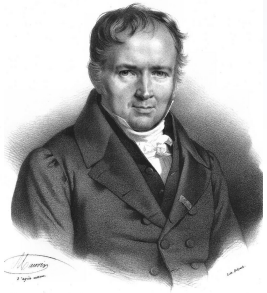
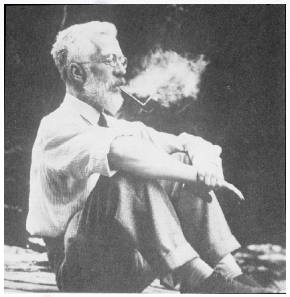
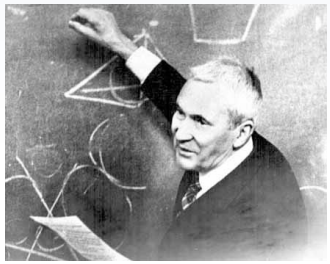
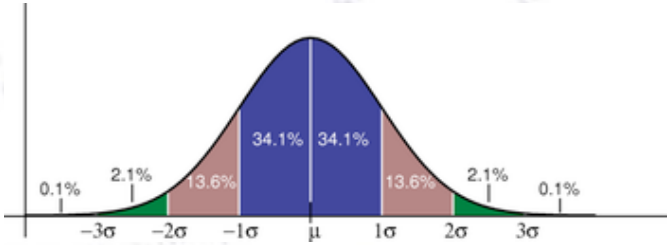
Applied ML

(Kernel) Principle Component Analysis



Troels C. Petersen (NBI)

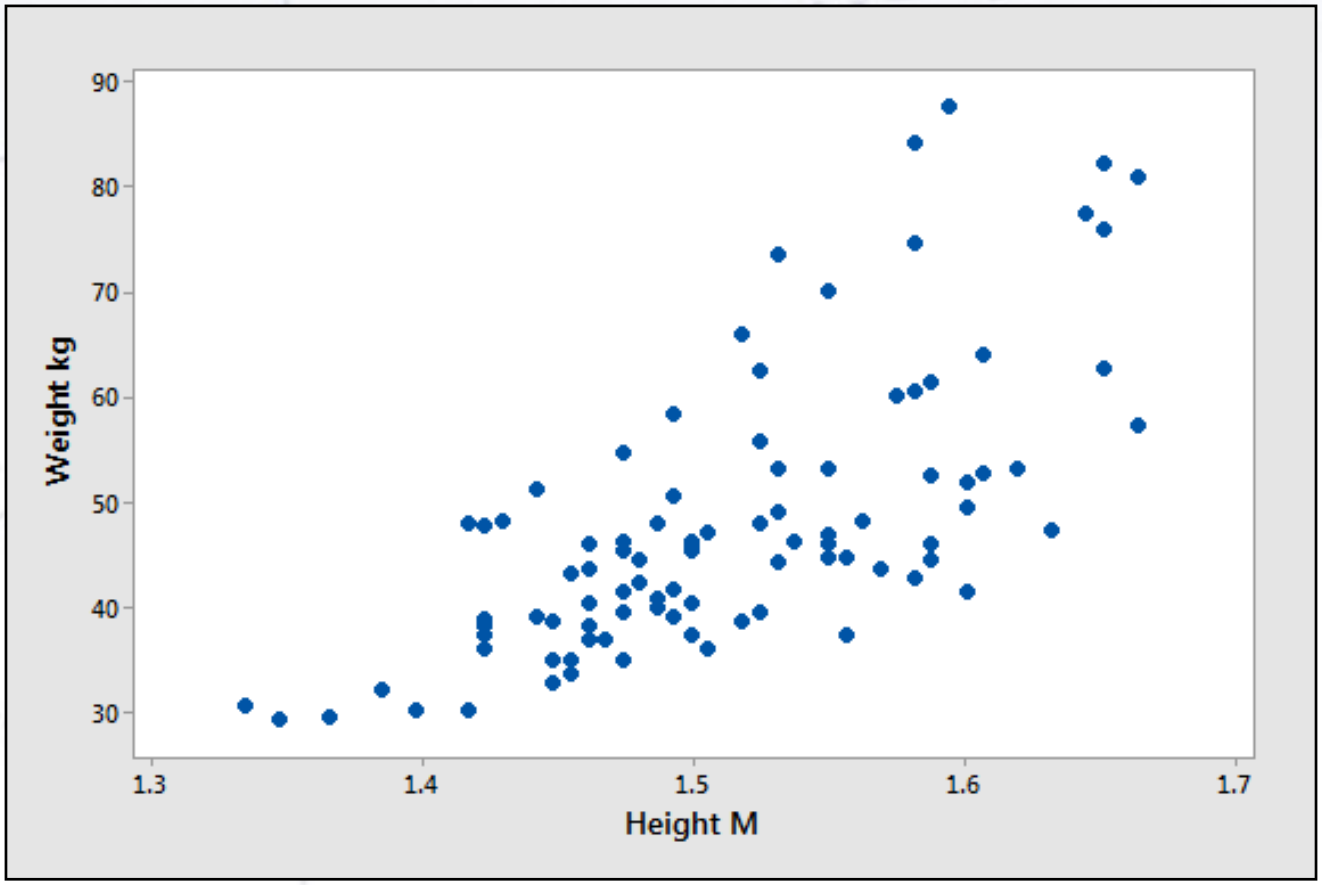


"Statistics is merely a quantisation of common sense - Machine Learning is a sharpening of it!"

PCA overview

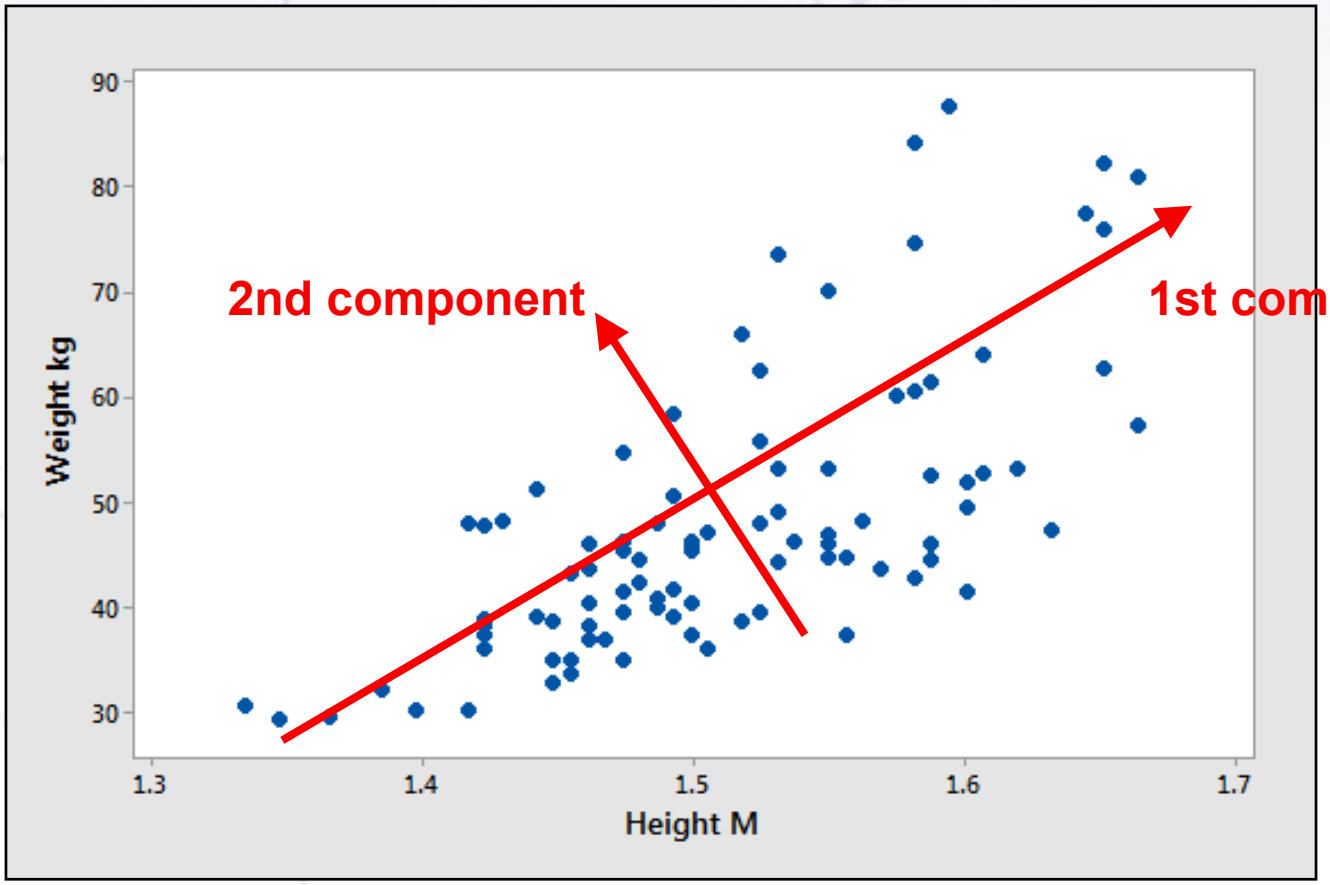
Consider data which have correlations, here in 2D (for visualisation), but potentially in (very) high dimension.

We want to apply a PCA to this data, to reduce dimensionality!



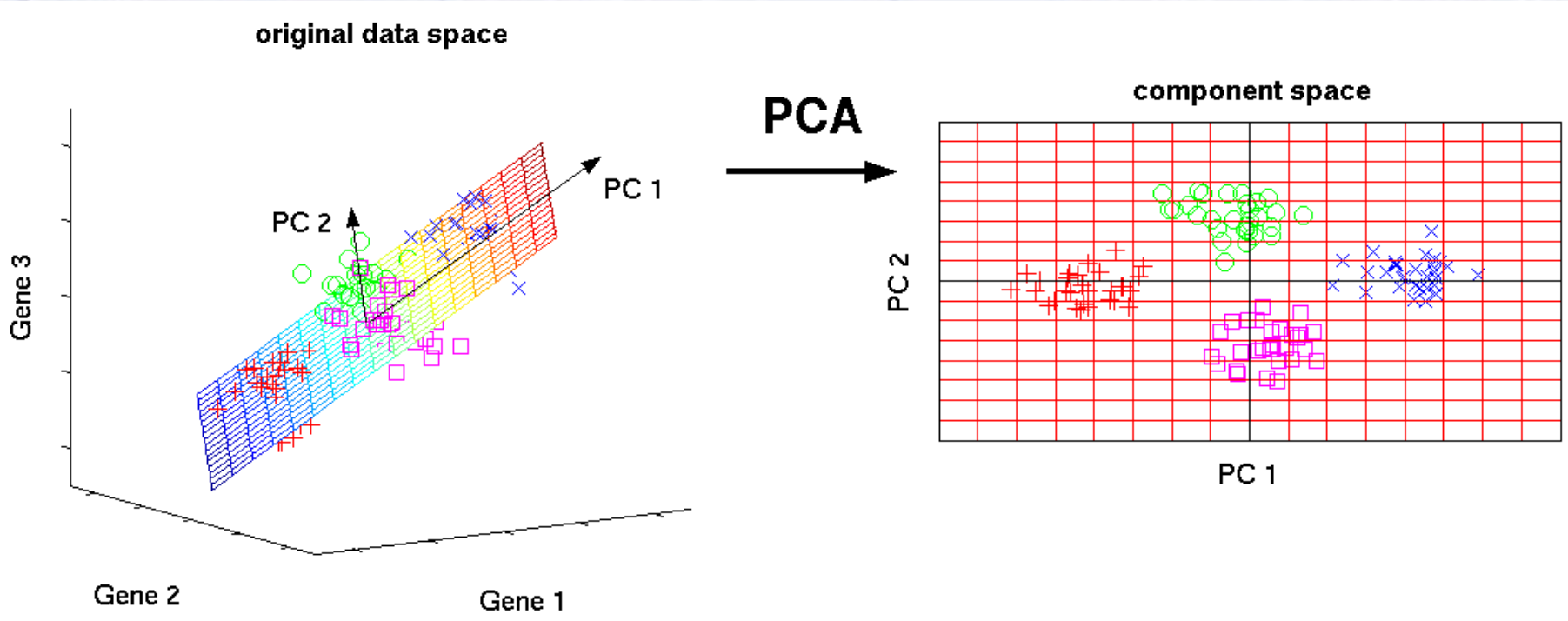
PCA overview

Find the direction, which has the maximum variance, i.e. “best along the direction of the data”.
The effective way to do this, is to find the eigenvectors and eigenvalues, and rank the eigenvectors (i.e. directions) according to eigenvalues.



PCA overview II

It is hard to illustrate the high dimensional cases, but here is an attempt at seeing 3D points reduced to 2D points by PCA.

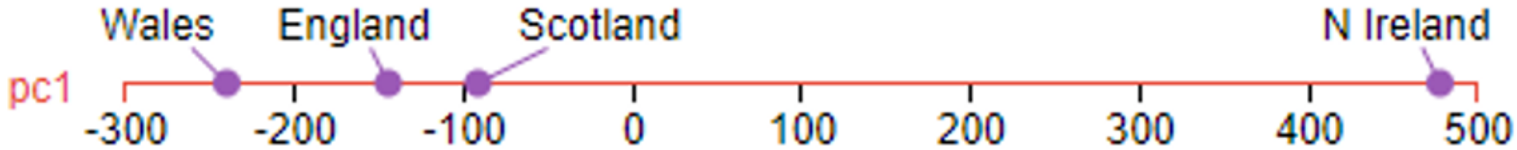


Essentially, one finds the two (orthogonal) directions, which approximates the data best, and "throw away" all the other dimensions in this new space.

17-dimensional PCA

Considering the diet of UK parts, the PCA approach (again) clearly shows structure:

	England	N Ireland	Scotland	Wales
Alcoholic drinks	375	135	458	475
Beverages	57	47	53	73
Carcase meat	245	267	242	227
Cereals	1472	1494	1462	1582
Cheese	105	66	103	103
Confectionery	54	41	62	64
Fats and oils	193	209	184	235
Fish	147	93	122	160
Fresh fruit	1102	674	957	1137
Fresh potatoes	720	1033	566	874
Fresh Veg	253	143	171	265
Other meat	685	586	750	803
Other Veg	488	355	418	570
Processed potatoes	198	187	220	203
Processed Veg	360	334	337	365
Soft drinks	1374	1506	1572	1256
Sugars	156	139	147	175



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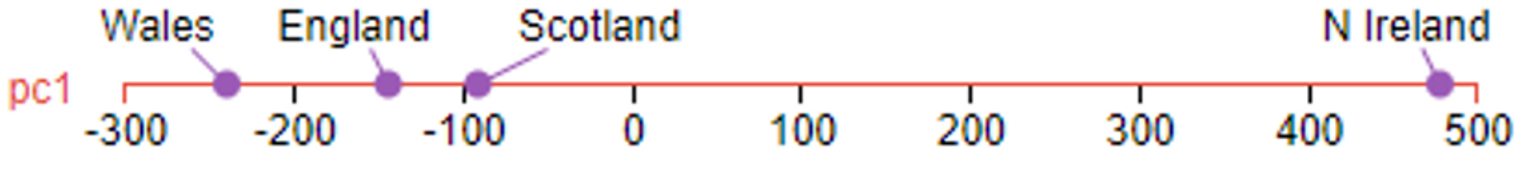

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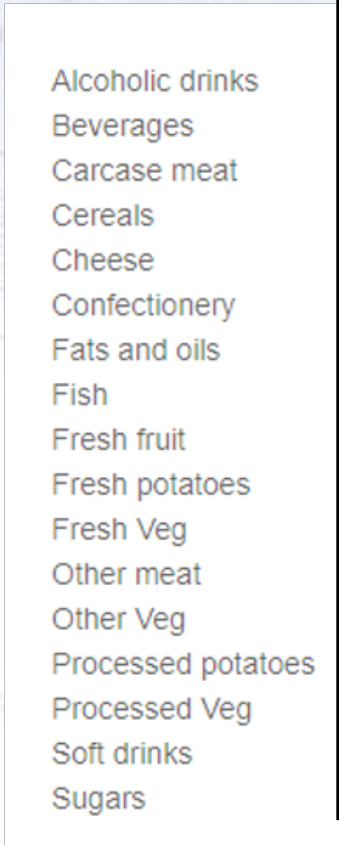
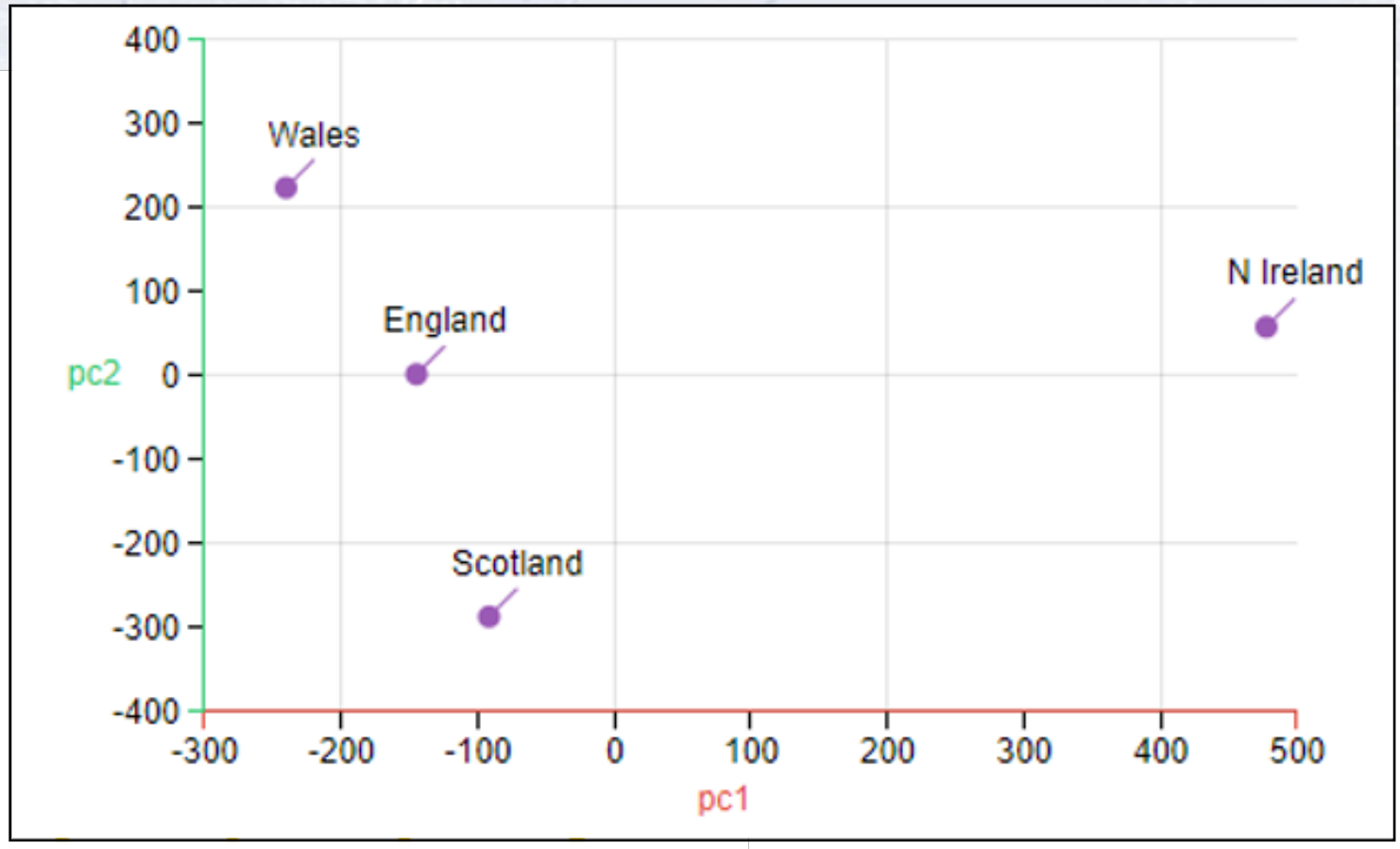
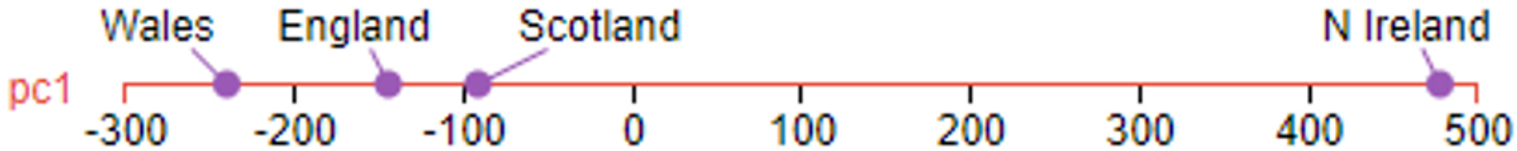
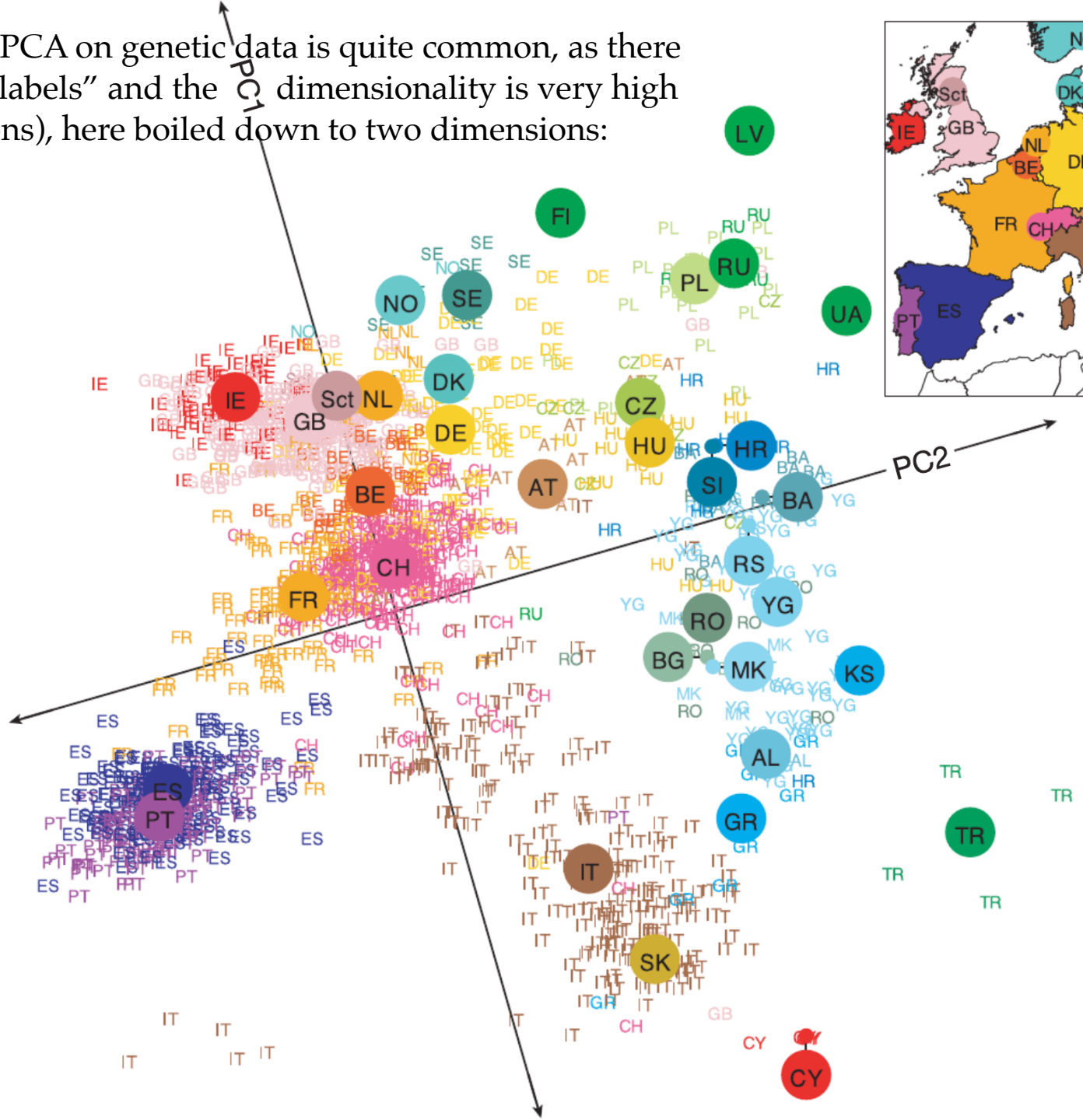


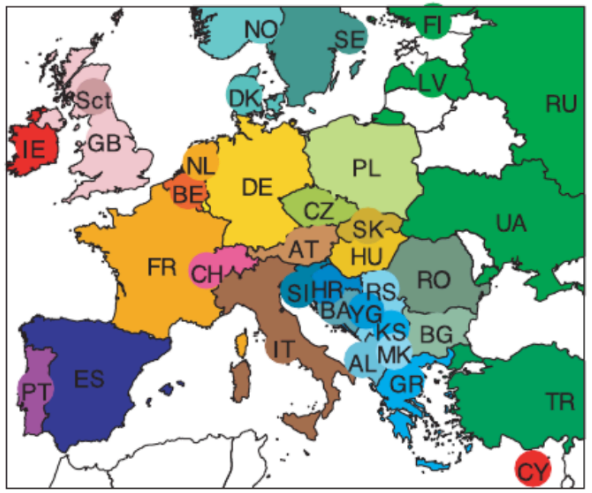




PCA example

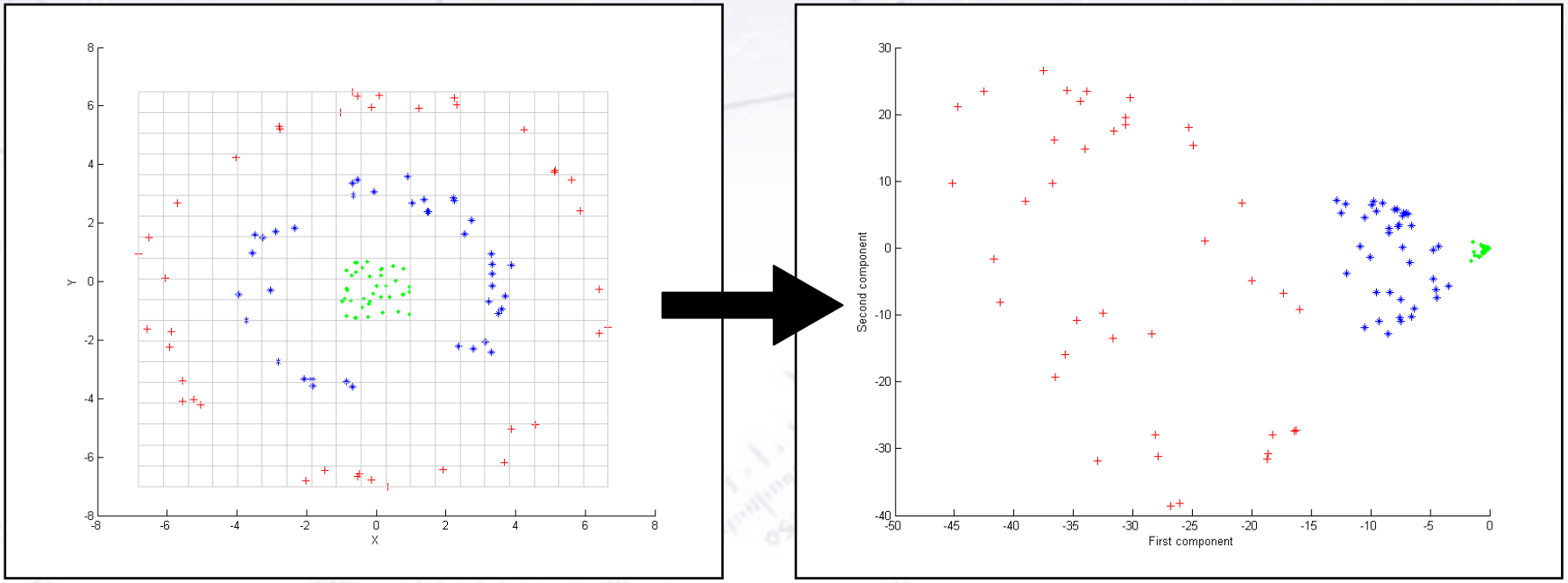
Using PCA on genetic data is quite common, as there is no "labels" and the dimensionality is very high (millions), here boiled down to two dimensions:





Kernel PCA

For non-linear problems, the kernel PCA might be the solution. Here, a (non-linear) kernel is applied before the PCA transformation. This is computationally heavy, but often works well as shown below:



There are other non-linear unsupervised methods, in particular t-SNE and UMAP have gained popularity from their performance.