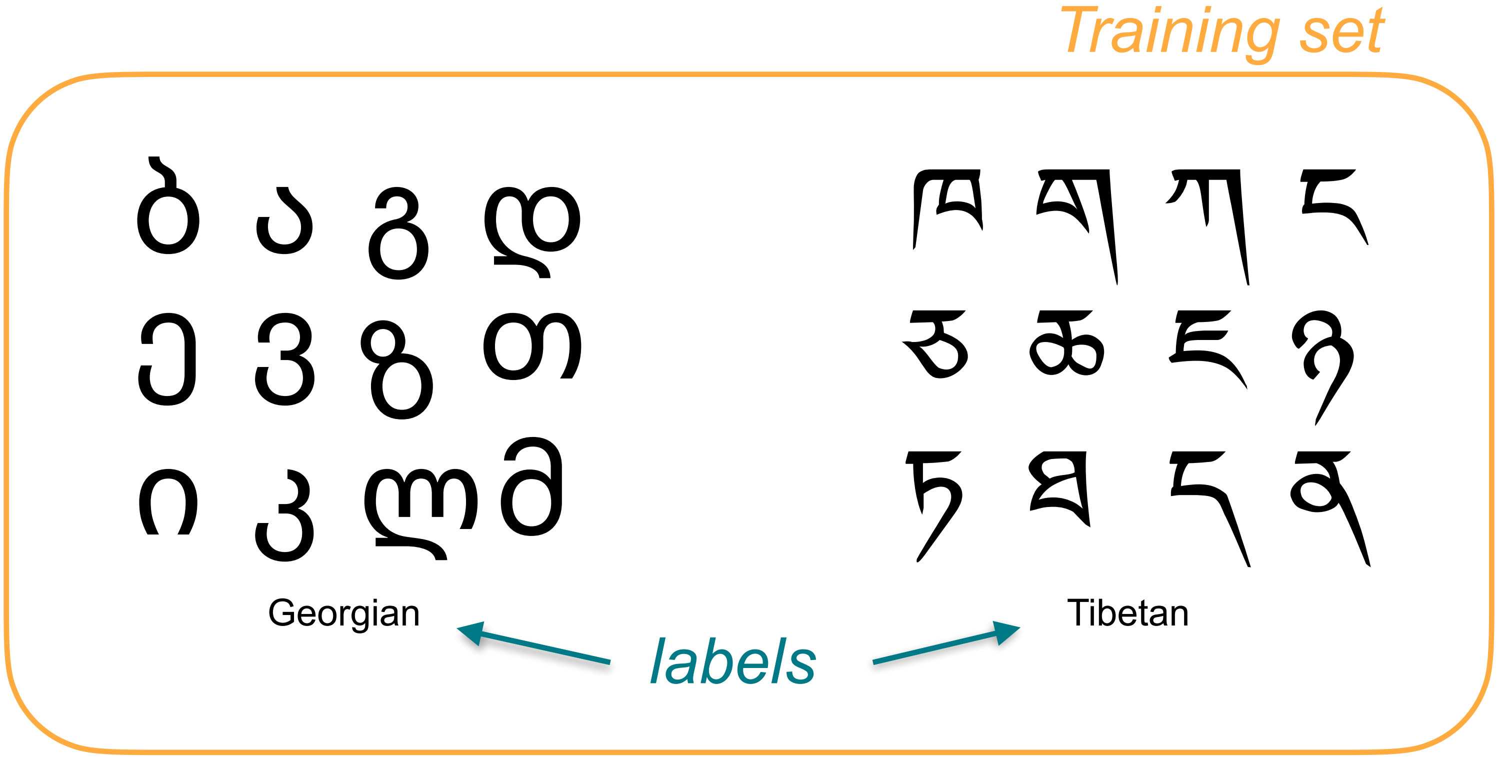


Supervised classification: training phase



Supervised classification: test phase

Which alphabet does each of these belong to?

Supervised classification: test phase

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Your guess	T	T	T	G	G

Supervised classification: test phase

Which alphabet does each of these belong to?

Labels	T	G	T	G	G
Your guess	T	T	T	G	G

Evaluation: accuracy 80%

Supervised classification: test phase

Which alphabet does each of these belong to?

Test set

Labels	T	G	T	G	G
Your guess	T	T	T	G	G

Evaluation: accuracy 80%

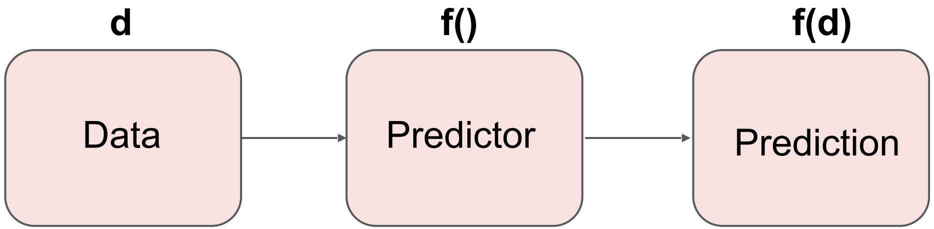
Reinforcement learning

- An "agent" exploring an environment

- Learning by trial and error instead of having examples

Types of data and representations

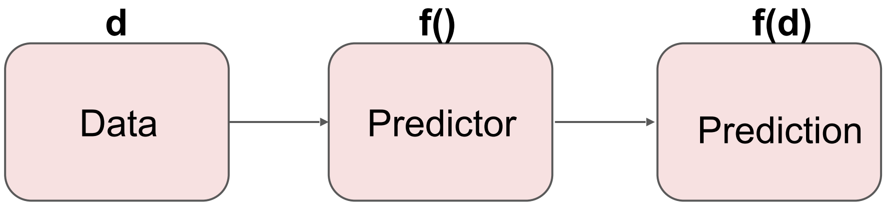
Representing data mathematically



Attribute-value pairs:

- categorical
- ordinal
- numeric

Representing data mathematically



Attribute-value pairs:

- categorical: cat, dog, giraffe, elephant
  - mutually exclusive
  - encoded as numbers, but mathematical operations not meaningful
- ordinal: poor, satisfactory, good, excellent
  - encoded as numbers, meaningful to compare
- numeric: 0/1, -54, 32
  - meaningful to do mathematical operations
  - usually good practice to normalize values

Example: wind power prediction

Attribute-value pairs:

- categorical
  - wind direction {north, south, west, east}
  - wind turbine type {horizontal-axis, vertical-axis}
- ordinal
  - day of the week {Monday, Tuesday,...}
  - capacity {<2 MW, 3-5 MW, >5 MW}
- numeric
  - wind speed {5 m/s}
  - outside temperature { 20°C}

How to pick good attributes?

Example: handwritten digits

Bitmap images with a lot of variation in style, pressure, pen type

Example: handwritten digits

Bitmap images with a lot of variation in style, pressure, pen type

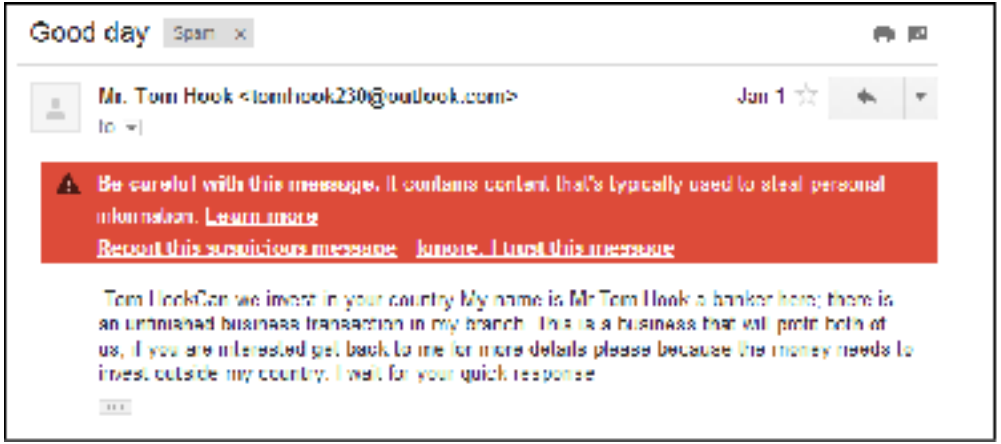
Representation:

- each pixel is a separate attribute
- 400 attributes for a 20x20 bitmap
- real number (degree of blackness) or binary
- preprocessing such that a pixel in different images has the same meaning (eg. centering)

Example: text classification

Detect spam in email classification:

- input: string of characters
- output: binary classification



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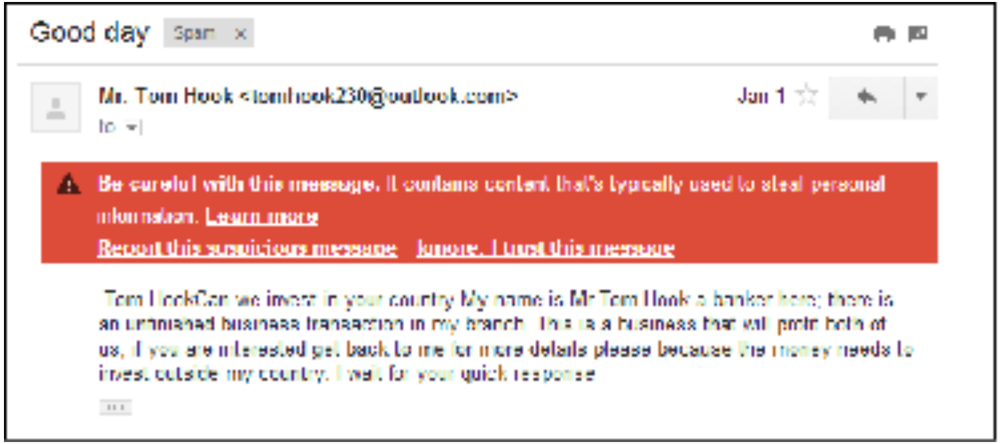
Naïve representation

- words as values



Example: text classification

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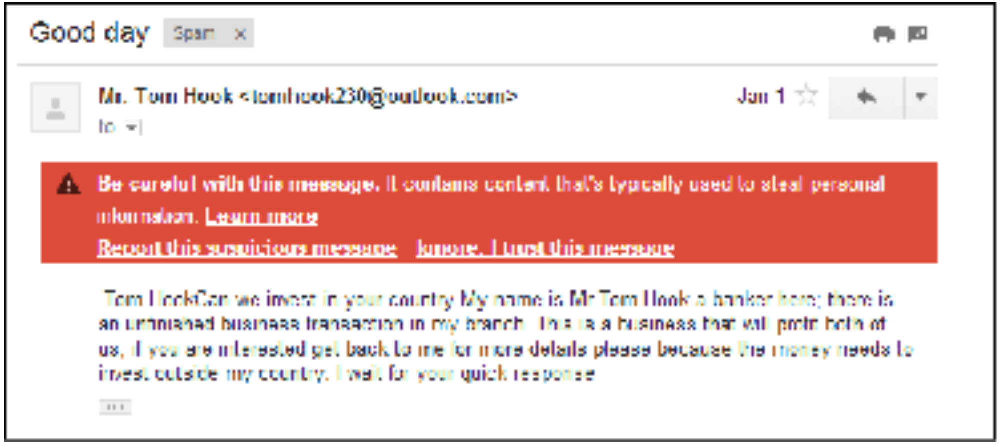
Naïve representation

- words as values

Better representation

- words as numeric attributes
- one attribute for each word
- many attributes, but binary

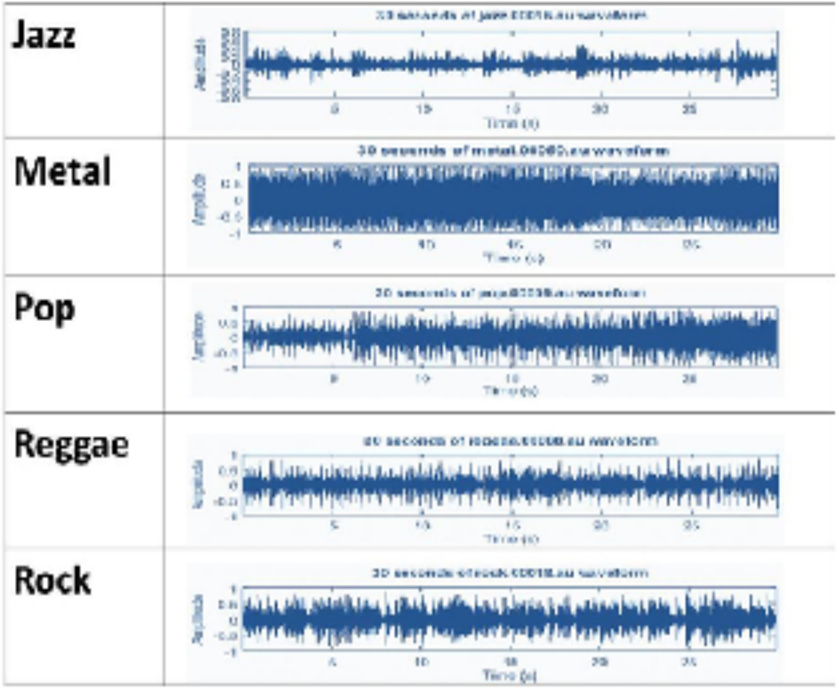


Example: music/speech

Time series - waveforms

Naïve representation:

- sample at regular intervals



Example: music/speech

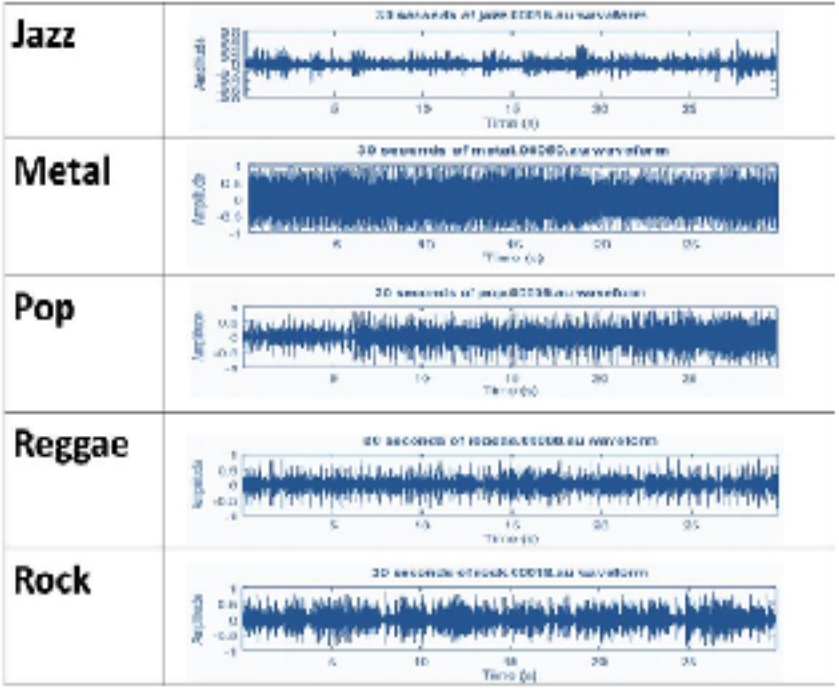
Time series - waveforms

Naïve representation:

- sample at regular intervals

Better representation:

- decompose signal as sine waves
- find base frequencies and their weights
- weights are the values for attributes



Summary: end-to-end ML

1. Define the task

2. Get the data
3. Choose the right representation
4. Get an overview
    - summary statistics (location, scale, shape, multivariate analysis)
    - visualizations
5. Prepare the data
    - data cleaning (missing values)
    - standardisation, outlier detection, transformations (polynomial, logarithmic)

6. Select a model
    - based on volume, complexity of data, assumptions about distributions and shape
7. Train and evaluate
    - on training set (cross-validation)
    - fine-tune model - optimize hyperparameters (grid search, randomized search)
8. Evaluate on test set
9. Launch, monitor, maintain

Reproducibility in machine learning

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Computational reproducibility can be defined as the process of obtaining consistent results using the same input data, computational methods, and conditions of analysis.

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Sources of stochasticity:

- Random initialization of layer weights
- Shuffling of datasets
- Changes in machine learning frameworks
- Noisy hidden layers

Reproducibility in ML

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Tools for reproducible ML:
- keeping track of model trainings (hyperparameters, etc)
- dataset versioning
- model sharing and management tools
- version control (git)
- model deployment tools

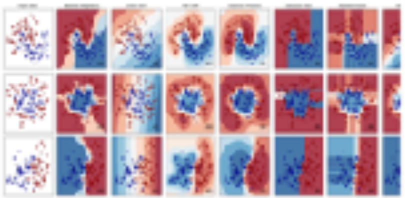
E.g. *wandb.ai*, *guild.ai*, ...

Introduction to scikit-learn

Classification

Identifying which category an object belongs to.

Applications: Spam detection, image recognition.
Algorithms: SVM, nearest neighbors, random forest, and more...

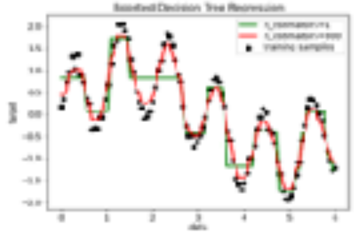


Examples

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.
Algorithms: SVR, nearest neighbors, random forest, and more...

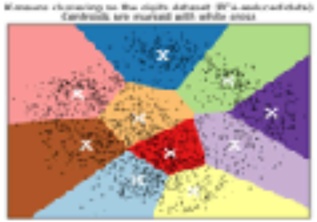


Examples

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: k-Means, spectral clustering, mean-shift, and more...

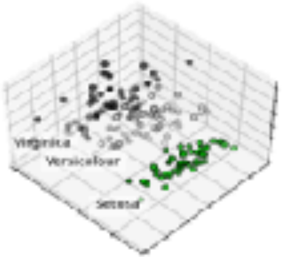


Examples

Dimensionality reduction

Reducing the number of random variables to consider.

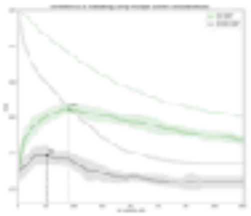
Applications: Visualization, Increased efficiency
Algorithms: k-Means, feature selection, non-negative matrix factorization, and more...



Model selection

Comparing, validating and choosing parameters and models.

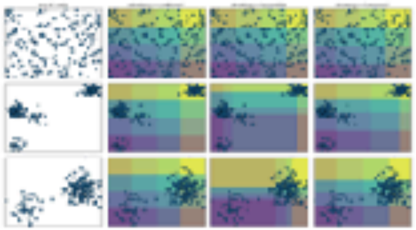
Applications: Improved accuracy via parameter tuning
Algorithms: grid search, cross validation, metrics, and more...



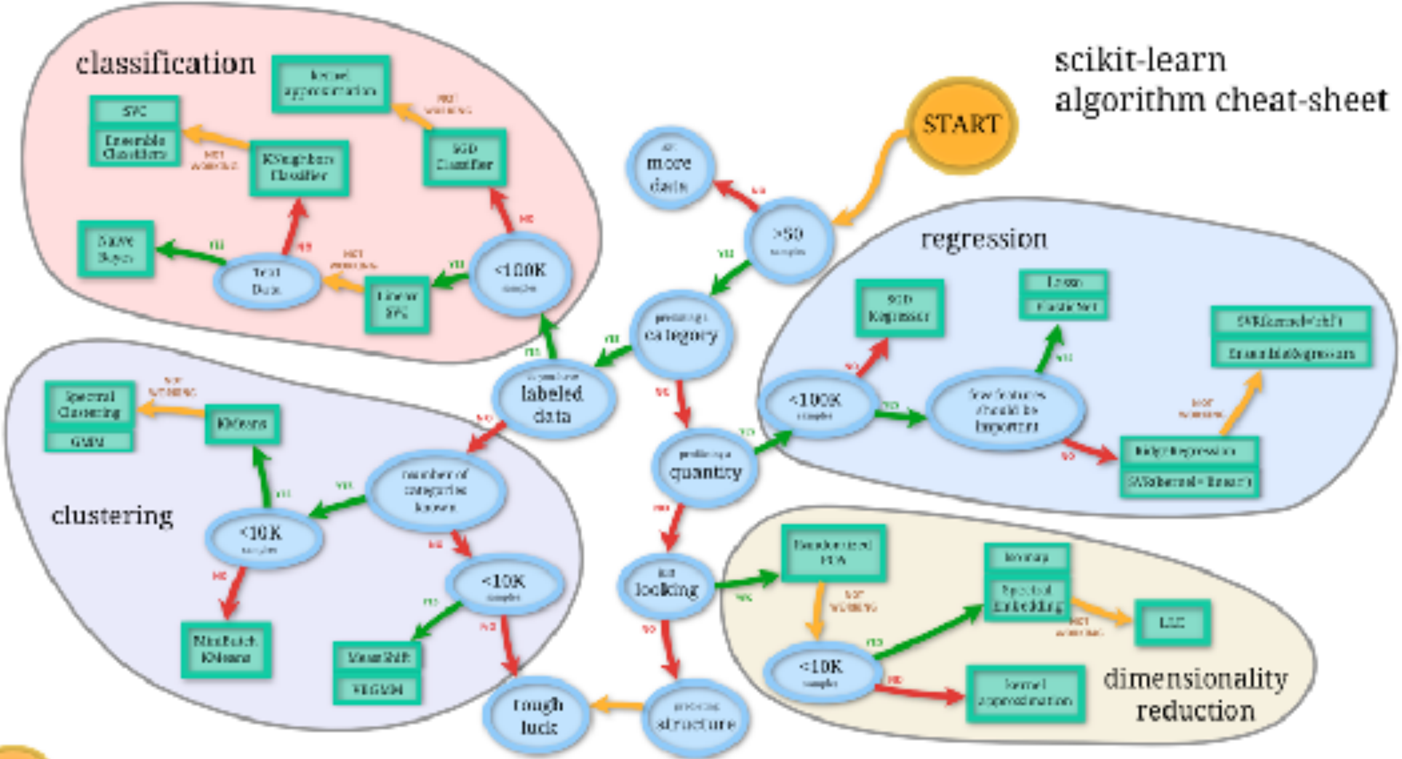
Preprocessing

Feature extraction and normalization.

Applications: Transforming input data such as text for use with machine learning algorithms.
Algorithms: preprocessing, feature extraction, and more...

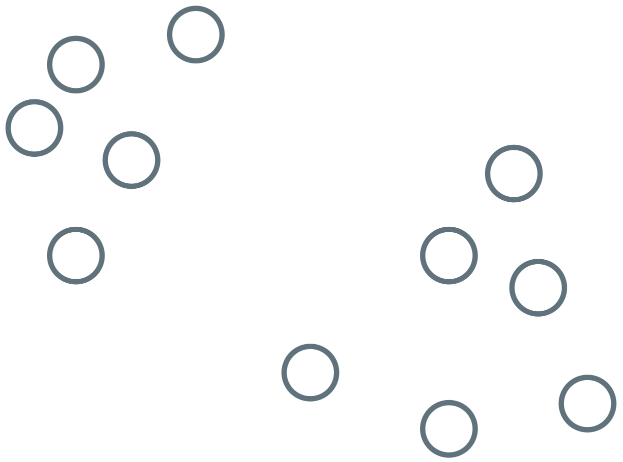


Choosing the right model

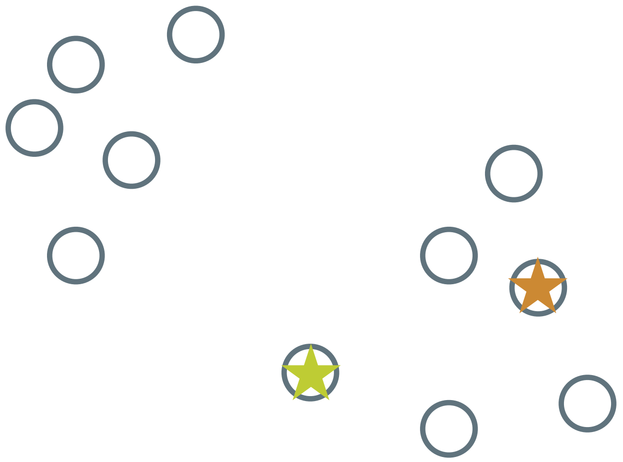


Clustering

How k-means works

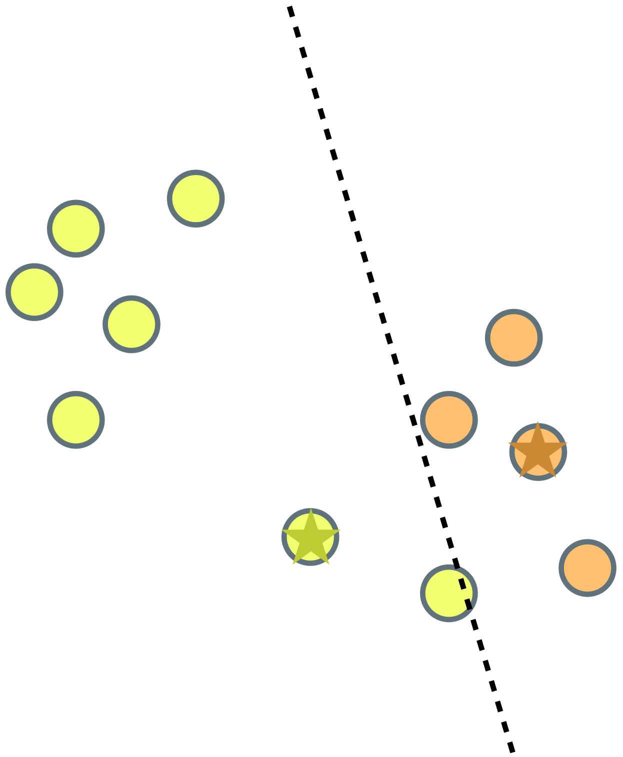


How k-means works



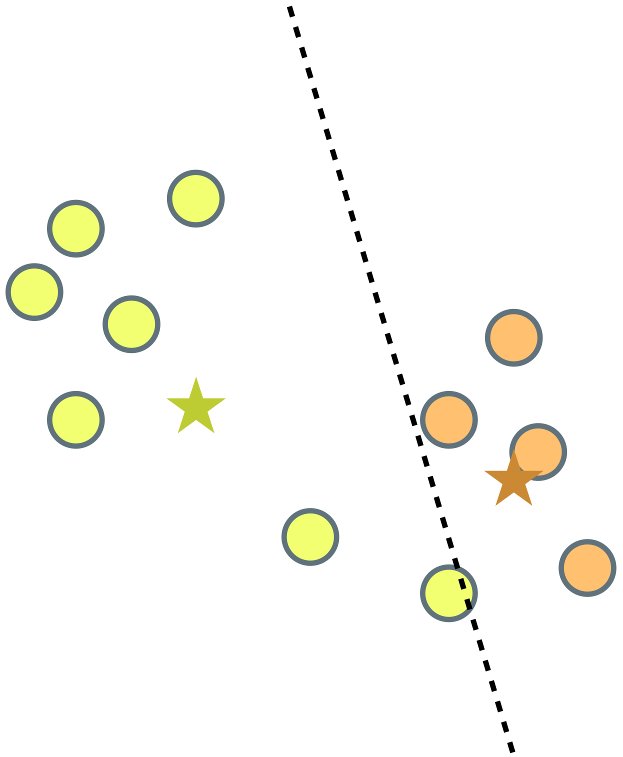
Place *k* centroids in correspondence with *k* random data points

How k-means works



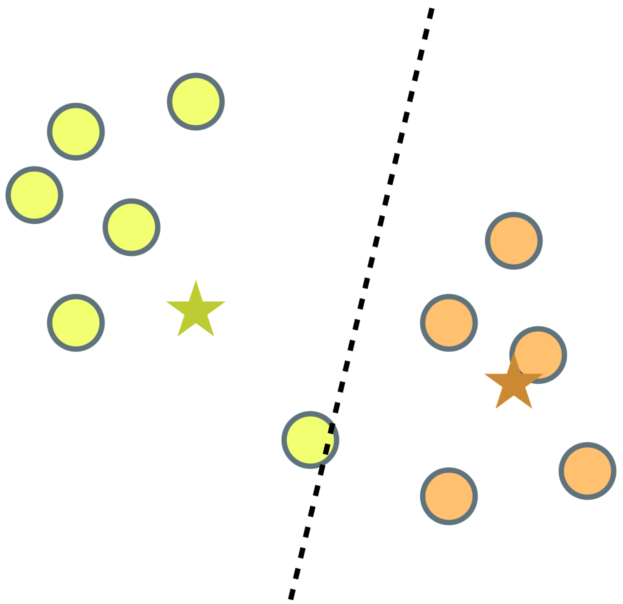
Assign each point to the nearest centroid

How k-means works



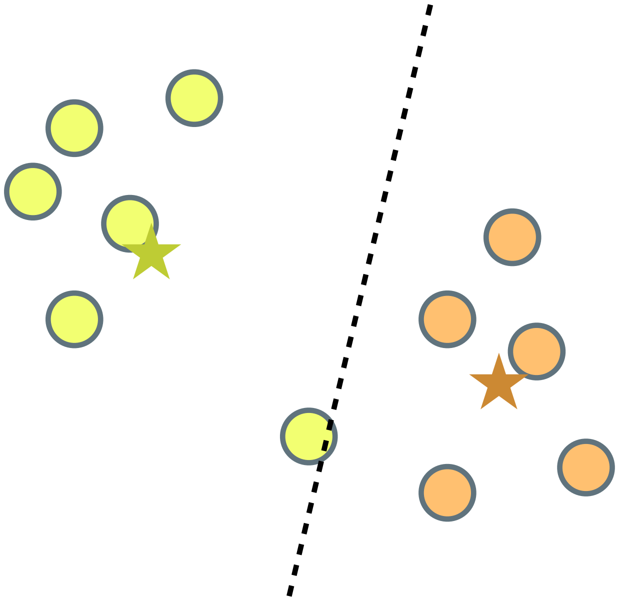
Move centroid to the center of mass of the datapoints assigned to it

How k-means works



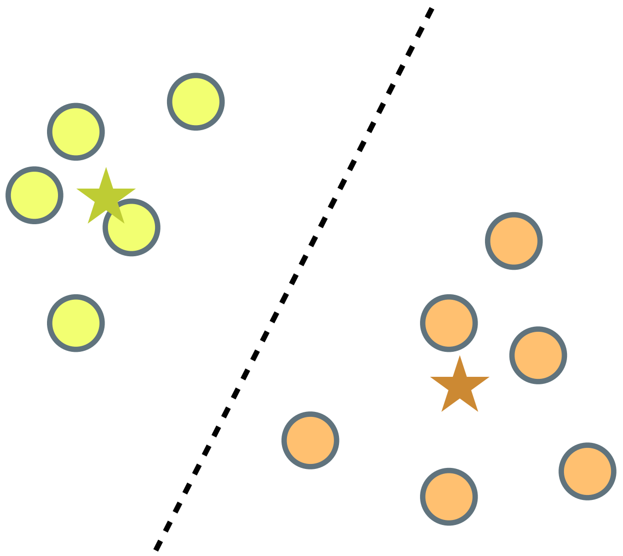
Repeat assignment
to nearest centroids

How k-means works



Repeat moving centroids to center of mass

How k-means works

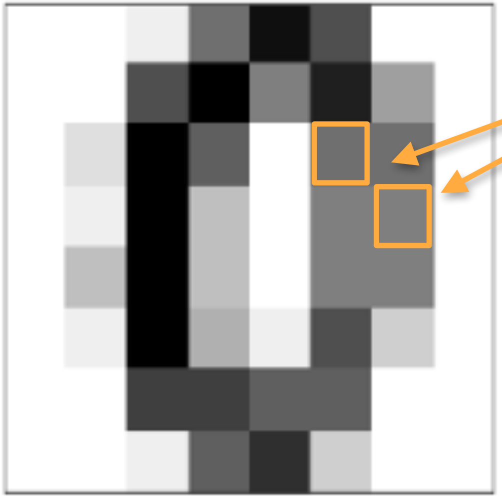


The algorithm converges

Dimensionality Reduction

How does PCA work?

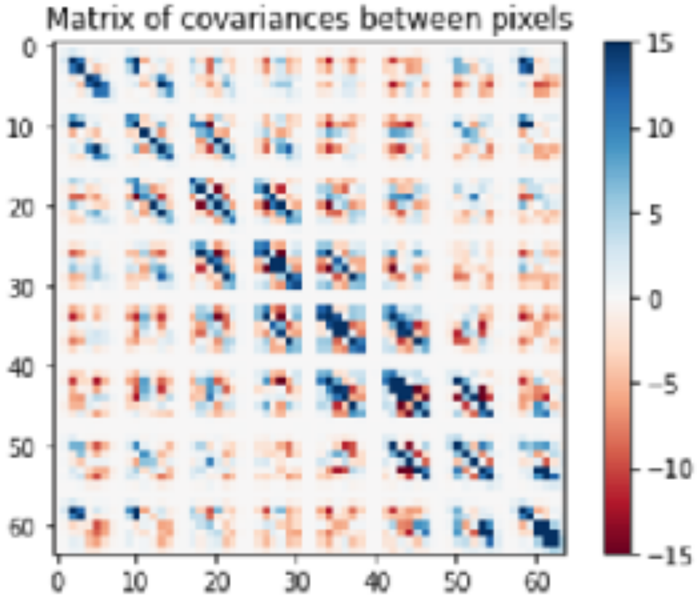
In all "natural" datasets, feature variables are normally correlated to each other.



Across the dataset, these two pixels are likely to be of similar colour.

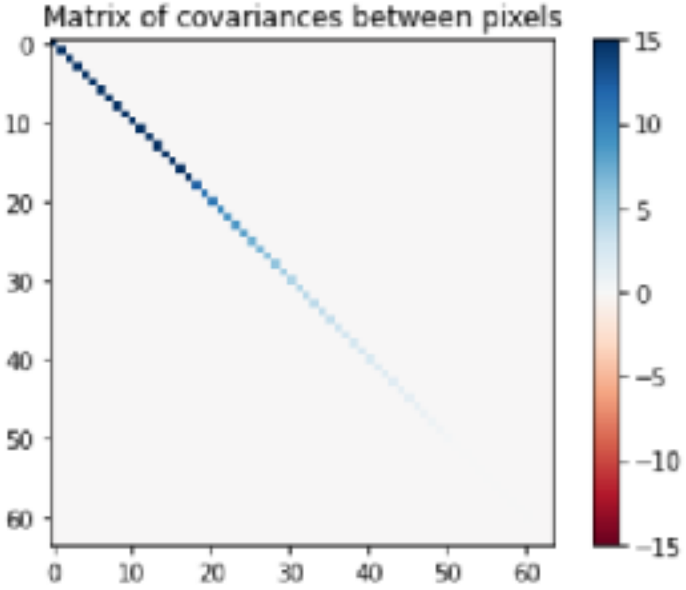
How does PCA work?

The matrix of covariances is symmetric and positive-definite.



We can therefore **diagonalise** it...

How does PCA work?

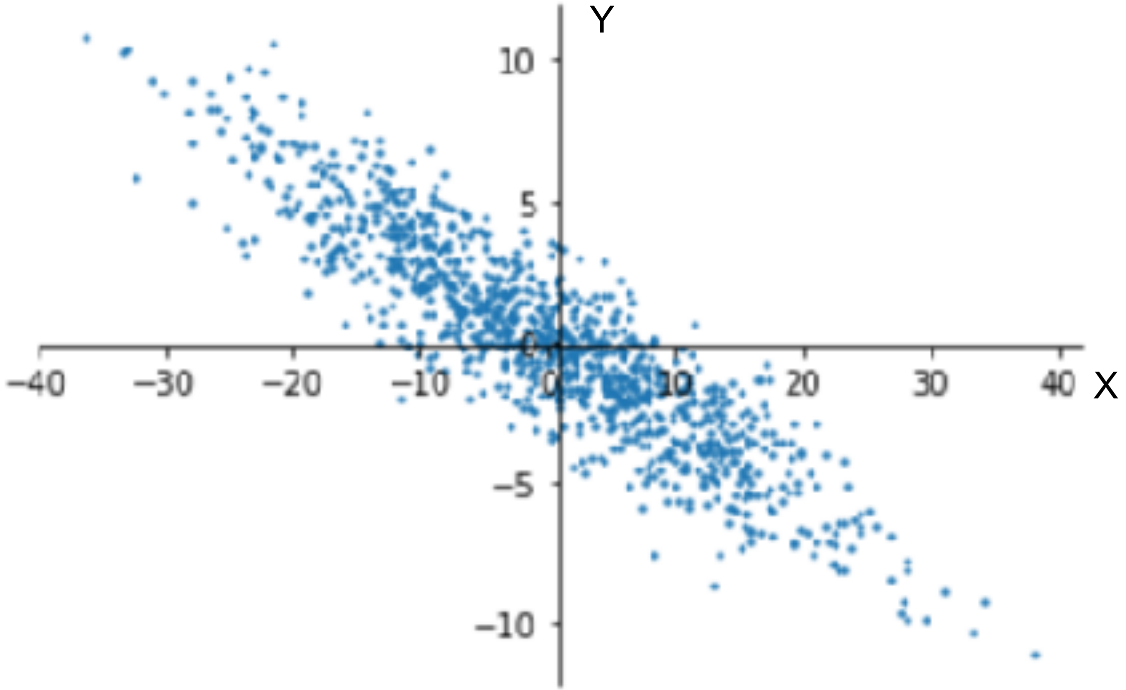


And move to a space of **statistically independent** feature variables.

The dimensions corresponding to **larger eigenvalues** have larger variance and thus describe the variability within the dataset better.

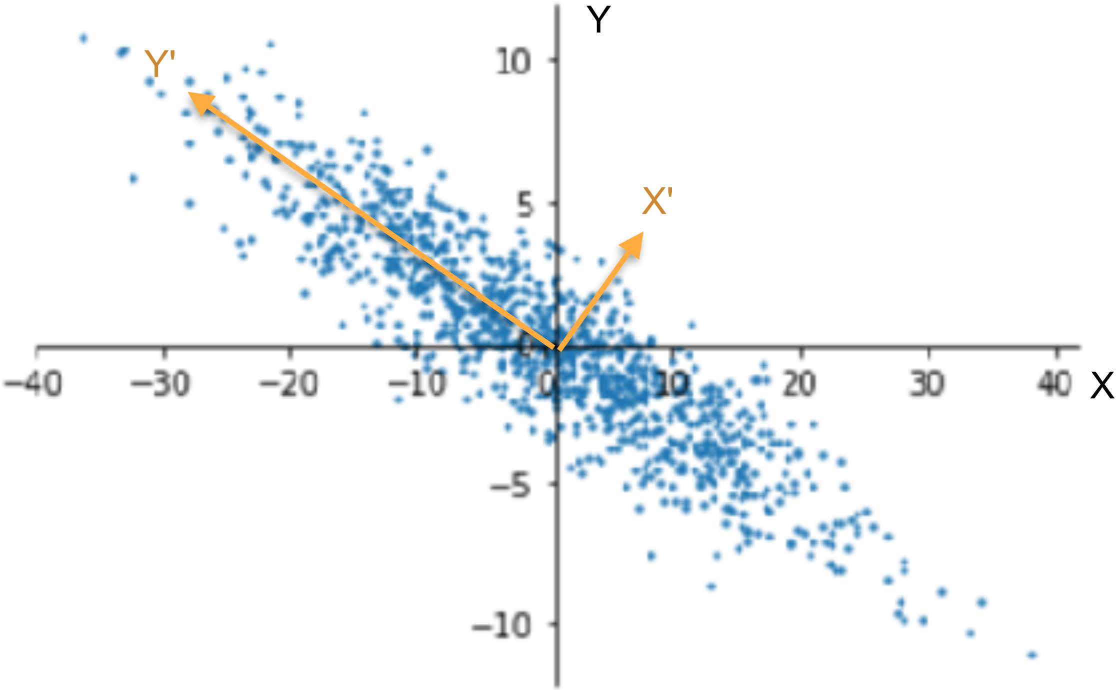
Wait... what?

Suppose we have data described by **2** variables X and Y:



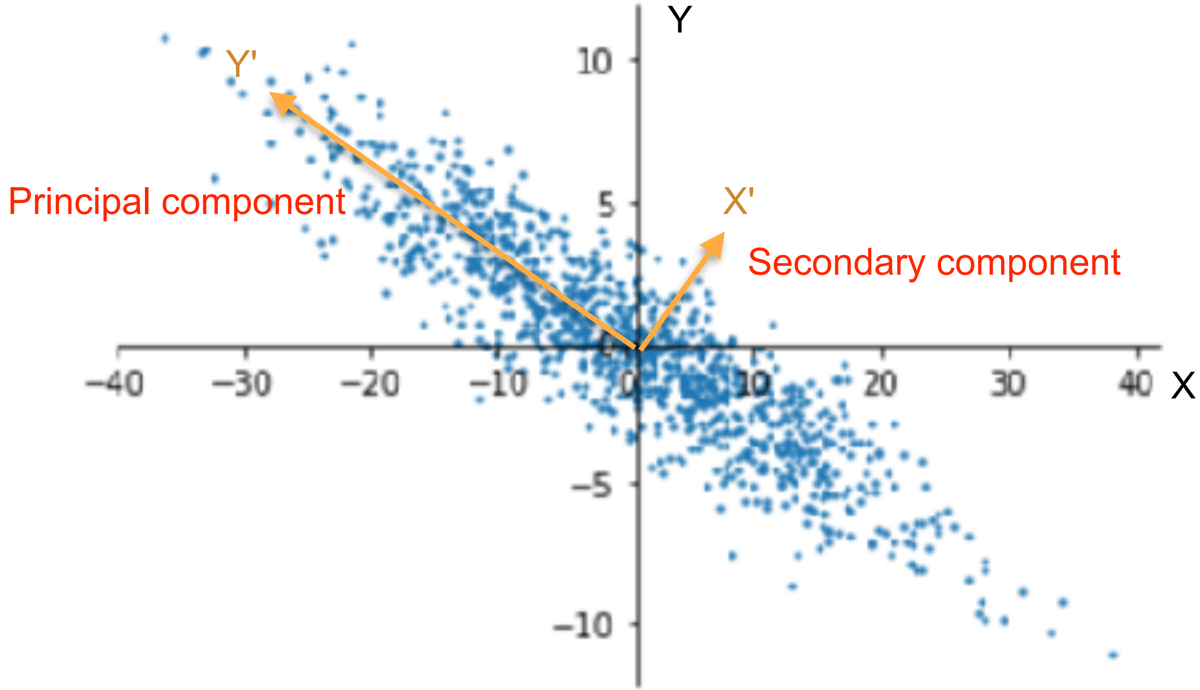
Wait... what?

PCA finds two new variables that are **uncorrelated**:



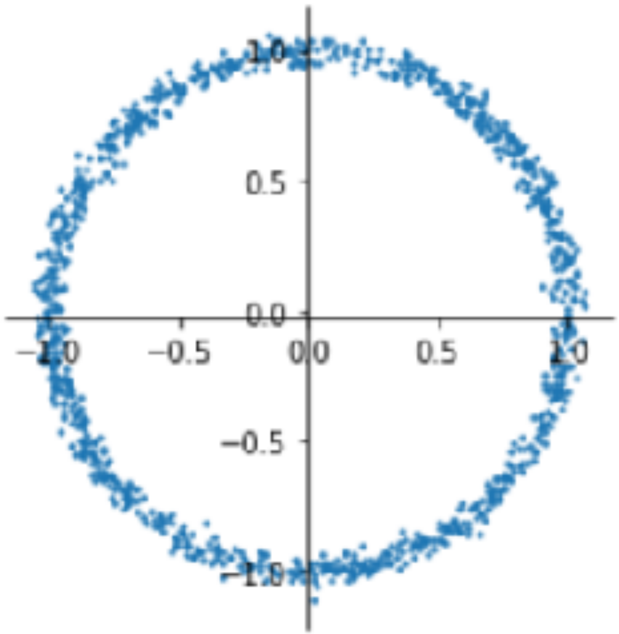
Wait... what?

... then selects the ones with **highest variance**, which capture the data variability:



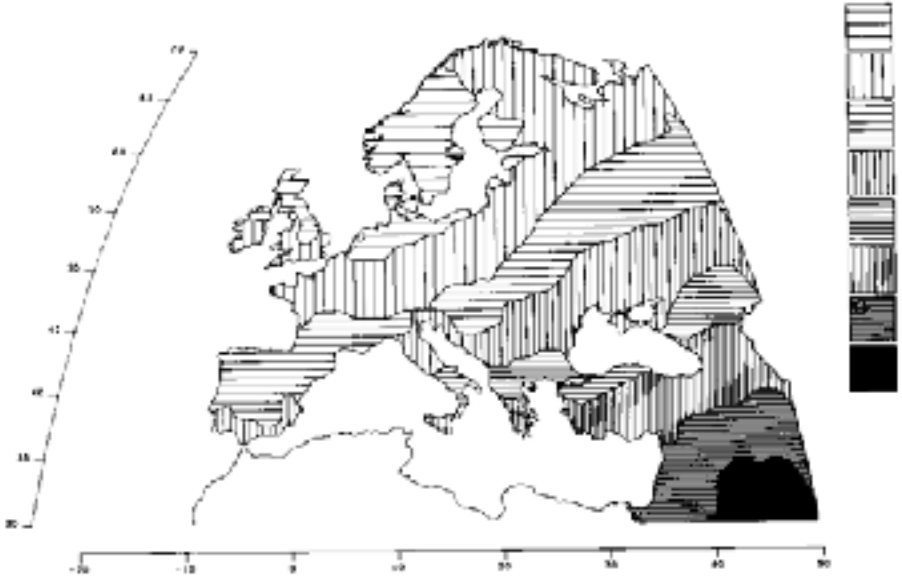
Failure case

- Data is not linearly correlated
- θ is a "principal" component, r a "secondary" component
- PCA will never find them.



Cool uses of dimensionality reduction

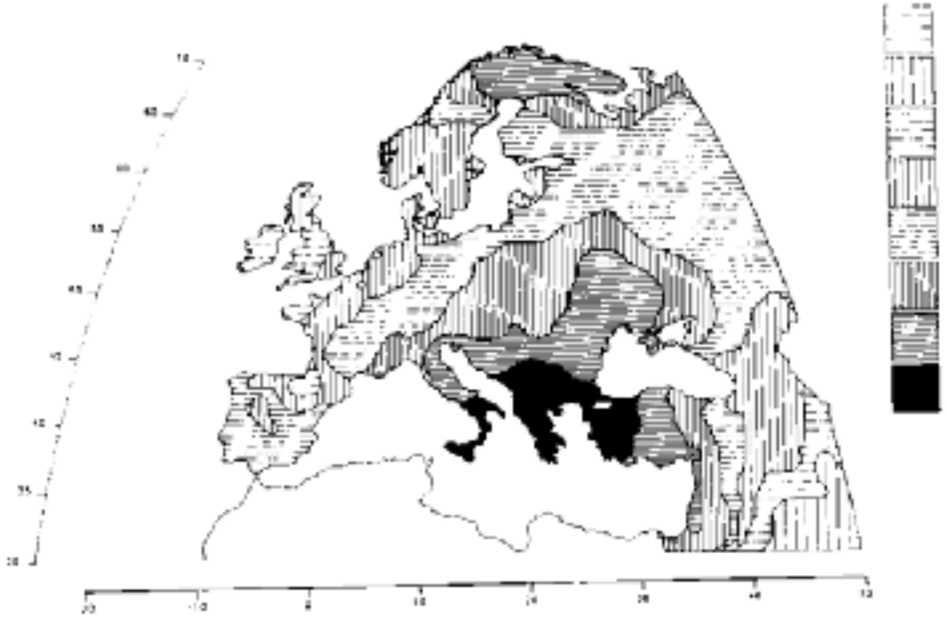
- DNA dimensionality is huge
- First PC of genetic variability in Europe: spread of agriculture



Cavalli Sforza, 1997

Cool uses of dimensionality reduction

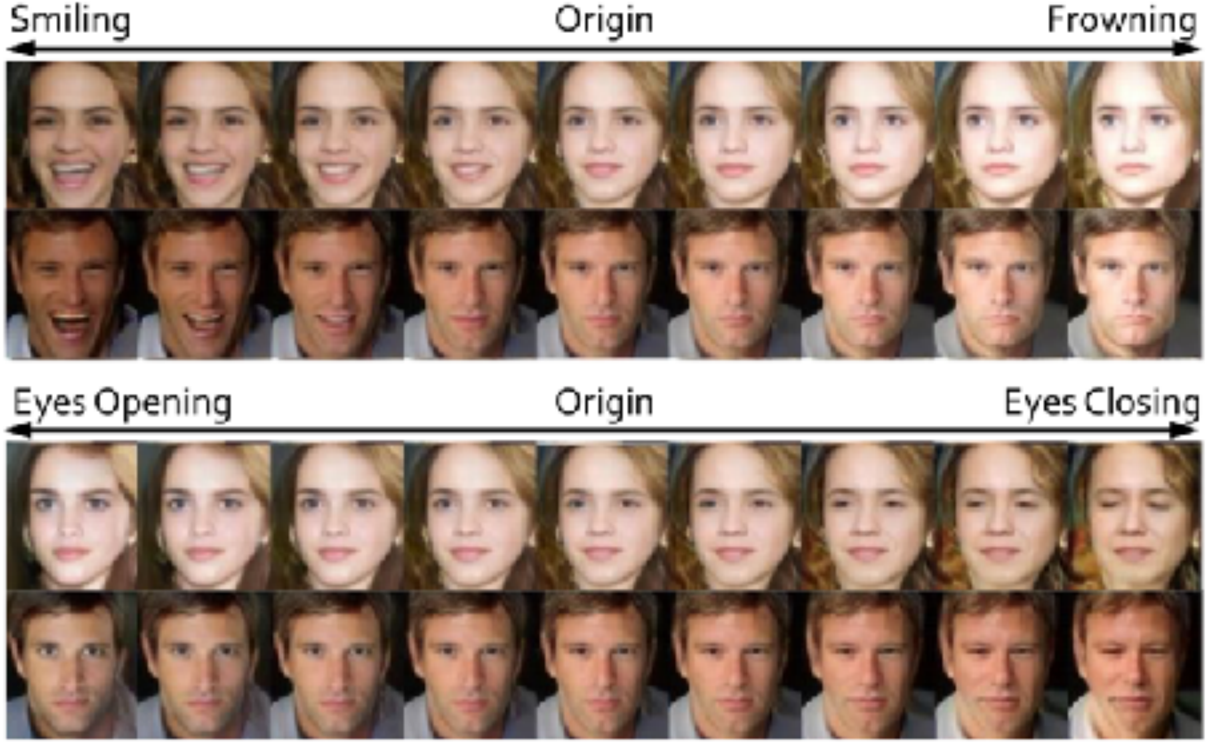
- DNA dimensionality is huge
- Third PC of genetic variability in Europe: Greek colonisation



Cavalli Sforza, 1997

Cool uses of dimensionality reduction

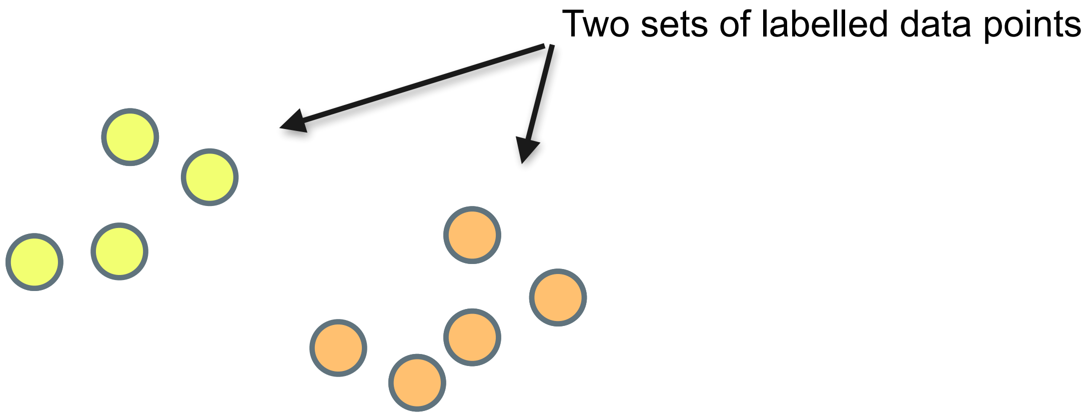
Finding semantically meaningful dimensions and interpolating



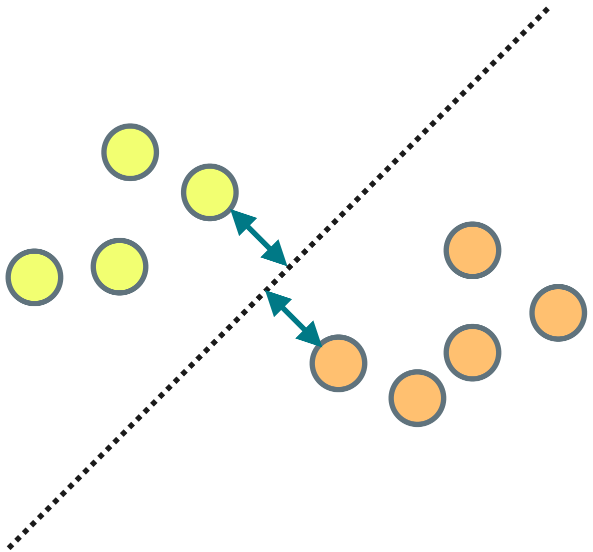
Liu et al. 2018, arXiv:1804.03487

Support Vector Machines

Intuitive understanding of SVM



Intuitive understanding of SVM

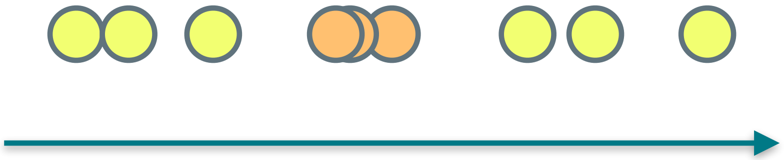


Linear SVM

Find the hyperplane that separates the two sets by the largest **margin** between the "support vectors".

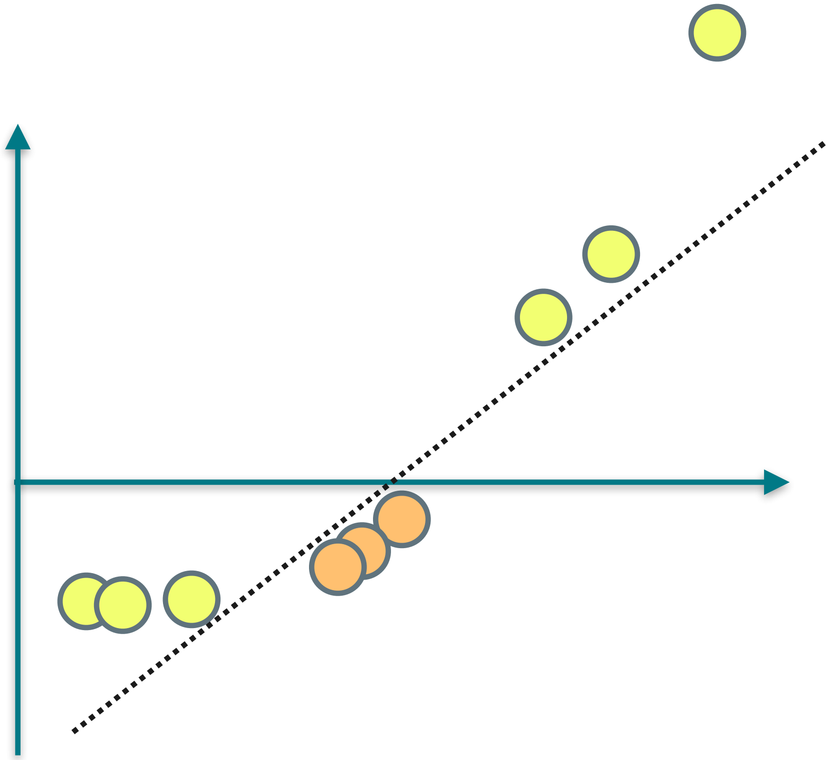
This is the line that separates the classes.

Intuitive understanding of SVM



If the data is **not linearly separable**...

Intuitive understanding of SVM



If the data is **not linearly separable**...

we project to more dimensions which are nonlinear functions of the original ones, so that we can now separate linearly.

The actual mathematical implementation is more efficient!