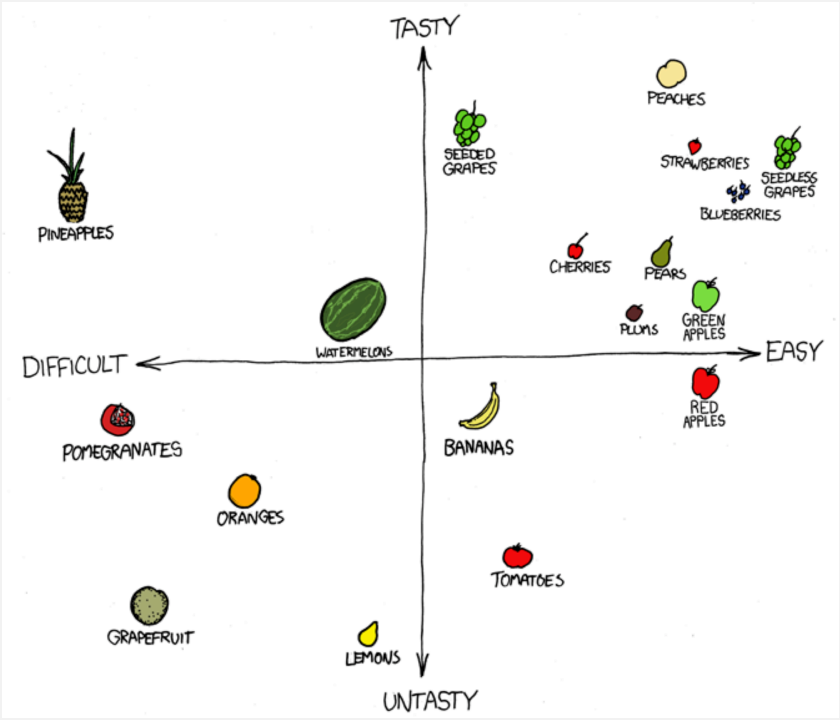
Dimensionality Reduction

Principal component analysis

Biology 683

Lecture 9

Heath Blackmon



Planning

Thursday (22 April): Class but just if you have questions about using Rmarkdown (otherwise you can skip). Final homework will post on Thursday it will cover doing a simple PCA.

Tuesday 27th Brief class to go over project assignment

- Inside of a single .Rmd file you will
- Read in a csv datafile
- Performing a statistical analysis
- Provide a publication quality plot
- Include text above and below each block of code that explains what you are doing.
- You will upload your .Rmd file and the CSV file that you use to a google folder.
- I will “knit” your file and grade the resulting html file.
- Contact me first if you are considering using any R packages we have not covered in class.

Thursday 29th Review class: Final will post after class and you can begin to work on it.

Tuesday 4th 5:00 PM Final will close.

Thanks to all of you for your flexibility and hard work this semester I know that the delivery format has been less than ideal for a class like this.

Why do we do dimensional reduction?

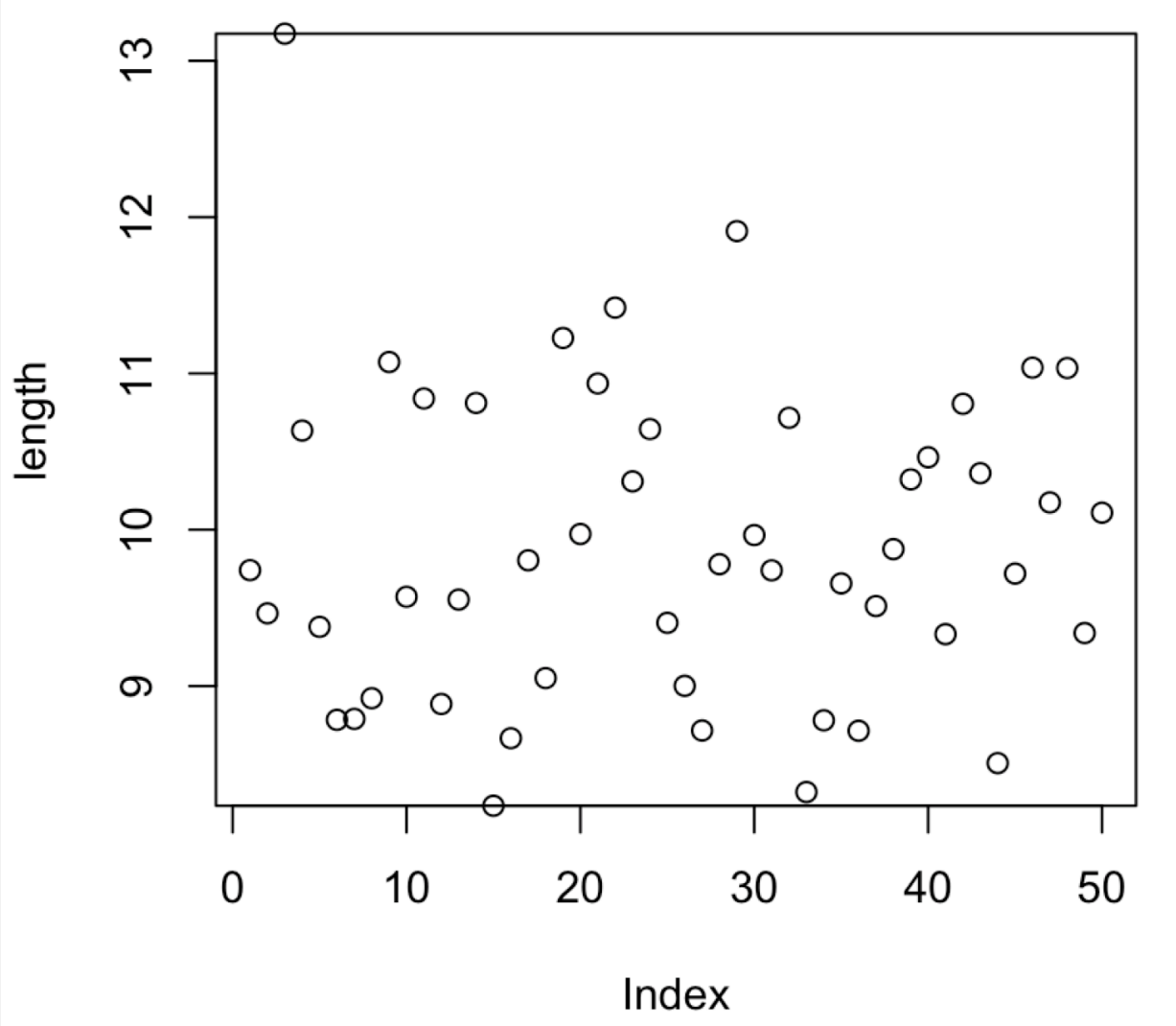
1. Datasets are getting bigger and bigger
2. Understanding our data is often the new bottleneck
3. We can’t think well beyond 3-4 dimensions
4. We can’t illustrate well beyond 2-3 dimensions

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.

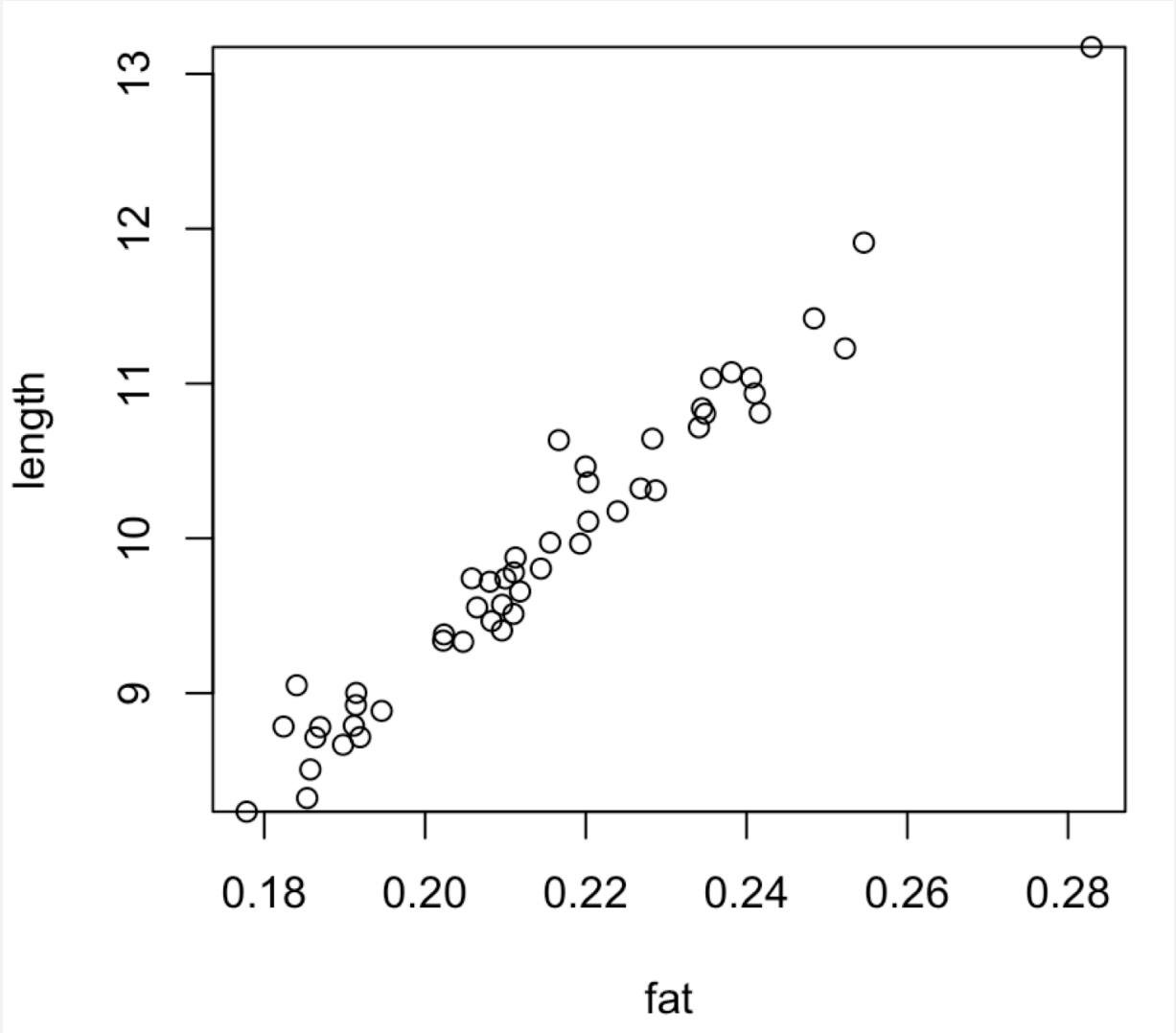
One dimensional data

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
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288	9.05	0.26
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466	11.42	0.21
400	10.31	0.23
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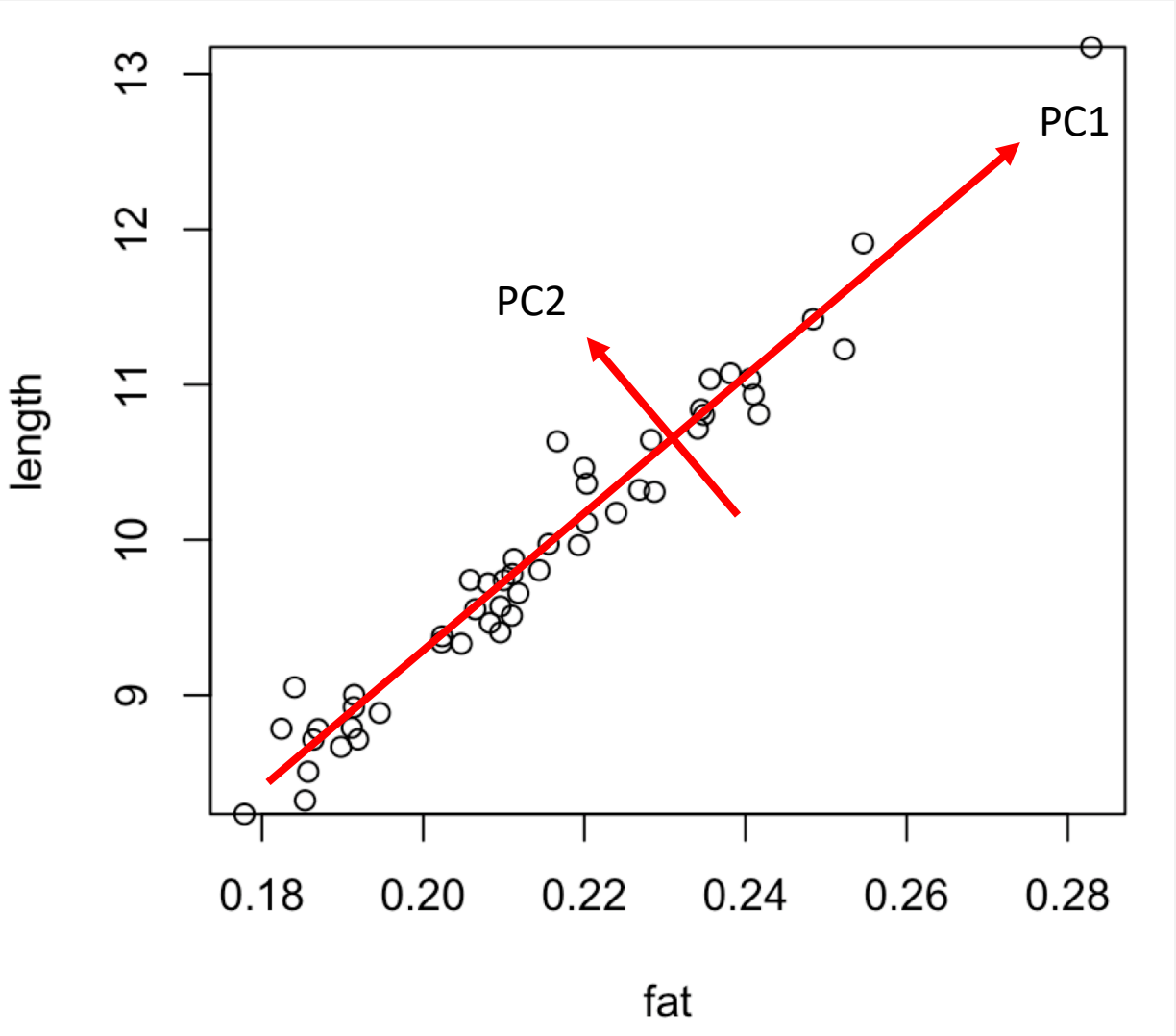

The math behind - PCA

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
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= X

nxm matrix

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

W = loadings mxm matrix

$$T = X \cdot W$$

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

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

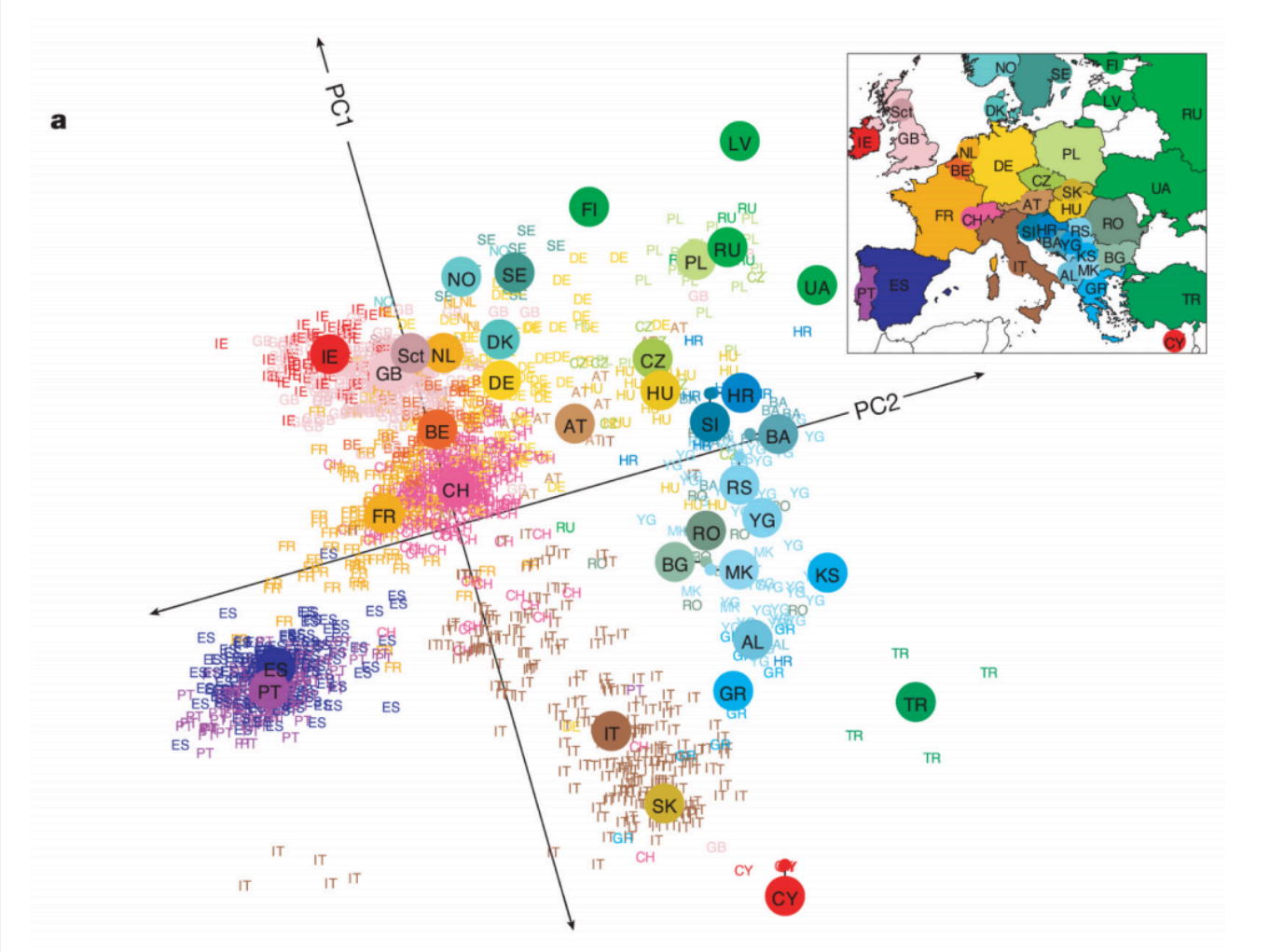
This is T a nxm matrix that has our PC scores. The first column of the matrix will be the one that captures the most variation.

How do people use PCA

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

3000 rows
500,000 columns

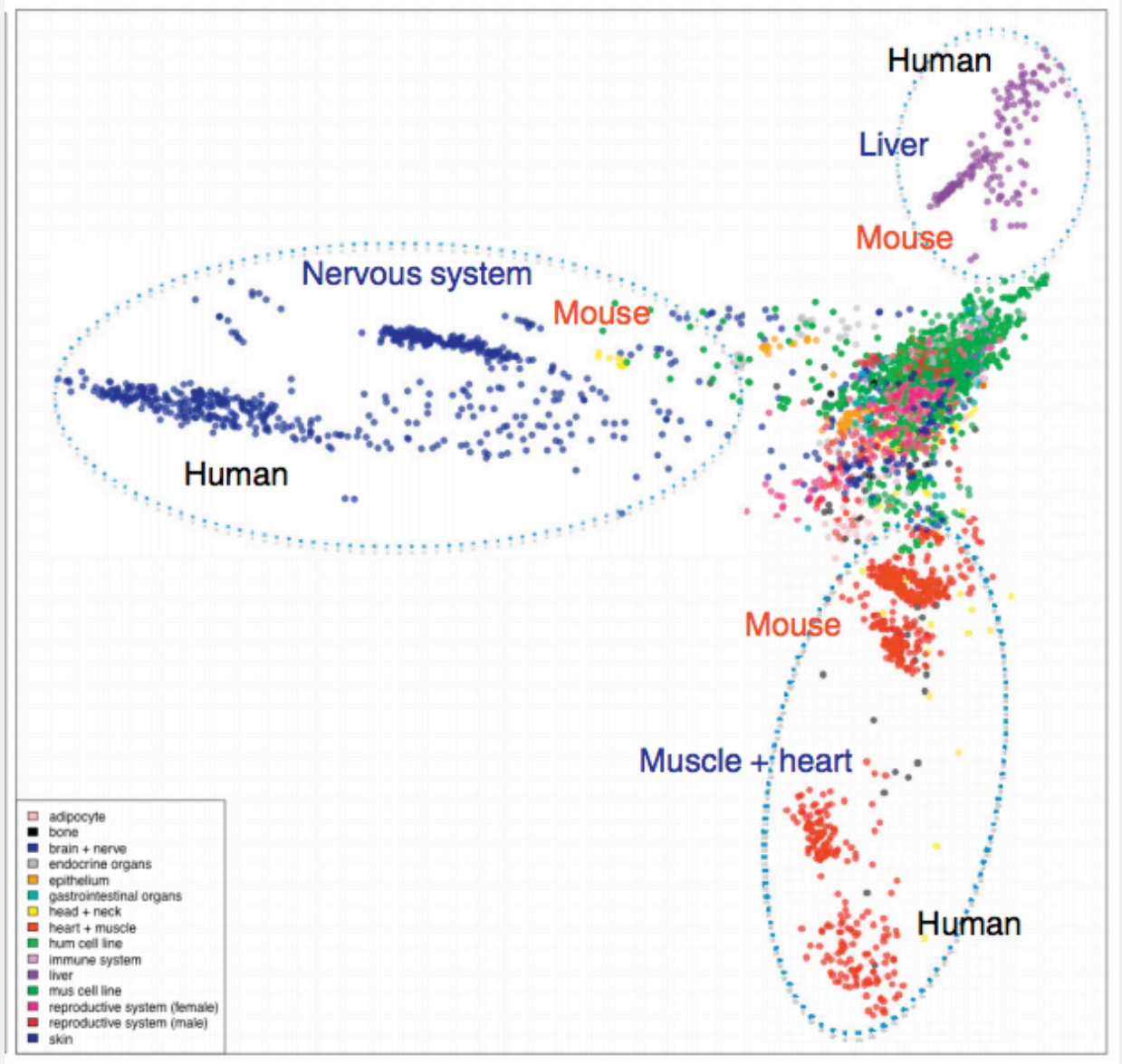
What are PC1 and PC2?



How do people use PCA

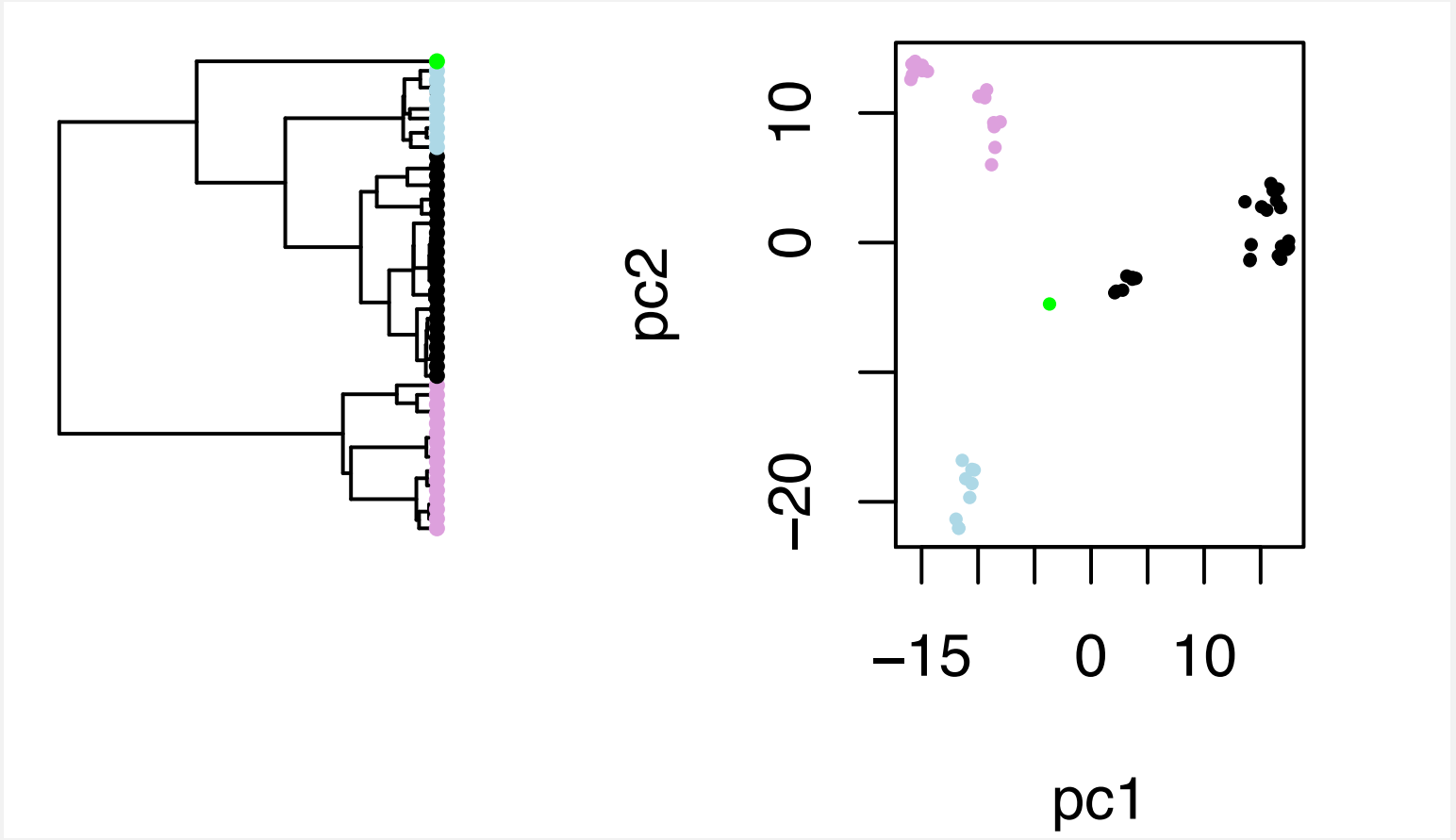
Input data:
Expression level for 1000s of genes
In 100s of cells (color indicates type of cell)

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



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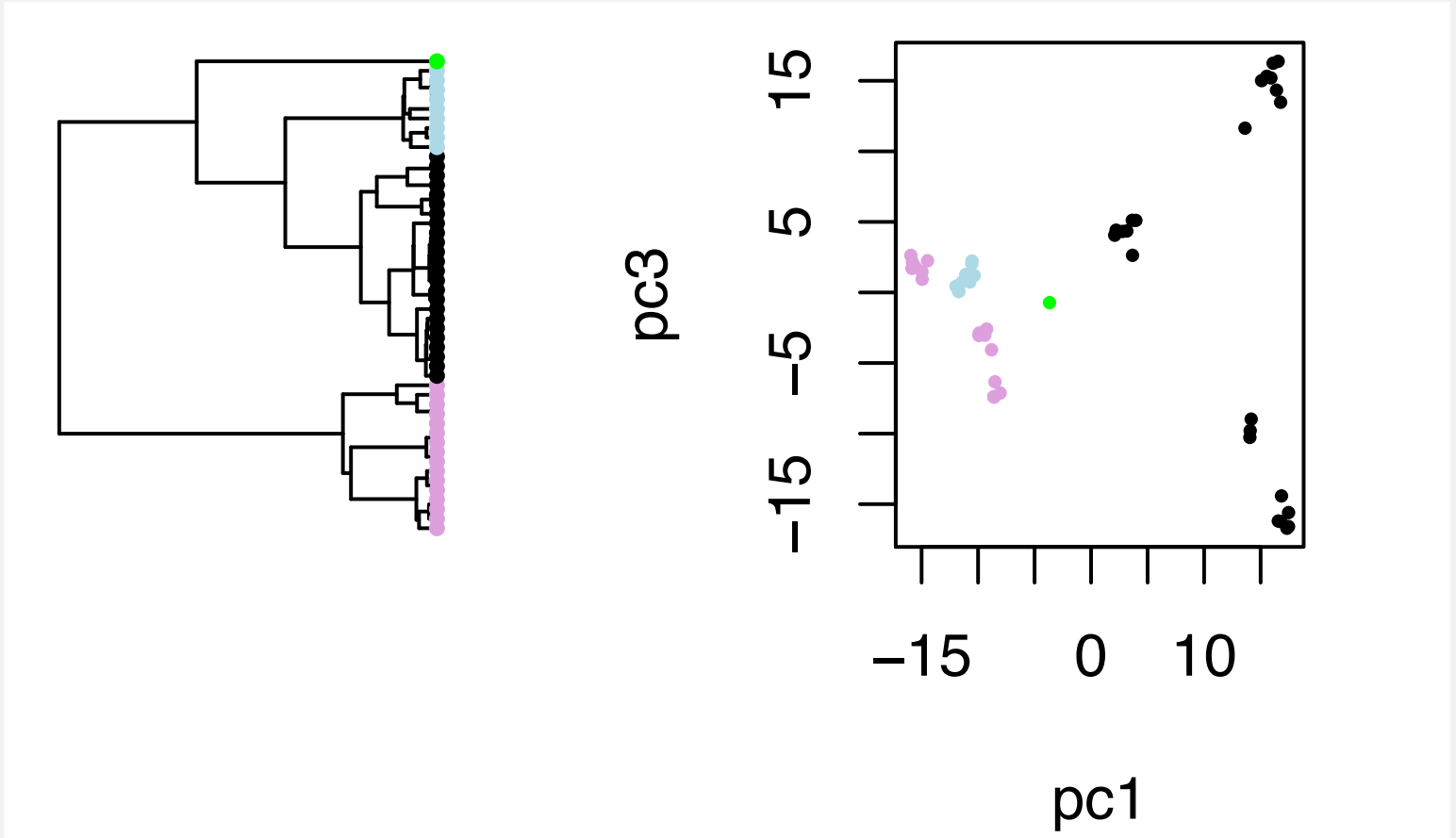
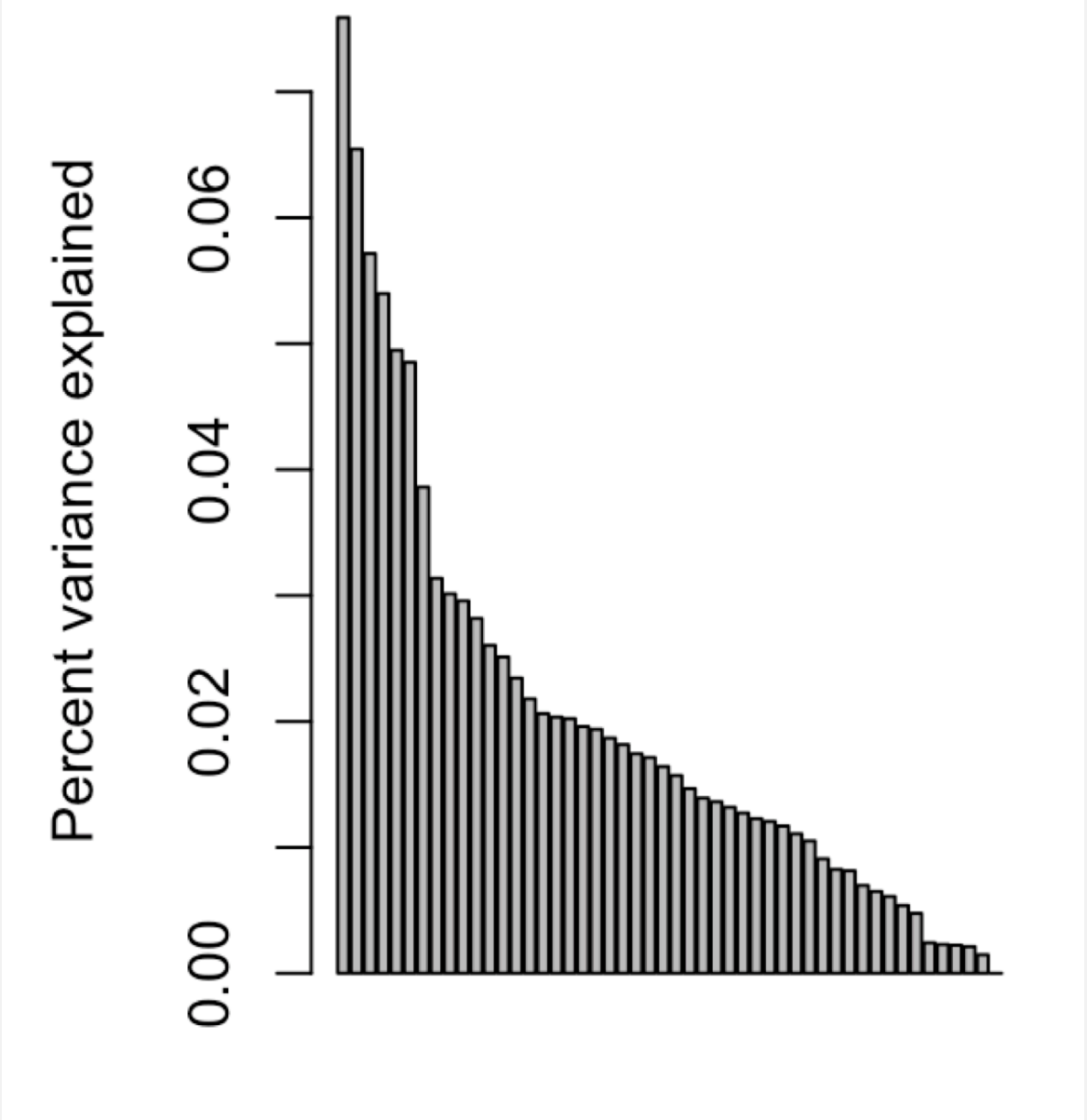


How informative is your PCA

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.

An example of useful and less useful dimensional reduction

Example in Rmarkdown

Standard Packages

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

New Packages

car – `data.ellipse` function

FactoMineR – `PCA` function