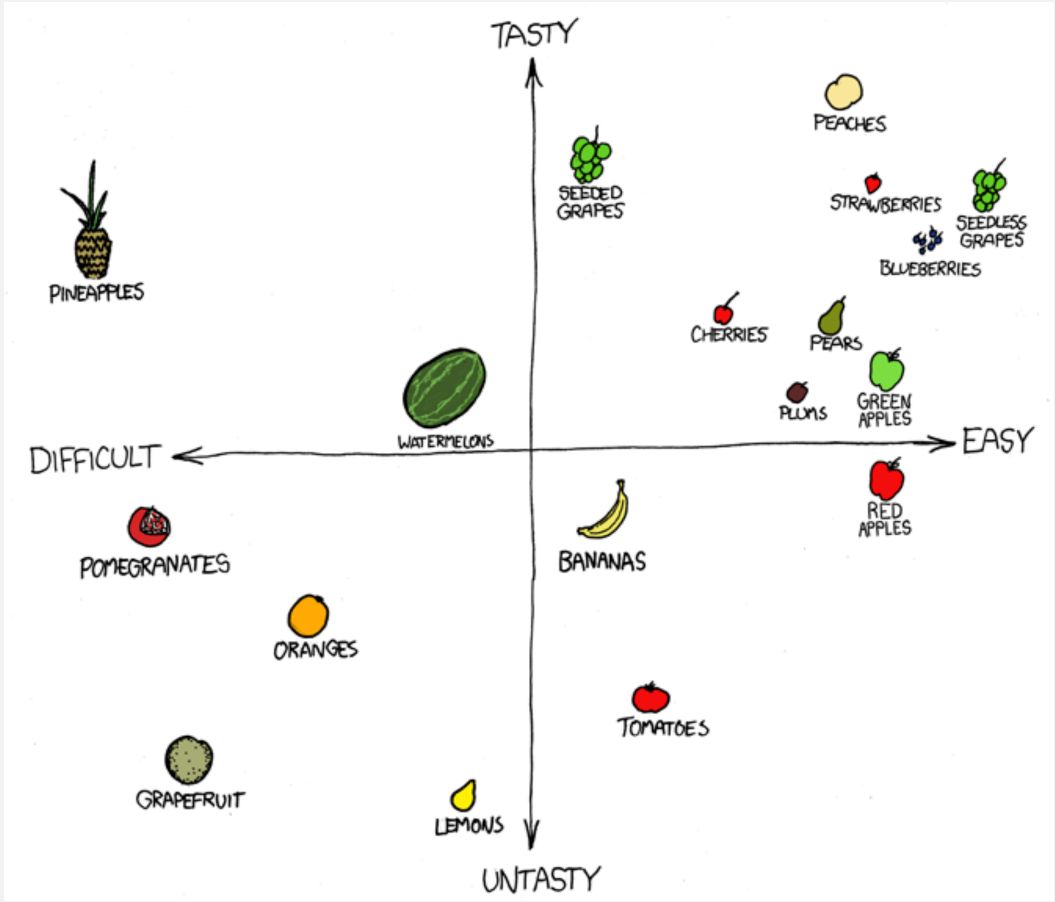
# Dimensionality Reduction

## Principal component analysis

## Corrections for multiple tests

## Biology 683




Heath Blackmon

# What are multiple comparisons/testing

| Horsebean | Linseed | Soybean | Sunflower | Meatmeal | Casein |
|---|---|---|---|---|---|
| 179 | 205 | 189 | 205 | 179 | 205 |
| 216 | 198 | 186 | 198 | 216 | 198 |
| 165 | 212 | 175 | 212 | 165 | 212 |
| 183 | 218 | 193 | 218 | 183 | 218 |
| 169 | 210 | 149 | 210 | 169 | 210 |

$$FWER = 1-(1-alpha)^{m}$$

Family wise error rate

$$FWER = 1-(1-0.05)^{15}$$

45% chance of false positive

# Bonferroni Correction

With the Bonferroni correctio method we divide alpha by number of comparisons being completed.

$$FWER = 1-(1-0.05)^{15}$$

45% chance of false positive

$$0.05/15 = 0.0033333$$

$$FWER = 1-(1-0.00333)^{15}$$

5% chance of false positive

# False Discovery Rate

An alternative approach is to decide what proportion of positive results we are ok with having be false positives. This is a common approach in genetic scans (GWAS). The math is bit more complicated but FDR approaches and Bonferroni methods are available in the p.adjust function.

# Why do we do dimensional reduction?

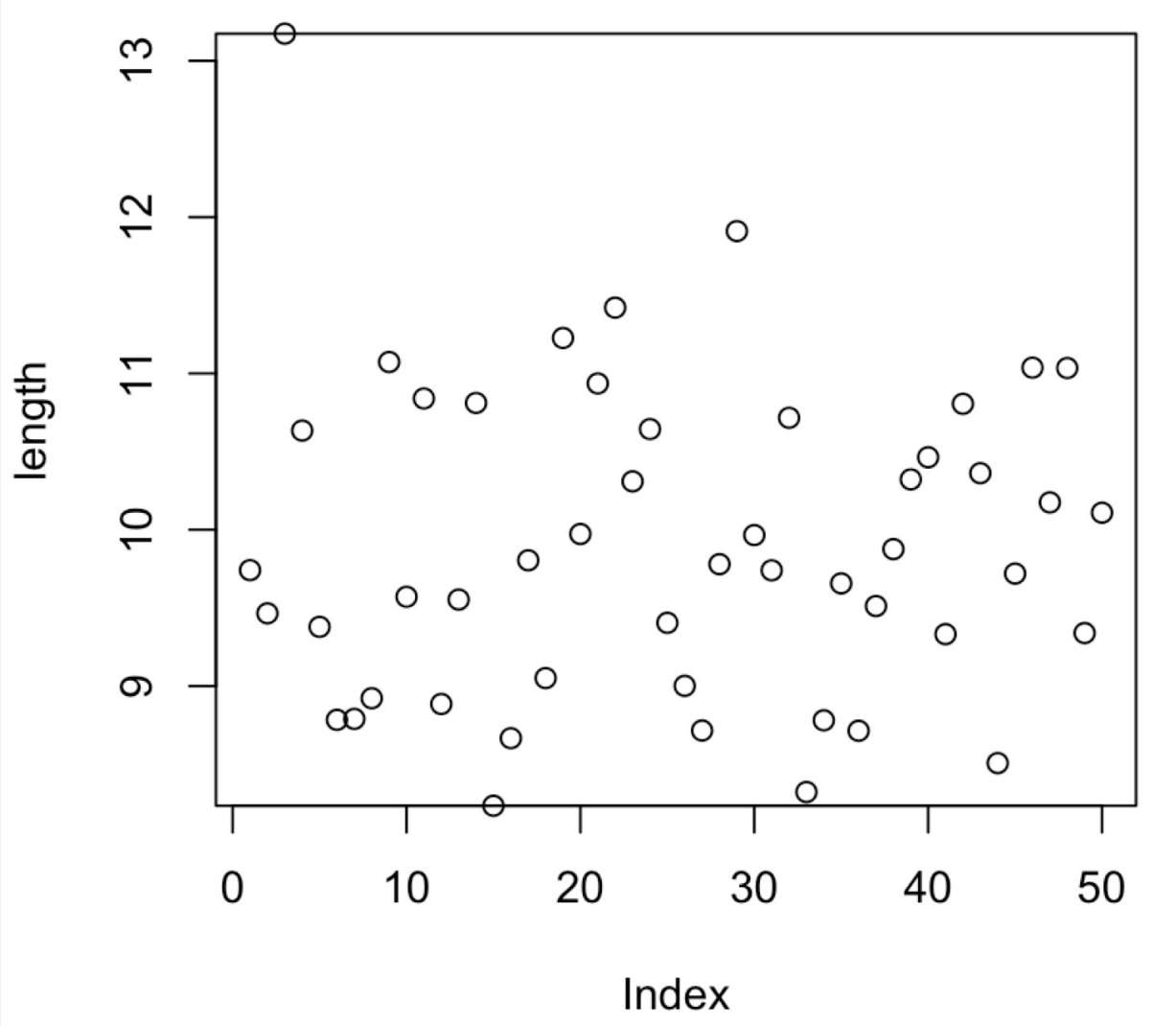
1. Datasets are getting bigger and bigger
2. Understanding our data is often the new bottleneck
3. We can’t think well beyond 3-4 dimensions
4. We can’t illustrate well beyond 2-3 dimensions

# What is principal component analysis

PCA is a dimensional reduction tool that takes many (possibly correlated) measurements and transforms it into a smaller set of uncorrelated measuerments.

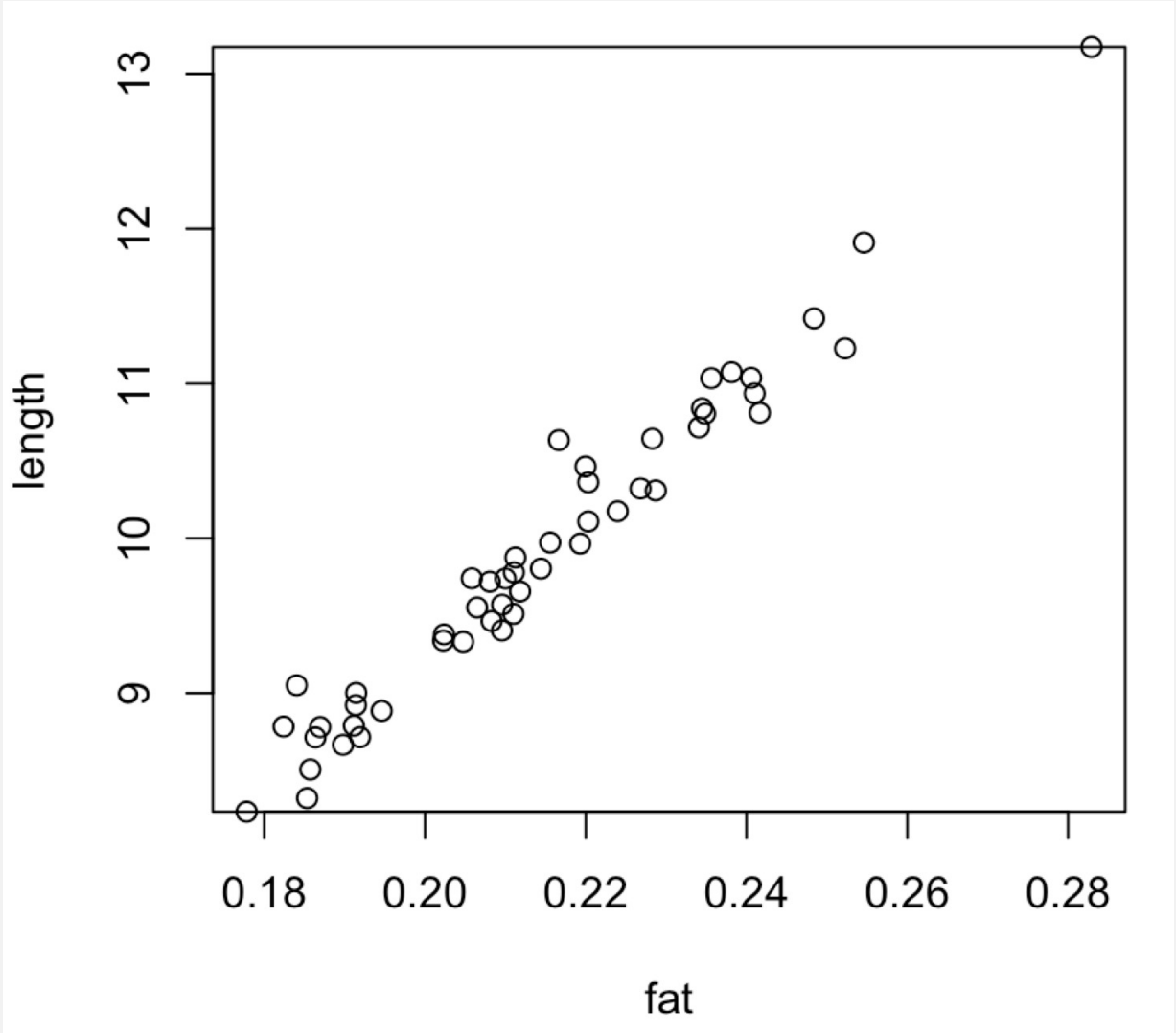
# One dimensional data

| fish_ID | length |
|---|---|
| 379 | 9.74 |
| 430 | 9.47 |
| 55 | 13.17 |
| 434 | 10.63 |
| 147 | 9.38 |
| 497 | 8.78 |
| 127 | 8.79 |
| 362 | 8.92 |
| 107 | 11.07 |
| 116 | 9.57 |
| 414 | 10.84 |
| 232 | 8.89 |
| 193 | 9.55 |
| 80 | 10.81 |
| 283 | 8.23 |
| 68 | 8.67 |
| 341 | 9.8 |
| 288 | 9.05 |
| 200 | 11.23 |
| 62 | 9.97 |
| 69 | 10.94 |
| 466 | 11.42 |
| 400 | 10.31 |
| 83 | 10.64 |
| 106 | 9.4 |
| 280 | 9 |



# Two-dimensional data

| fish_ID | length | fat |
|---|---|---|
| 379 | 9.74 | 0.21 |
| 430 | 9.47 | 0.2 |
| 55 | 13.17 | 0.28 |
| 434 | 10.63 | 0.22 |
| 147 | 9.38 | 0.28 |
| 497 | 8.78 | 0.26 |
| 127 | 8.79 | 0.24 |
| 362 | 8.92 | 0.25 |
| 107 | 11.07 | 0.24 |
| 116 | 9.57 | 0.25 |
| 414 | 10.84 | 0.26 |
| 232 | 8.89 | 0.17 |
| 193 | 9.55 | 0.23 |
| 80 | 10.81 | 0.32 |
| 283 | 8.23 | 0.24 |
| 68 | 8.67 | 0.25 |
| 341 | 9.8 | 0.19 |
| 288 | 9.05 | 0.26 |
| 200 | 11.23 | 0.23 |
| 62 | 9.97 | 0.22 |
| 69 | 10.94 | 0.18 |
| 466 | 11.42 | 0.21 |
| 400 | 10.31 | 0.23 |
| 83 | 10.64 | 0.19 |



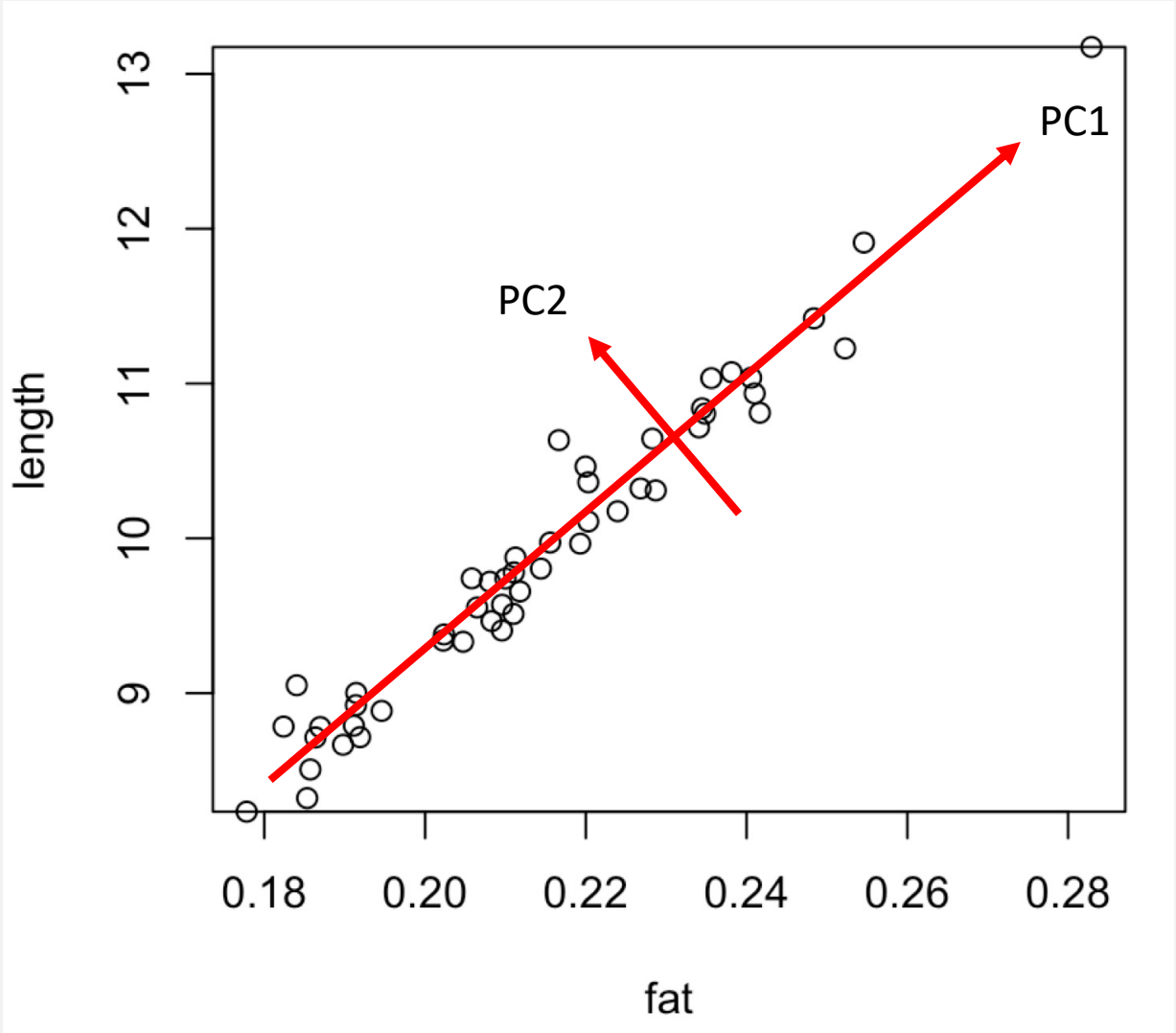
# High dimensional data

| fish_ID | length | fat | m3 | m4 | m5 | m6 | m7 |
|---|---|---|---|---|---|---|---|
| 379 | 9.74 | 0.21 | 9.74 | 0.21 | 0.27 | 1.45 | 2.97 |
| 430 | 9.47 | 0.2 | 9.47 | 0.2 | 4.28 | 0.83 | 1.57 |
| 55 | 13.17 | 0.28 | 13.17 | 0.28 | 7.01 | 1.25 | 4.59 |
| 434 | 10.63 | 0.22 | 10.63 | 0.22 | 15.33 | 0.89 | 2.09 |
| 147 | 9.38 | 0.28 | 9.38 | 0.28 | 5.77 | 0.77 | 2.03 |
| 497 | 8.78 | 0.26 | 8.78 | 0.26 | 18.81 | 0.61 | 1.39 |
| 127 | 8.79 | 0.24 | 8.79 | 0.24 | 8.92 | 1.24 | 2.62 |
| 362 | 8.92 | 0.25 | 8.92 | 0.25 | 0.44 | 0.98 | 2.19 |
| 107 | 11.07 | 0.24 | 11.07 | 0.24 | 16.89 | 0.84 | 2.24 |
| 116 | 9.57 | 0.25 | 9.57 | 0.25 | 13.55 | 1.26 | 3.02 |
| 414 | 10.84 | 0.26 | 10.84 | 0.26 | 11.23 | 0.2 | 0.57 |
| 232 | 8.89 | 0.17 | 8.89 | 0.17 | 2.02 | 0.94 | 1.42 |
| 193 | 9.55 | 0.23 | 9.55 | 0.23 | 5.24 | 1.05 | 2.32 |
| 80 | 10.81 | 0.32 | 10.81 | 0.32 | 6.04 | 0.79 | 2.73 |
| 283 | 8.23 | 0.24 | 8.23 | 0.24 | 0.12 | 0.07 | 0.13 |
| 68 | 8.67 | 0.25 | 8.67 | 0.25 | 2.76 | 0.41 | 0.89 |
| 341 | 9.8 | 0.19 | 9.8 | 0.19 | 9.73 | 1.59 | 2.97 |
| 288 | 9.05 | 0.26 | 9.05 | 0.26 | 15.31 | 0.49 | 1.16 |
| 200 | 11.23 | 0.23 | 11.23 | 0.23 | 3.04 | 1.26 | 3.24 |
| 62 | 9.97 | 0.22 | 9.97 | 0.22 | 13.14 | 0.28 | 0.61 |
| 69 | 10.94 | 0.18 | 10.94 | 0.18 | 5.23 | 0.14 | 0.28 |
| 466 | 11.42 | 0.21 | 11.42 | 0.21 | 6.11 | 0.3 | 0.71 |
| 400 | 10.31 | 0.23 | 10.31 | 0.23 | 2.78 | 0.43 | 1.02 |
| 83 | 10.64 | 0.19 | 10.64 | 0.19 | 10.93 | 0.86 | 1.73 |

What are our options?

# Dimensionality reduction - PCA

| fish_ID | length | fat |
|---|---|---|
| 379 | 9.74 | 0.21 |
| 430 | 9.47 | 0.2 |
| 55 | 13.17 | 0.28 |
| 434 | 10.63 | 0.22 |
| 147 | 9.38 | 0.28 |
| 497 | 8.78 | 0.26 |
| 127 | 8.79 | 0.24 |
| 362 | 8.92 | 0.25 |
| 107 | 11.07 | 0.24 |
| 116 | 9.57 | 0.25 |
| 414 | 10.84 | 0.26 |
| 232 | 8.89 | 0.17 |
| 193 | 9.55 | 0.23 |
| 80 | 10.81 | 0.32 |
| 283 | 8.23 | 0.24 |
| 68 | 8.67 | 0.25 |
| 341 | 9.8 | 0.19 |
| 288 | 9.05 | 0.26 |
| 200 | 11.23 | 0.23 |
| 62 | 9.97 | 0.22 |
| 69 | 10.94 | 0.18 |
| 466 | 11.42 | 0.21 |
| 400 | 10.31 | 0.23 |
| 83 | 10.64 | 0.19 |



# The math behind - PCA

M measurements

N samples

| fish_ID | length | fat | m3 | m4 | m5 | m6 | m7 |
|---|---|---|---|---|---|---|---|
| 379 | 9.74 | 0.21 | 9.74 | 0.21 | 0.27 | 1.45 | 2.97 |
| 430 | 9.47 | 0.2 | 9.47 | 0.2 | 4.28 | 0.83 | 1.57 |
| 55 | 13.17 | 0.28 | 13.17 | 0.28 | 7.01 | 1.25 | 4.59 |
| 434 | 10.63 | 0.22 | 10.63 | 0.22 | 15.33 | 0.89 | 2.09 |
| 147 | 9.38 | 0.28 | 9.38 | 0.28 | 5.77 | 0.77 | 2.03 |
| 497 | 8.78 | 0.26 | 8.78 | 0.26 | 18.81 | 0.61 | 1.39 |

**= X**

nxm matrix

PCA is an Eigendecomposition of $(X^T X)$

$W$ = loadings mxm matrix

$$T = X \cdot W$$

```
pca <- prcomp(X)
pca$x
```

| fish_ID | PC1 | PC2 | PC3 | PC4 | PC5 | PC6 | PC7 |
|---|---|---|---|---|---|---|---|
| 379 | 0.48401035 | 0.3204638 | 0.86441909 | 0.75599341 | 0.19841263 | 0.29382035 | 0.87356767 |
| 430 | 0.92864946 | 0.7321531 | 0.17546787 | 0.22461749 | 0.50242958 | 0.66343818 | 0.82559145 |
| 55 | 0.12804522 | 0.03920335 | 0.59362519 | 0.39215655 | 0.9883746 | 0.92951871 | 0.26687076 |
| 434 | 0.2062225 | 0.21152673 | 0.47047215 | 0.66007816 | 0.71549665 | 0.89006466 | 0.31692619 |
| 147 | 0.85635814 | 0.17733842 | 0.94029393 | 0.11666265 | 0.10601835 | 0.18949868 | 0.42276984 |
| 497 | 0.78104386 | 0.88445893 | 0.45355361 | 0.61294154 | 0.02441031 | 0.3948512 | 0.08124852 |

**= T**

nxm matrix

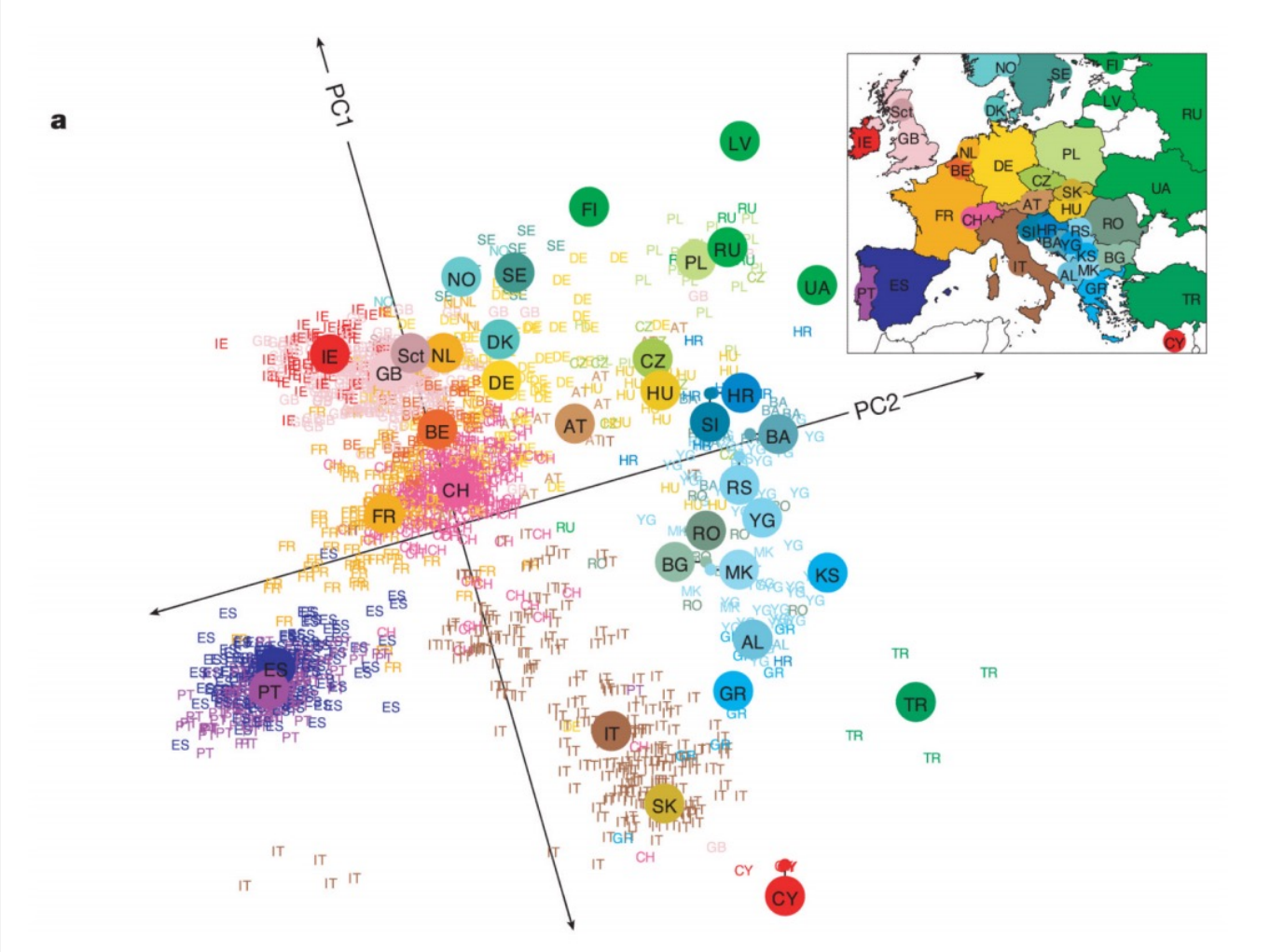
This is T a nxm matrix that has our PC scores. The first column of the matrix will be the one that captures the most variation.

# How do people use PCA

Input data: 500,000 SNP genotypes for 3000 Europeans.

3000 rows
500,000 columns

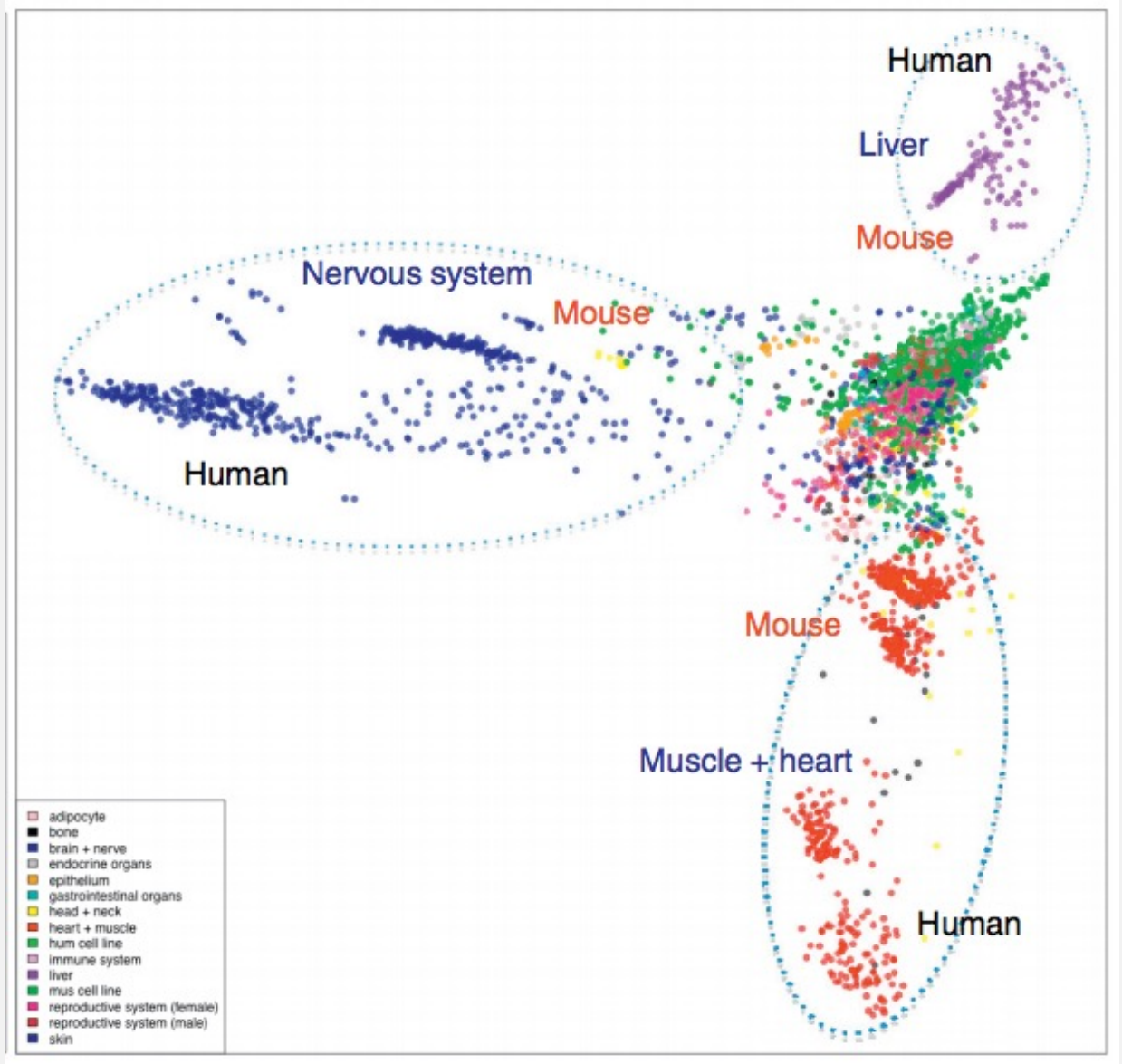
What are PC1 and PC2?



# How do people use PCA

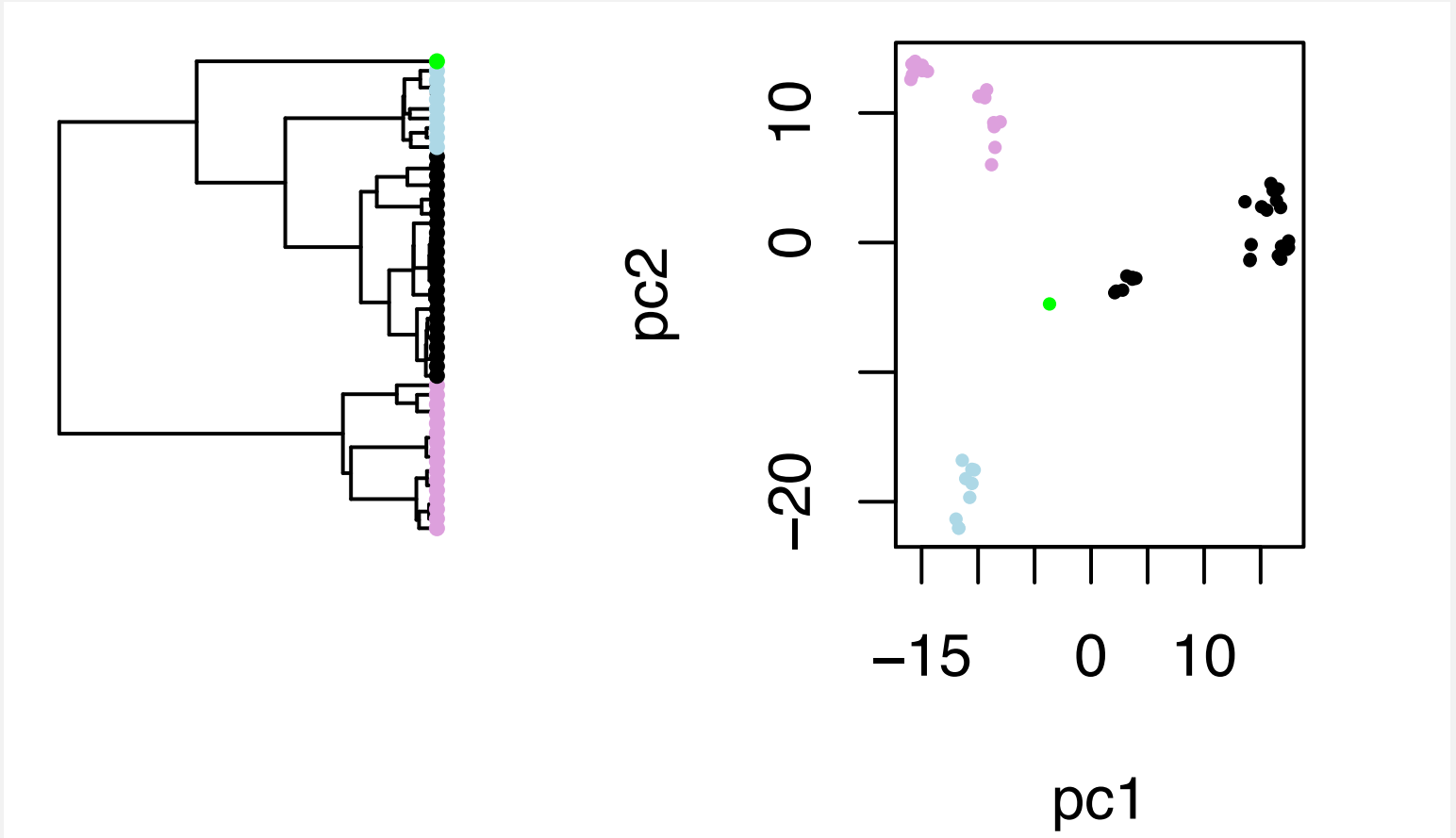
Input data:
Expression level for 1000s of genes
In 100s of cells (color indicates type of cell)

What are the PCs here?



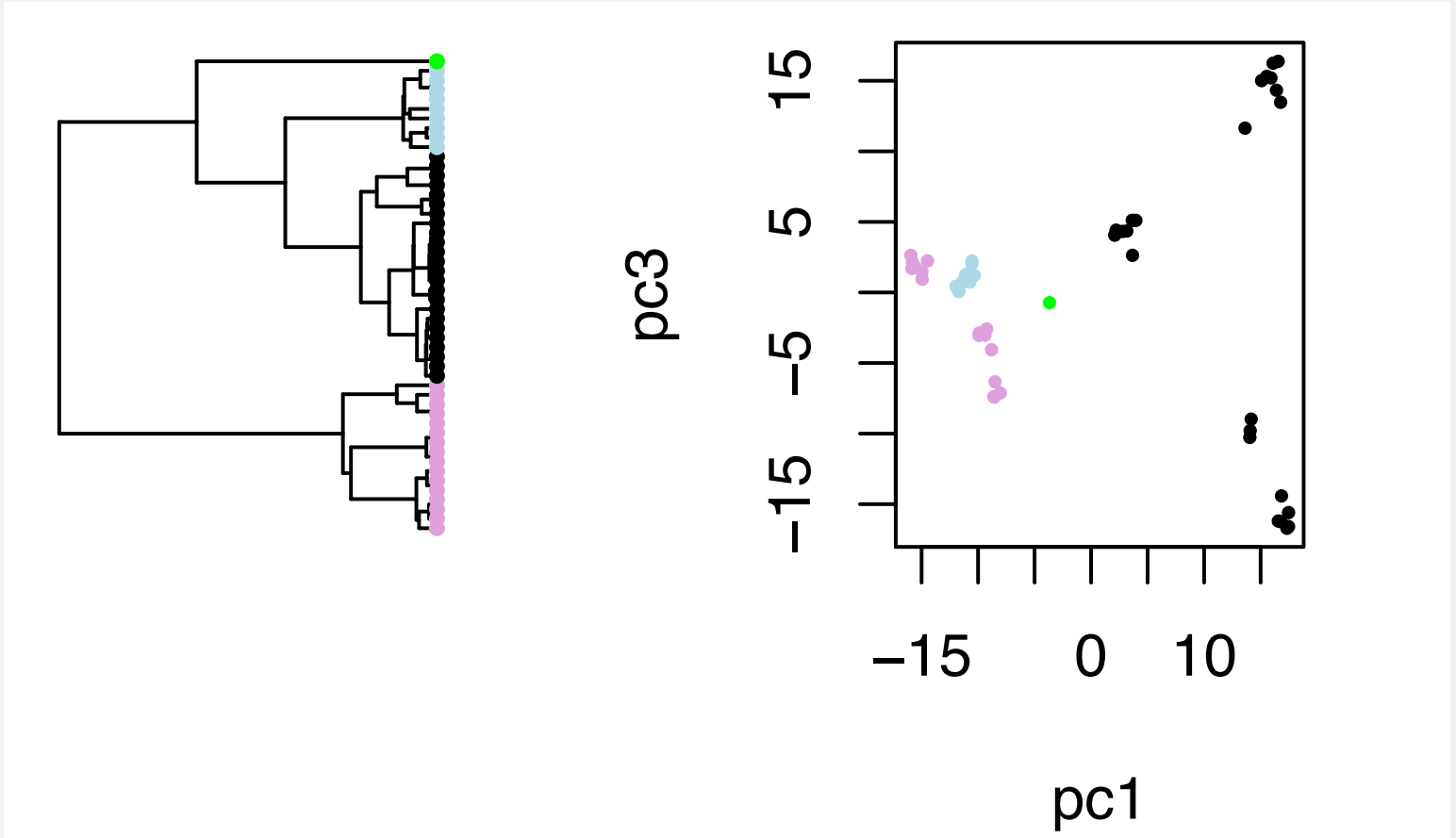
# How do people use PCA

Input data:
Radseq data (genotypes at 100s of loci)
For a large number of species or strains



# How do people use PCA

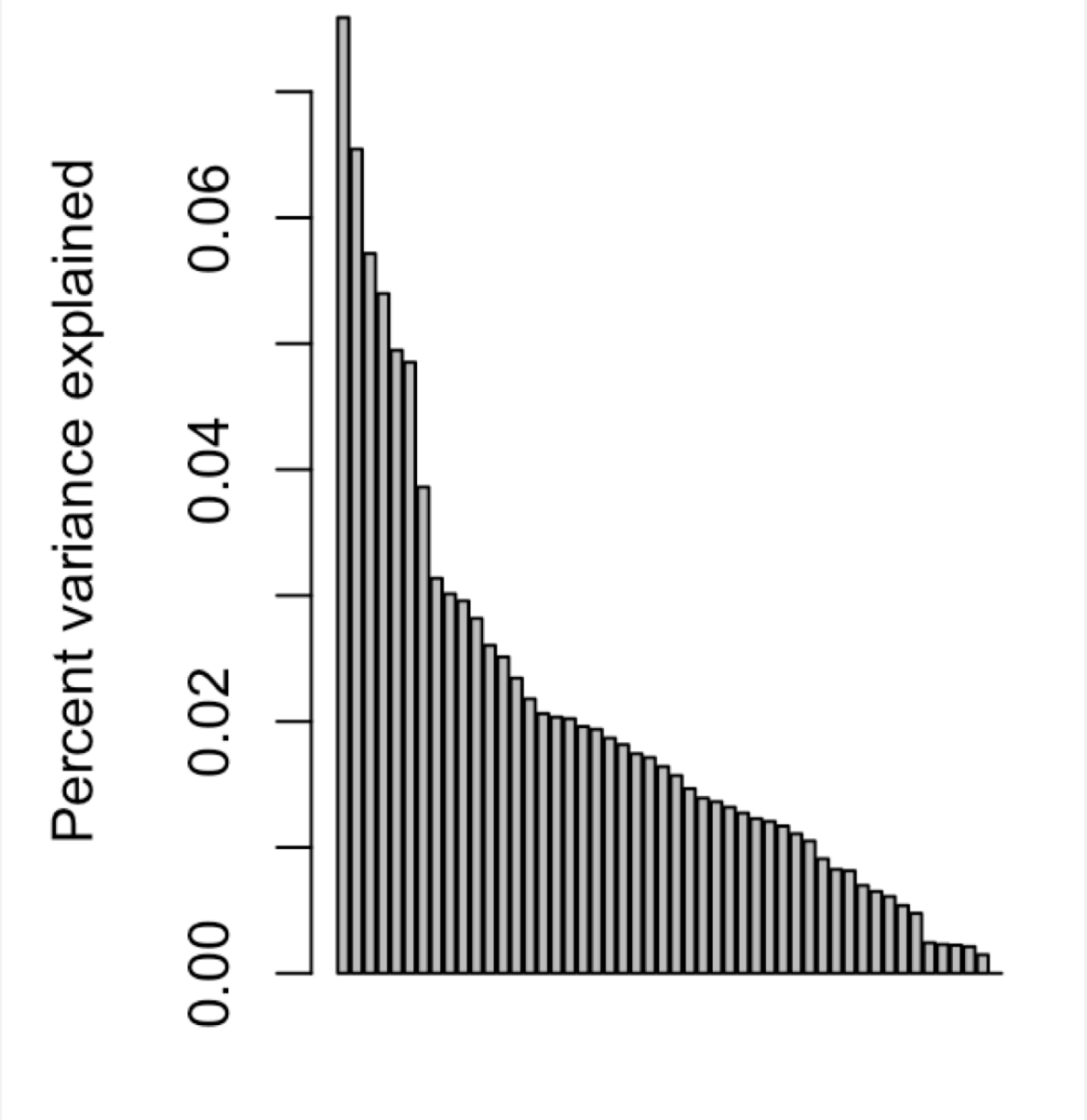
Input data:
Radseq data (genotypes at 100s of loci)
For a large number of species or strains



# How informative is your PCA

Scree Plot: A plot that illustrates the proportion of total variance that is captured by each principal component.

Steep means you can greatly reduce dimensionality without losing information



# Alternatives

**Discriminate function analysis**: This is similar to PCA but you assign groupings to the data first and the discriminating components best parse your assigned groups from one another.

# Doing PCA in R

## Standard Packages

stats – this is part of the base install and has the function `prcomp`

## New Packages

car – `data.ellipse` function

FactoMineR – `PCA` function