

session 3:
Unsupervised learning

M. Kundegorski

13th December 2019

IAFIG-RMS - Bioimage Analysis With Python
Cambridge Bioinformatics Training Centre



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

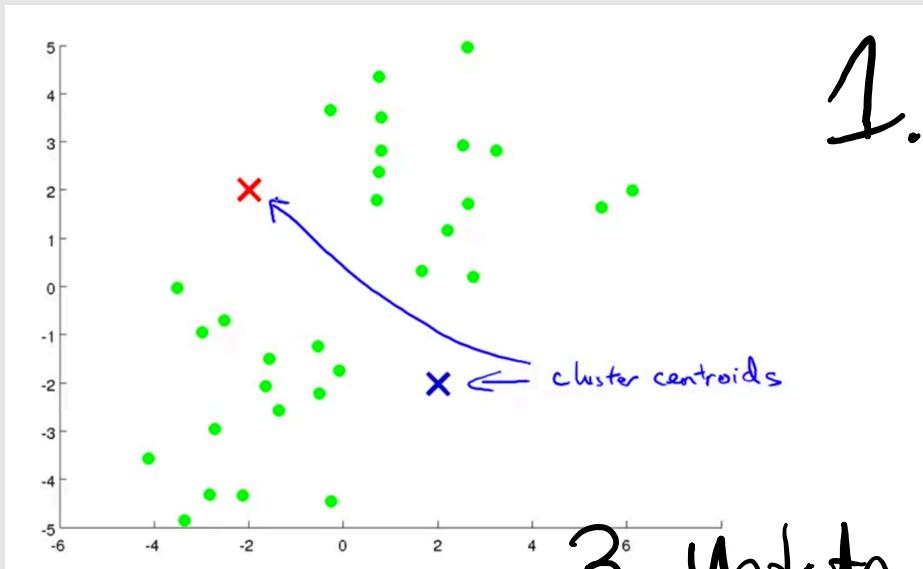
Principles

- 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.

Clustering: finding data similarity

k-means

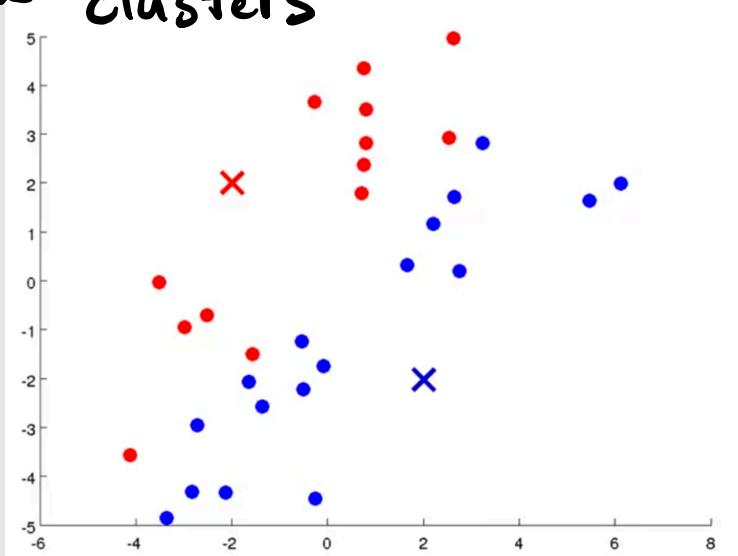
$K = 2$



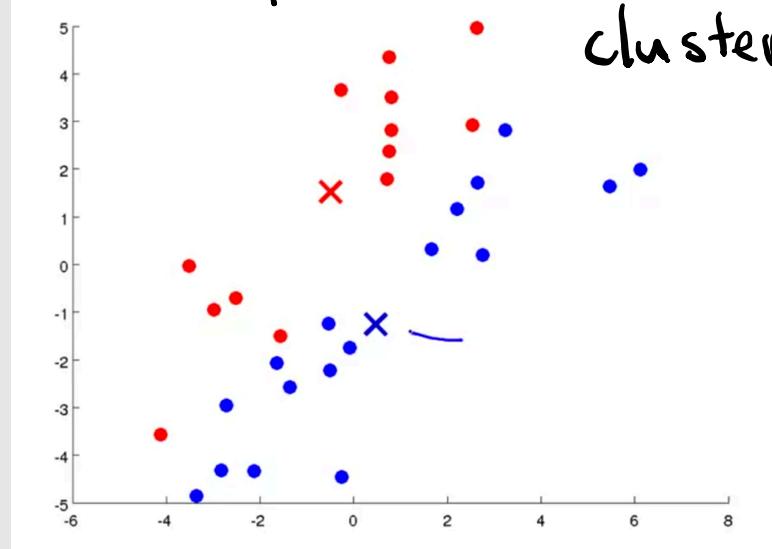
1.

random
initialisation

2. find
clusters

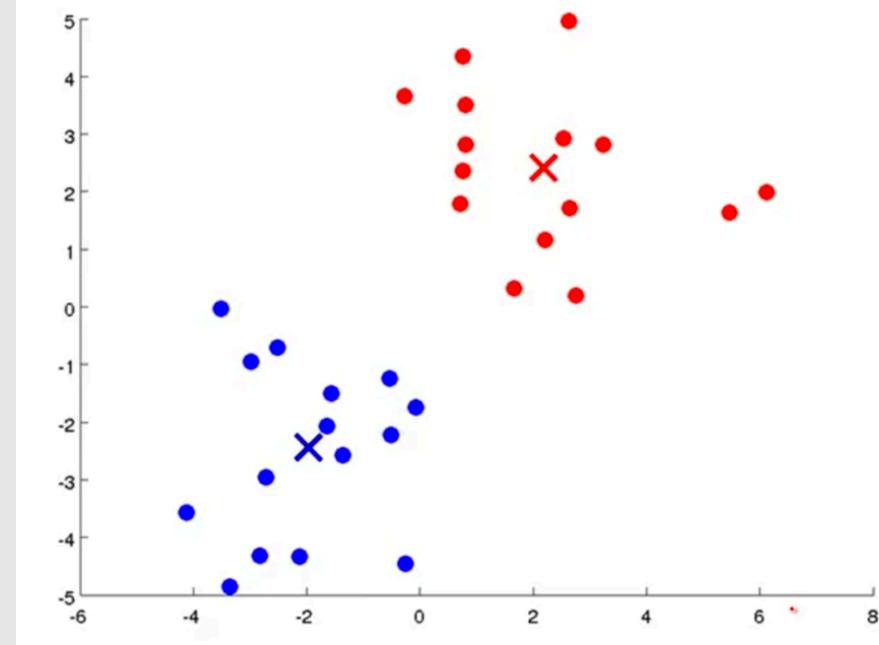
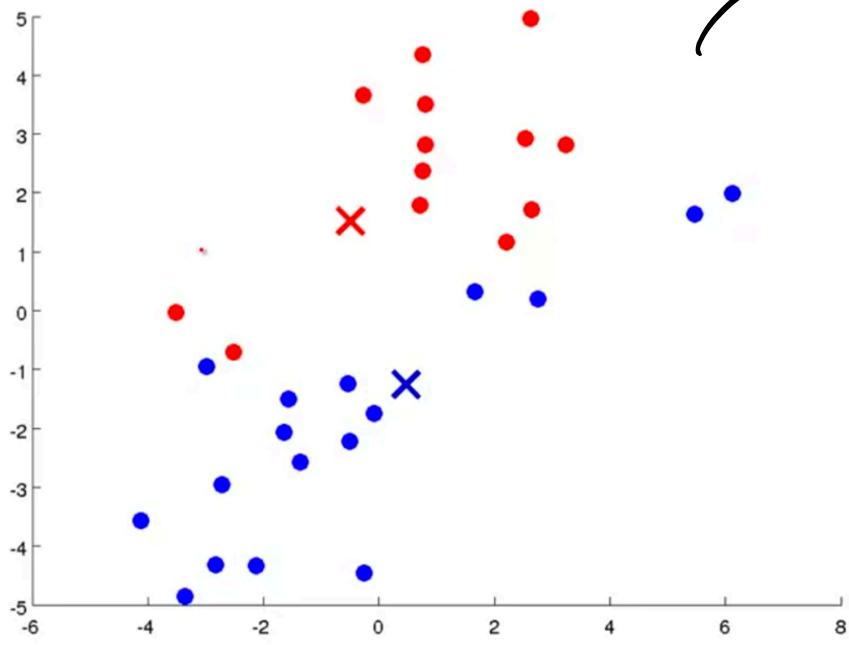


3. Update mean of
clusters



k means

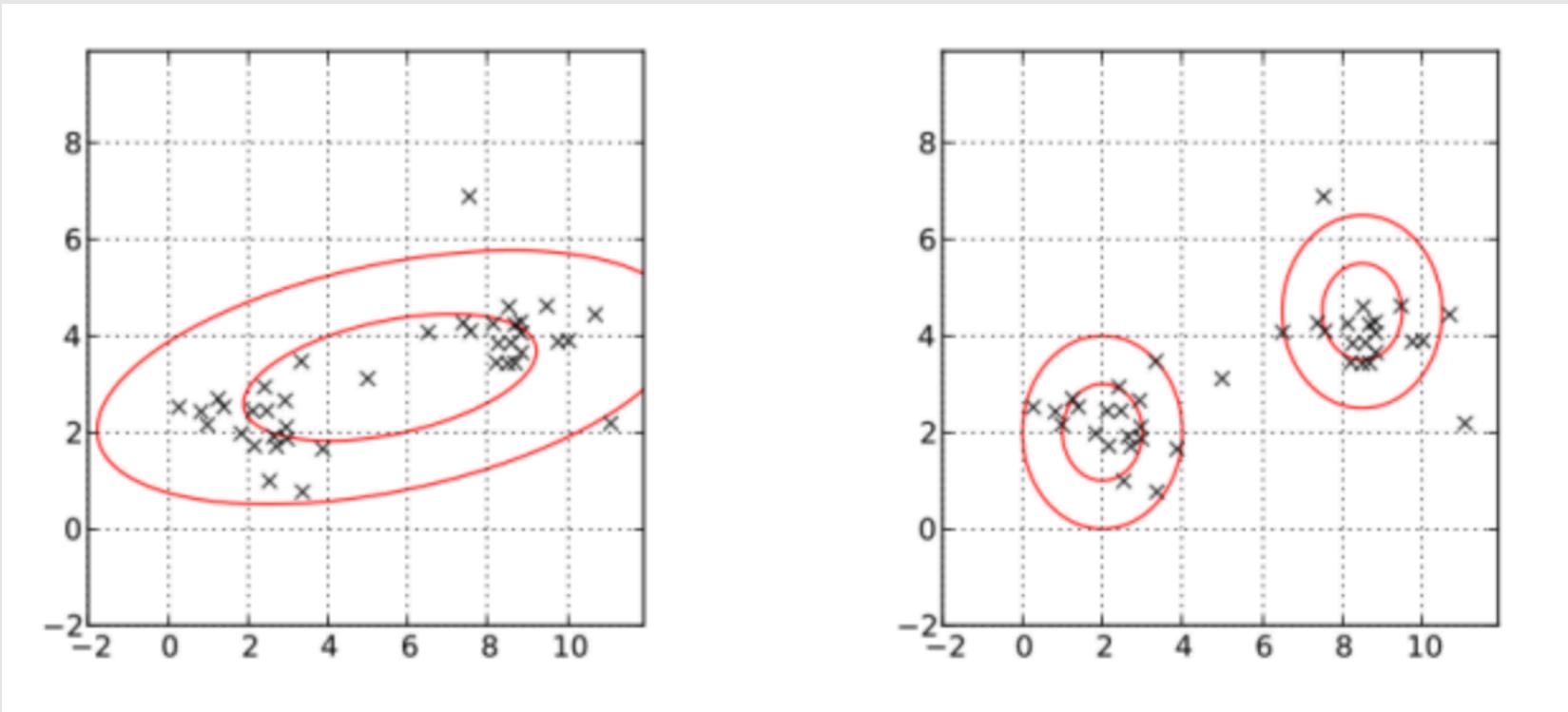
convergence



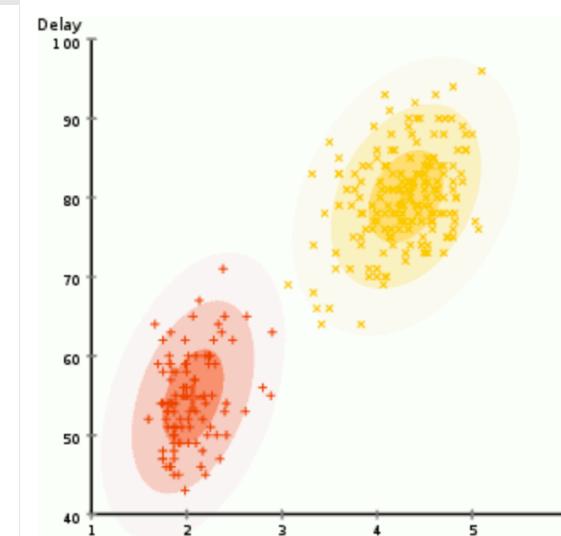
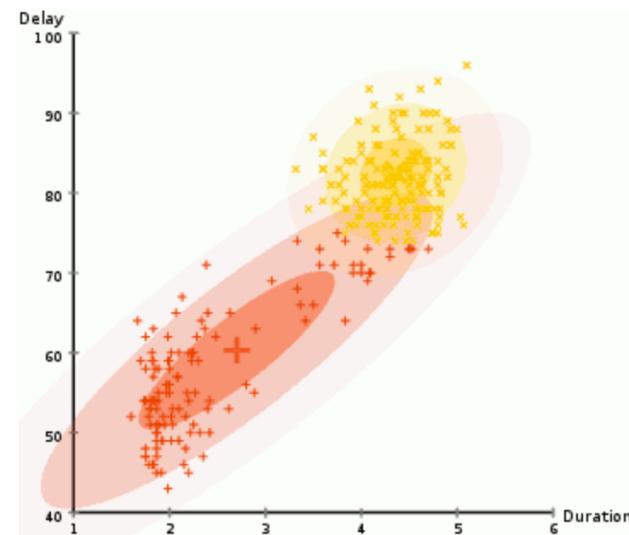
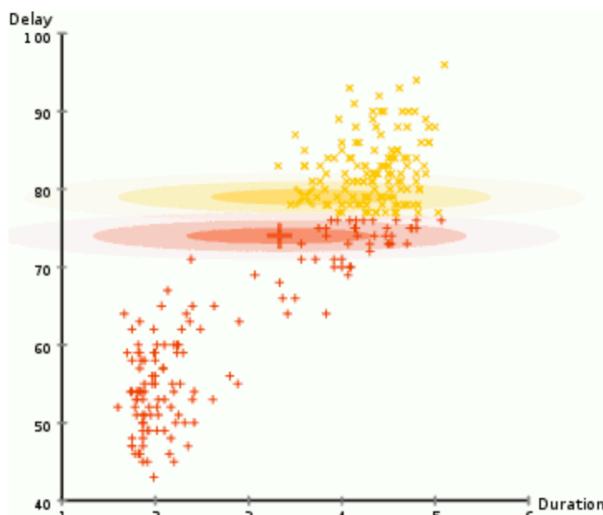
k-medoids

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

Mixture of Gaussians



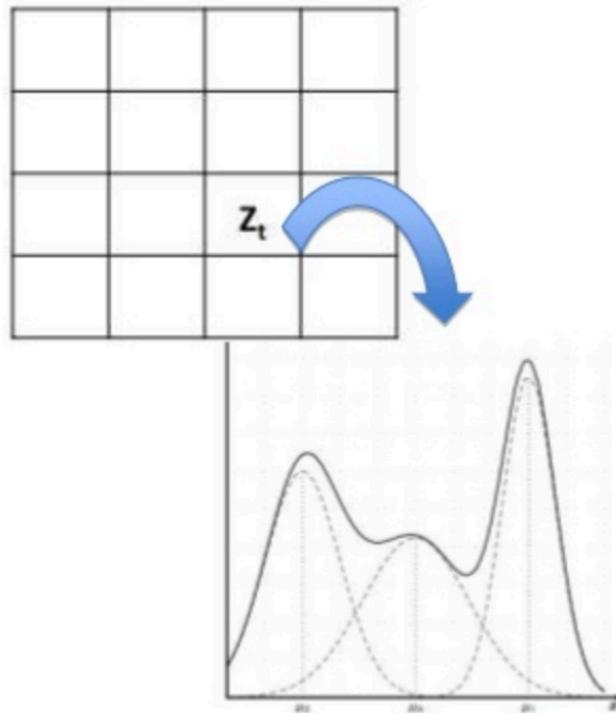
Expectation-Maximisation



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

Gaussian Mixture Model

Gaussian Mixture Model (GMM)



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

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

Example:



Mean-shift segmentation

790

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

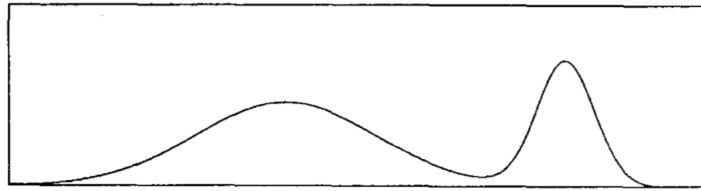
- KDE + gradient ascent

Mean Shift, Mode Seeking, and Clustering

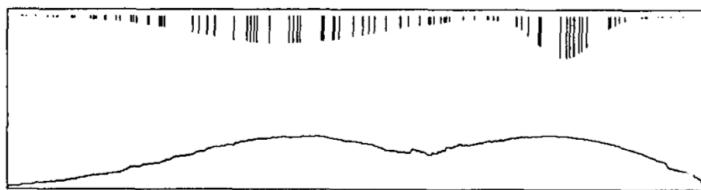
Yizong Cheng

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 is shown that mean shift is a mode-seeking process on a surface “shadowed” by a weight function. The shadowing analysis is used to prove that mean shift is equivalent to gradient ascent on the density estimated with a shadow of its. Convergence and its rate is the subject of Section IV. The last section discusses the applications of mean shift to global optimization, mode seeking, and clustering.

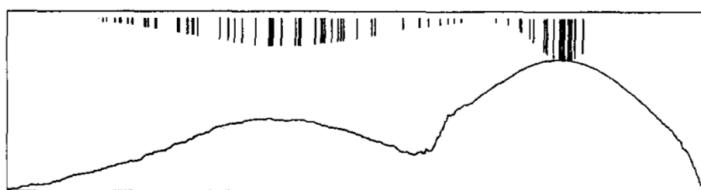
A relation among kernels called “shadow” will be defined in Section III. It will be proved that mean shift on any kernel is equivalent to gradient ascent on the density estimated with a shadow of its. Convergence and its rate is the subject of Section IV. The last section discusses the applications of mean shift to global optimization, mode seeking, and clustering.



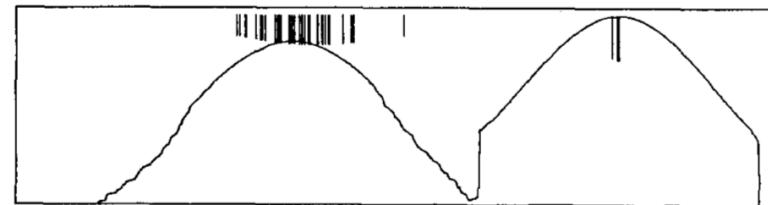
(a)



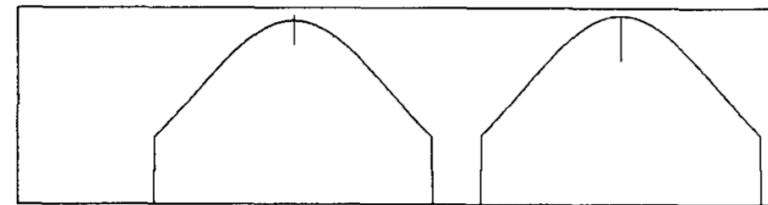
(b)



(c)



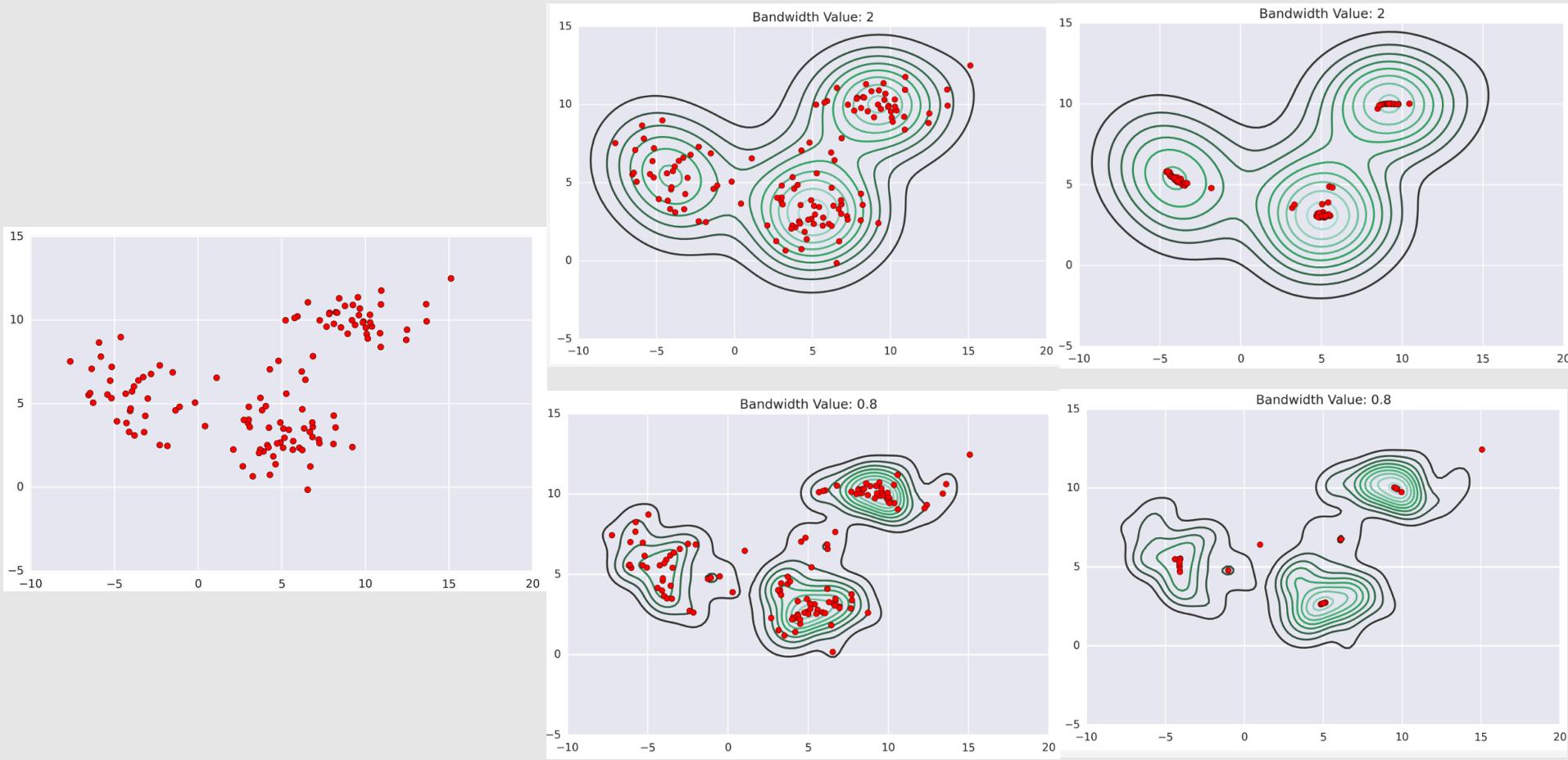
(d)



(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 .

Mean-shift segmentation



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

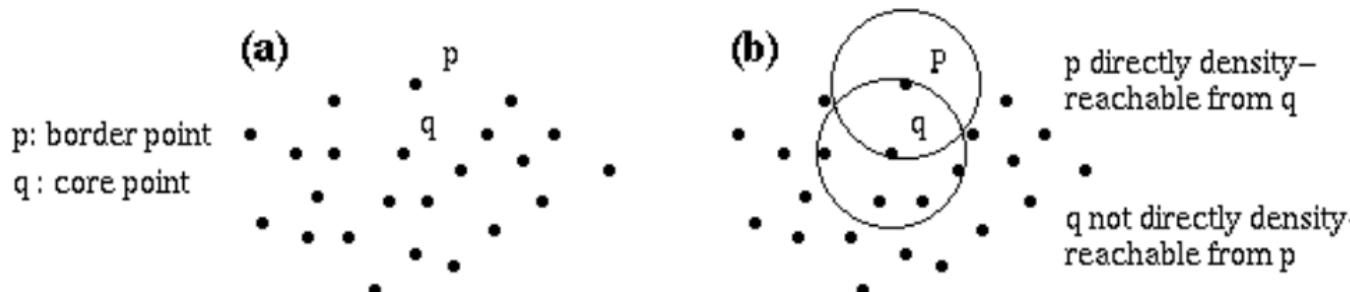


figure 2: core points and border points

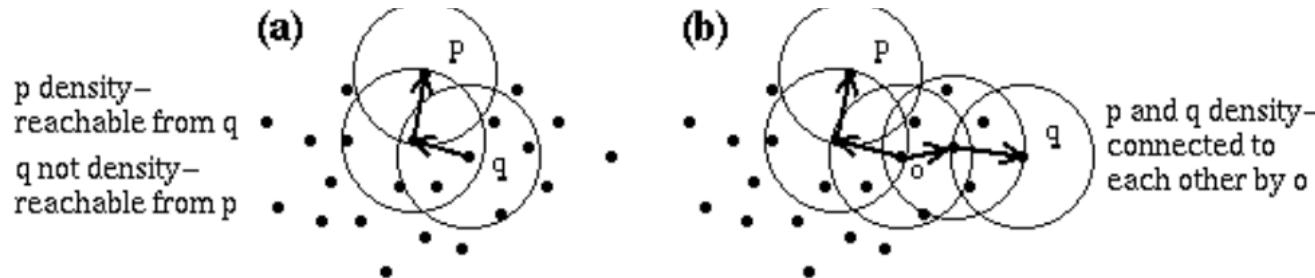
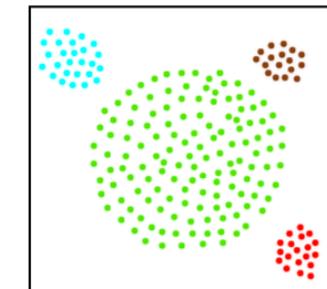
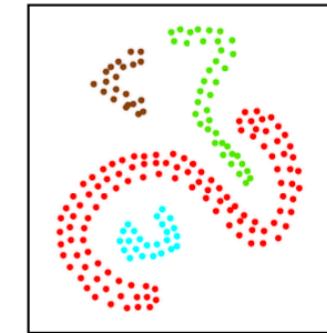
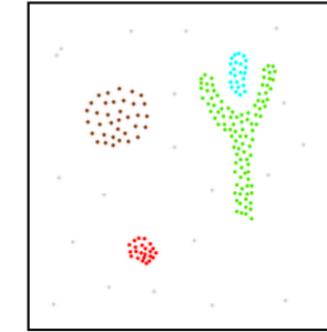


figure 3: density-reachability and density-connectivity



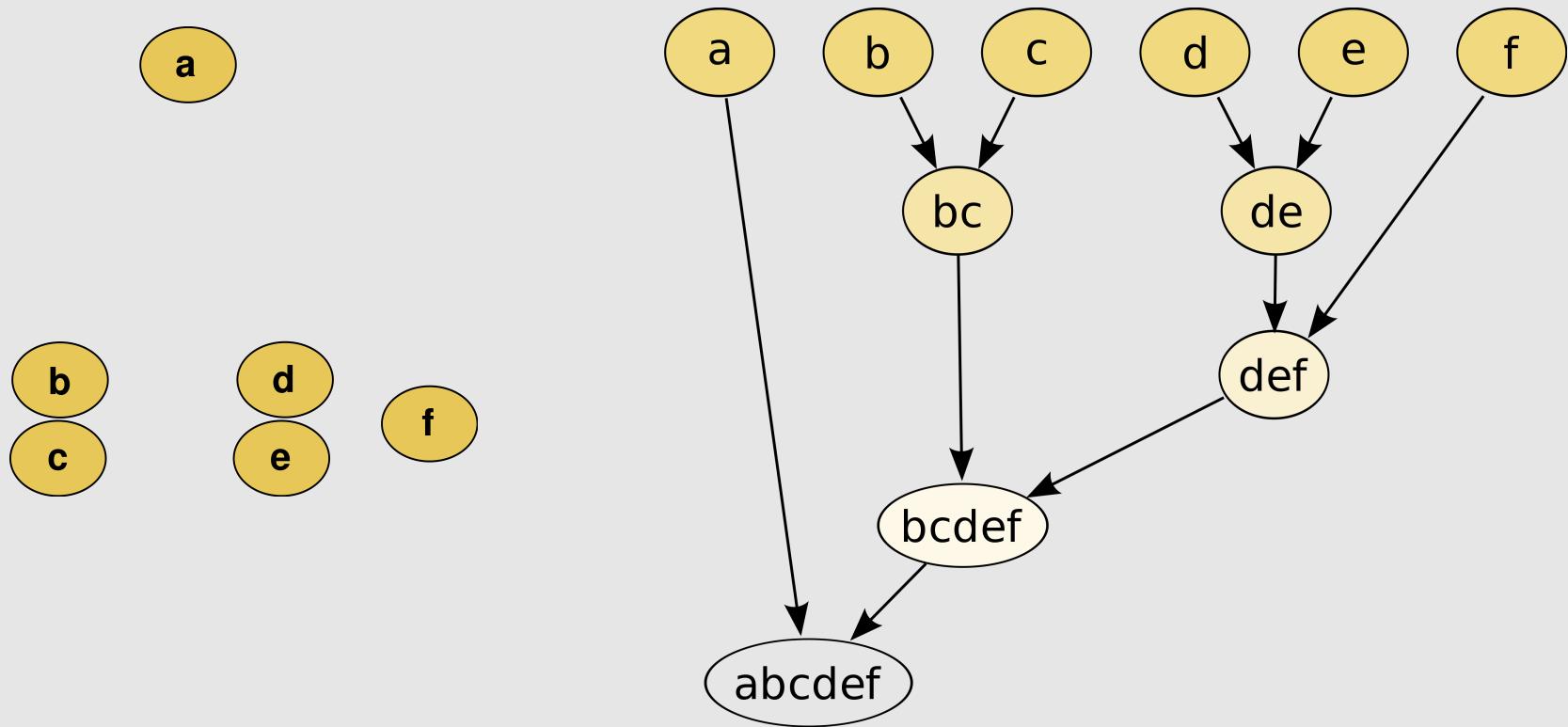
database 3

database 2

database 1

figure 6: Clusterings discovered by DBSCAN

Hierarchical clustering



Component Analysis: feature selection, dimensionality reduction, encoding...

Principle Component Analysis

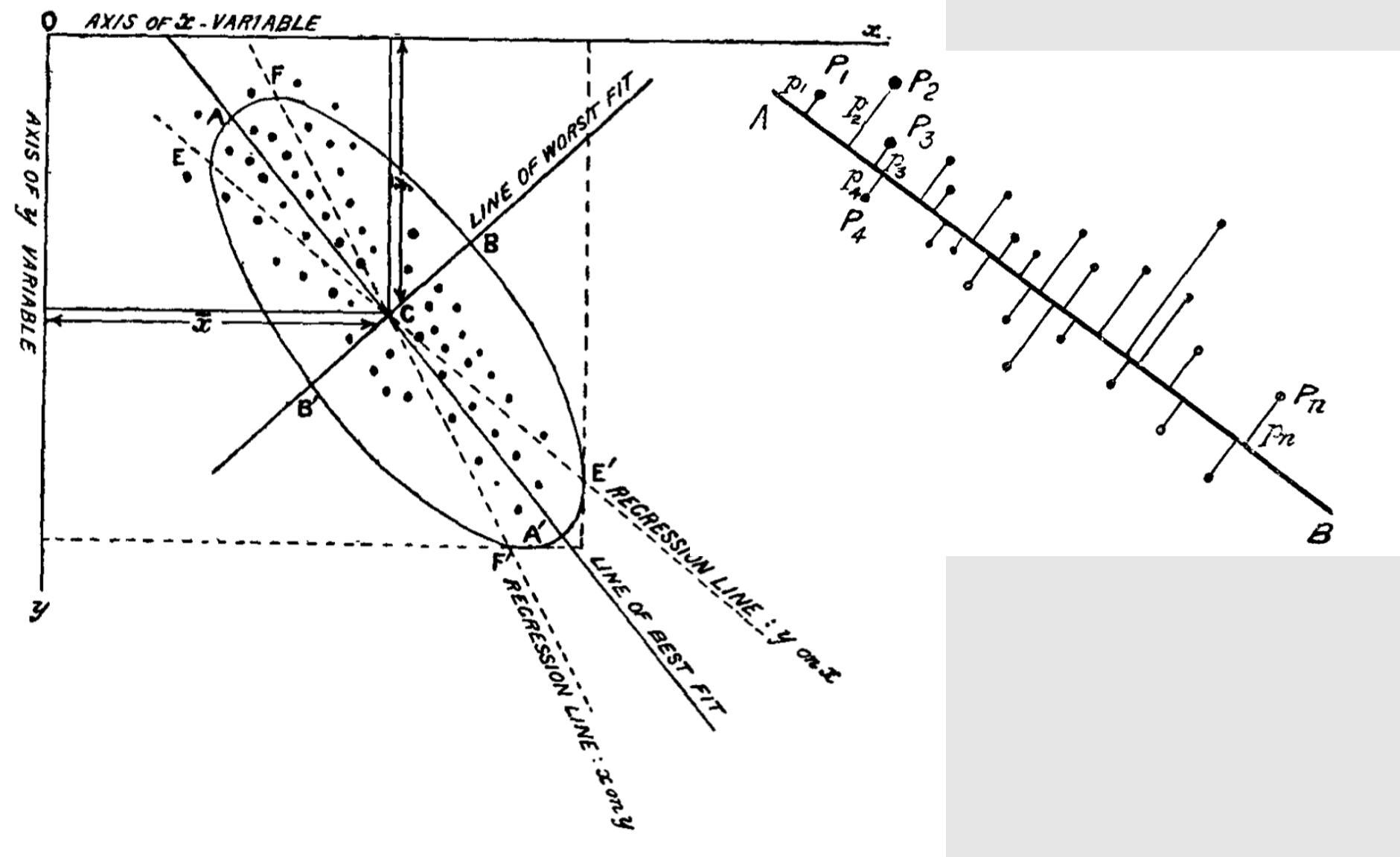
[559]

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

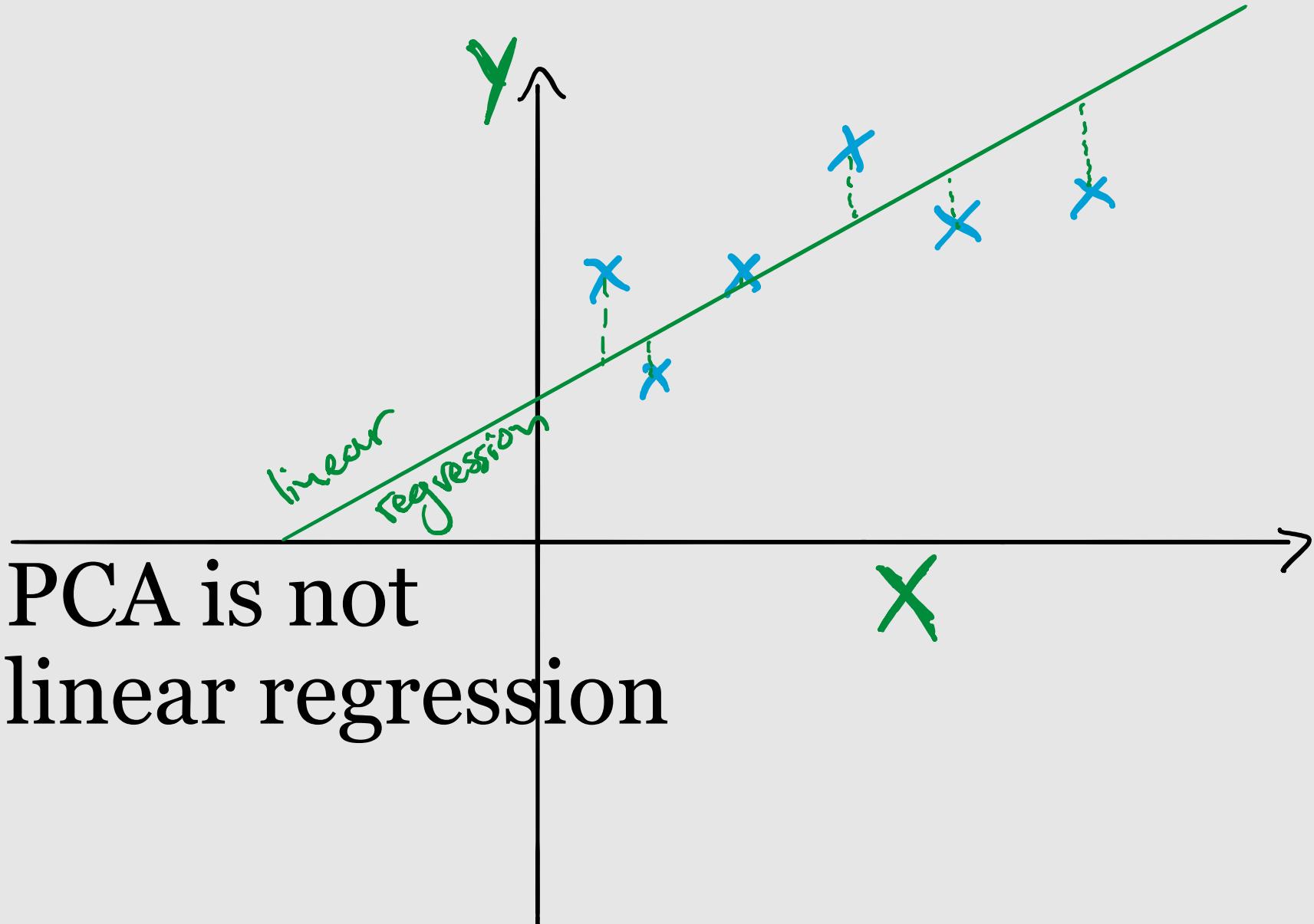
(1) In many physical, statistical, and biological investigations it is desirable to represent a system of points in plane, three, or higher dimensioned space by the "best-fitting" straight line or plane. Analytically this consists in taking

$$y = a_0 + a_1 x, \quad \text{or} \quad z = a_0 + a_1 x + b_1 y,$$
$$\text{or} \quad z = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + \dots + a_n x_n,$$

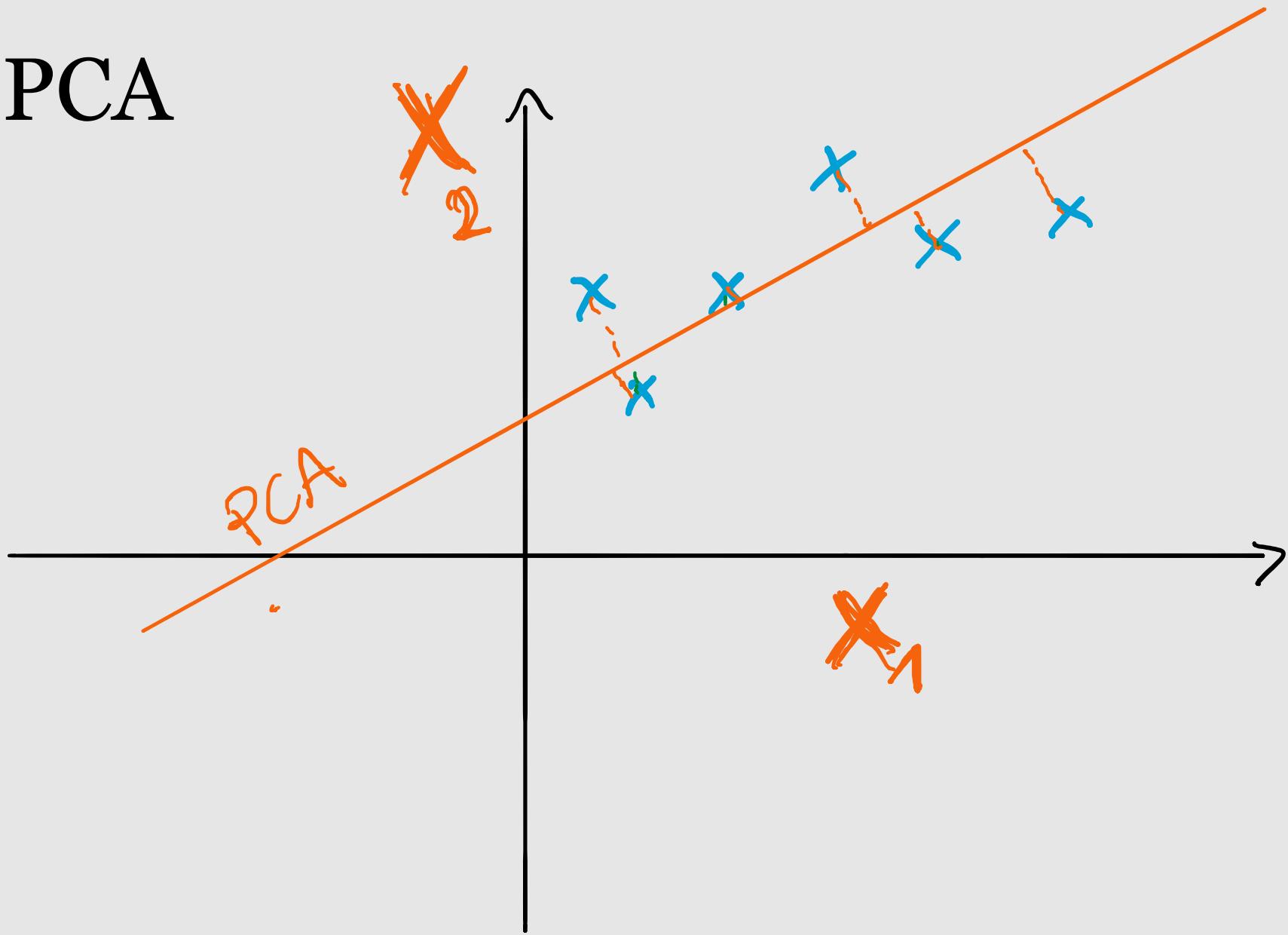
where y , x , z , x_1 , x_2 , \dots , x_n are variables, and determining the "best" values for the constants a_0 , a_1 , b_1 , a_0 , a_1 , a_2 , a_3 , \dots , a_n



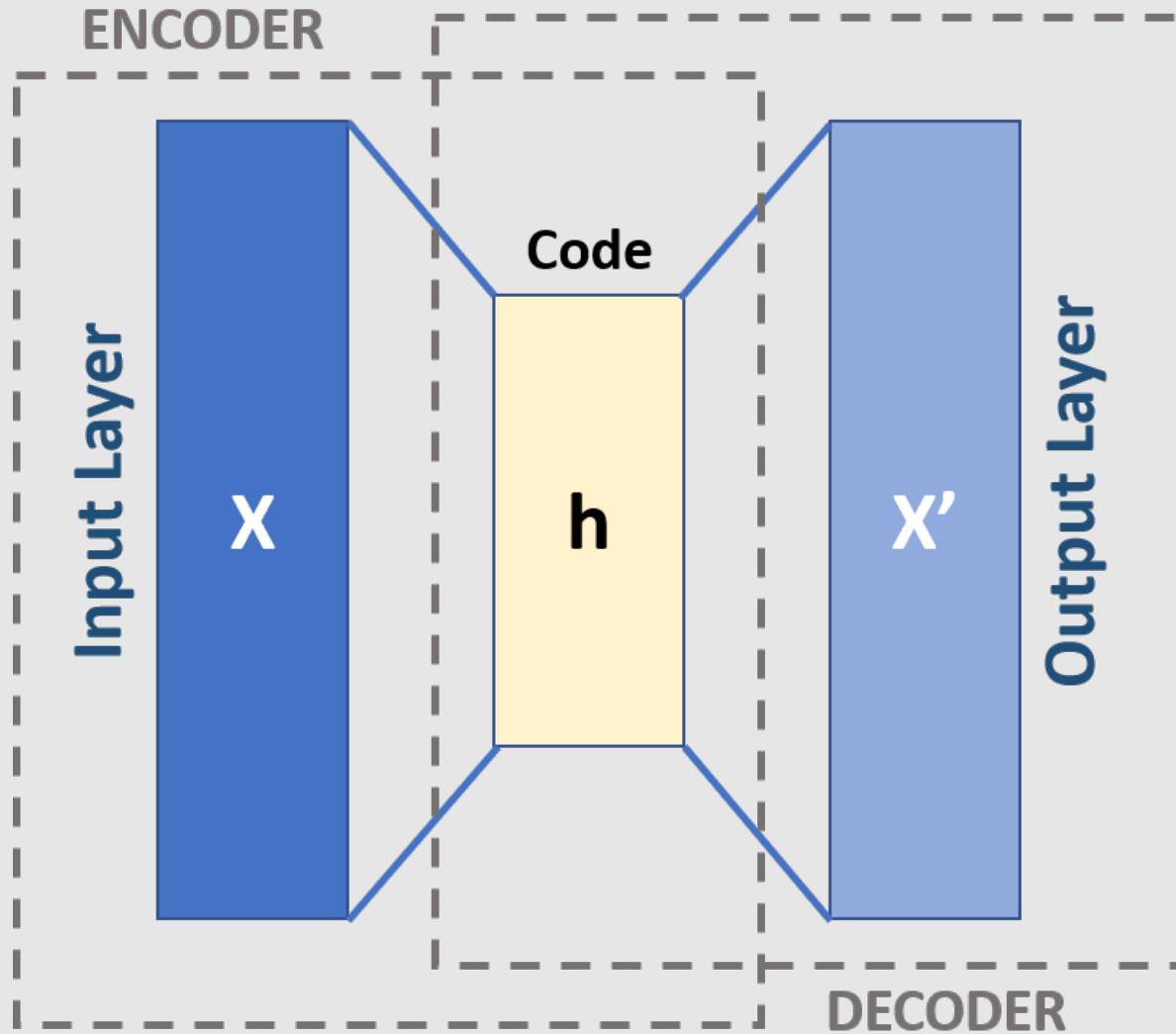
**PCA is not
linear regression**



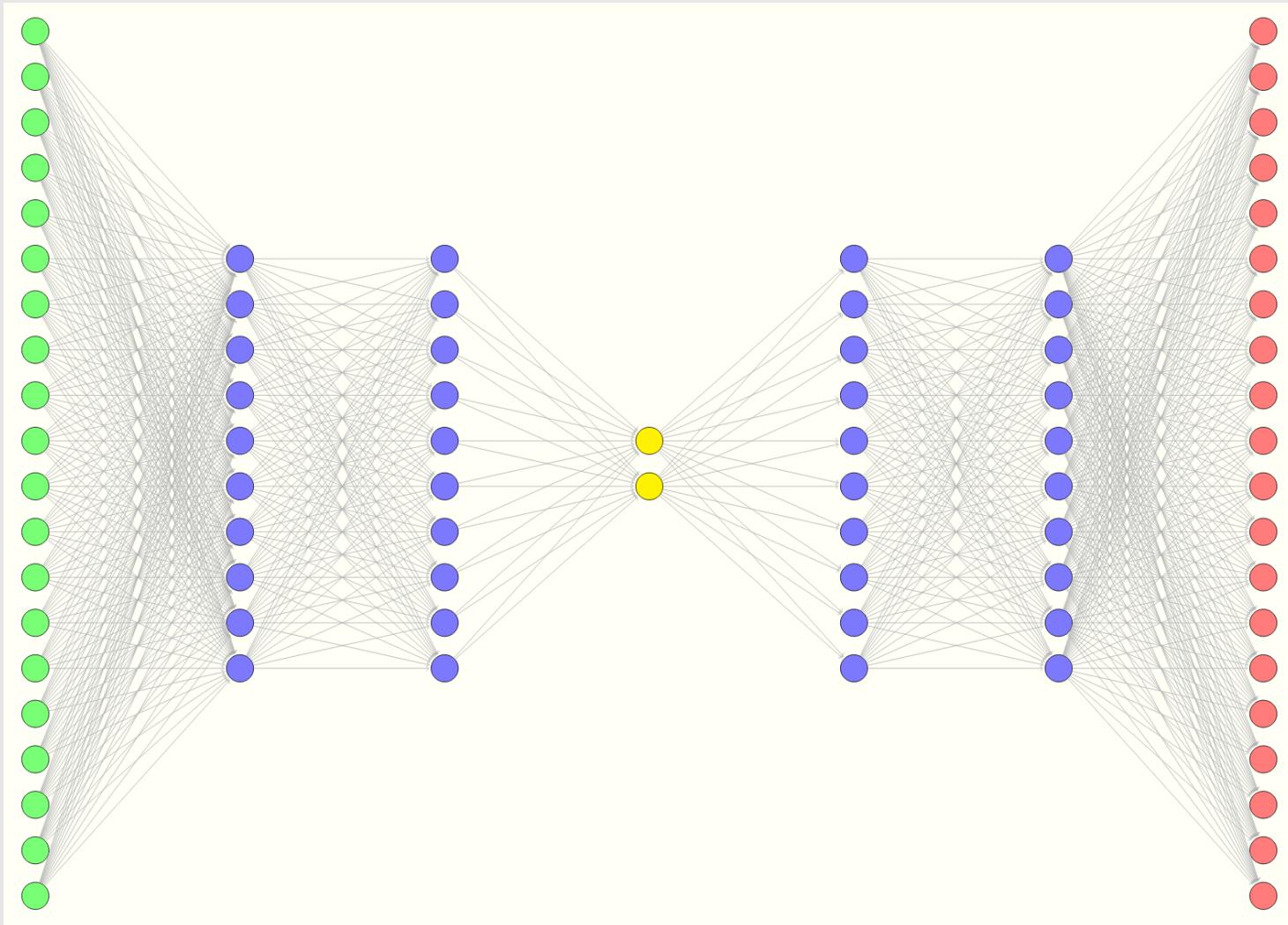
PCA



Autoencoder



Autoencoder



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

Visualizing Data using t-SNE

Laurens van der Maaten

TiCC

Tilburg University

P.O. Box 90153, 5000 LE Tilburg, The Netherlands

LVDMAATEN@GMAIL.COM

t-SNE

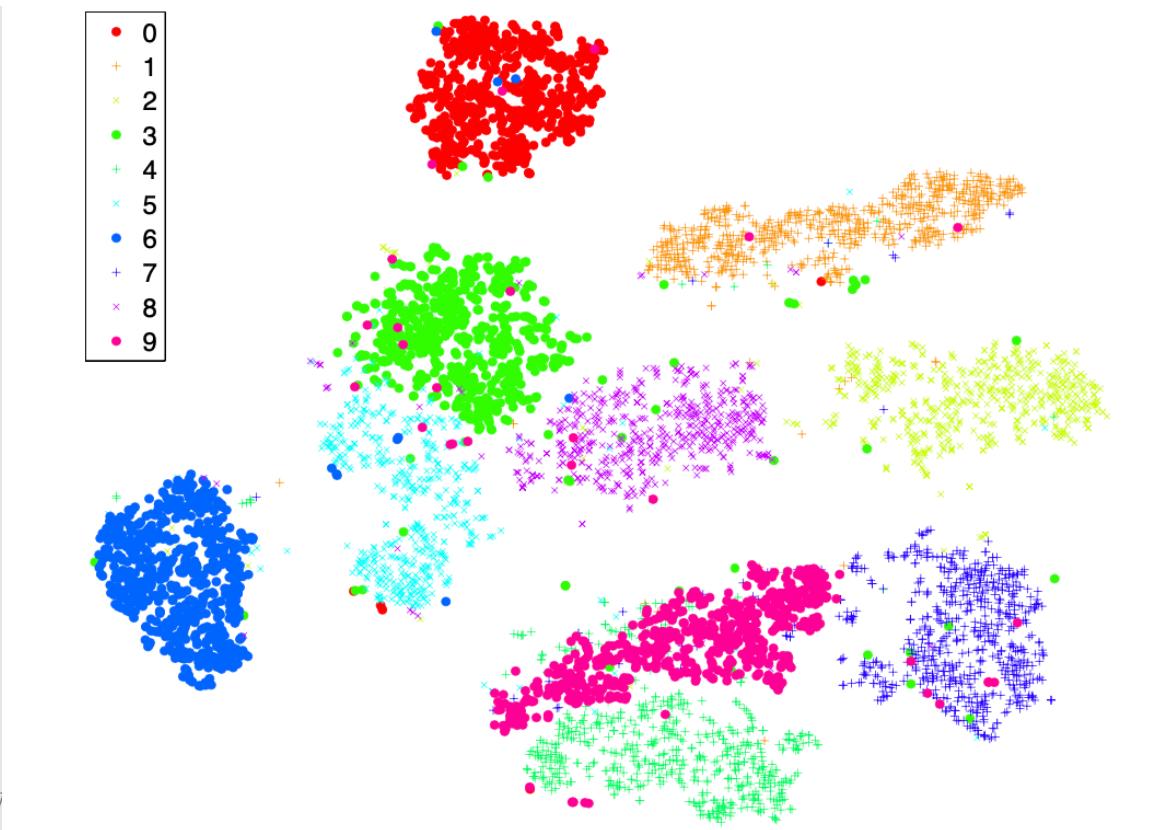
Geoffrey Hinton

Department of Computer Science

University of Toronto

6 King's College Road, M5S 3G4 Toronto, ON, Canada

HINTON@CS.TORONTO.EDU



Example

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

Philip T. Jackson¹, Yinhai Wang², Sinead Knight², Hongming Chen²,
Thierry Dorval², Martin Brown², Claus Bendtsen², Boguslaw Obara¹

¹Department of Computer Science, Durham University

²IMED Biotech Unit, AstraZeneca

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

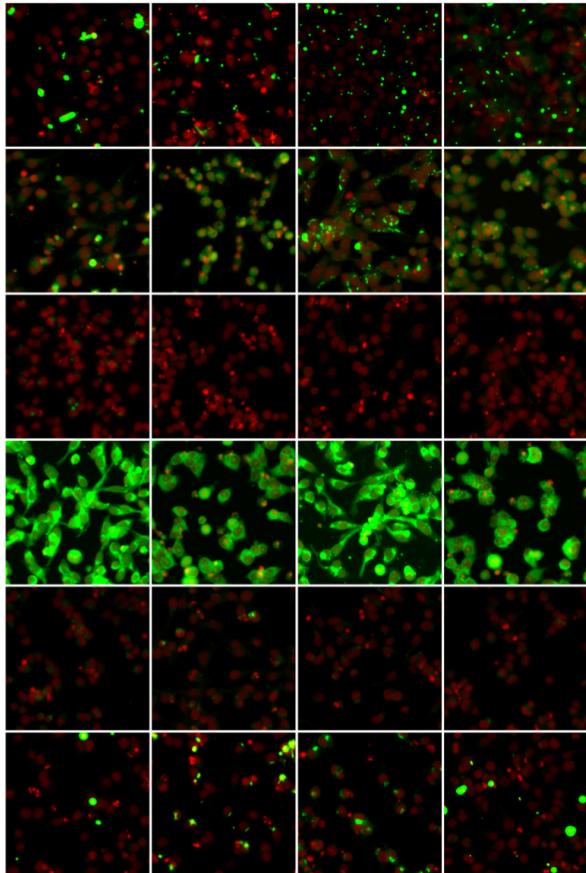


Figure 4. Samples from six of the 70 phenotypic clusters detected by k-means. Each row shows four example images from a single cluster. Rows 2 and 4 show genuine GFP expression.

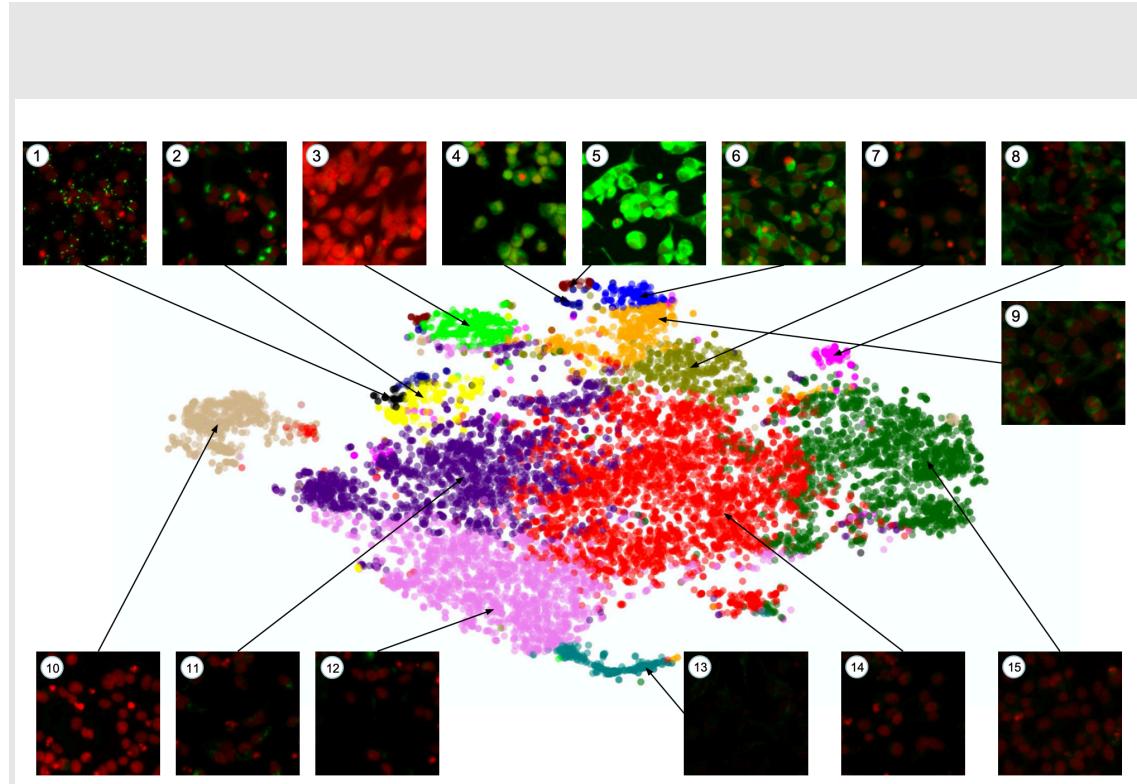


Figure 5. A t-sne embedding of our dataset, with colours showing phenotypic clusters discovered by k-means. For visualization purposes, we set $k = 15$ here.