BIOST 546: Machine Learning for Biomedical Big Data

Ali Shojaie

Lecture 10: Dimension Reduction - Part II
Spring 2017

Recap

- Dimension reduction
- PCA basics

Today's Class

- PCA, continued
- MDS

PCA and Dimension Reduction

Recall the USArrests data:

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> pc.out <- prcomp(USArrests, scale=TRUE)
> print(pc.out$rot)
                PC1        PC2        PC3         PC4
Murder   -0.5358995  0.4181809 -0.3412327  0.64922780
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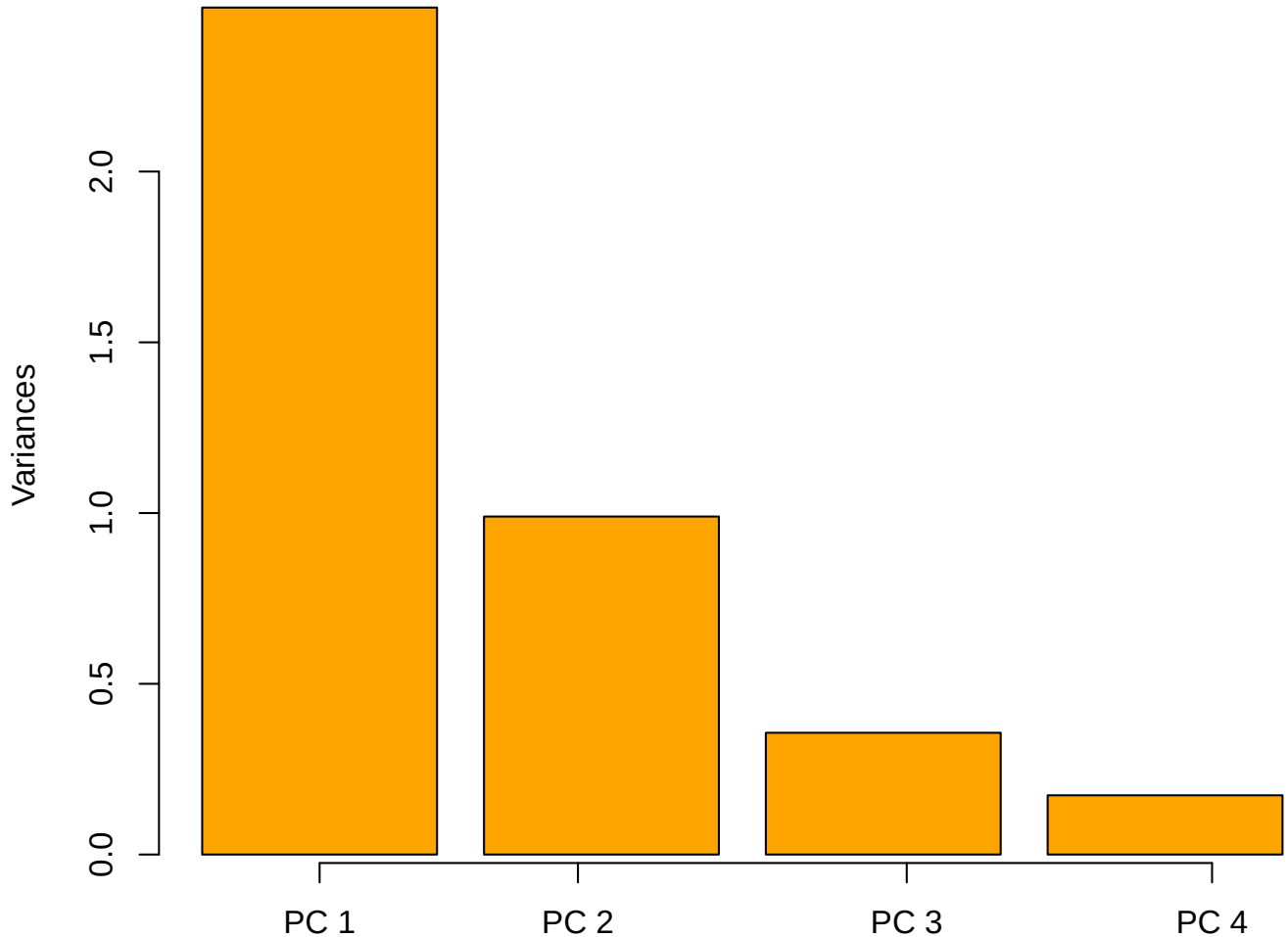
Q: With 4 PC's again have a 4 dimensional space, just as the original data, so why is PCA a dimension reduction technique?

A: Not if we use all 4 PC's! The **dimension reduction** in PCA comes from the fact that often few PC's explain most of the variation in the data.

Variances Explained by Each PC

```
pc.out <- prcomp(USArrests, scale=TRUE, retx=TRUE)
screeplot(pc.out)
```



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- In general, we would like to know, “how much of the information in the data is lost by projecting the observations onto the first M principal components”.
- In other words, “how much of the variance in the data is not contained in the first M principal components”?
- To answer these question, we need to know the proportion of variance explained (PVE) by each principal component.

The Proportion of Variance Explained (ctd.)

- The total variance in the data set (assuming that the variables have been centered to have mean zero) is defined as

$$\sum_{i=1}^{n}\sum_{j=1}^{p} X_{ij}^2$$

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- So, the proportion of variance explained by each principal component loading vector is:

$$\frac{\sum_{i=1}^{n}\left(\sum_{j=1}^{p} X_{ij}w_j\right)^2}{\sum_{i=1}^{n}\sum_{j=1}^{p} X_{ij}^2}$$

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Consider the transformation matrix

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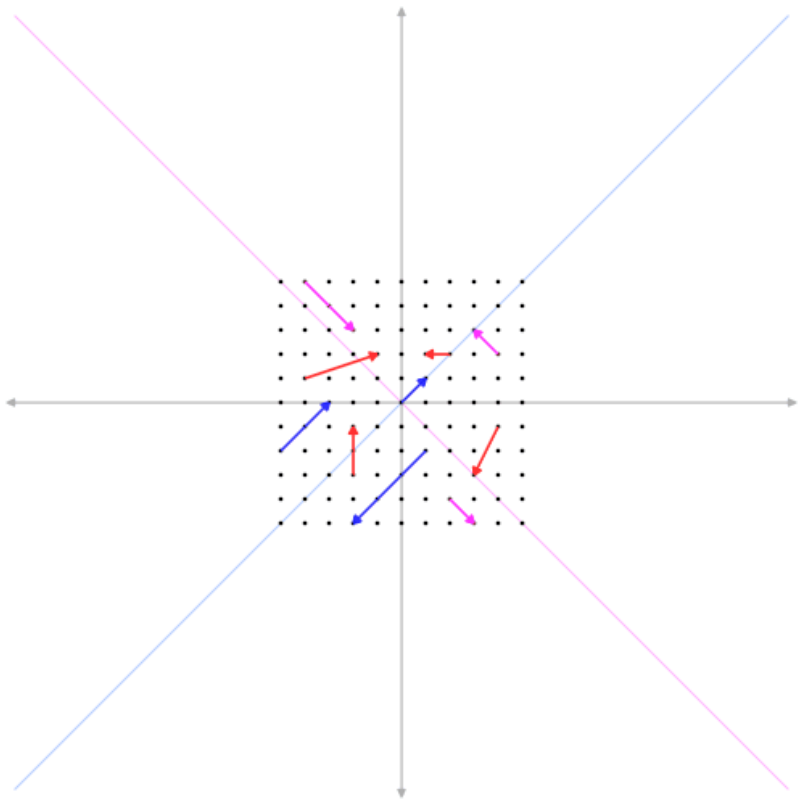

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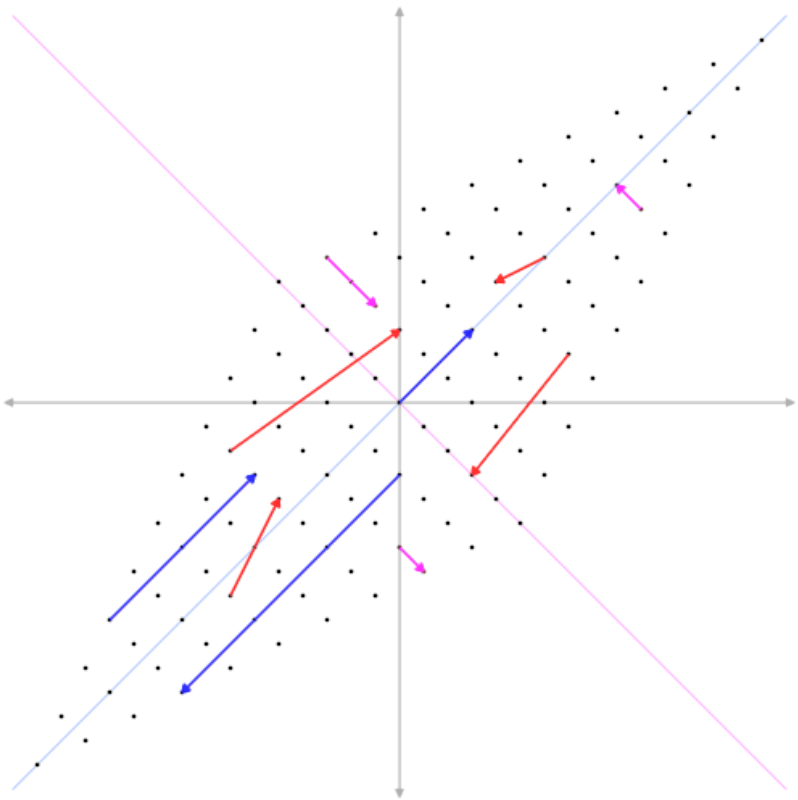

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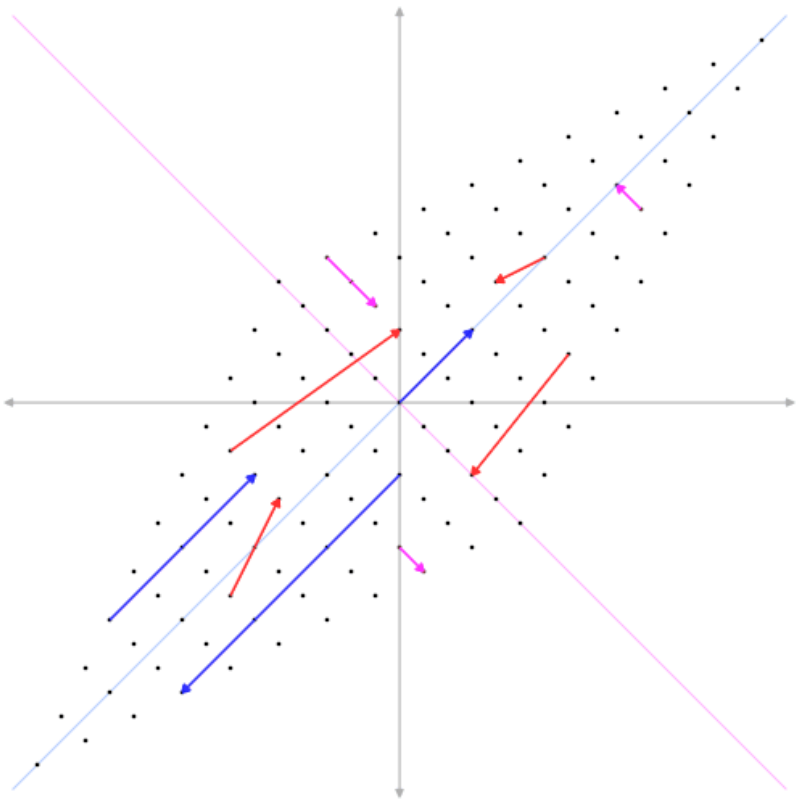

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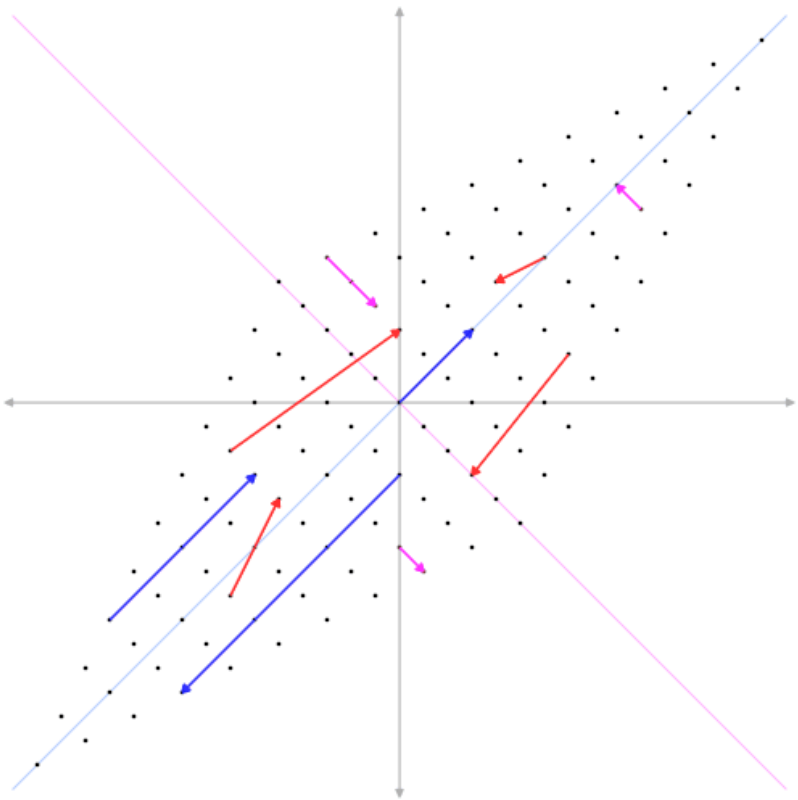

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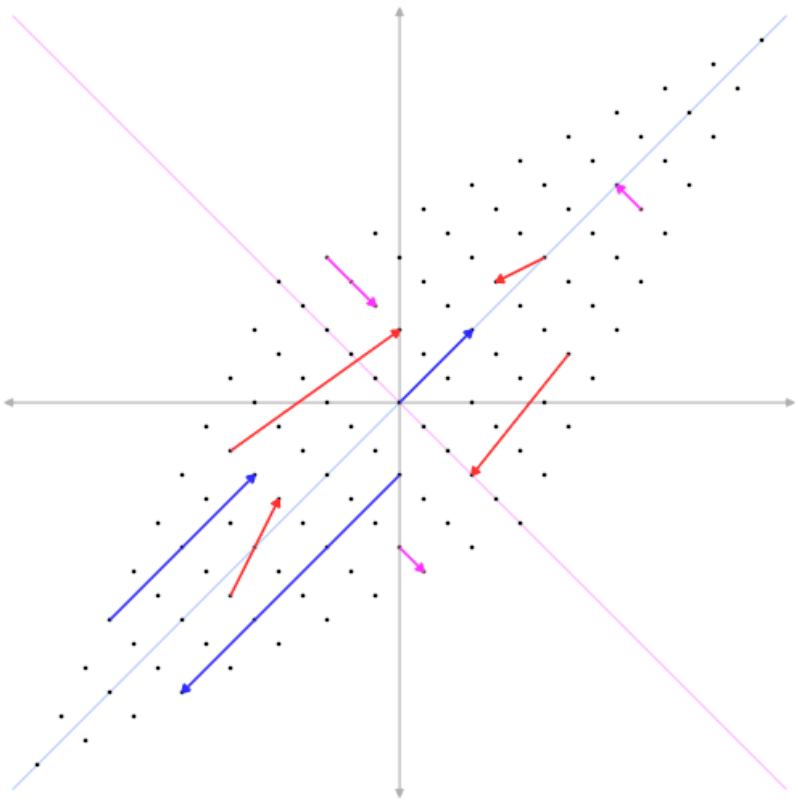
- The length of purple vectors does not change, so $\lambda_w = 1$.



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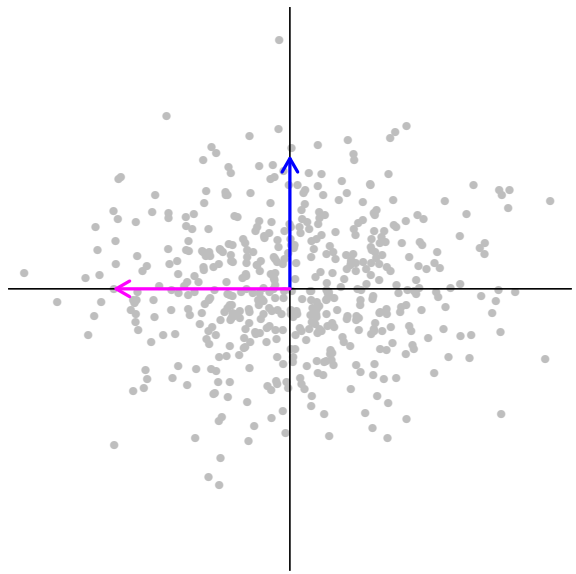
- $\Sigma = I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, i.e., uncorrelated data
  - Here, eigenvectors are $\binom{0}{1}$ and $\binom{-1}{0}$ and the eigenvalues are 1 and 1.



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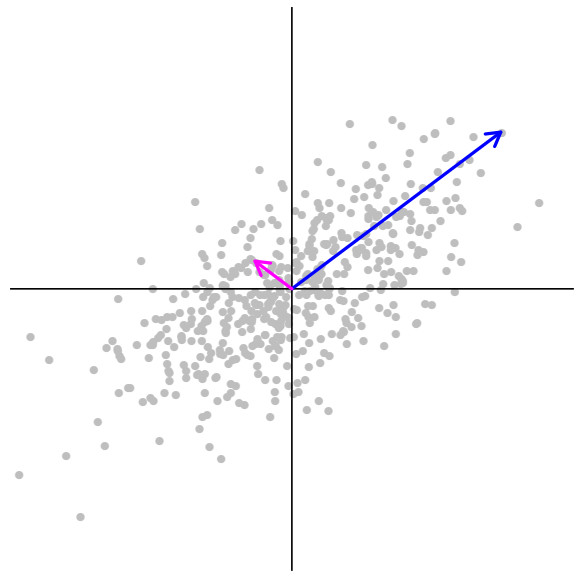
- $\Sigma = \begin{bmatrix} 1 & 0.7 \\ 0.7 & 1 \end{bmatrix}$, i.e., cor $= 0.7$
  - Here, eigenvectors are $\begin{pmatrix} 0.7 \\ 0.7 \end{pmatrix}$ and $\begin{pmatrix} -0.7 \\ 0.7 \end{pmatrix}$ and the eigenvalues are 1.7 and 0.3.



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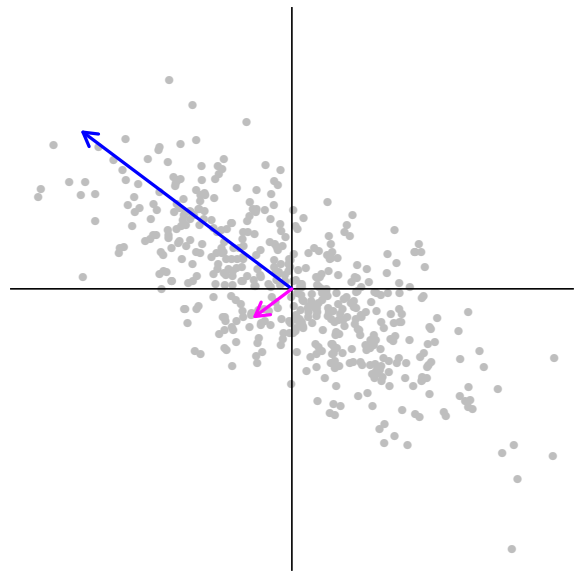

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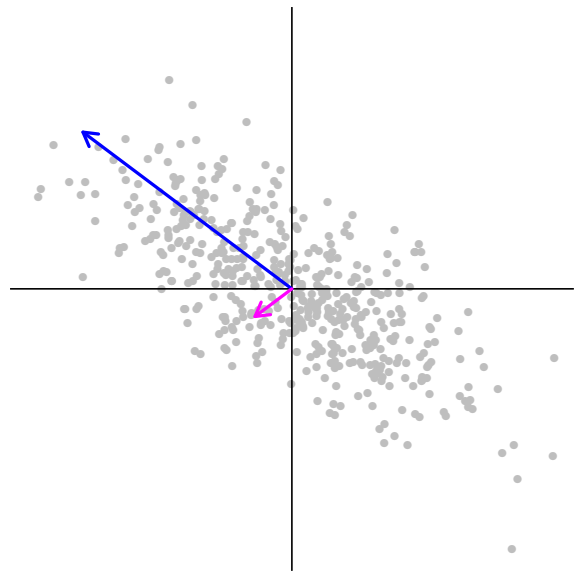

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$\Rightarrow$ PC loadings are eigenvectors of the covariance matrix.

Variances Explained by Each PC

- Let's look at the variances for each of the PC's:

Variance	PC1	PC2	PC3	PC4
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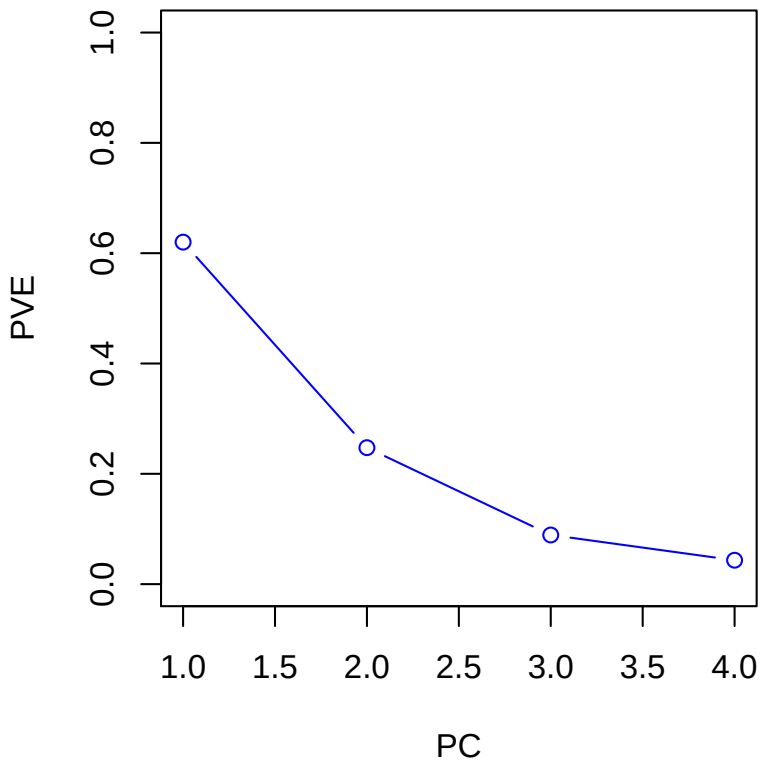
	0.620	0.247	0.089	0.043

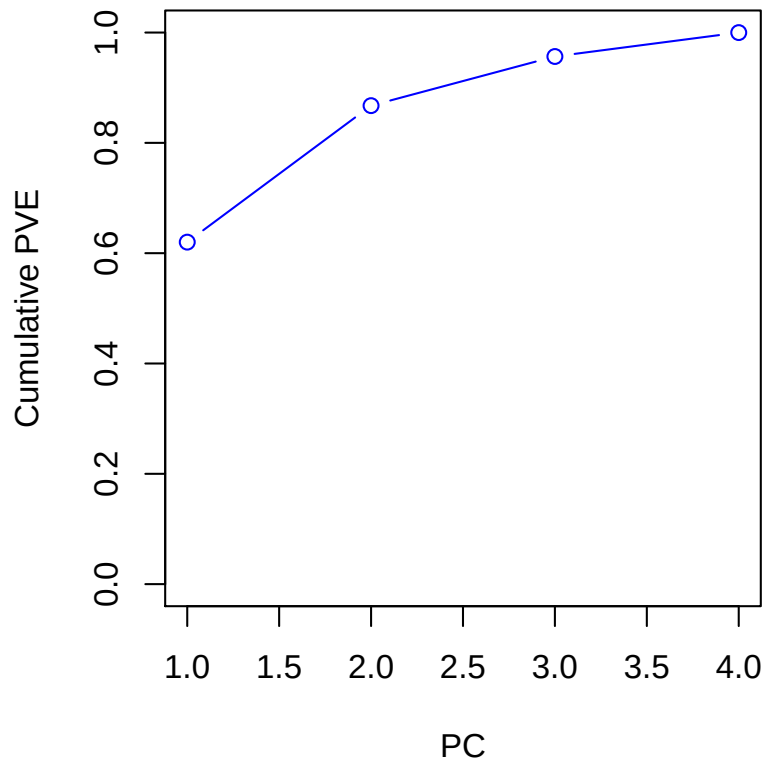
- We can see that the first 2 PC's explain 87% of the variance in the data.

Scree Plots

- We can plot the PVE as well as the cumulative PVE:

```
plot((pc.out$sdev^2)/sum(pc.out$sdev^2), xlab="PC",
     ylab="PVE", ylim=c(0, 1), type='b')
plot(cumsum(pc.out$sdev^2)/sum(pc.out$sdev^2), xlab="PC",
    ylab="Cumulative PVE", ylim=c(0, 1), type='b')
```





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- On the other hand, if we use too many PC's, we don't get the benefits of dimension reduction (e.g. in visualization and prediction).
- We want to use the smallest number of PC's that would give us a "good" understanding of the data.
- Unfortunately, like many other questions in unsupervised learning, there is no easy answer to this question.

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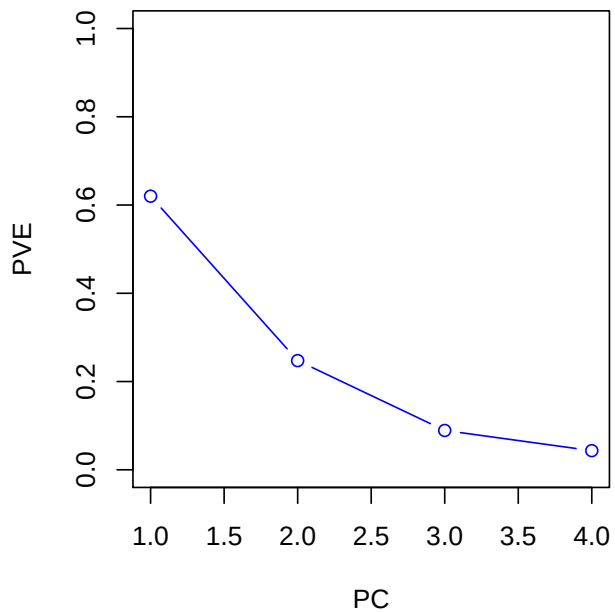

PCA in High Dimensions: NCI60 Data

- The dataset includes gene expression data for 6830 genes from 64 cancer samples (from different cancer subtypes)
- Data can be downloaded form
  `http://www-stat.stanford.edu/~tibs/ElemStatLearn/`
- Missing values have been imputed
- For this analysis (and to simplify the plots), I have removed 5 subtypes with only 1 samples:
  `UNKNOWN, K562B-repro, K562A-repro, MCF7A-repro, MCF7D-repro`
- Let's perform PCA on this data!

PCA in High Dimensions: NCI60 Data

- First, which one of these datasets should we use?

```
> dat.1 <- read.table('nci-mod.data')
> dim(dat.1)
[1] 6830   59
> dat.2 <- t(dat.1)      #transposing the data
> dim(dat.2)
[1]   59 6830
```

- How many PC's will we get from applying PCA to `dat.1`? How about `dat.2`?
- What's the difference? Which one should we use?

PCA in High Dimensions: NCI60 Data (ctd.)

Let's try both!

```
> pc.1 <- prcomp(dat.1, scale=TRUE, retx=TRUE)
> pc.2 <- prcomp(dat.2, scale=TRUE, retx=TRUE)

> dim(pc.1$rot)
[1] 59 59
> dim(pc.1$x)
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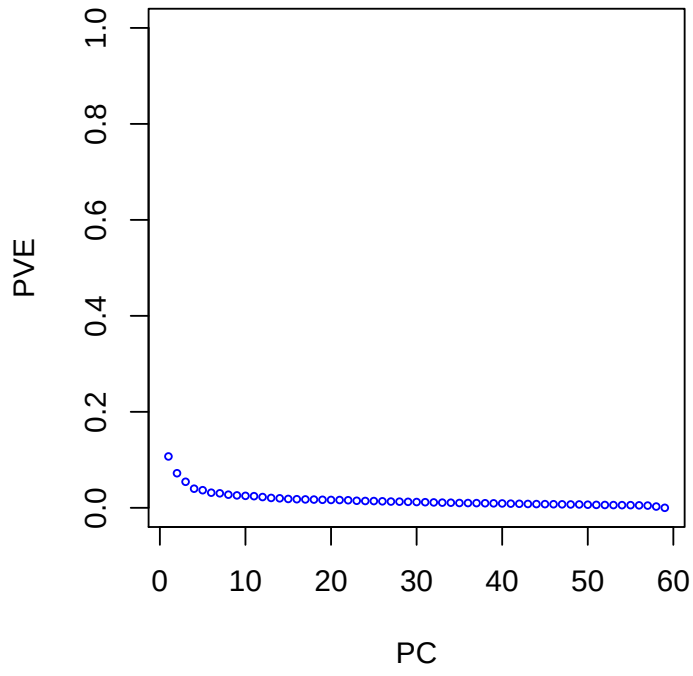
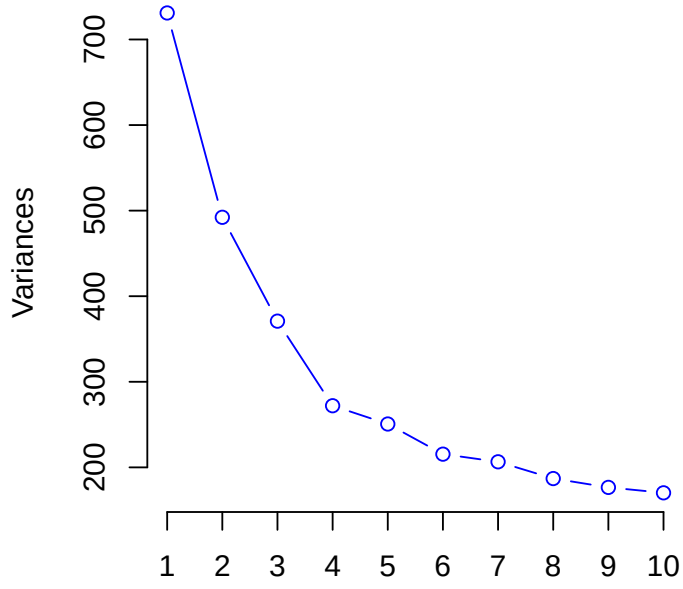
Remarks:

- Each PC loading should be of the same length as the number of variables! (each column of `$rot` is a PC loading)
- There are at most $\min(n,p)$ PC loadings; for $p \gg n$, we have at most n PC's.
- Variables should always be in columns of X!

How Many PC's?

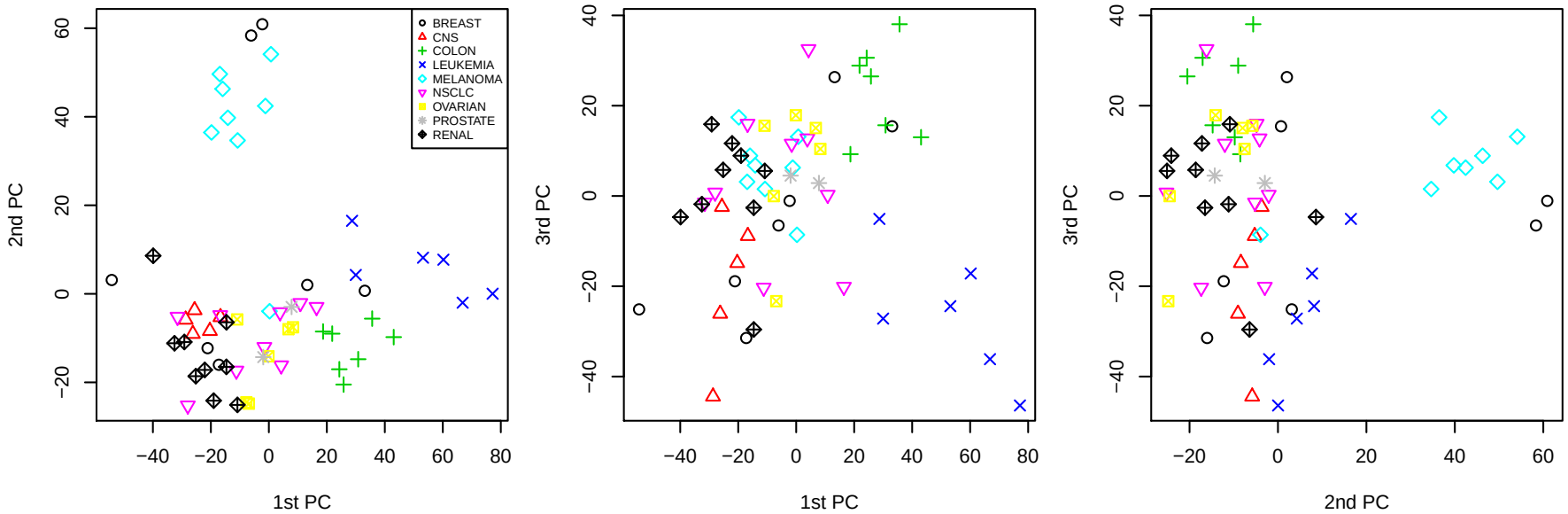
- In high dimensions, the proportion of variance explained for each PC is often small.
- However, the first few PC's usually provide a good projection, and we can usually find an "elbow" in the scree plot. Here, 4 PC's seems to be a good choice.





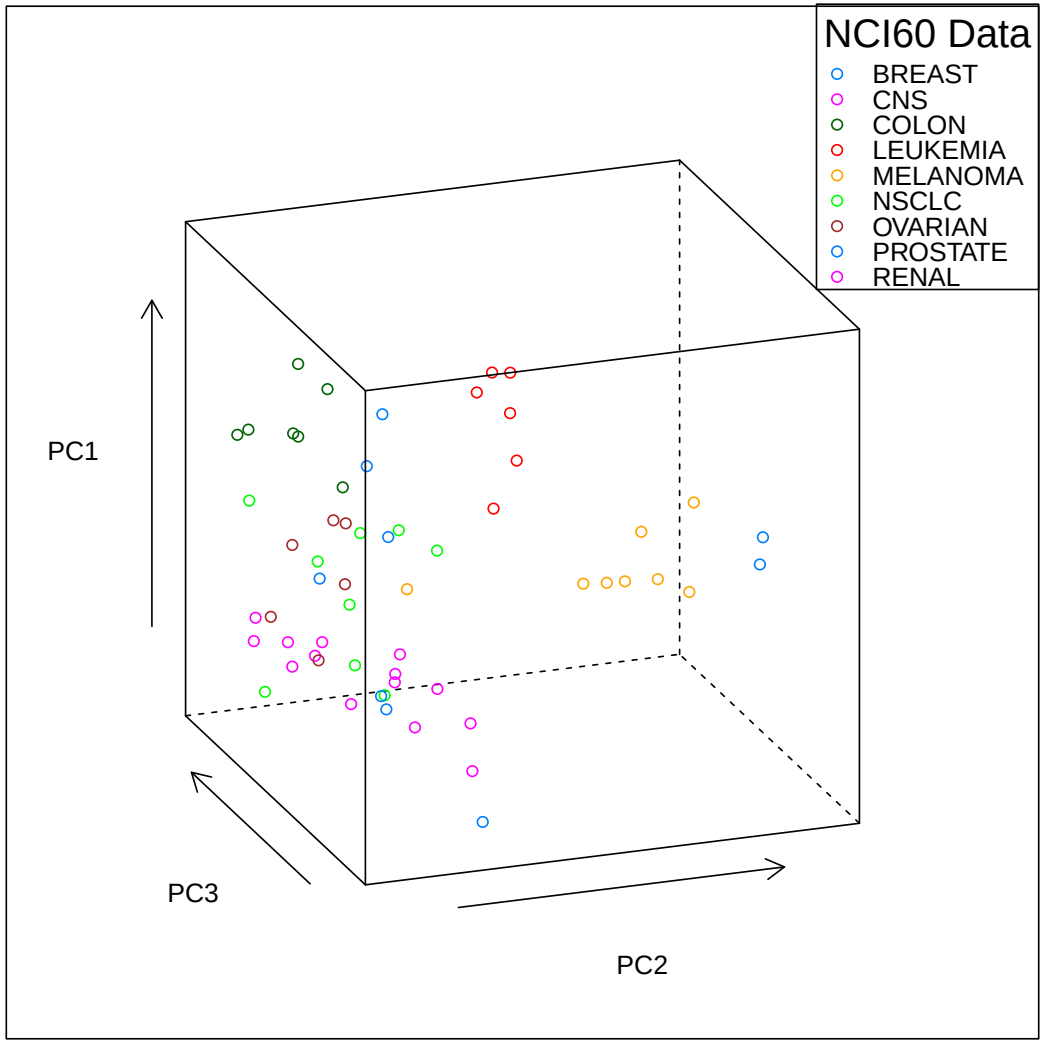
Projecting Samples into the PC Space

- Let's look at the space of the first 3 PC's



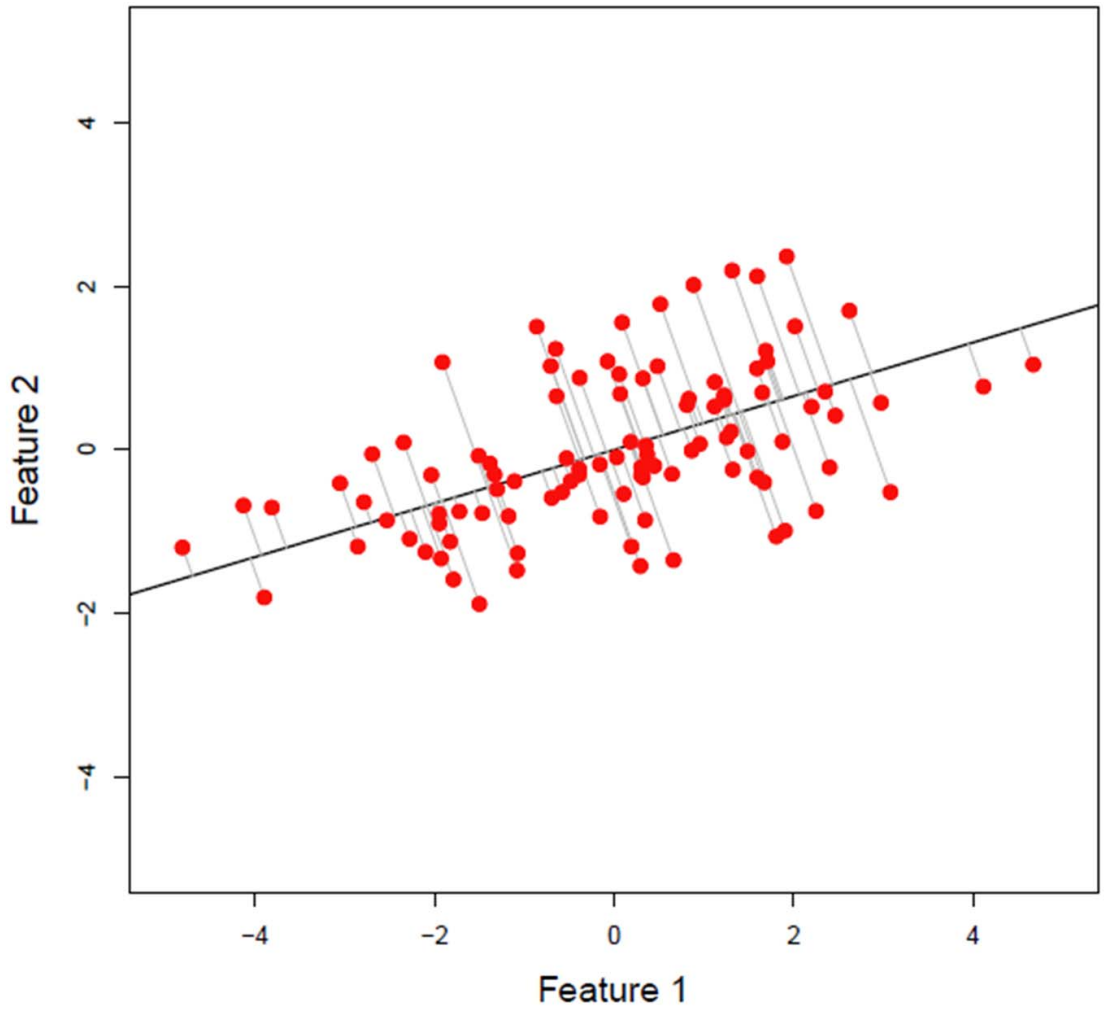
- After projecting the samples into the space of PC's, we can perform clustering or classification in the new space.

A Different View



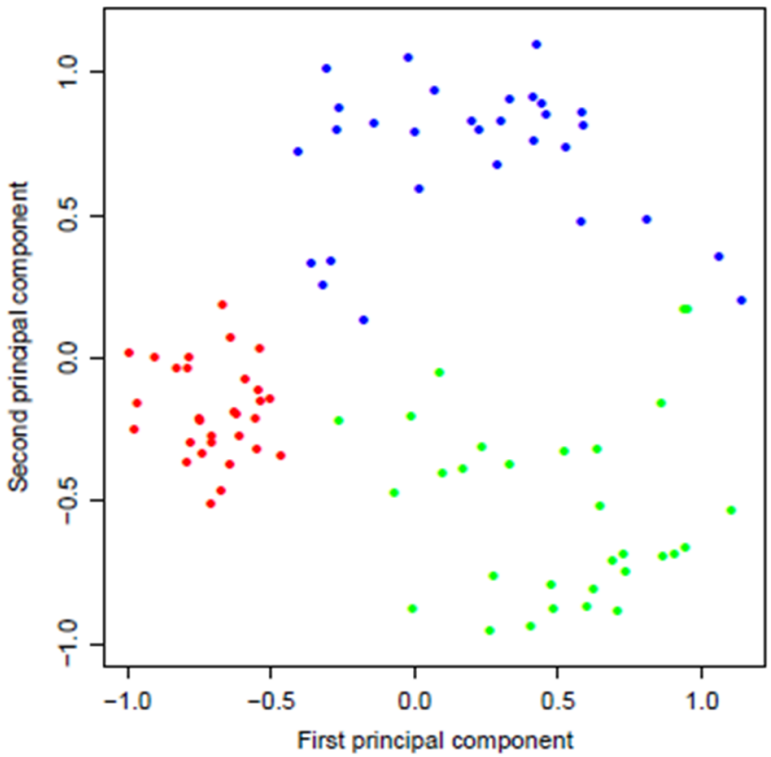
Another look at PCA

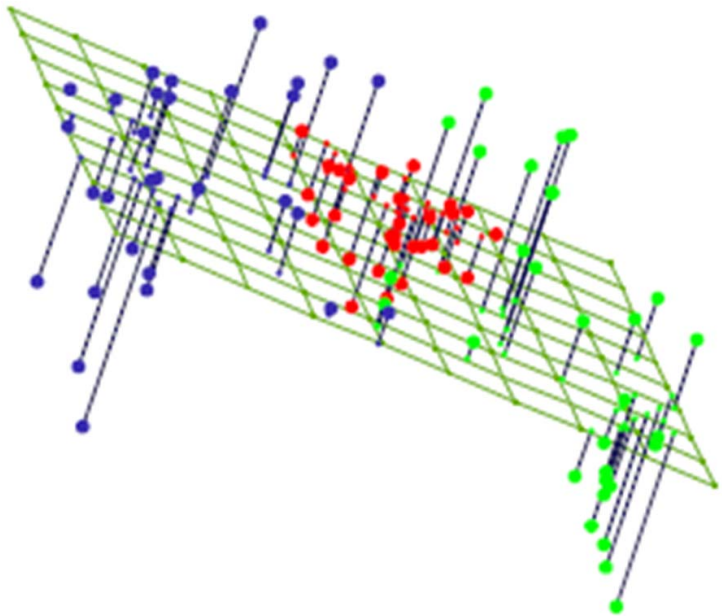
The first PC gives the direction with minimum orthogonal distance from the observations.



Another look at PCA

In general, the PCA Solution finds a *hyperplane* that is closest to the data in terms of squared orthogonal distance.





The PCA Solution

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$$w_m = \max_{w:\|w\|=1} \mathrm{Var}(w^\mathsf{T} X) \text{ and } w_m \perp \{w_1, \ldots w_{m-1}\}.$$

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- This is a well-known problem in mathematics, and its solution is known to be given by the eigenvectors of Σ (i.e. PC loadings are eigenvectors of the covariance matrix).

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  - Here, Λ is a diagonal matrix of eigenvalues.
  - The matrix of eigenvectors V gives the PC loading vectors.
  - The eigenvalues give the amount of variance explained by each eigenvector
  - For symmetric matrices, the eigenvectors are orthogonal: $v_j^{\mathsf{T}} v_k = 0, j \neq k$

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- The `R` function `prcomp` solves the PCA problem using the SVD of X.
- However, there is another function in R for PCA: `princomp`, which solves the PCA problem by finding the eigen-decomposition of X.
- In most cases, these functions produce identical results. However, the method of estimation of PC's in the two functions is different.

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- And finally, remember that this is unsupervised learning!

Be Careful!

nature genetics

Interpreting principal component analyses of spatial population genetic variation

John Novembre[1,3] & Matthew Stephens[1,2]

Nearly 30 years ago, Cavalli-Sforza *et al.* pioneered the use of principal component analysis (PCA) in population genetics and used PCA to produce maps summarizing human genetic variation across continental regions[1]. They interpreted gradient and wave patterns in these maps as signatures of specific migration events[1–3]. These interpretations have been controversial[4–7], but influential[8], and the use of PCA has become widespread in analysis of population genetics data[9–13]. However, the behavior of PCA for genetic data showing continuous spatial variation, such as might exist within human continental groups, has been less well characterized. Here, we find that gradients and waves observed in Cavalli-Sforza *et al.*'s maps resemble sinusoidal mathematical artifacts that arise generally when PCA is applied to spatial data, implying that the patterns do not necessarily reflect specific migration events. Our findings aid interpretation of PCA results and suggest how PCA can help correct for continuous population structure in association studies.

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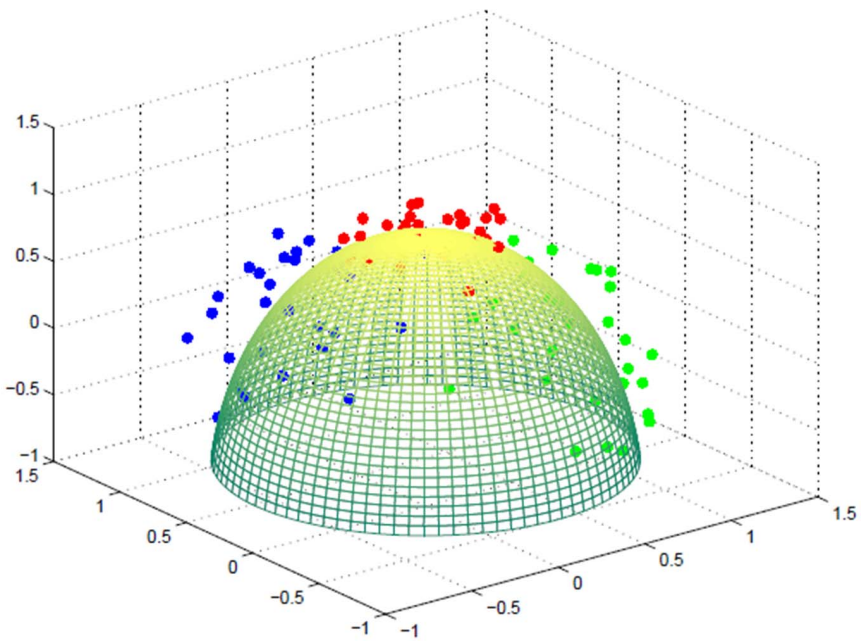

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- More formally, MDS tries to find n vectors of length m, $z_i, i = 1, \ldots, n$, that minimize the following *stress function*:

$$S_M(z_1, z_2, \ldots, z_n) = \sum_{i \neq i'} (d_{ii'} - \|z_i - z_{i'}\|)^2$$

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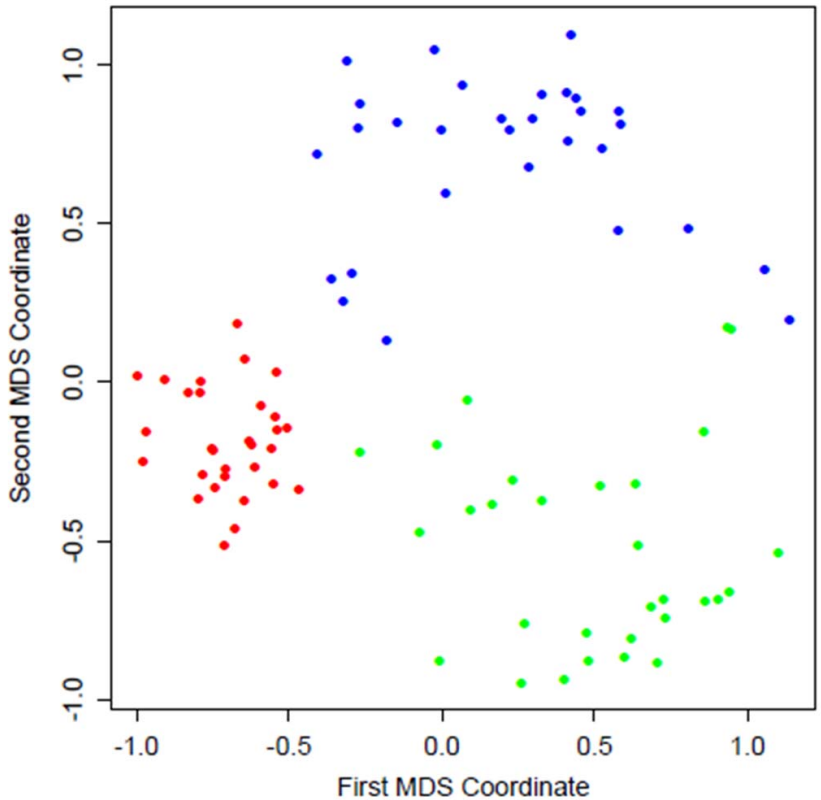
- We can also use rankings instead of distances which gives rise to *non-metric* MDS

MDS Applied to the Half-Sphere Data

In the new space, the points are well separated from each other:



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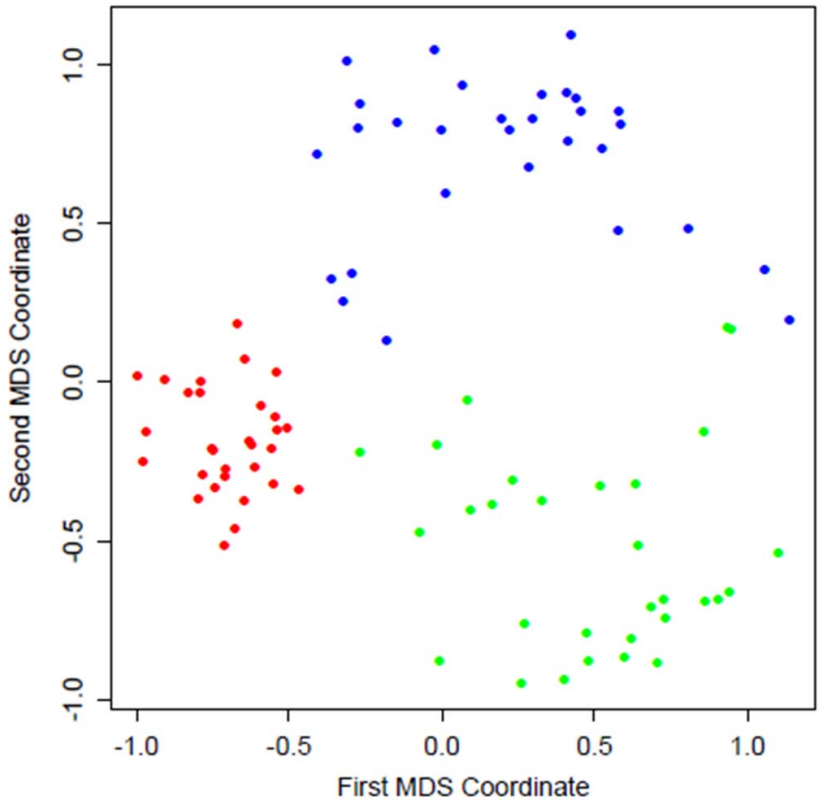

MDS can be very useful if we believe nonlinear distances represent the data better, for instance in ecology, where we can incorporate the phylogenetic tree to define more informative distances

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- The function `cmdscale()` gives the "classic" MDS; `isoMDS()` gives a non-metric (rank-based) MDS

MDS for the `USArrests` Data

```
> dist.1=daisy(USArrests); mds.1=cmdscale(dist.1)
> dist.2=daisy(USArrests, metric="manhattan"); mds.2=cmdscale(dist.2)
>
> x=mds.1[,1]
> y=mds.1[,2]
>
> plot(x, y, xlab = "Coordinate 1", ylab = "Coordinate 2",
xlim = range(x)*1.2, type = "n", main='Euclidean Dist')
> text(x, y, labels = rownames(USArrests), col='blue', cex=0.7)
```

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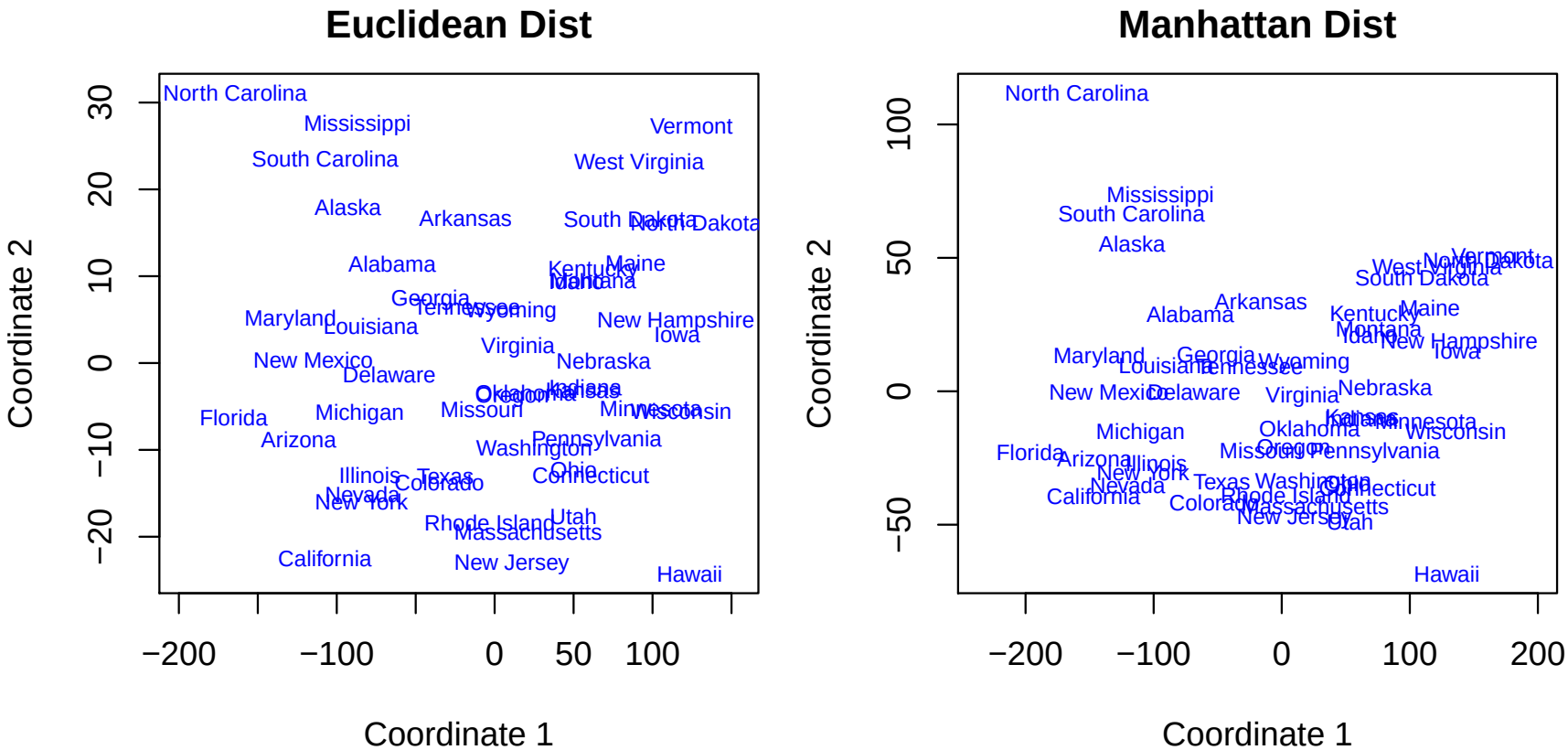
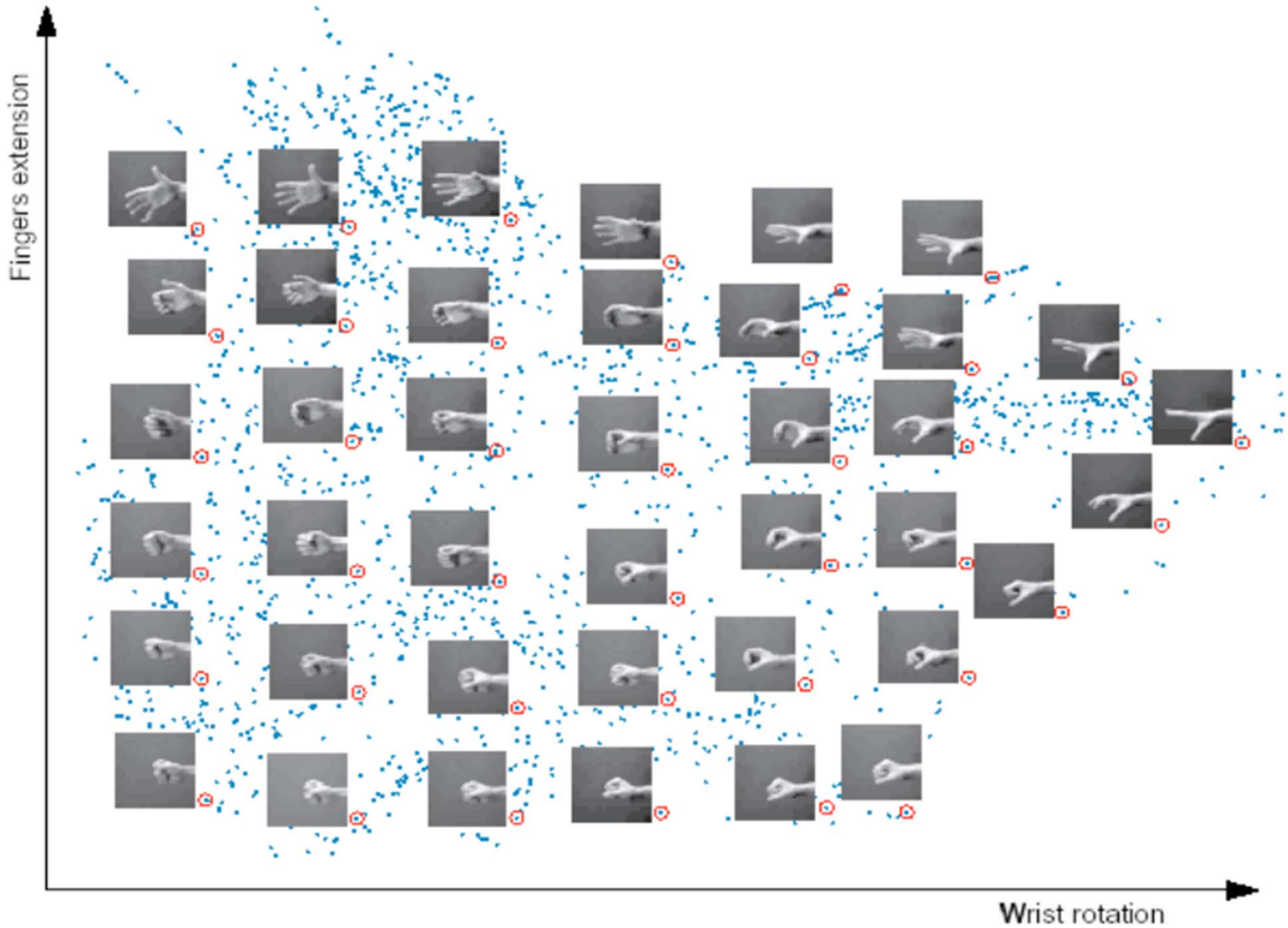


`isoMDS` gives slightly better results in this case!

An Interesting Application



From *Tenenbaum et. al.*

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- Therefore, it is important to be cautious about interpreting the results of unsupervised learning; it is often easy to get excited with some aspects of the study!