session 3:

Unsupervised learning

M. Kundegorski

3rd March 2020

Centre for Ecological Sciences
Indian Institute of Science

Bengaluru, India

Unsupervised learning

What can you do when you have no answers?

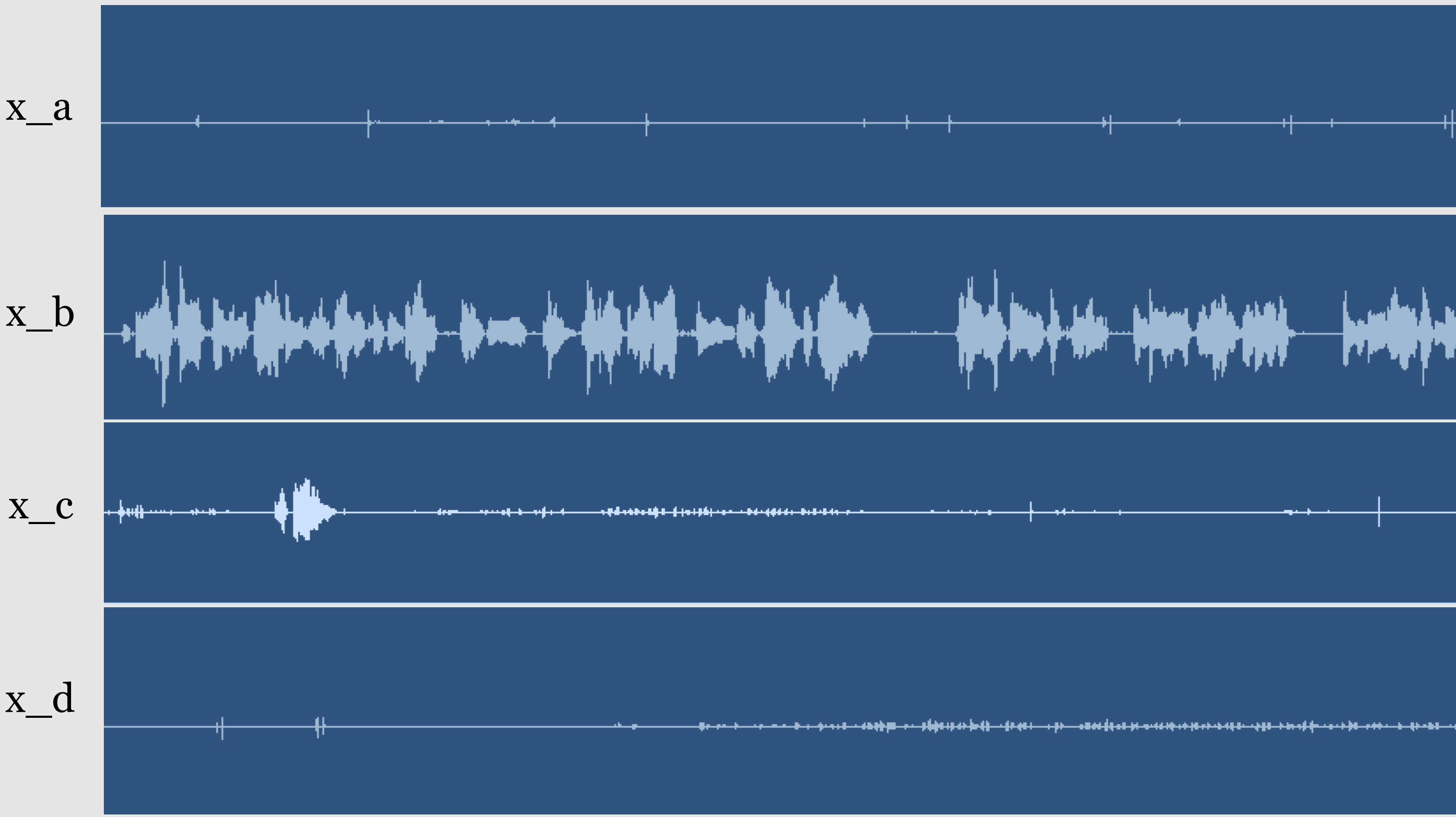
Uses of unsupervised learning

- pre-processing (sparse features clustering)
- simplifying data for supervised algorithms
- clustering for data exploration:
  - sparse data
  - big data
  - data for which we lack intuition to choose a statistical model
- label-free segmentation

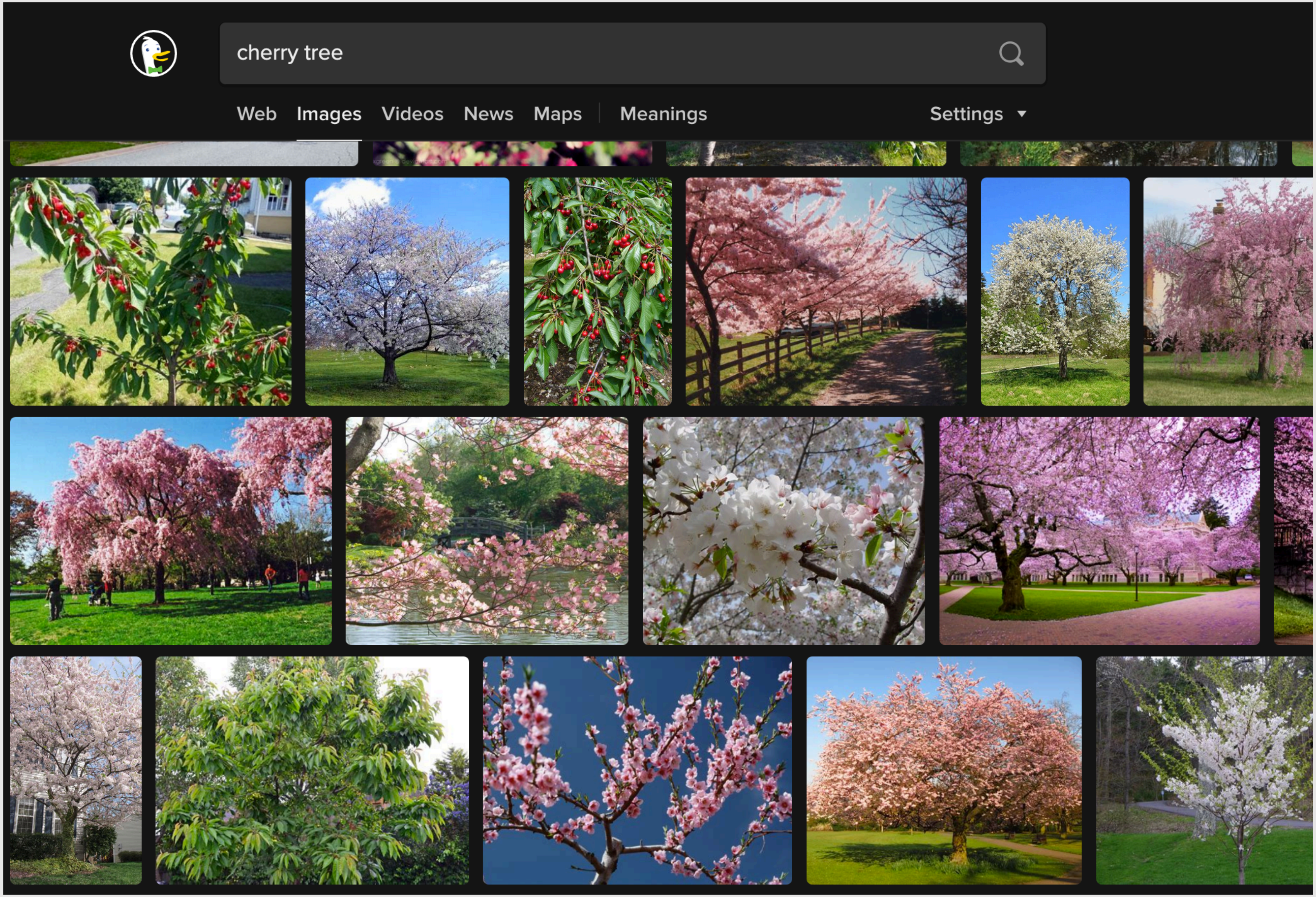
Principles

- exploration of variable space in looking for emerging patterns of similarity
- there is no provided ground truth, and in fact often it is not available at all.
- often used with huge amounts of data
- provided: knowledge of the feature space - for instance a definition of distance in feature space - that allows to draw some outcomes from provided data.

Variable selection



Unstructured data



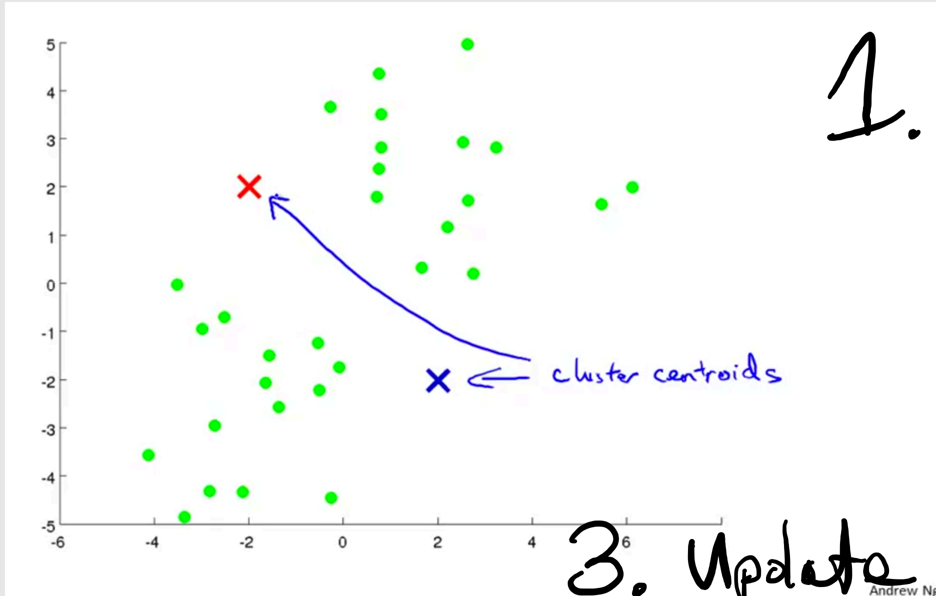
Clustering: finding data similarity

source: https://www.coursera.org/learn/machine-learning

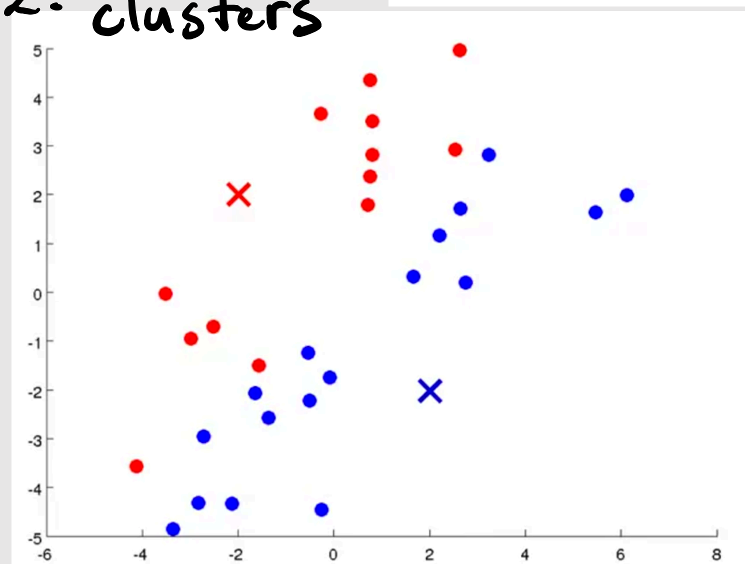
k-means

K = 2

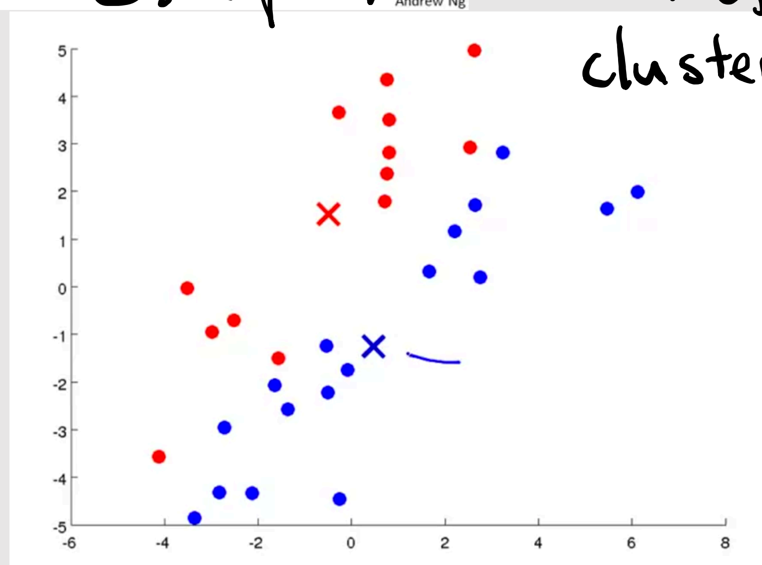
1. random initialisation



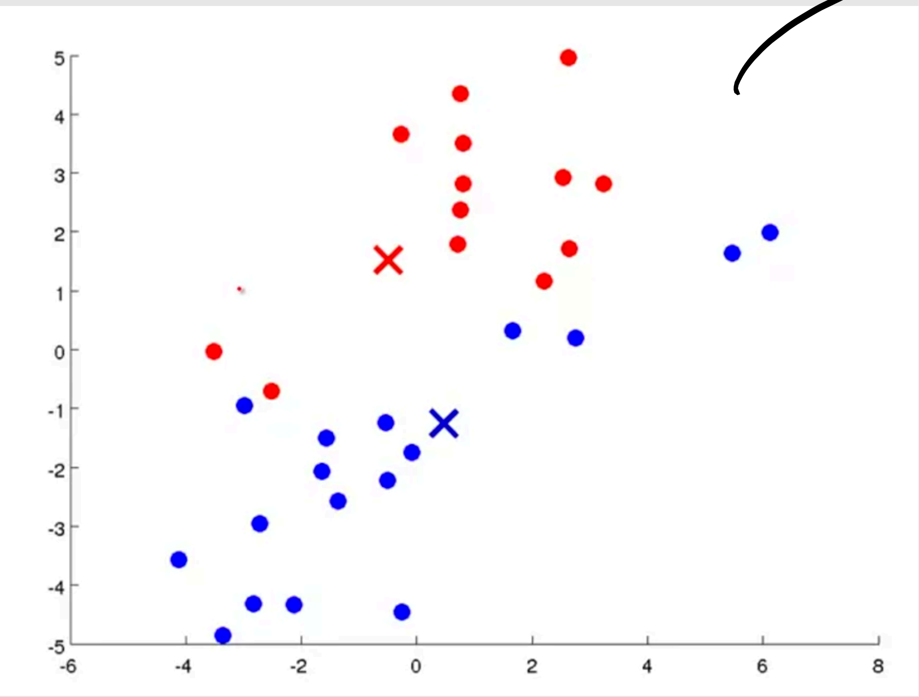
2. find clusters



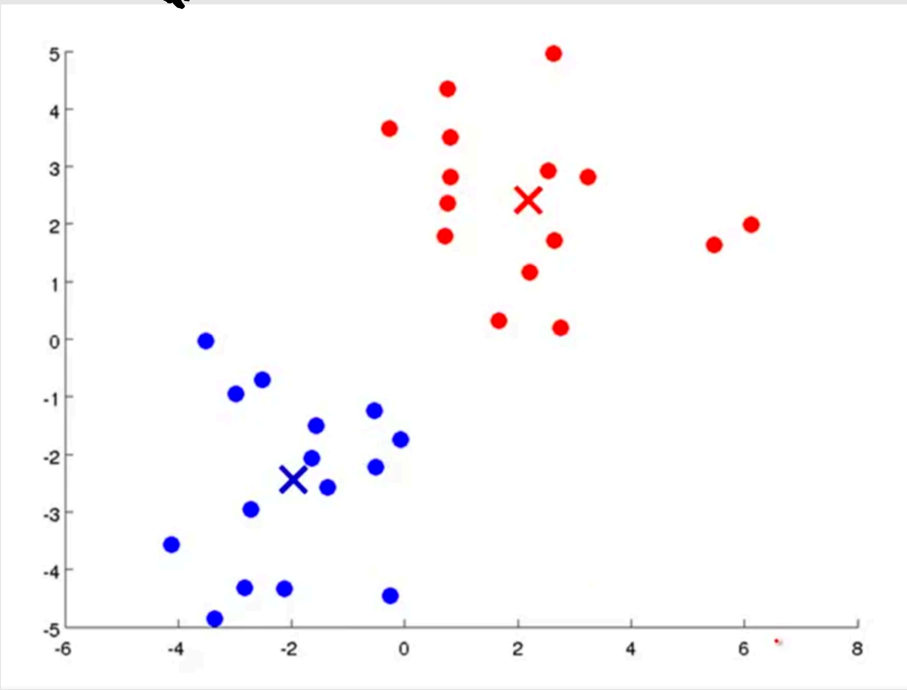
3. Update mean of clusters



k means



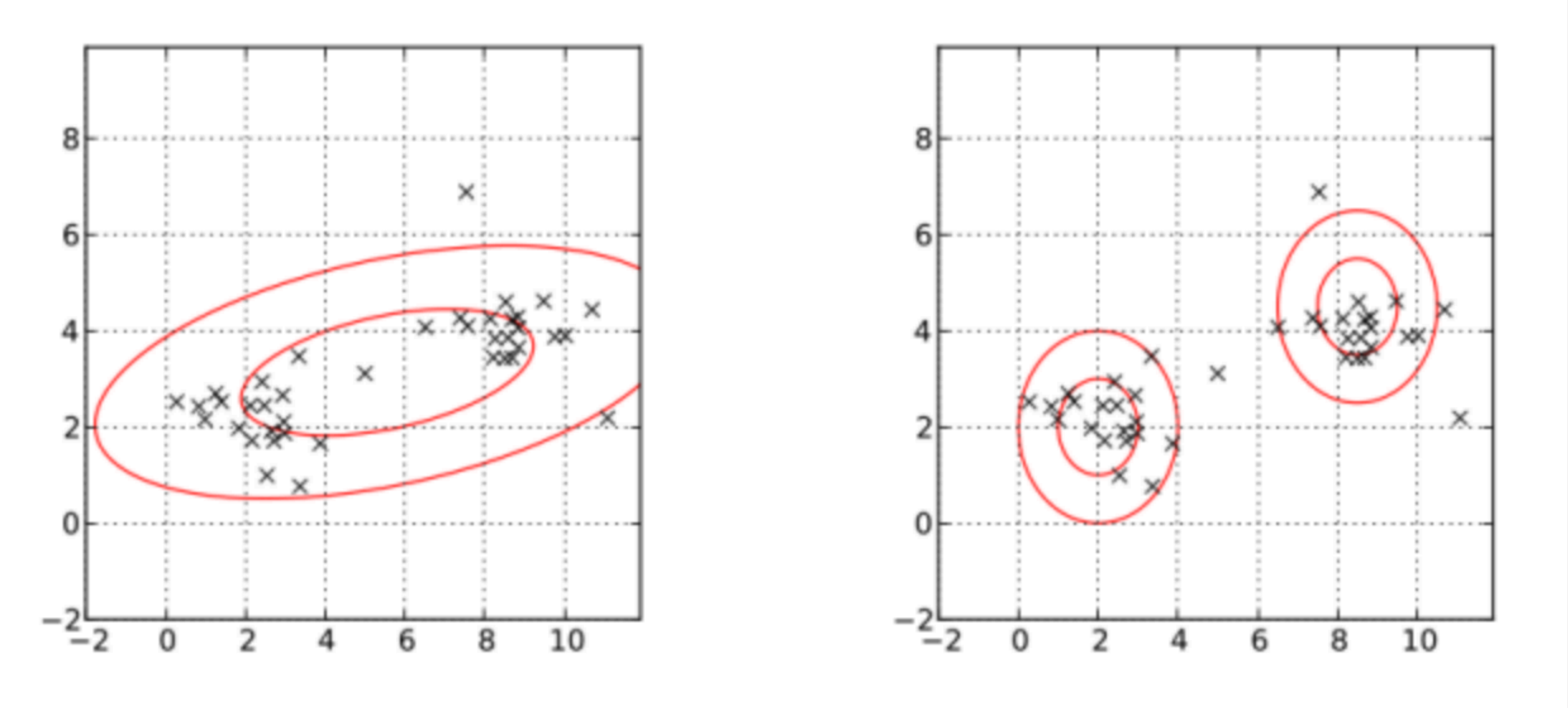
convergence



k-medoids

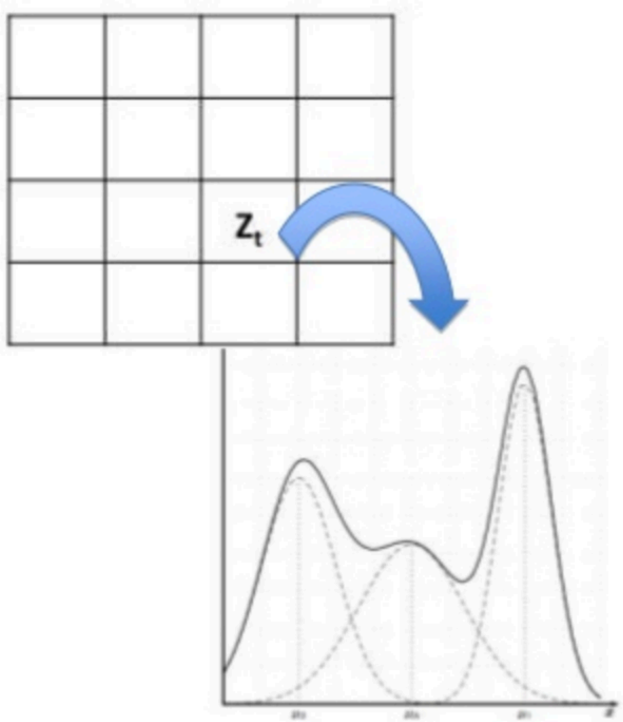
- Just like k-means but choosing median data point as centre

Gaussian Mixture Model



Background subtraction

Gaussian Mixture Model (GMM)

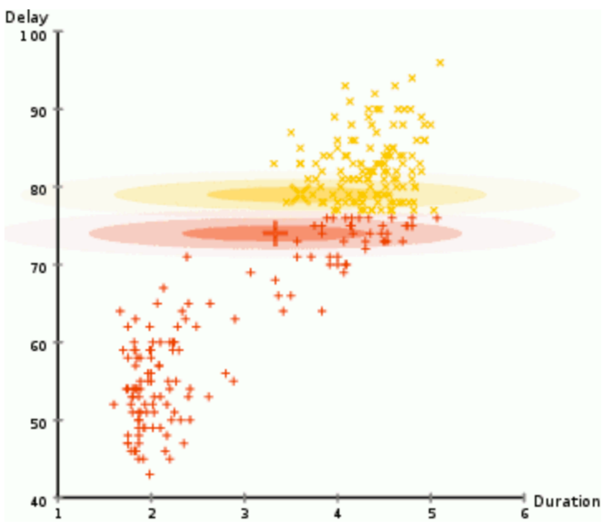


- A GMM is a mixture pdf which is a linear combination of K Gaussian pdfs.
- $\Sigma w_i = 1$
- each pixel is given one GMM

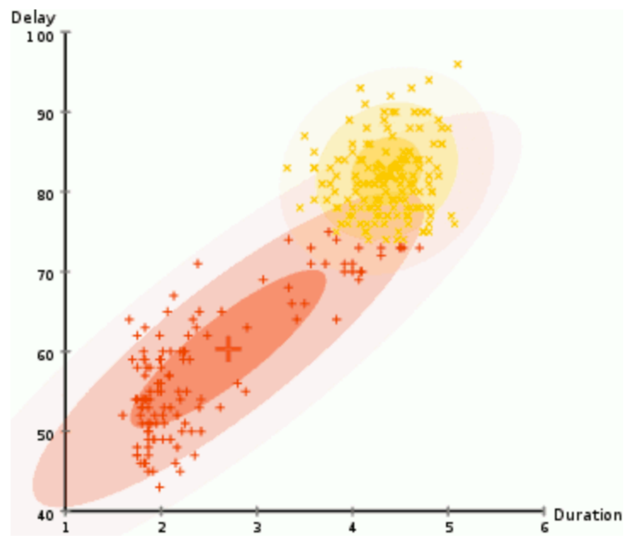
source: Zivkovic , 2004. Improved adaptive gaussian mixture model for background subtraction. Figure by Raviraj singh shekhawat

Example:

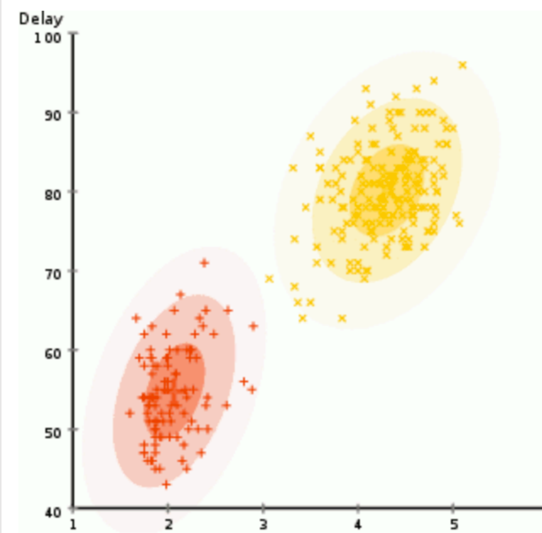
Algorithm for GMM: Expectation-Maximisation



The EM algorithm updating the parameters of a two-component bivariate Gaussian mixture model.[2]



The EM algorithm updating the parameters of a two-component bivariate Gaussian mixture model.[2]

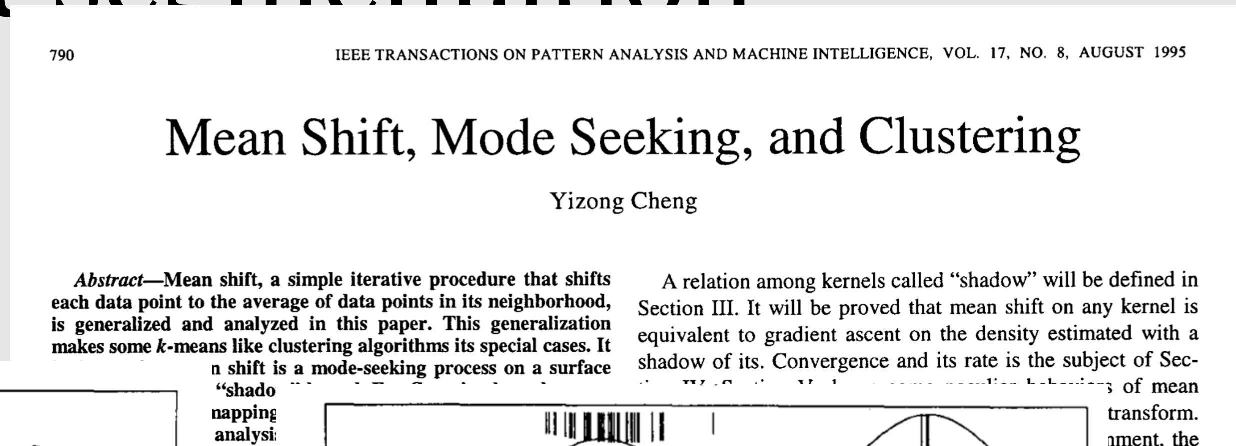


The EM algorithm updating the parameters of a two-com bivariate Gaussian mixture model.[2]

https://commons.wikimedia.org/wiki/File:EM_Clustering_of_Old_Faithful_data.gif

Mean-shift segmentation

- KDE + gradient ascent



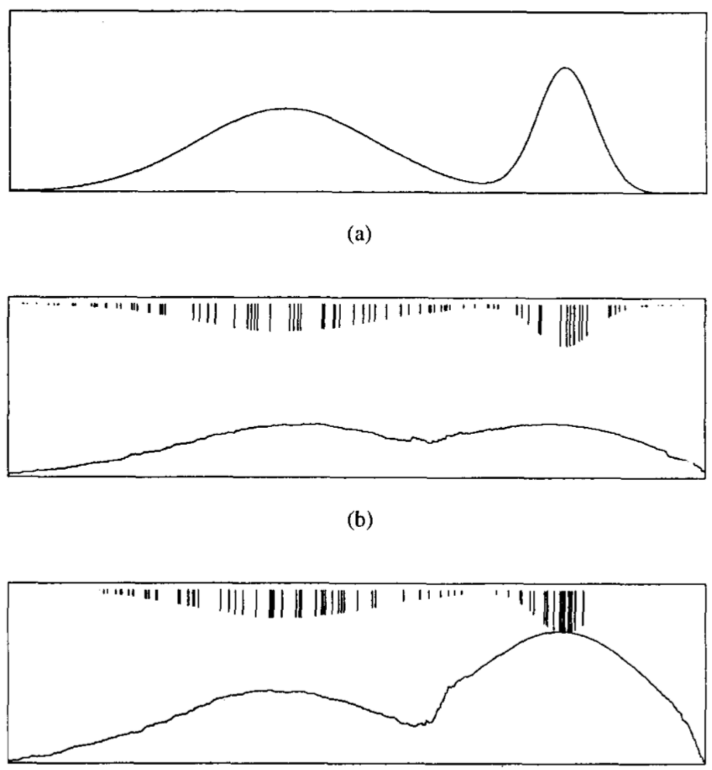
790 IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. 17, NO. 8, AUGUST 1995

Mean Shift, Mode Seeking, and Clustering

Yizong Cheng

Abstract—**Mean shift, a simple iterative procedure that shifts each data point to the average of data points in its neighborhood, is generalized and analyzed in this paper. This generalization makes some *k*-means like clustering algorithms its special cases. It ... n shift is a mode-seeking process on a surface ... "shado... napping ... analysi...**

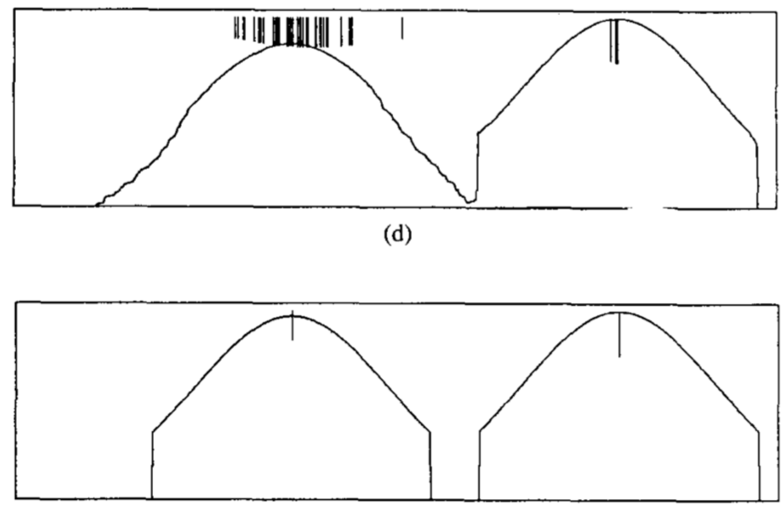
A relation among kernels called "shadow" will be defined in Section III. It will be proved that mean shift on any kernel is equivalent to gradient ascent on the density estimated with a shadow of its. Convergence and its rate is the subject of Sec- ... of mean ... transform. ... ment, the



(a)

(b)

(c)



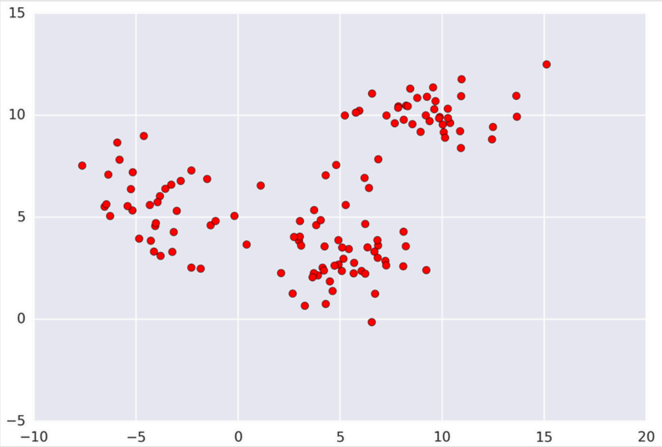
(d)

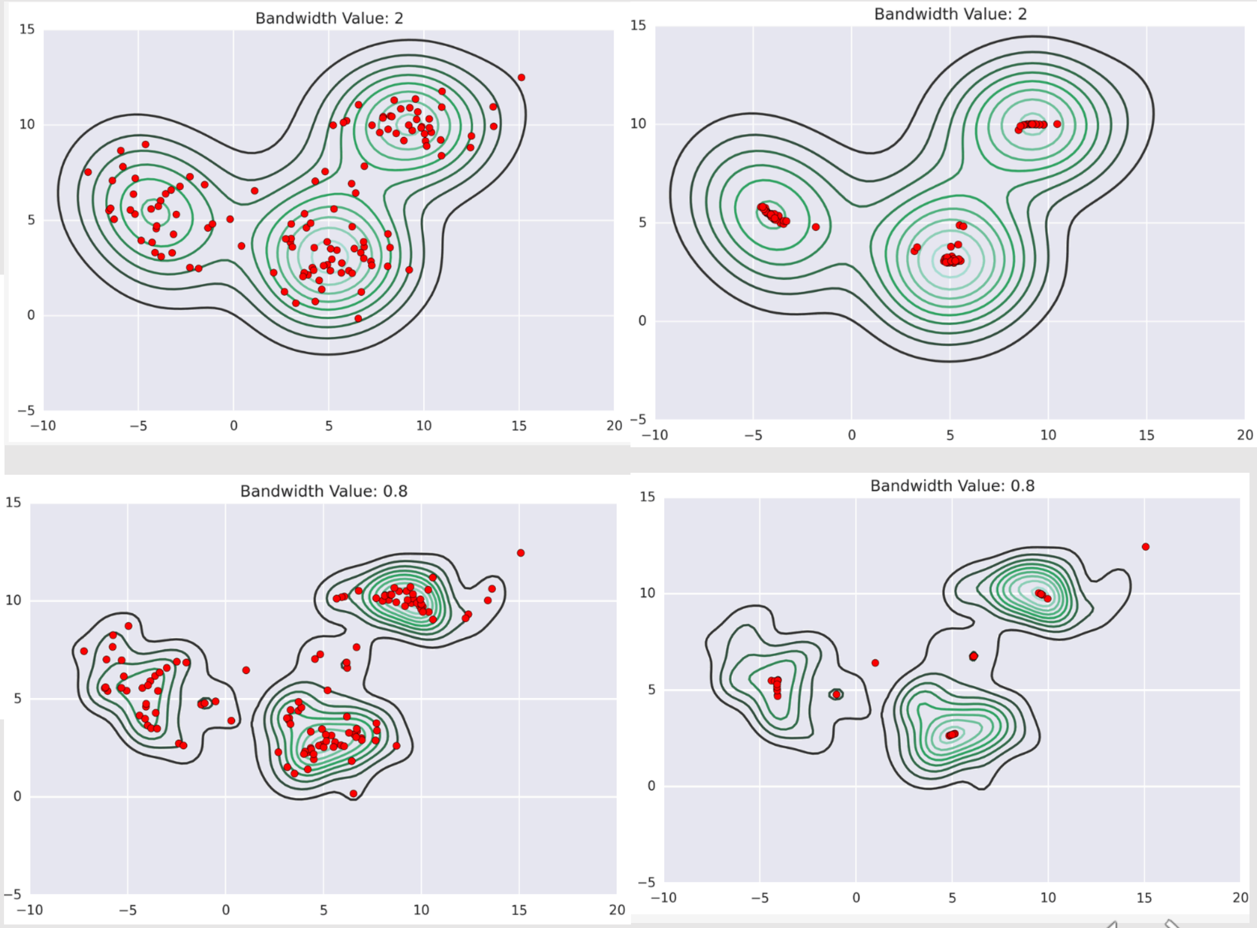
(e)

Fig. 8. Multistart global optimization using blurring. (a) shows the function f, whose global maximum is to be found. The next four figures show the mean shift of S, at the (b) initial, (c) first, (d) third, and (e) fifth iterations of a blurring process when f is used as the weight function. In each of these four figures, the vertical bars show the positions and f values of the S points, and the curve shows the q function, whose local maxima locations approximate those of f.

source: https://spin.atomicobject.com/2015/05/26/mean-shift-clustering/

Mean-shift segmentation





EM vs mean-shift?

Gaussian mean shift is an EM algorithm

Miguel Á. Carreira-Perpiñán
Dept. of Computer Science & Electrical Engineering
OGI School of Science & Engineering, Oregon Health & Science University
20000 NW Walker Road, Beaverton, OR 97006, USA
Email: `miguel@csee.ogi.edu`

August 23, 2006

Abstract

The mean-shift algorithm, based on ideas proposed by Fukunaga and Hostetler (1975), is a hill-climbing algorithm on the density defined by a finite mixture or a kernel density estimate. Mean-shift can be used as a nonparametric clustering method and has attracted recent attention in computer vision applications such as image segmentation or tracking. We show that, when the kernel is Gaussian, mean-shift is an expectation-maximisation (EM) algorithm, and when the kernel is non-gaussian, mean-shift is a generalised EM algorithm. This implies that mean-shift converges from almost any starting point and that, in general, its convergence is of linear order. For Gaussian mean-shift we show: (1) the rate of linear convergence approaches 0 (superlinear convergence) for very narrow or very wide kernels, but is often close to 1 (thus extremely slow) for intermediate widths, and exactly 1 (sublinear convergence) for widths at which modes merge; (2) the iterates approach the mode along the local principal component of the data points from the inside of the convex hull of the data points; (3) the convergence domains are nonconvex and can be disconnected and show fractal behaviour. We suggest ways of accelerating mean-shift based on the EM interpretation.

Keywords: mean-shift algorithm, Gaussian mixtures, kernel density estimators, EM algorithm, clustering

DBSCAN – industry standard

Published in Proceedings of 2nd International Conference on Knowledge Discovery and Data Mining (KDD-96)

A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise

Martin Ester, Hans-Peter Kriegel, Jörg Sander, Xiaowei Xu

Institute for Computer Science, University of Munich
Oettingenstr. 67, D-80538 München, Germany
{ester | kriegel | sander | xwxu}@informatik.uni-muenchen.de

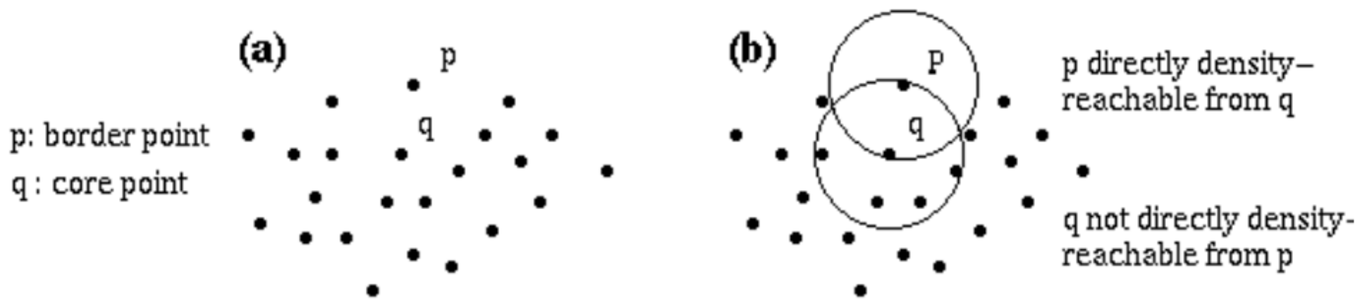


figure 2: core points and border points

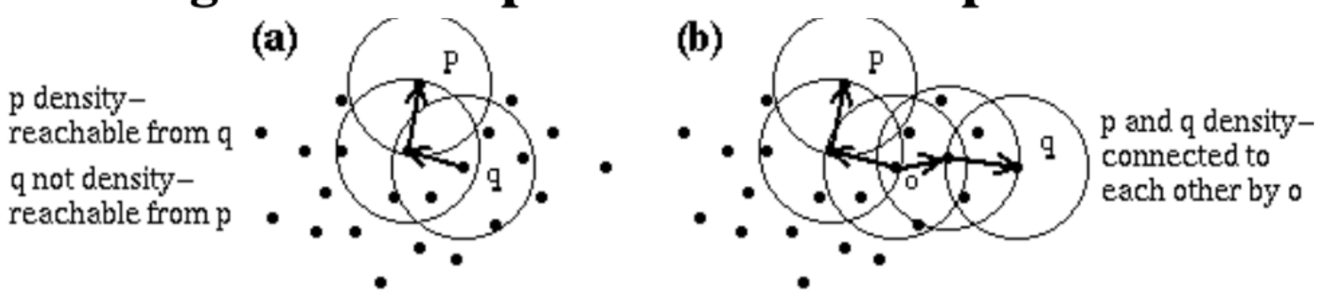


figure 3: density-reachability and density-connectivity

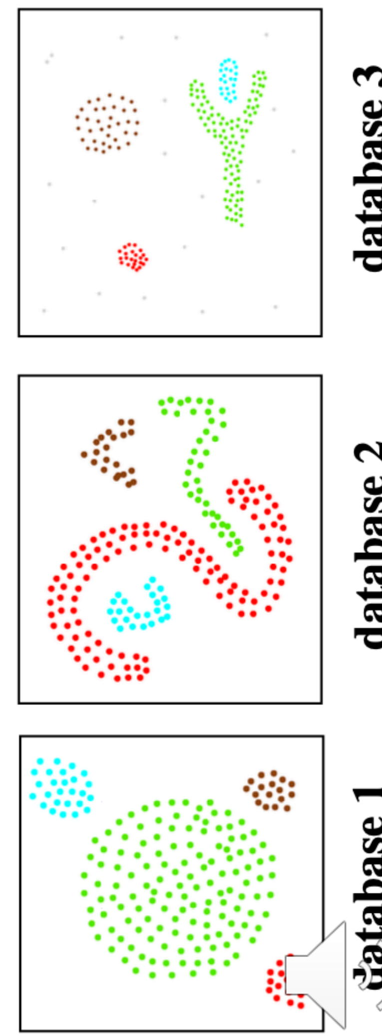
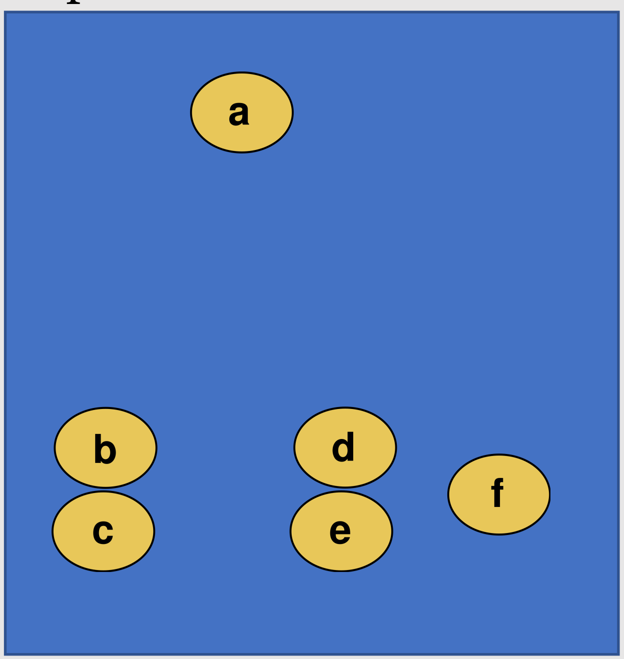
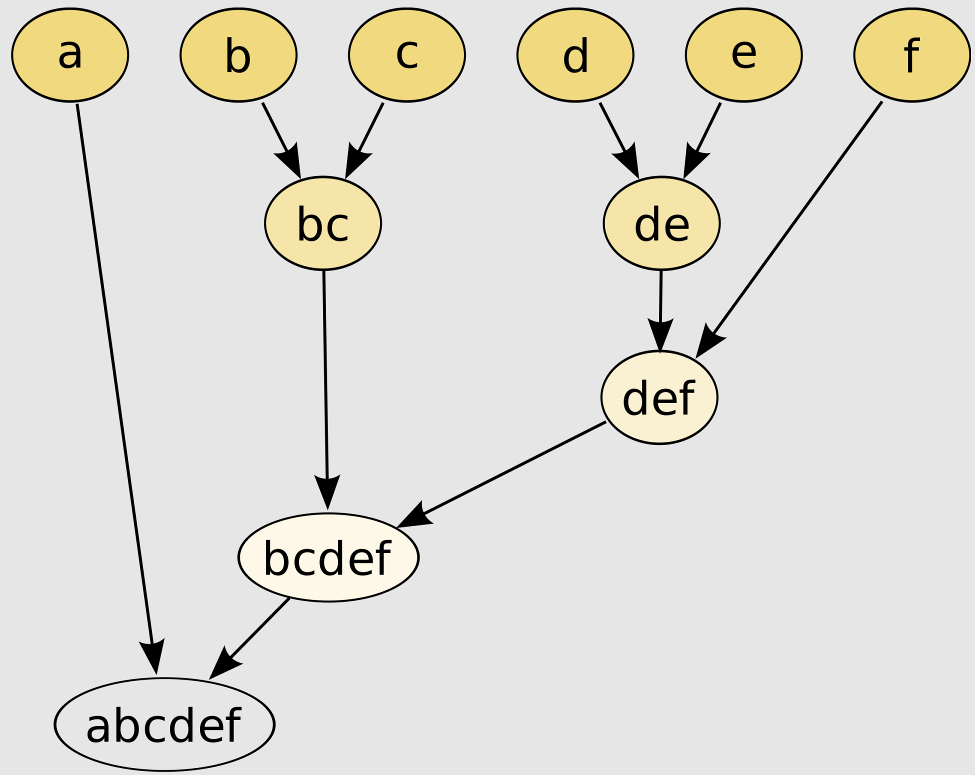


figure 6: Clusterings discovered by DBSCAN

Hierarchical clustering

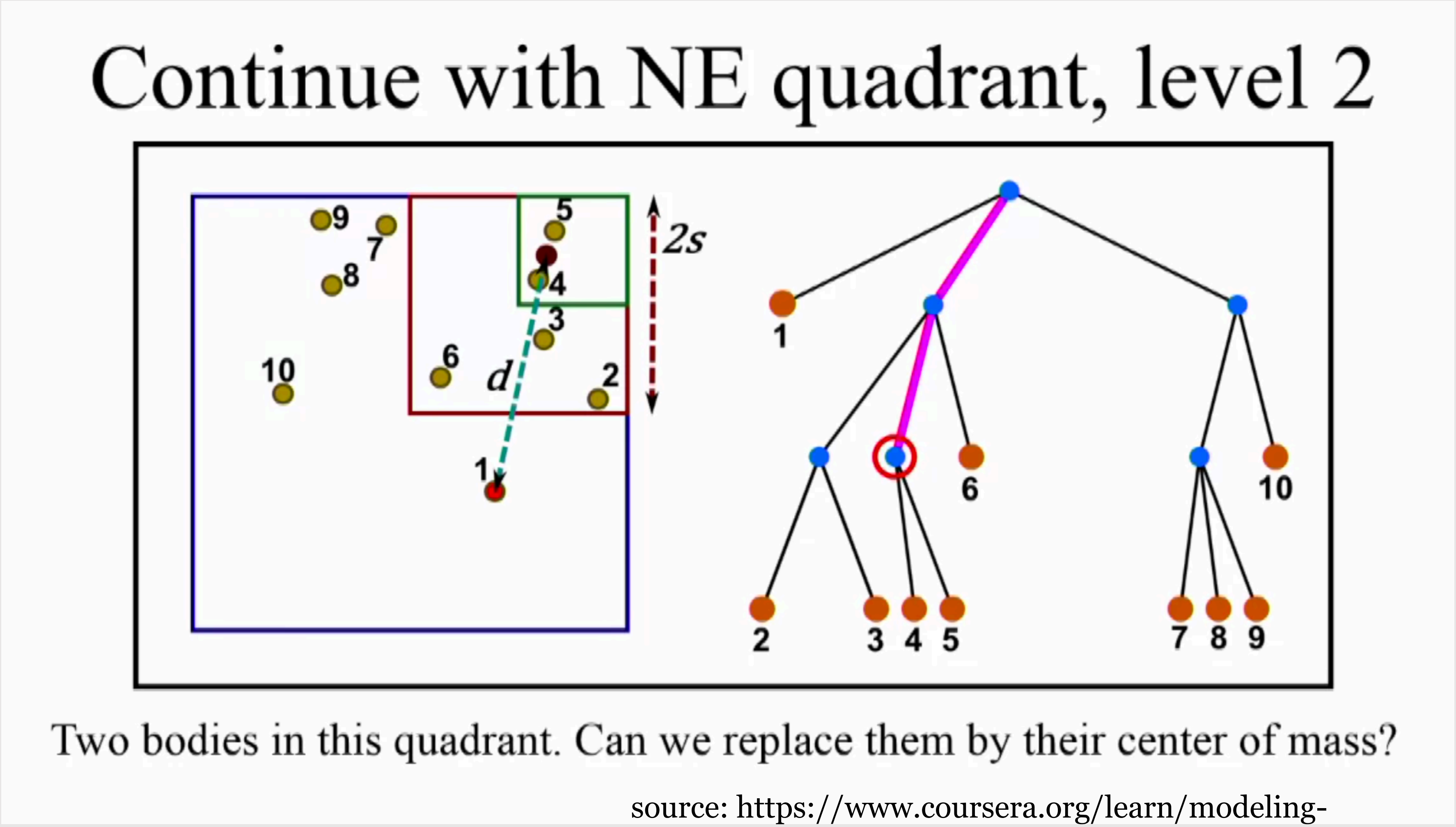
space Ω





https://en.wikipedia.org/wiki/Hierarchical_clustering

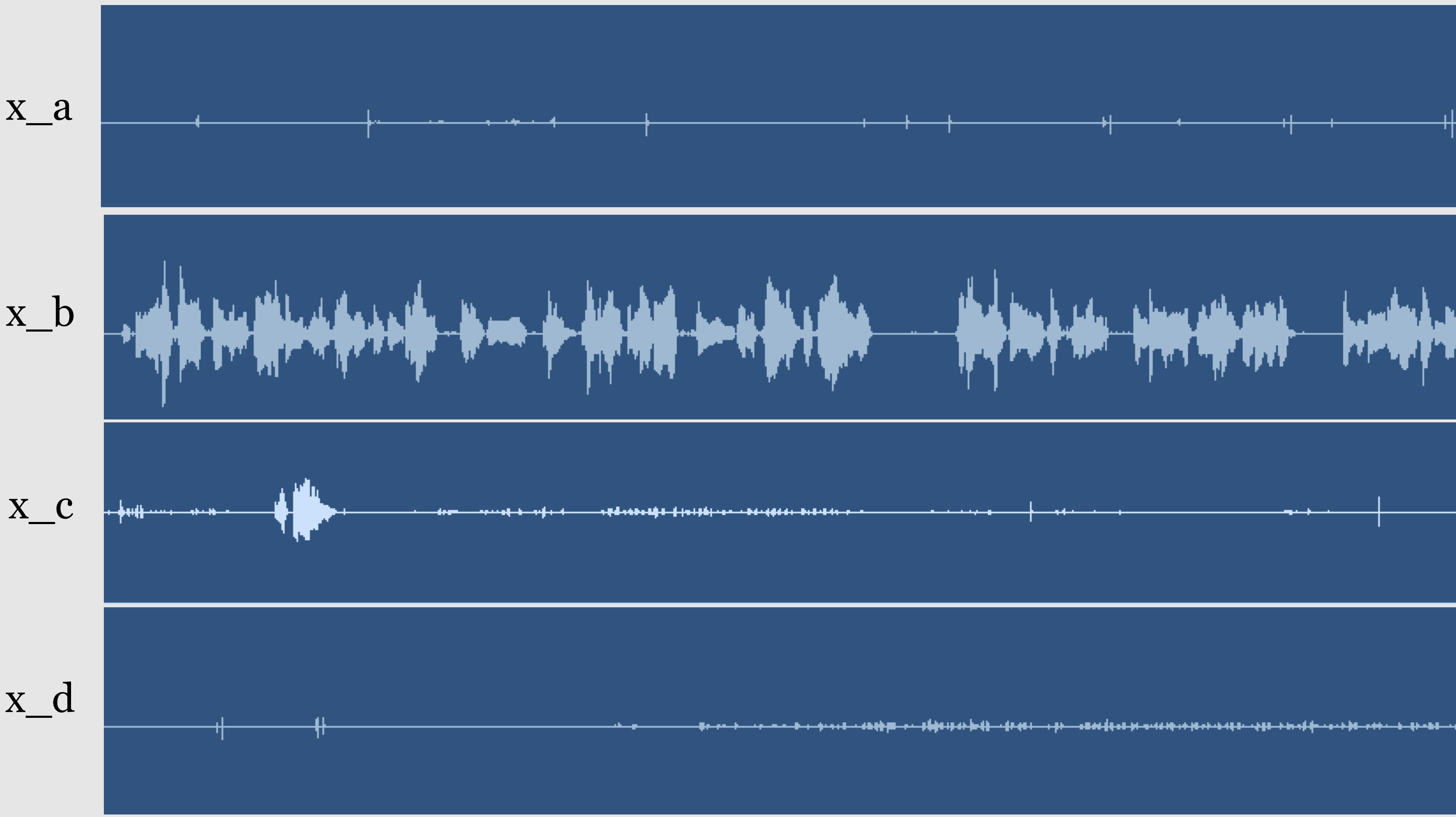
Barnes-Hut algorithm: using the quadtree



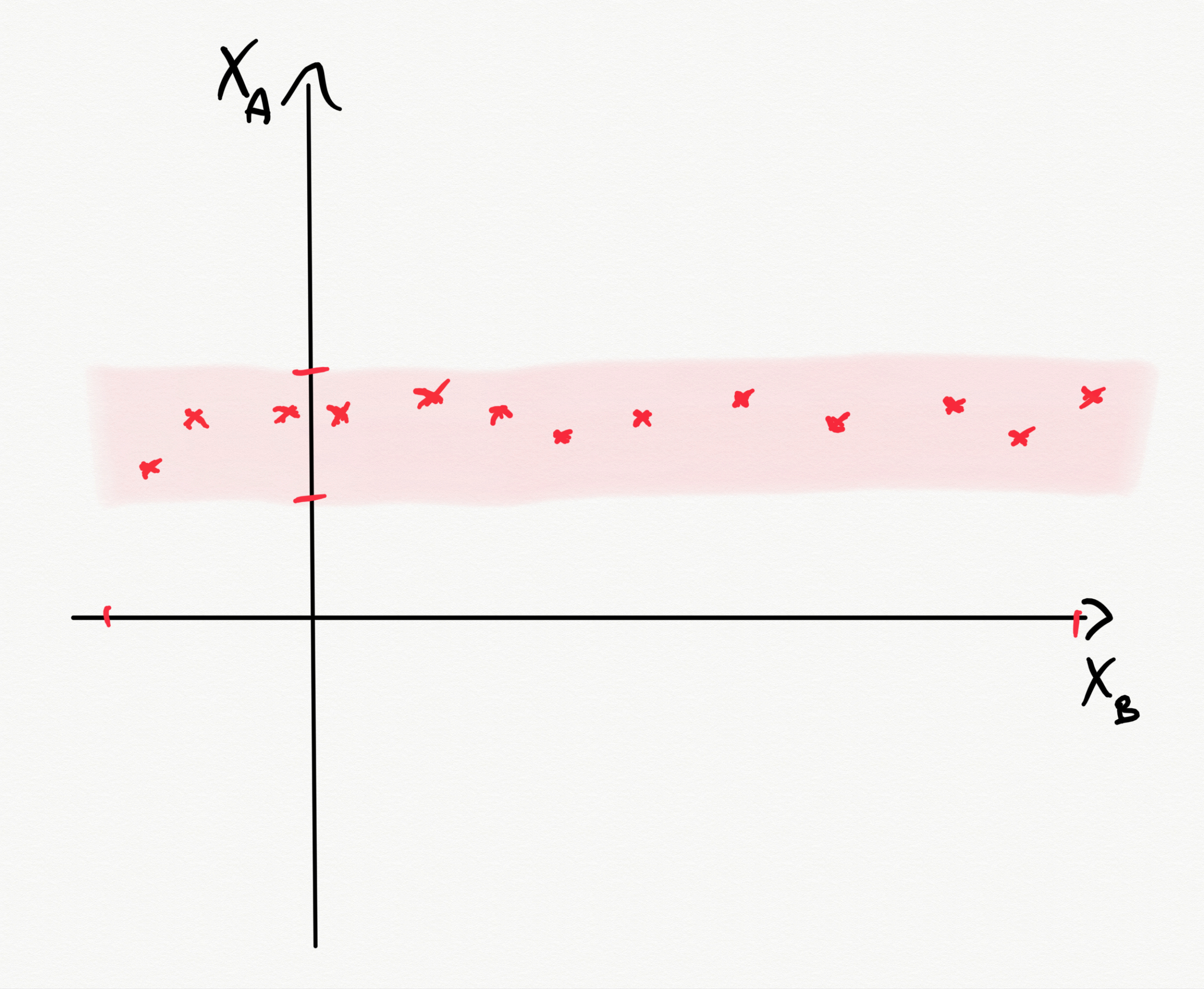
source: https://www.coursera.org/learn/modeling-simulation-natural-processes

Component Analysis: feature selection, dimensionality reduction, encoding…

Variable selection



Variable selection



Priniciple Component Analysis

[559]

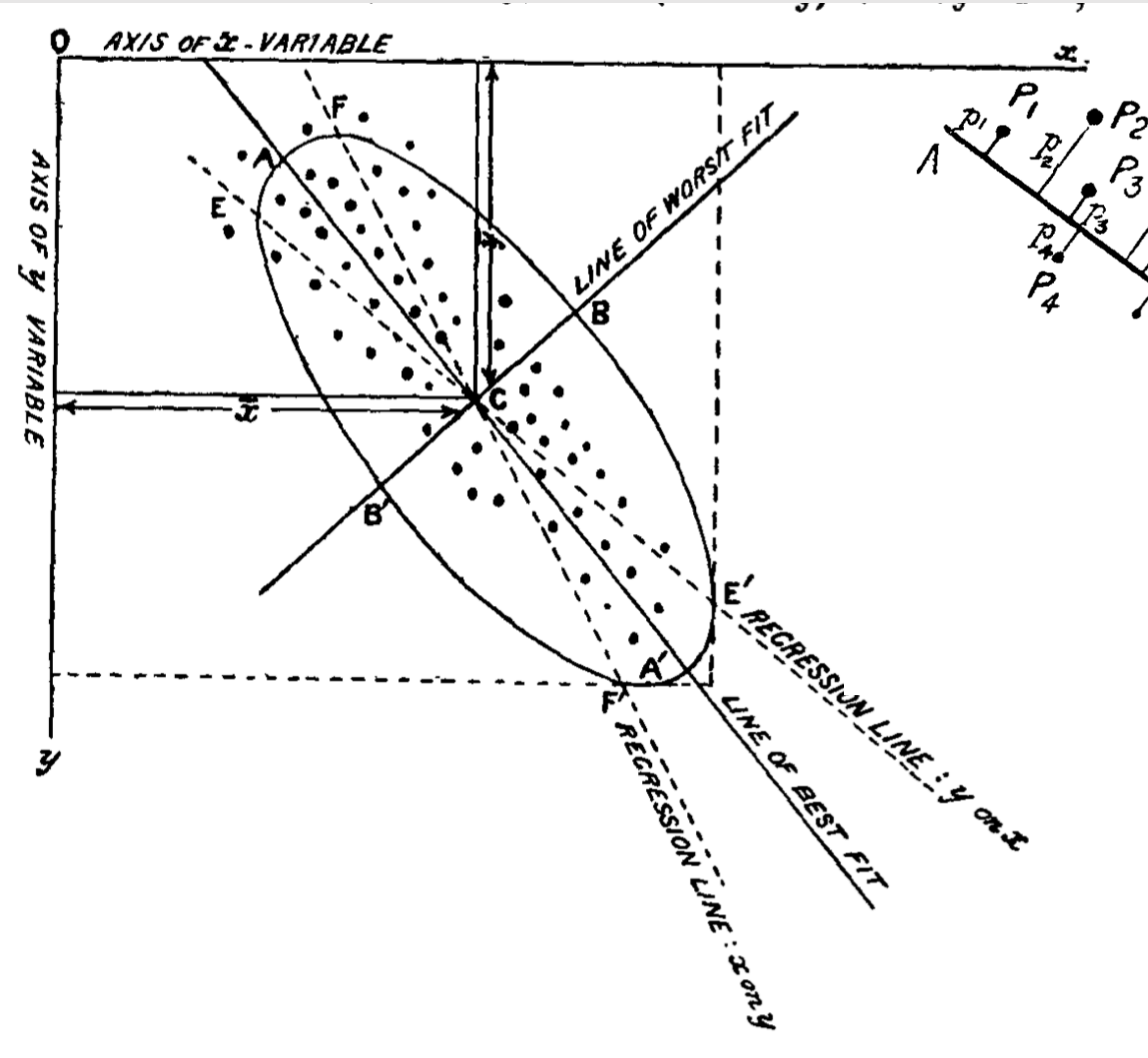
LIII. *On Lines and Planes of Closest Fit to Systems of Points in Space.* *By* KARL PEARSON, *F.R.S., University College, London* *.

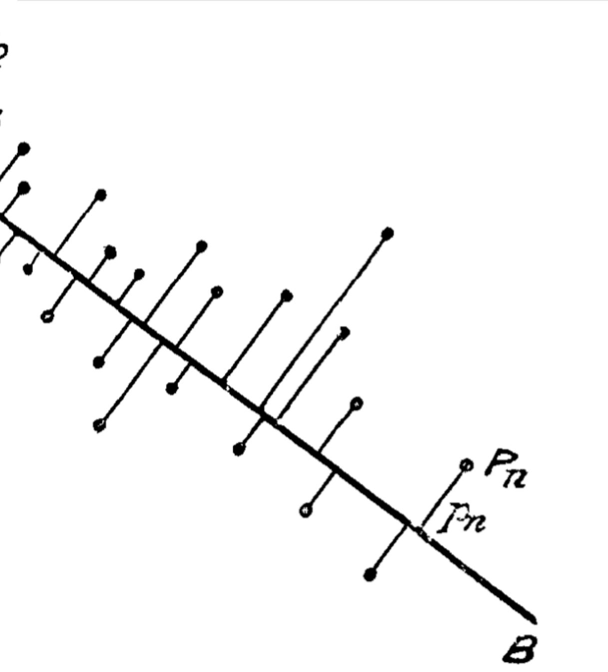
(1) IN many physical, statistical, and biological investigations it is desirable to represent a system of points in plane, three, or higher dimensioned space by the "best-fitting" straight line or plane. Analytically this consists in taking

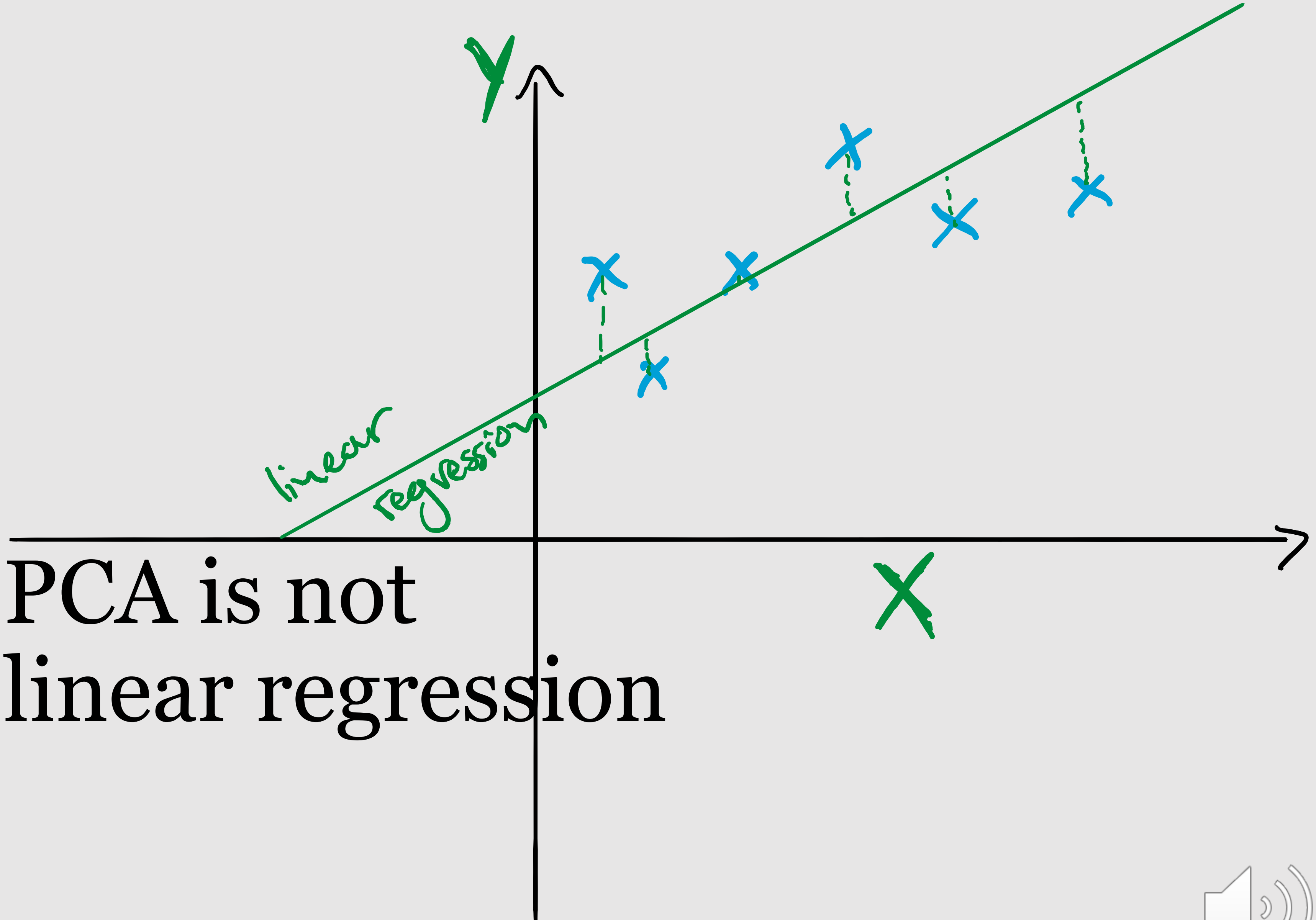
$$y = a_0 + a_1 x, \quad \text{or} \quad z = a_0 + a_1 x + b_1 y,$$

$$\text{or} \quad z = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + \ldots + a_n x_n,$$

where y, x, z, x_1, x_2, $\ldots x_n$ are variables, and determining the "best" values for the constants a_0, a_1, b_1, a_0, a_1, a_2, a_3, $\ldots$ a_n

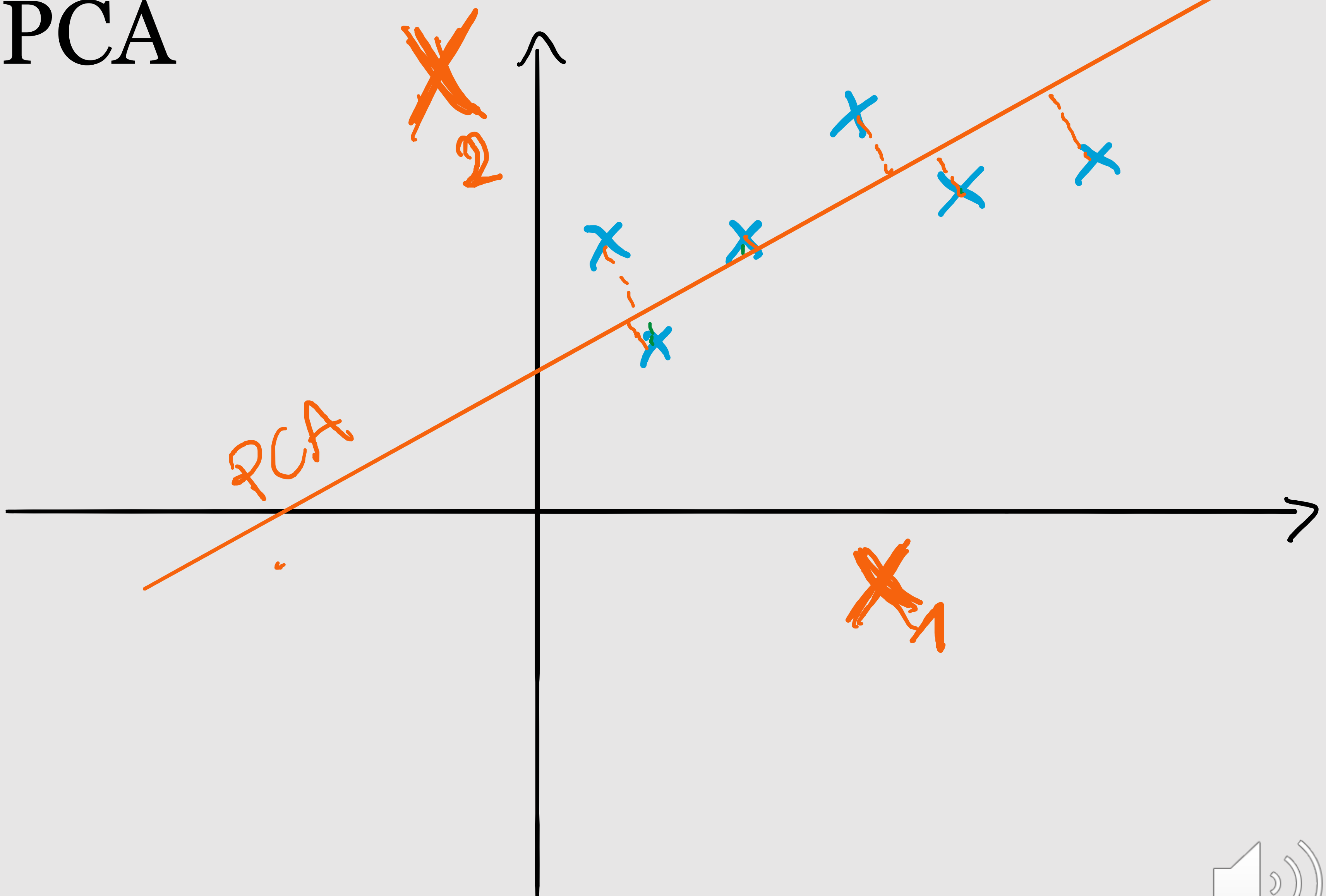

O
AXIS OF x - VARIABLE
x
AXIS OF y VARIABLE
y
LINE OF WORST FIT
LINE OF BEST FIT
REGRESSION LINE : y on x
REGRESSION LINE : x on y
A
B
C
E
F
B'
A'
E'
F'


A
B
P1
P2
P3
P4
Pn
p1
p2
p3
p4
pn

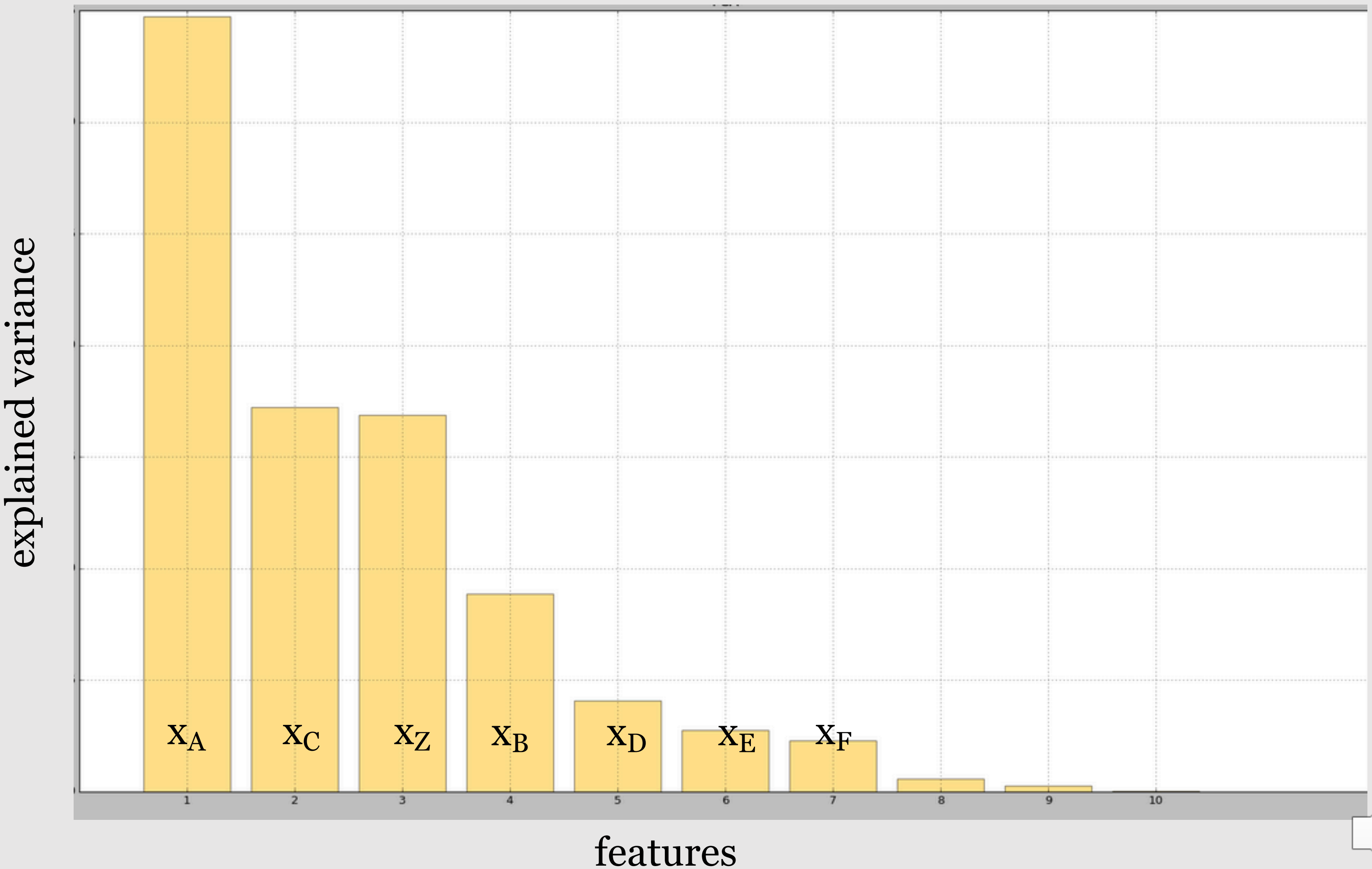


PCA is not linear regression

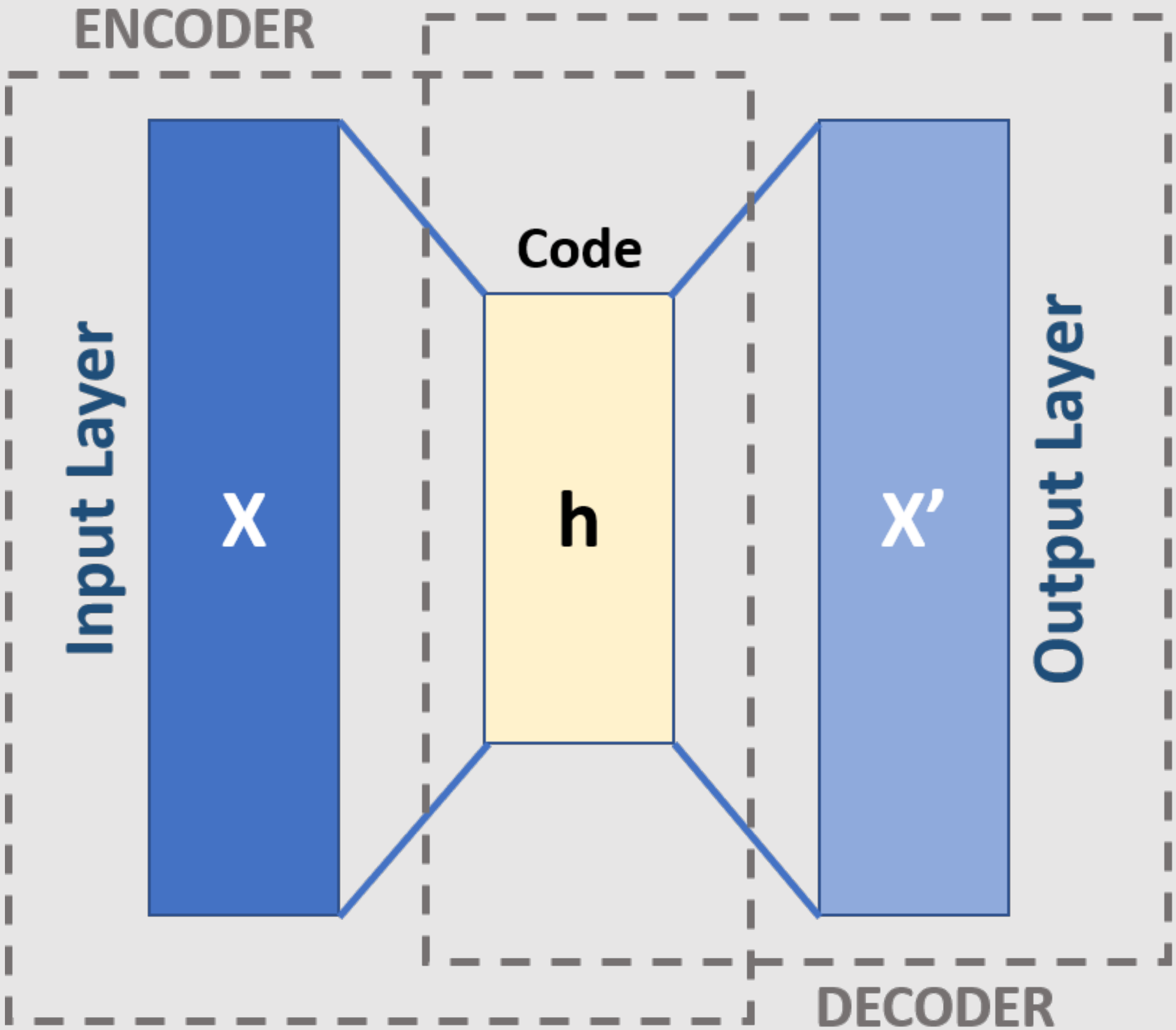
PCA



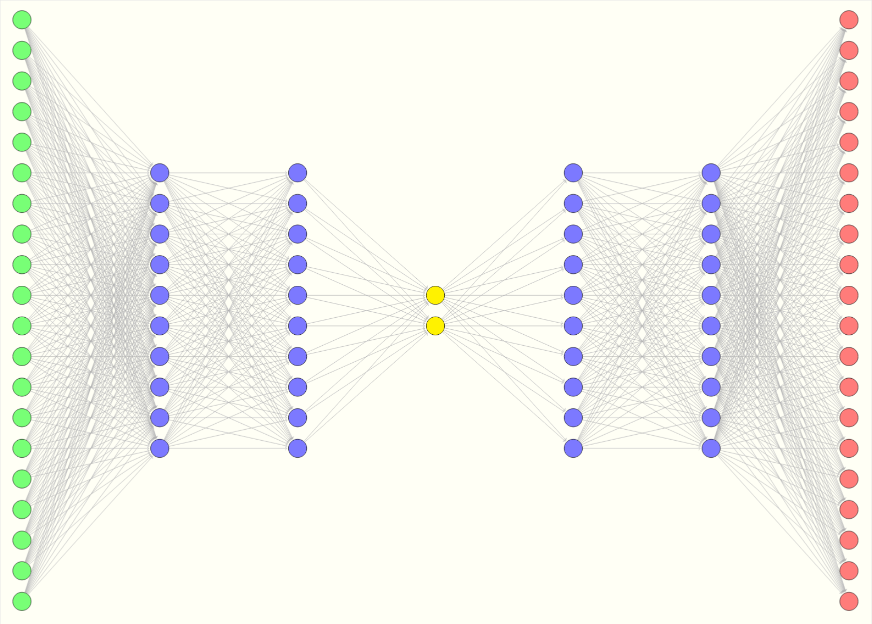
PCA – feature selection



Autoencoder



Autoencoder



source: https://gertjanvandenburg.com/blog/autoencoder/

An overfitting algorithm

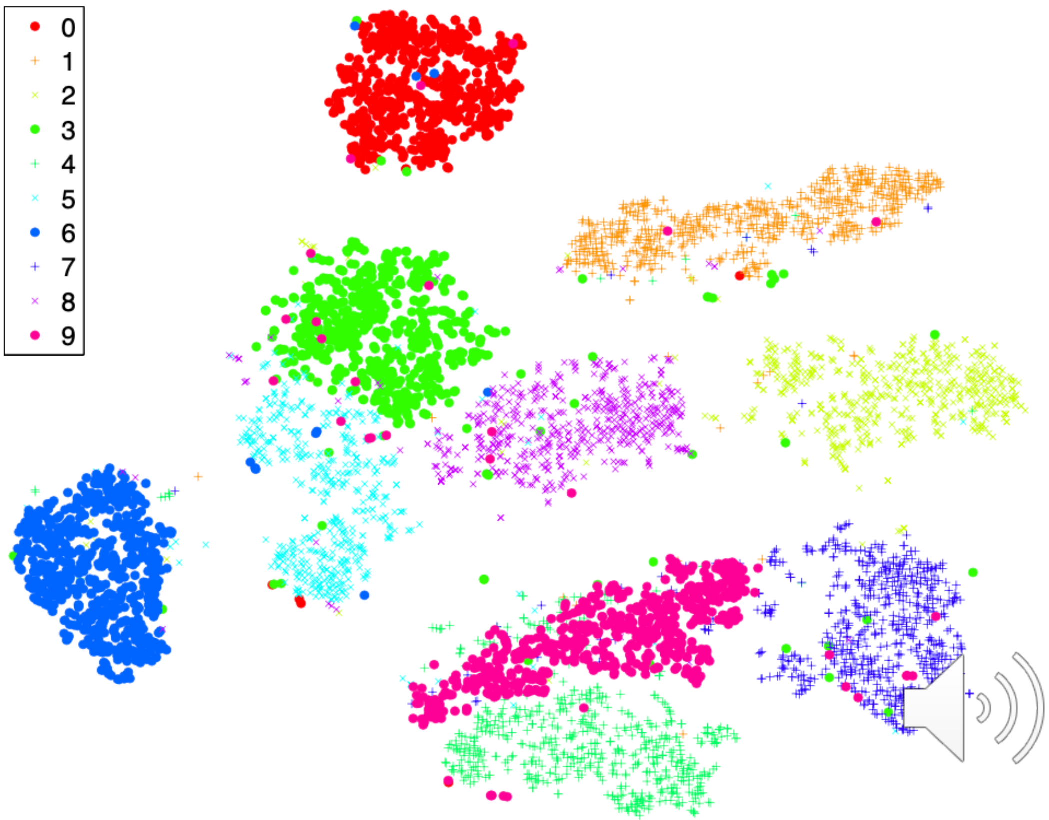
Finding the simplest function allowing reconstruction of the data within some margin of error

Visualizing Data using t-SNE

Laurens van der Maaten LVDMAATEN@GMAIL.COM
TiCC
Tilburg University
P.O. Box 90153, 5000 LE Tilburg, The Netherlands

Geoffrey Hinton HINTON@CS.TORONTO.EDU
Department of Computer Science
University of Toronto
6 King's College Road, M5S 3G4 Toronto, ON, Canada

t-SNE



github.com/mixmixmix/learnmachine

Example

Phenotypic Profiling of High Throughput Imaging Screens with Generic Deep Convolutional Features

Philip T. Jackson[1], Yinhai Wang[2], Sinead Knight[2], Hongming Chen[2], Thierry Dorval[2], Martin Brown[2], Claus Bendtsen[2], Boguslaw Obara[1]

[1]Department of Computer Science, Durham University [2]IMED Biotech Unit, AstraZeneca

claus.bendtsen@astrazeneca.com, boguslaw.obara@durham.ac.uk

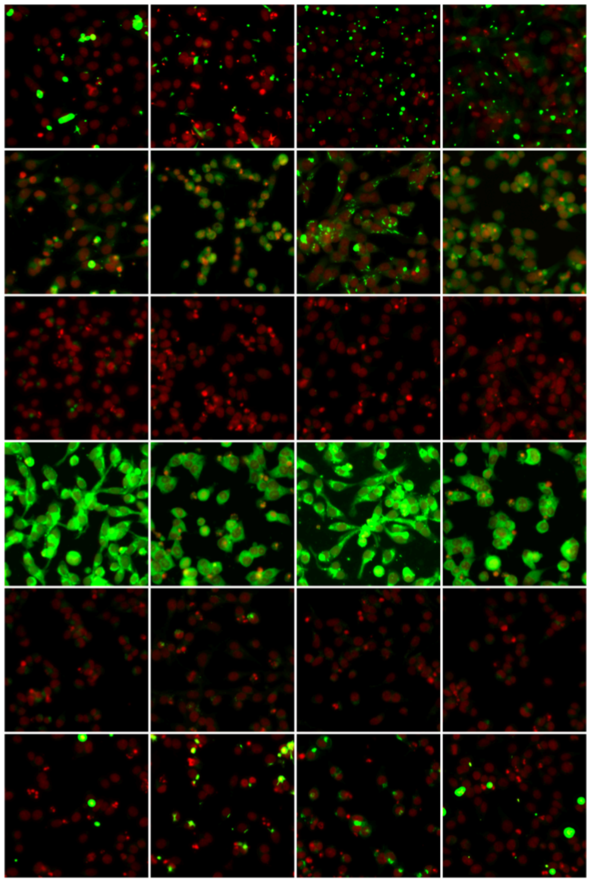


Figure 4. Samples from six of the 70 phenotypic clusters detected by k-means. Each row shows four example images from a single cluster. Rows 2 and 4 show genuine GFP expression.

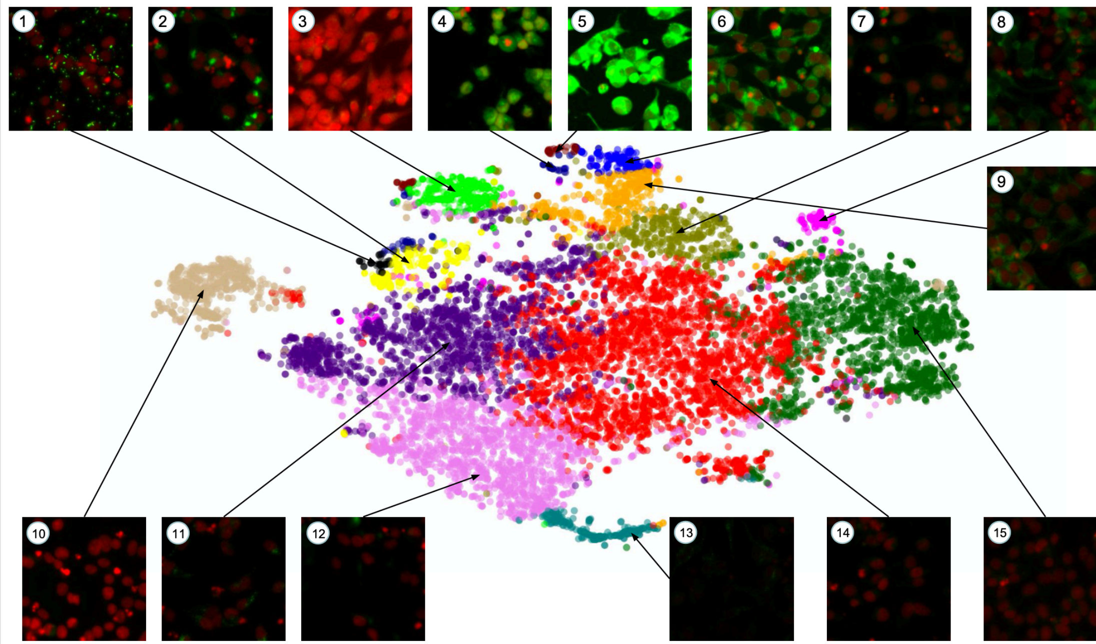


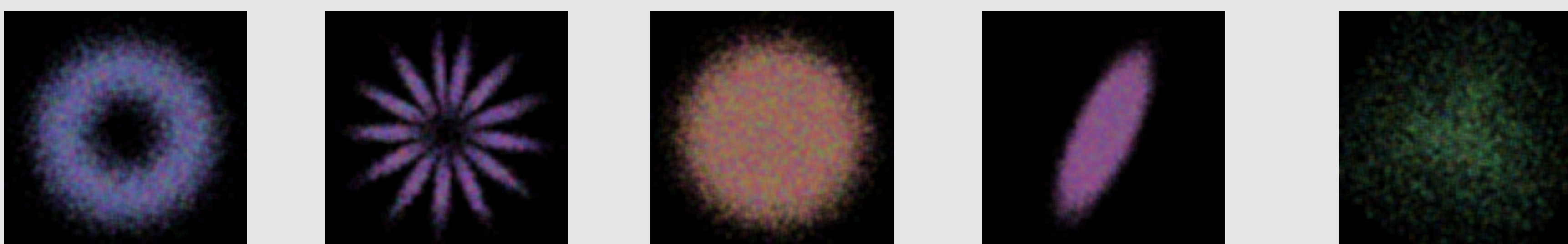
Figure 5. A t-sne embedding of our dataset, with colours showing phenotypic clusters discovered by k-means. For visualization purposes, we set $k = 15$ here.

gi

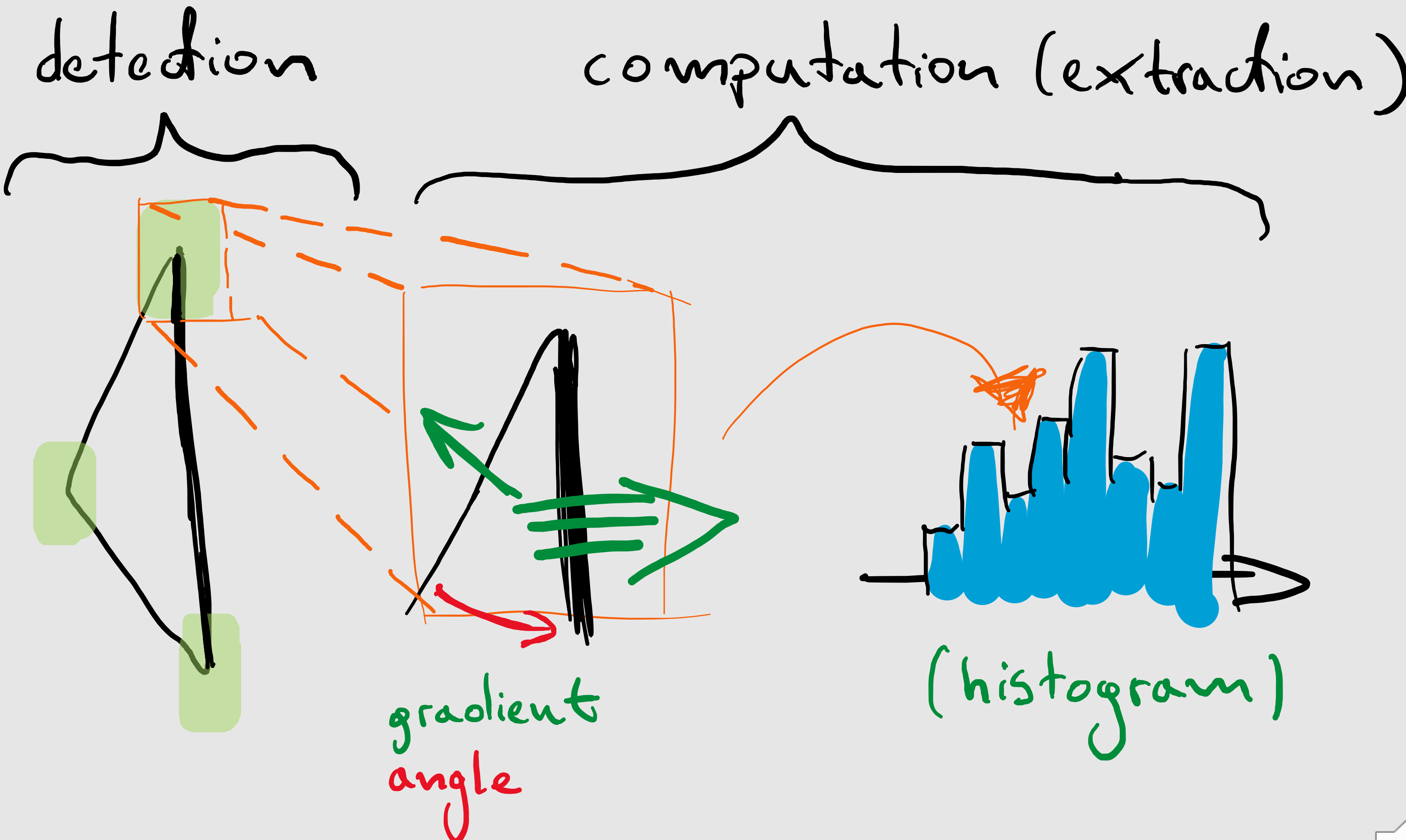
Problem representation

Basic features

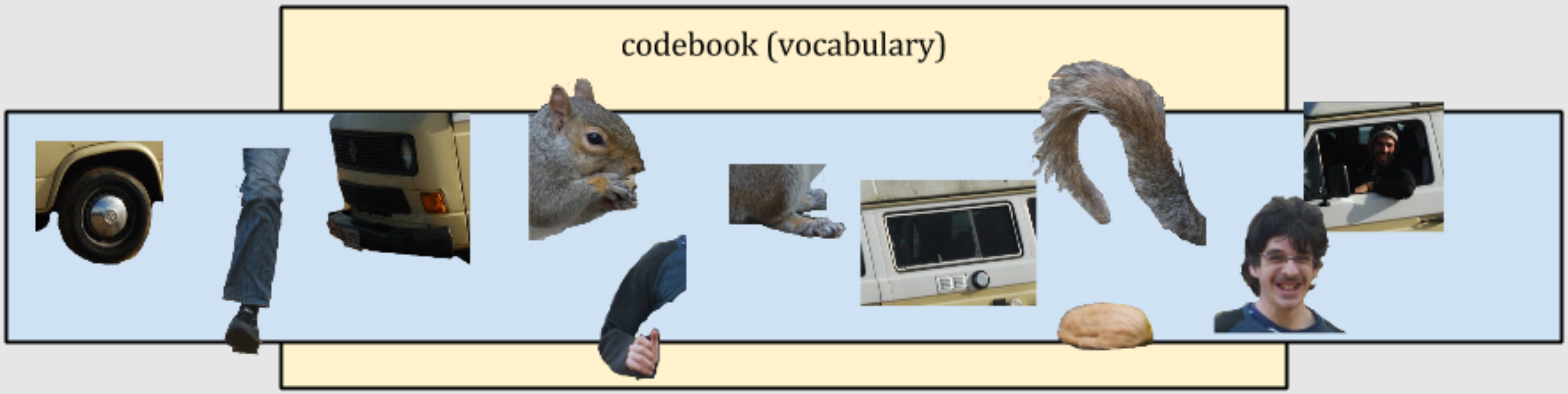
- colour statistics (over whole or part of the image)
- edges and gradients
- corners
- shapes (convolution/autocorrelation)

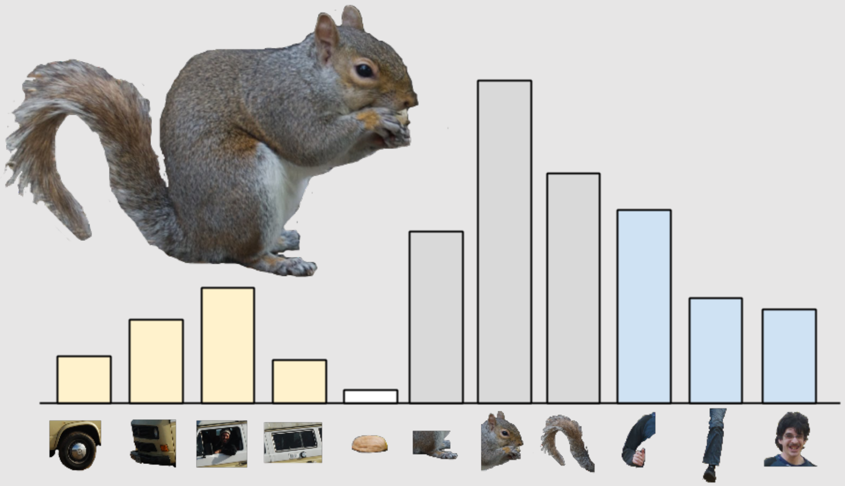


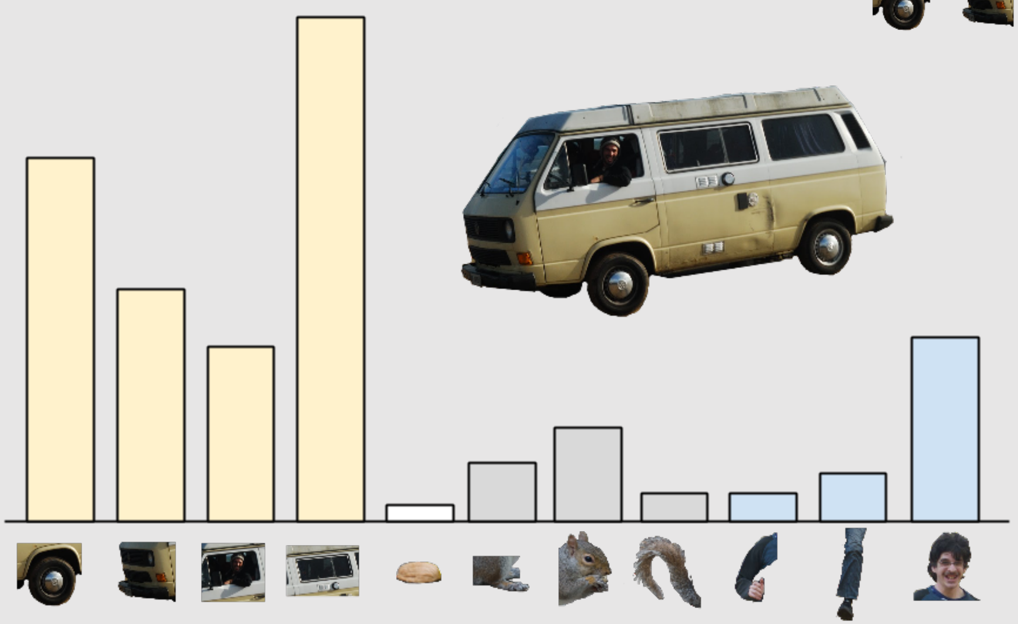
Sparse Features



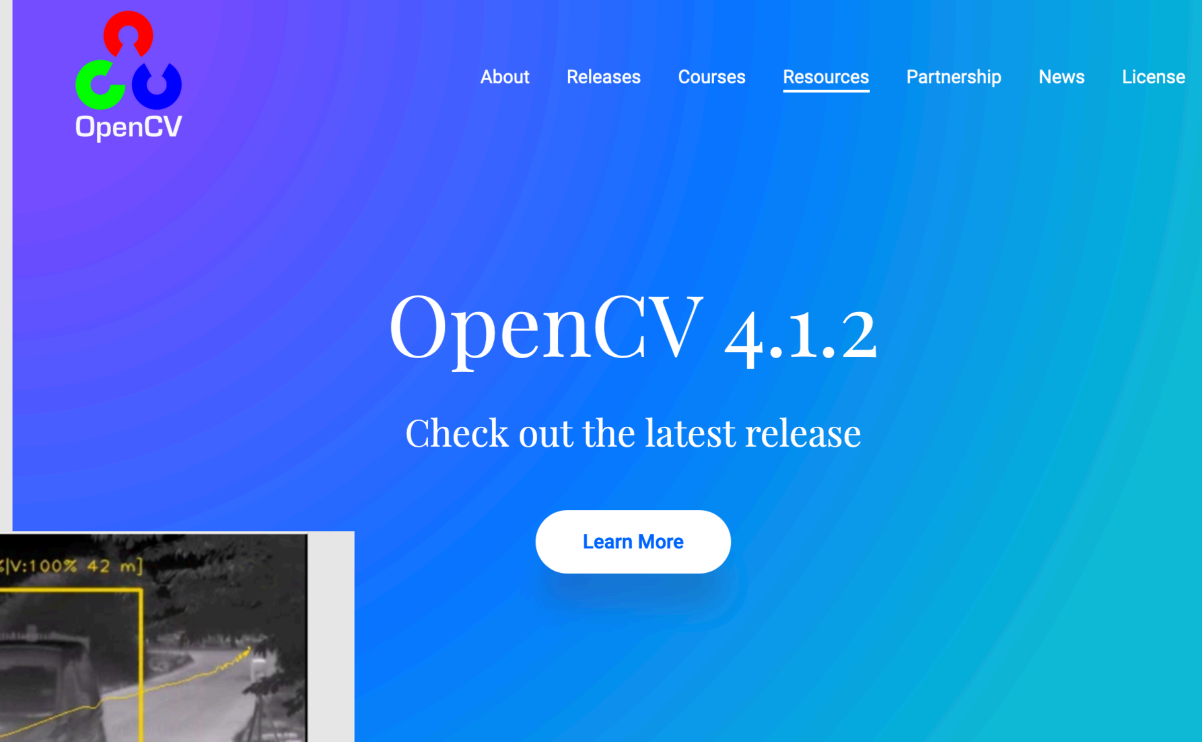
Bag of Visual Words


codebook (vocabulary)





OpenCV
C++ library



computer vision and robotics with Python bindings

OpenCV vs Scikit Learn

	OpenCV	Scikit Learn
Use	Industry and academia: from robotics to business analytics	Science and statistics
Language	C++/Java/Python	Python
Current version:	4.1.2	0.17
	Industry proven but at times poorly documented and inconsistent. Many well tested famous algorithms.	Excellent tutorials and examples, much easier to use and pythonesque.