Plan:
1. Work through two conceptual examples
2. Explain screeplots and loadings

# PCA: Examples

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# Stock Price returns for Chevron (CVX) and ExxonMobil (XOM)

PC1 and PC2 are the dotted lines on the plot

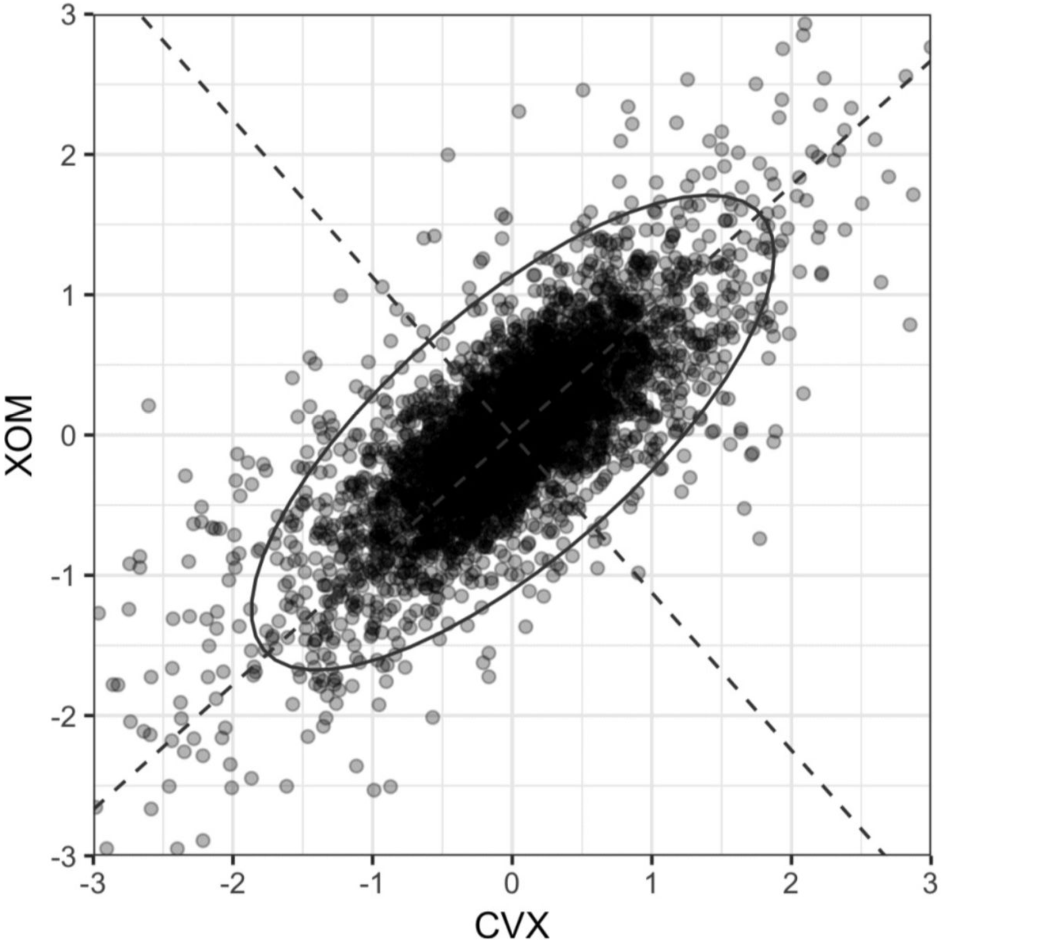



*Figure 7-1. The principal components for the stock returns for Chevron and ExxonMobil*

# Principal Component Analysis (PCA)

But....PCA shines when you're dealing with high-dimensional data. So we have to move *beyond* two predictors to many predictors....

**Step 1**: Combine all predictors in linear combination

**Step 2**: Assign weights that optimize the collection of the covariation to the first PC ($Z_1$) (maximizes the % total variance explained)

**Step 3**: Repeat Step 2 to generate new predictor $Z_2$ (second PC) with different weights. By definition $Z_1$ and $Z_2$ are uncorrelated. Continue until you have as many new variables (PCs) as original predictors

**Step 4**: Retain as many components as are needed to account for *most* of the variance.

Source: Practical Statistics for Data Scientists (Bruce & Bruce)

# S&P 500 Data:  5648 days (1993-2015) x 517 stocks

| | ADS | CA | MSFT | RHT | CTSH | CSC | EMC | IBM | XRX | ALTR | ADI | AVGO | BRCM | FSLR | INTC | LLTC | MCHP | MU | NVDA |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1/29/93 | 0 | 0.06012444 | -0.0220998 | 0 | 0 | 0.01889746 | 0.00736807 | 0.0921652 | 0.25914009 | -0.0071053 | -0.0157849 | 0 | 0 | 0 | -0.0504878 | -0.0898696 | 0 | 0.03702057 | 0 |
| 2/1/93 | 0 | -0.180389 | 0.02762115 | 0 | 0 | 0.01888884 | 0.01842489 | 0.11520651 | -0.1007745 | 0.06389288 | -0.0157929 | 0 | 0 | 0 | 0.09536733 | 0.0449348 | 0 | 0.03702038 | 0 |
| 2/2/93 | 0 | -0.1202566 | 0.03589987 | 0 | 0 | -0.0755726 | 0.02948172 | -0.0230413 | 0.02879553 | -0.0141924 | 0.0473628 | 0 | 0 | 0 | 0 | 0.0674022 | 0 | 0.12340155 | 0 |
| 2/3/93 | 0 | 0.0601242 | -0.024857 | 0 | 0 | -0.151128 | 0.00368875 | -0.2534543 | -0.04319 | -0.0071053 | 0.20523612 | 0 | 0 | 0 | -0.050495 | 0.0224674 | 0 | -0.0123403 | 0 |
| 2/4/93 | 0 | -0.3607697 | -0.0607567 | 0 | 0 | 0.11335029 | -0.0221136 | 0.0698618 | 0 | -0.0070962 | -0.0315699 | 0 | 0 | 0 | 0 | 0.0224674 | 0 | -0.0740409 | 0 |
| 2/5/93 | 0 | 0.03005777 | 0.09389247 | 0 | 0 | 0.09445283 | -0.0479066 | 0.04657454 | 0.17276006 | -0.0212976 | -0.0631478 | 0 | 0 | 0 | -0.0476873 | -0.0674022 | 0 | -0.0123403 | 0 |
| 2/8/93 | 0 | 0.03006643 | -0.0607498 | 0 | 0 | -0.1133503 | -0.0110568 | 0.11643635 | -0.04319 | 0.00709618 | 0 | 0 | 0 | 0 | -0.0196321 | -0.1235743 | 0 | -0.0617008 | 0 |
| 2/9/93 | 0 | -0.0901902 | -0.063521 | 0 | 0 | -0.1322391 | -0.0147456 | 0.06986181 | -0.115169 | 0.04969143 | -0.0157929 | 0 | 0 | 0 | -0.0112235 | 0.0224674 | 0 | 0 | 0 |
| 2/10/93 | 0 | 0.12025657 | 0.02209981 | 0 | 0 | 0.09445283 | 0.01474557 | -0.2561599 | 0.01439448 | 0.02838473 | 0.01578495 | 0 | 0 | 0 | 0.04487956 | 0.11233699 | 0 | 0.07404095 | 0 |
| 2/11/93 | 0 | 0.03005825 | -0.0220927 | 0 | 0 | -0.0188975 | 0.01474556 | -0.1397236 | -0.04319 | 0.02129762 | -0.0315699 | 0 | 0 | 0 | -0.0532953 | 0.06740222 | 0 | -0.0246804 | 0 |
| 2/12/93 | 0 | -0.0901901 | -0.0358999 | 0 | 0 | -0.0377863 | -0.0073681 | -0.0698618 | -0.1871546 | 0 | -0.0473628 | 0 | 0 | 0 | -0.0336561 | -0.112337 | 0 | -0.0370204 | 0 |
| 2/16/93 | 0 | -0.6313411 | -0.0607497 | 0 | 0 | -0.0377863 | -0.0479066 | -0.0931491 | -0.04319 | -0.0283938 | -0.1262955 | 0 | 0 | 0 | -0.098175 | -0.1460417 | 0 | -0.0246803 | 0 |
| 2/17/93 | 0 | 0.12025657 | -0.0165712 | 0 | 0 | -0.1700254 | -0.0110568 | 0.04657453 | -0.08638 | -0.0142015 | 0.03157785 | 0 | 0 | 0 | 0.04487955 | 0 | 0 | -0.0123403 | 0 |
| 2/18/93 | 0 | -0.1803808 | 0.00828562 | 0 | 0 | -0.0566751 | 0.00368875 | -0.0931491 | -0.08638 | 0 | -0.0157849 | 0 | 0 | 0 | -0.0168315 | 0.0224674 | 0 | 0.03702056 | 0 |
| 2/19/93 | 0 | 0.03006595 | -0.0469427 | 0 | 0 | 0 | 0.00736807 | -0.0232873 | 0.115169 | 0.01419237 | 0.03157785 | 0 | 0 | 0 | 0.10378311 | 0.15727183 | 0 | 0.14808196 | 0 |
| 2/22/93 | 0 | 0.03005825 | -0.0662782 | 0 | 0 | -0.1322477 | -0.0184249 | 0.13972361 | 0 | 0.02839382 | -0.0631557 | 0 | 0 | 0 | -0.0168317 | -0.0674022 | 0 | 0 | 0 |
| 2/23/93 | 0 | -0.0300583 | 0.03314266 | 0 | 0 | 0 | -0.0479066 | -0.0698618 | -0.1439645 | -0.0070962 | 0.03157785 | 0 | 0 | 0 | -0.0336631 | -0.0337047 | 0 | -0.0493606 | 0 |
| 2/24/93 | 0 | 0.15031459 | 0.10769942 | 0 | 0 | 0.01888884 | 0.04421782 | 0.1397236 | 0.08638003 | 0.00709618 | 0 | 0 | 0 | 0 | 0.11781411 | -0.0224674 | 0 | 0.09872137 | 0 |
| 2/25/93 | 0 | 0.15032277 | 0.04142827 | 0 | 0 | 0.01888884 | -0.0110568 | 0.37259628 | 0 | 0.02839382 | 0 | 0 | 0 | 0 | 0.0112163 | 0.15727183 | 0 | -0.0370205 | 0 |
| 2/26/93 | 0 | -0.0300659 | -0.0193286 | 0 | 0 | -0.0188888 | 0.01105682 | 0.06986181 | 0.05759106 | 0 | 0.01578495 | 0 | 0 | 0 | -0.028055 | -0.0224674 | 0 | -0.074041 | 0 |
| 3/1/93 | 0 | -0.180381 | -0.0497068 | 0 | 0 | -0.0944614 | -0.0073681 | 0 | 0.04358505 | 0.00709618 | 0.09472561 | 0 | 0 | 0 | -0.0336631 | 0.0224674 | 0 | 0 | 0 |
| 3/2/93 | 0 | 0 | 0.06351413 | 0 | 0 | 0.15113659 | 0.00368875 | -0.0698618 | 0.116229 | 0 | 0.11051053 | 0 | 0 | 0 | 0.09537435 | -0.0449348 | 0 | 0.12340155 | 0 |
| 3/3/93 | 0 | 0.12025658 | 0 | 0 | 0 | -0.0566751 | 0.03684977 | 0.16301088 | 0.02905891 | -0.0070962 | 0 | 0 | 0 | 0 | 0.01402383 | -0.112337 | 0 | -0.0370204 | 0 |
| 3/4/93 | 0 | -0.1503146 | -0.0220927 | 0 | 0 | 0.0377863 | 0.00367932 | -0.0698618 | -0.1452879 | -0.0070962 | -0.015785 | 0 | 0 | 0 | -0.0252473 | -0.0674022 | 0 | 0.01234016 | 0 |
| 3/5/93 | 0 | 0.03005825 | -0.0165714 | 0 | 0 | -0.0944614 | 0.00368875 | -0.0232873 | 0 | 0.03549001 | 0 | 0 | 0 | 0 | -0.0617041 | 0.0449348 | 0 | 0.02468042 | 0 |
| 3/8/93 | 0 | 0.06012444 | 0.02209275 | 0 | 0 | 0.01888884 | -0.025793 | 0.11643634 | 0.21792524 | 0 | 0.04736279 | 0 | 0 | 0 | 0.06731932 | 0.13480441 | 0 | 0.09872114 | 0 |
| 3/9/93 | 0 | 0.09019015 | 0.00552151 | 0 | 0 | 0.09446144 | 0.00736807 | 0.09314908 | -0.0290523 | -0.0070962 | -0.0157849 | 0 | 0 | 0 | 0.0112163 | 0.0898696 | 0 | 0 | 0 |
| 3/10/93 | 0 | 0.03006595 | 0.01104991 | 0 | 0 | 0 | 0.01105681 | -0.1862981 | 0.02905891 | -0.0141924 | -0.0157849 | 0 | 0 | 0 | -0.0196321 | -0.0449348 | 0 | 0 | 0 |
| 3/11/93 | 0 | -0.0300583 | 0.02761408 | 0 | 0 | 0.22670058 | 0 | -0.1862982 | -0.0581112 | 0.00709618 | 0.06314774 | 0 | 0 | 0 | -0.0196392 | 0.01123011 | 0 | 0 | 0 |
| 3/12/93 | 0 | 0 | 0.06627822 | 0 | 0 | -0.0188975 | 0.01474556 | 0.30273448 | -0.1452813 | 0.02839381 | 0.06314774 | 0 | 0 | 0 | 0.02524749 | 0.01123729 | 0 | 0.13574153 | 0 |

For this example: we'll focus on 16 top companies

Source: Practical Statistics for Data Scientists (Bruce & Bruce)

# Screeplot

The vernacular definition of “scree” is an accumulation of loose stones or rocky debris lying on a slope or at the base of a hill or cliff.

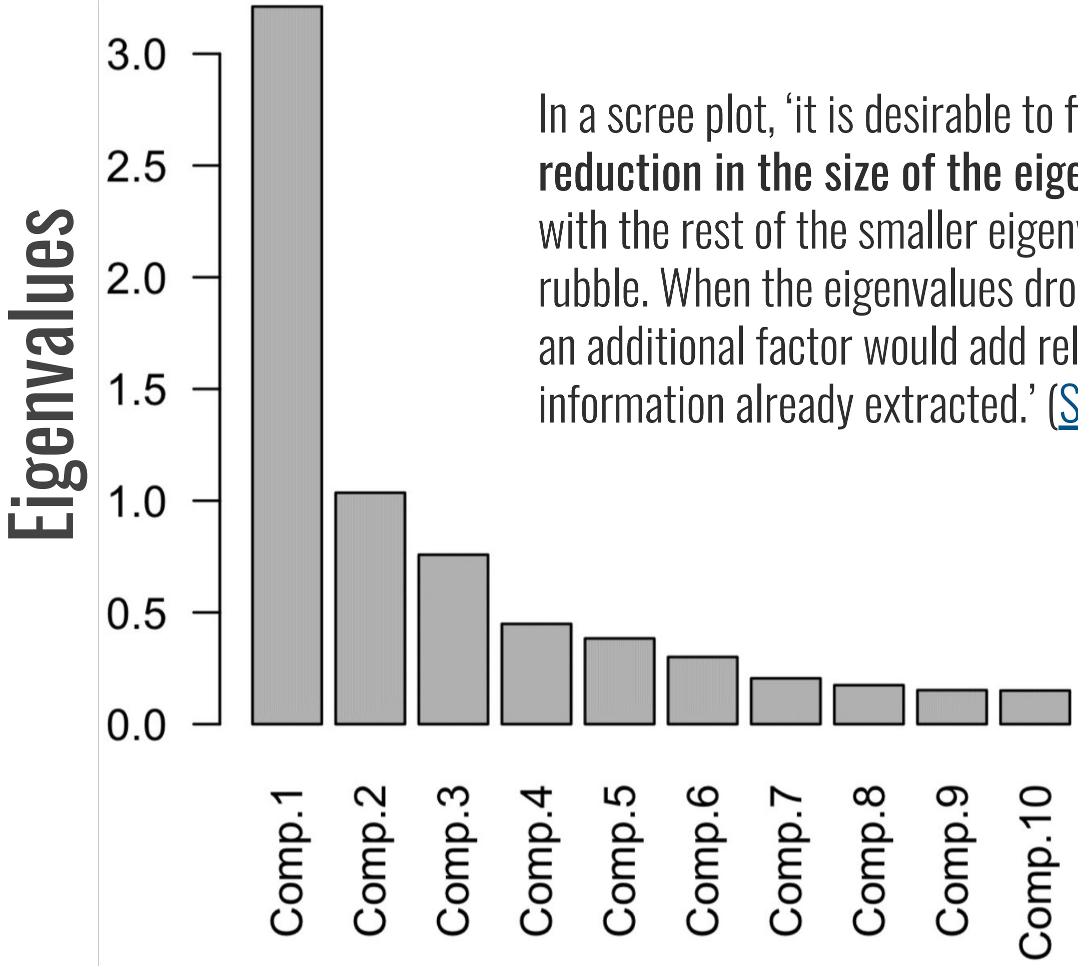



*Figure 7-2. A screeplot for a PCA of top stocks from the S&P 500*

In a scree plot, ‘it is desirable to find a **sharp reduction in the size of the eigenvalues** (like a cliff), with the rest of the smaller eigenvalues constituting rubble. When the eigenvalues drop dramatically in size, an additional factor would add relatively little to the information already extracted.’ (Source)

# Loading of PCs 1-5

PC1: Overall stock market trend

PC2: Price change of energy stocks

PC3: movements of Apple and CostCo.

PC4: movements of Schlumberger to other stocks

PC5: Financial companies

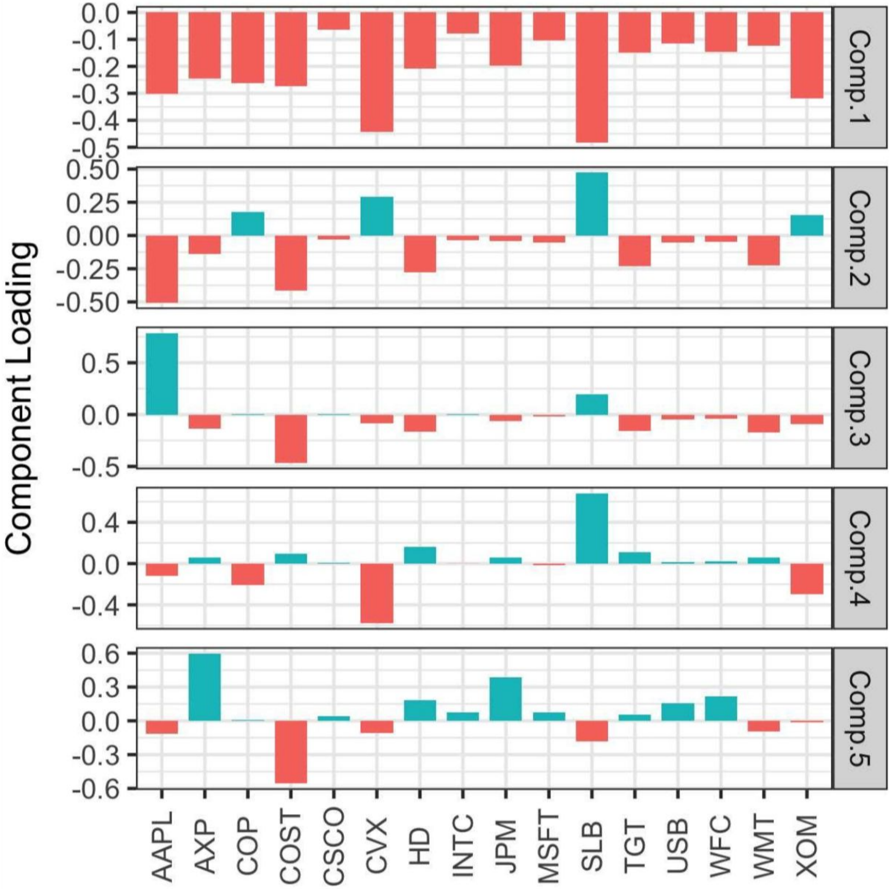



*Figure 7-3. The loadings for the top five principal components of stock price returns*

# How many PCs to select?

Option 1: Visually through the **screeplot**

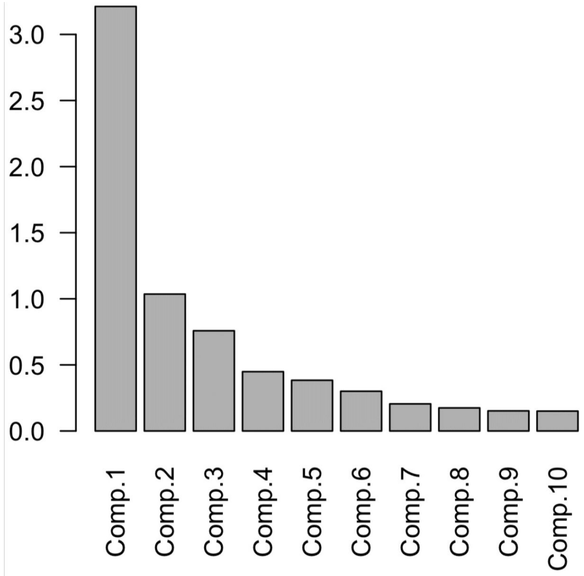



*Figure 7-2. A screeplot for a PCA of top stocks from the S&P 500*

Option 2: % Variance explained (i.e. 80% variance explained)

Option 3: Inspect loadings for an intuitive interpretation

Option 4: Cross-validation

# PCA : Key Ideas

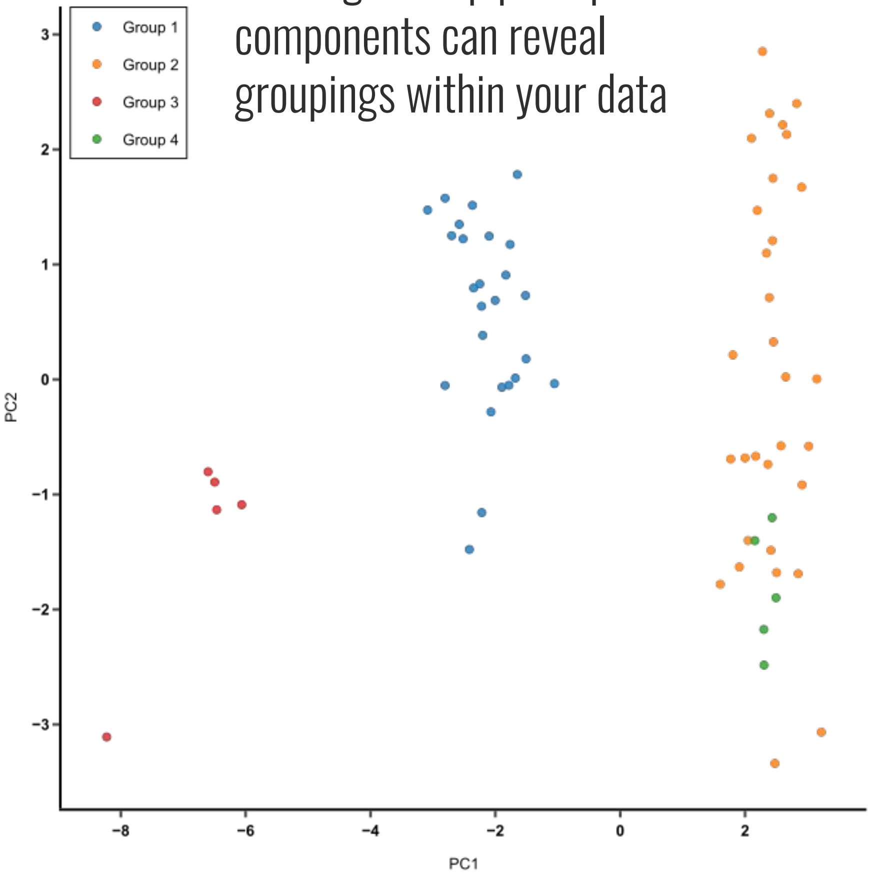
1. PCs are linear combinations of the predictor variables (numeric data only)
2. Calculated to minimize correlation between components (minimizes redundancy)
3. A limited number of components will typically explain most of the variance in the outcome variable
4. Limited set of PCs can be used in place of original predictors (dimensionality reduction)

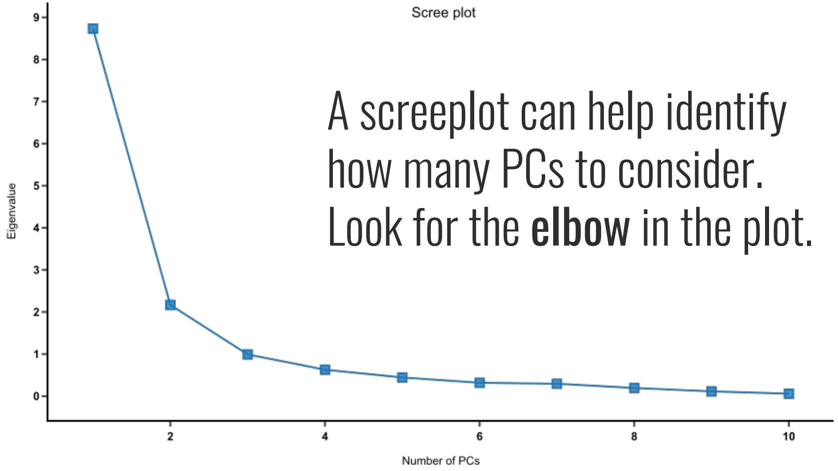
For more on PCA:

- https://blog.bioturing.com/2018/06/14/principal-component-analysis-explained-simply/
- http://setosa.io/ev/principal-component-analysis/

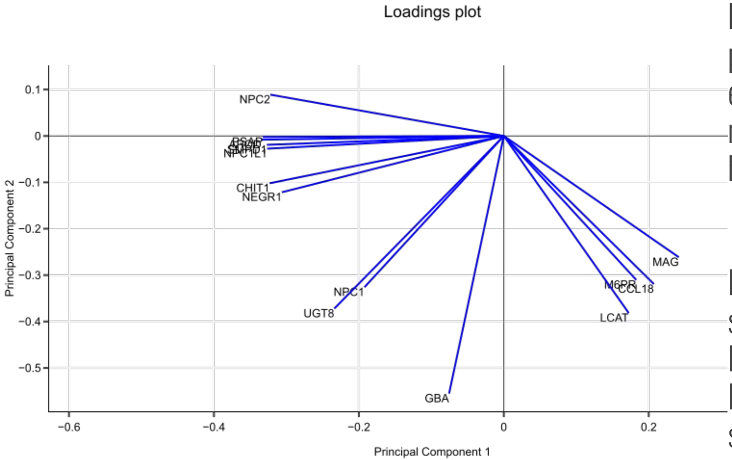
Source: Practical Statistics for Data Scientists (Bruce & Bruce)

# Plotting the top principal components can reveal groupings within your data




A screeplot can help identify how many PCs to consider. Look for the **elbow** in the plot.




**Loadings plot:** project values on each PC show how much weight they have on that PC

In this example, NPC2 and CHIT1 strongly influence PC1, while GBA and LCAT have more say in PC2

https://blog.bioturing.com/2018/06/18/how-to-read-pca-biplots-and-scree-plots/

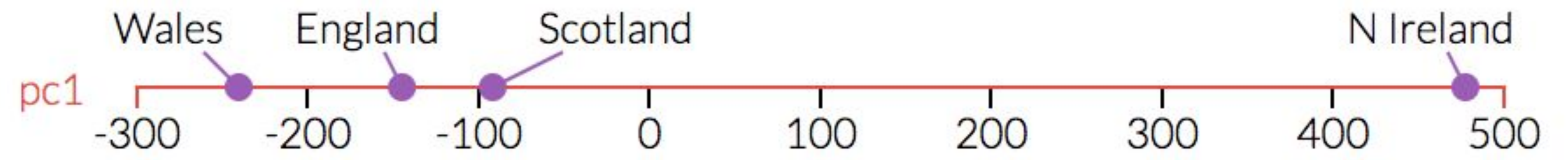
# Case Study: Diet in the UK

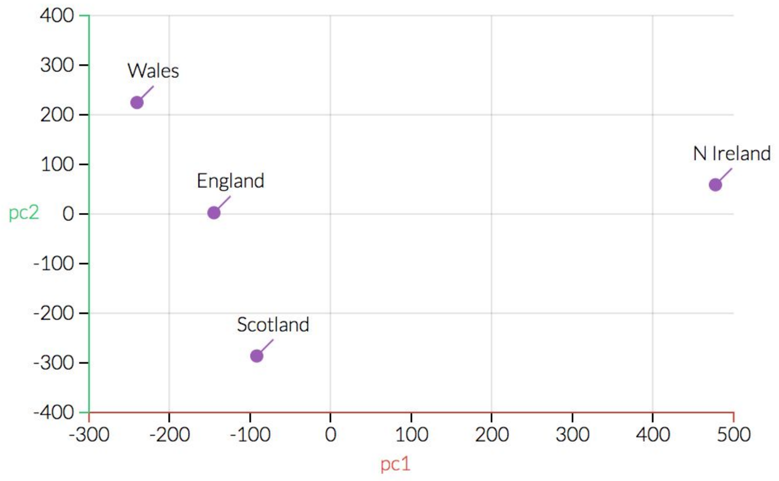
| | England | N Ireland | Scotland | Wales |
|---|---|---|---|---|
| Alcoholic drinks | 375 | 135 | 458 | 475 |
| Beverages | 57 | 47 | 53 | 73 |
| Carcase meat | 245 | 267 | 242 | 227 |
| Cereals | 1472 | 1494 | 1462 | 1582 |
| Cheese | 105 | 66 | 103 | 103 |
| Confectionery | 54 | 41 | 62 | 64 |
| 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 |

17 foods x 4 countries

http://setosa.io/ev/principal-component-analysis/

# PCA: Diet in the K




Can already tell that N Ireland is distinct

If we look back at the raw data Northern Ireland, eats way more fresh potatoes and way fewer fresh fruits, cheese, & fish. This reflects real world geography...

http://setosa.io/ev/principal-component-analysis/


Source: Denver Public Library

# Case Study: Genetics and Geography

Letter | Published: 31 August 2008

## Genes mirror geography within Europe

John Novembre, Toby Johnson, Katarzyna Bryc, Zoltán Kutalik, Adam R. Boyko, Adam Auton, Amit Indap, Karen S. King, Sven Bergmann, Matthew R. Nelson, Matthew Stephens & Carlos D. Bustamante

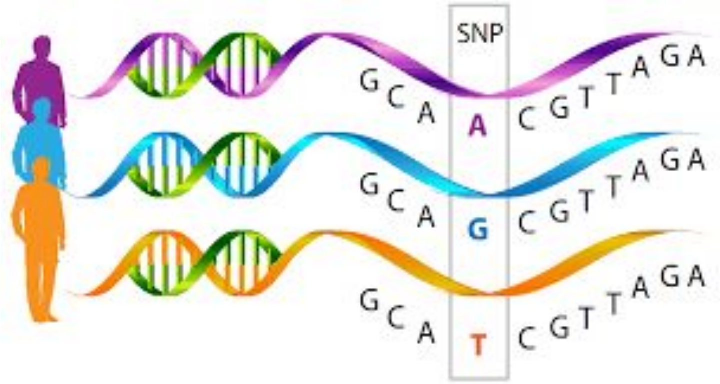
*Nature* **456**, 98–101 (06 November 2008) | Download Citation

The Data: 1,387 Europeans x 500,000 SNPs

https://www.nature.com/articles/nature07331

# SNP (Single Nucleotide Polymorphism)

- Reminder: Your DNA is made up of four bases: G, C, T, & As
- A **SNP** is a position in one's DNA that varies between individuals (appears in at least 1% of the population)
    - This results from normal human variation
    - Some contribute to disease, but many are just differences between humans
    - These are used by companies like 23andMe and Ancestry.com



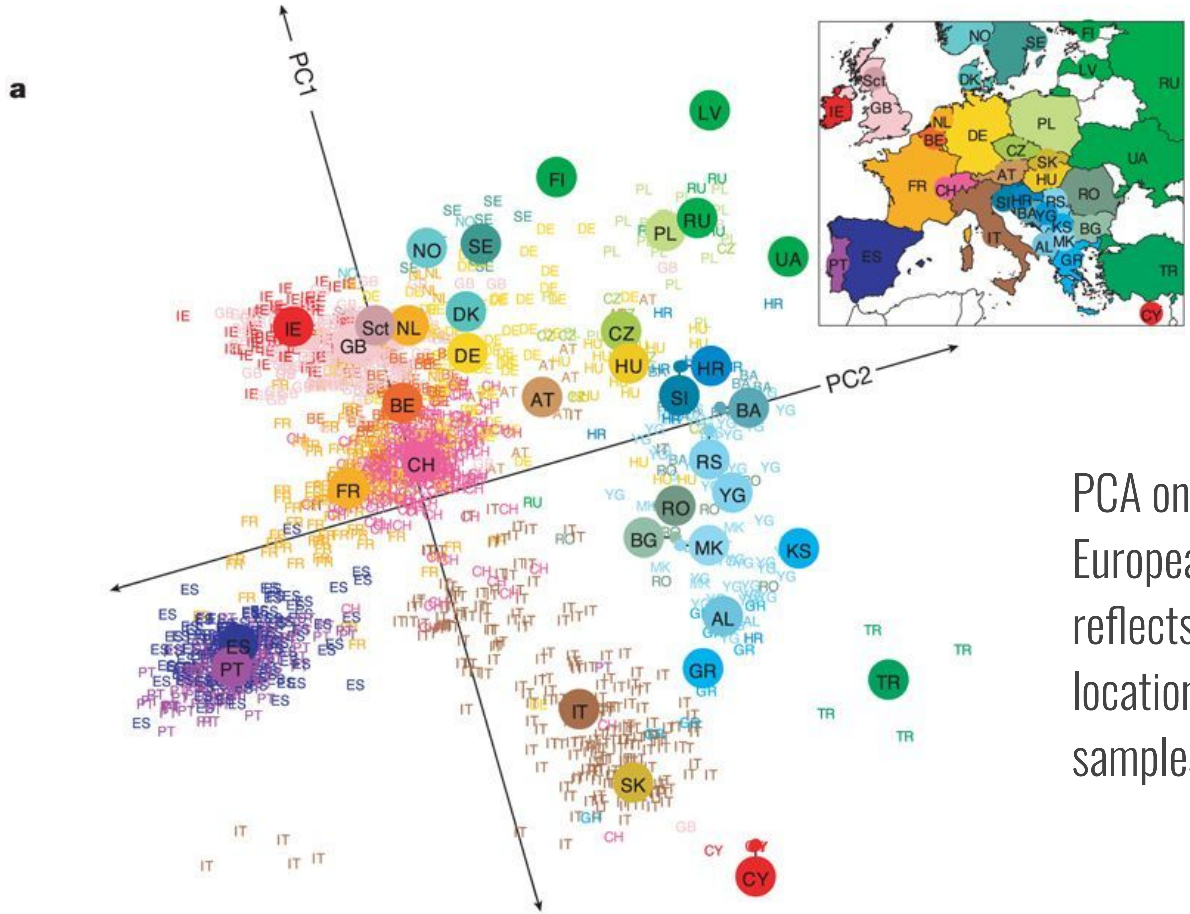
# The Data: 1,387 Europeans x 500,000 SNPs

**Step 1:** Measure genotype (GCTA) at 500,000 positions (SNPs) along the genome in 1387 European individuals

**Step 2:** Calculate PCs from 500,000 SNPs

**Step 3:** Plot PC1 and PC2 (each point is an individual)

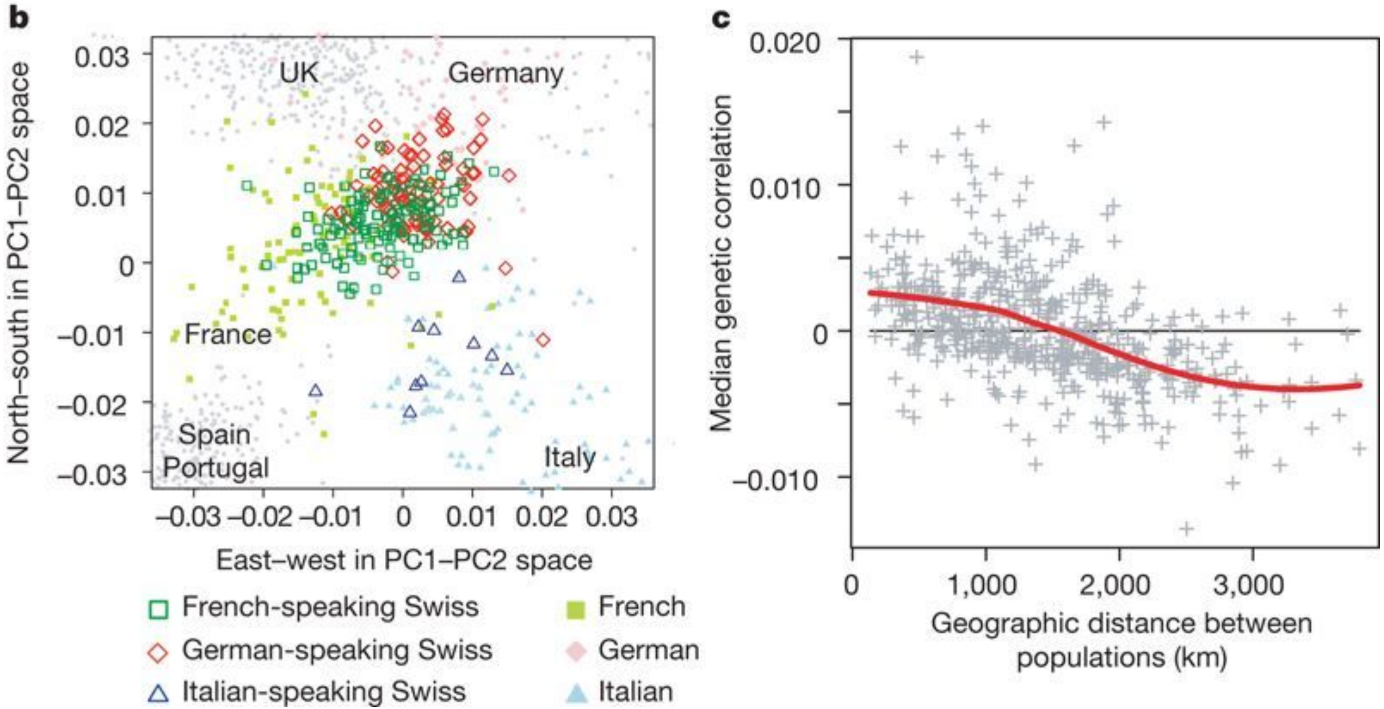
**Step 4**: Compare to the map of Europe




PCA on SNP data for European samples reflects geographic location of where samples came from

https://www.nature.com/articles/nature07331

# PC1 is East-West ; PC2 is North-South




https://www.nature.com/articles/nature07331

# Dimensionality Reduction with PCA: Pros & Cons

Pros:

- Helps compress data; reduced storage space.
- reduces computation time.
- helps remove redundant features (if any)
- Identifies outliers in the data

Cons:

- may lead to some amount of data loss.
- tends to find linear correlations between variables, which is sometimes undesirable.
- fails in cases where mean and covariance are not enough to define datasets.
- may not know how many principal components to keep
- highly affected by outliers in the data

https://www.geeksforgeeks.org/dimensionality-reduction/