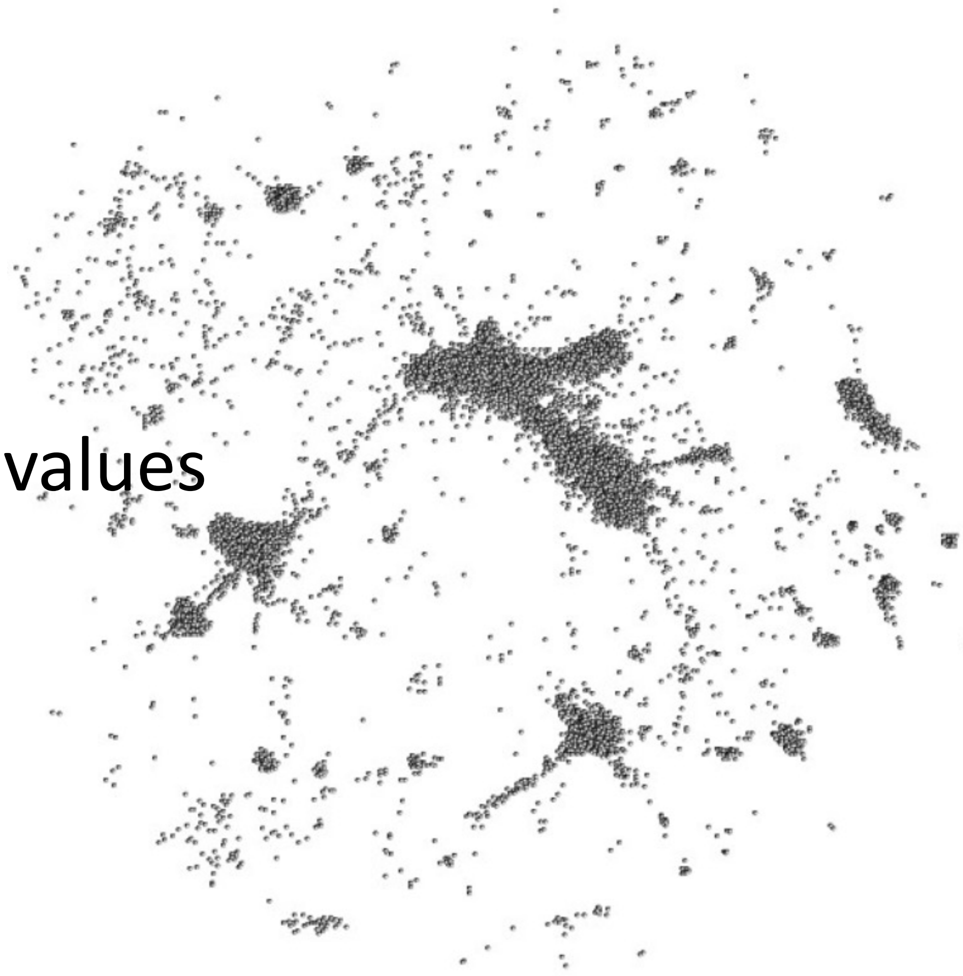
# SVD, PCA, and dimension reduction

# Roadmap

- Dimension reduction
- Absolute essentials of eigenvectors and eigenvalues
- SVD and PCA
- Examples



# Consider genotype data

## Individuals (few 1000s)

Genetic loci (few 100k)

| | HGDP00448 | HGDP00479 | HGDP00985 | HGDP00611 | HGDP00623 | HGDP00557 | HGDP00569 | HGDP00581 |
|---|---|---|---|---|---|---|---|---|
| MitoA10045G | AA | AA | AA | AA | AA | AA | AA | AA |
| MitoA10551G | AA | AA | AA | AA | AA | AA | -- | -- |
| MitoA11252G | AA | AA | AA | AA | GG | AA | AA | AA |
| MitoA11468G | AA | AA | AA | AA | AA | AA | GG | GG |
| MitoA11813G | AA | AA | AA | AA | AA | AA | AA | AA |
| MitoA12309G | AA | AA | AA | AA | AA | AA | -- | GG |
| MitoA13106G | GG | GG | GG | AA | AA | AA | AA | AA |
| MitoA13264G | AA | AA | AA | AA | AA | AA | AA | AA |
| MitoA13781G | AA | AA | AA | AA | AA | AA | AA | AA |
| rs10000543 | CC | CC | TC | CC | CC | CC | TT | CC |
| rs10000918 | GG | AG | GG | AG | AG | AG | AA | AG |
| rs10000929 | AG | AA | AA | AA | AA | AG | AA | AA |
| rs10001378 | TT | CC | TT | TC | TC | TT | TT | TC |
| rs10001548 | TC | TT | TC | TT | TC | TC | TT | CC |
| rs10002472 | GG | AG | GG | GG | AG | GG | GG | GG |
| rs10004399 | AA | AA | AA | AG | AG | AA | AA | AG |
| rs1000459 | TT | TC | TC | CC | CC | CC | [illegible] | [illegible] |
| rs10005550 | GG | GG | GG | GG | GG | GG | GG | GG |

https://hagsc.org/hgdp/files.html

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| MitoA13781G | AA | AA | AA | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] |
| rs10000543 | CC | CC | TC | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] |
| rs10000918 | GG | AG | GG | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] |
| rs10000929 | AG | AA | AA | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] |
| rs10001378 | TT | CC | TT | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] |
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- Convert to numbers
- compare columns ?
- Would like to visualize in 2 dimesions:
  - 1000 x 2 ?

# Suppose your data looks like genotype data

Individuals (few 1000s)

Genetic loci (few 100k)

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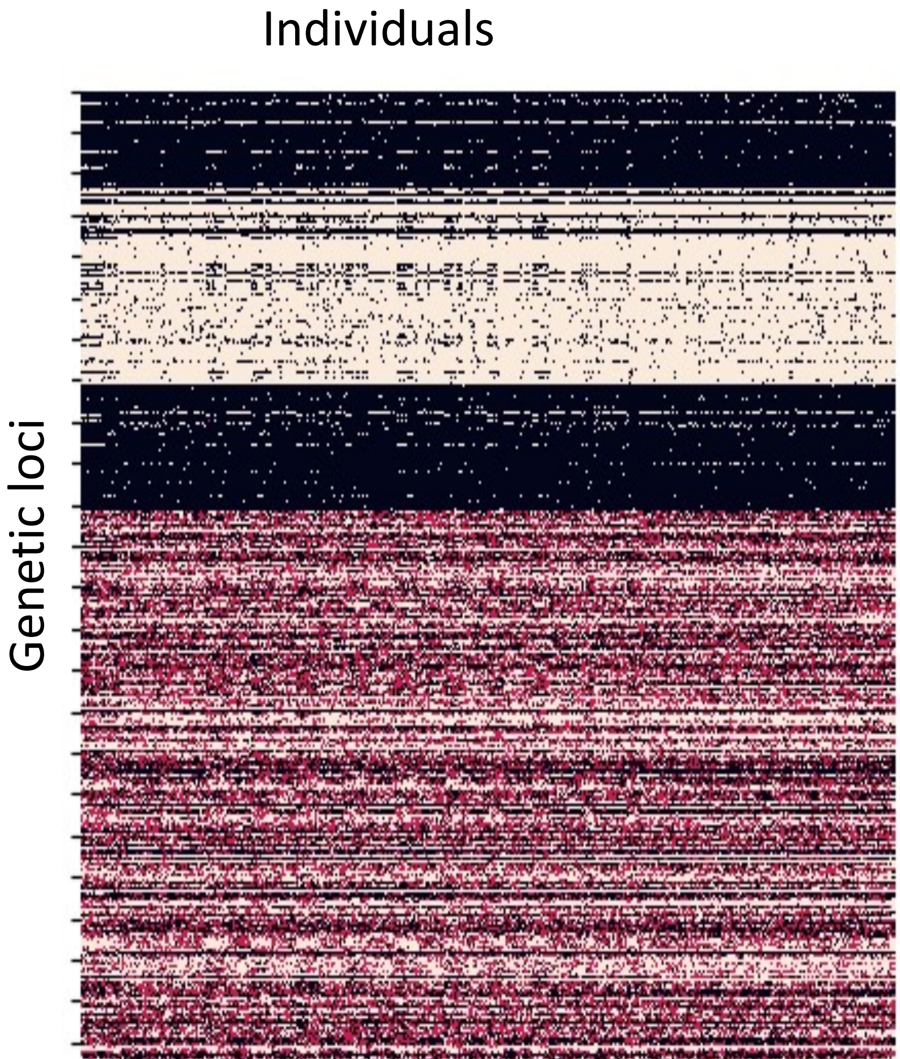
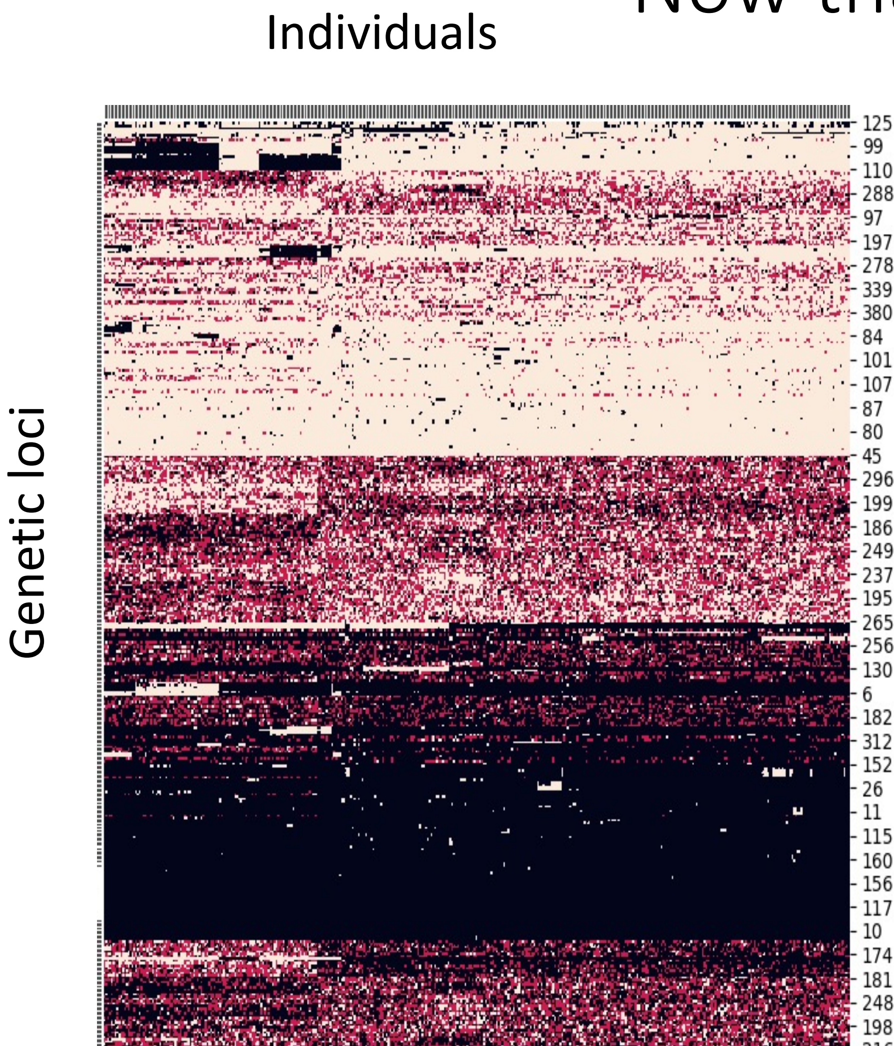



- Some rows are similar to each other, some columns are similar to each other
- The data are in some way “predictable”
- Can we build a low-complexity object that explains most of the data matrix.

# Now that looks like structure

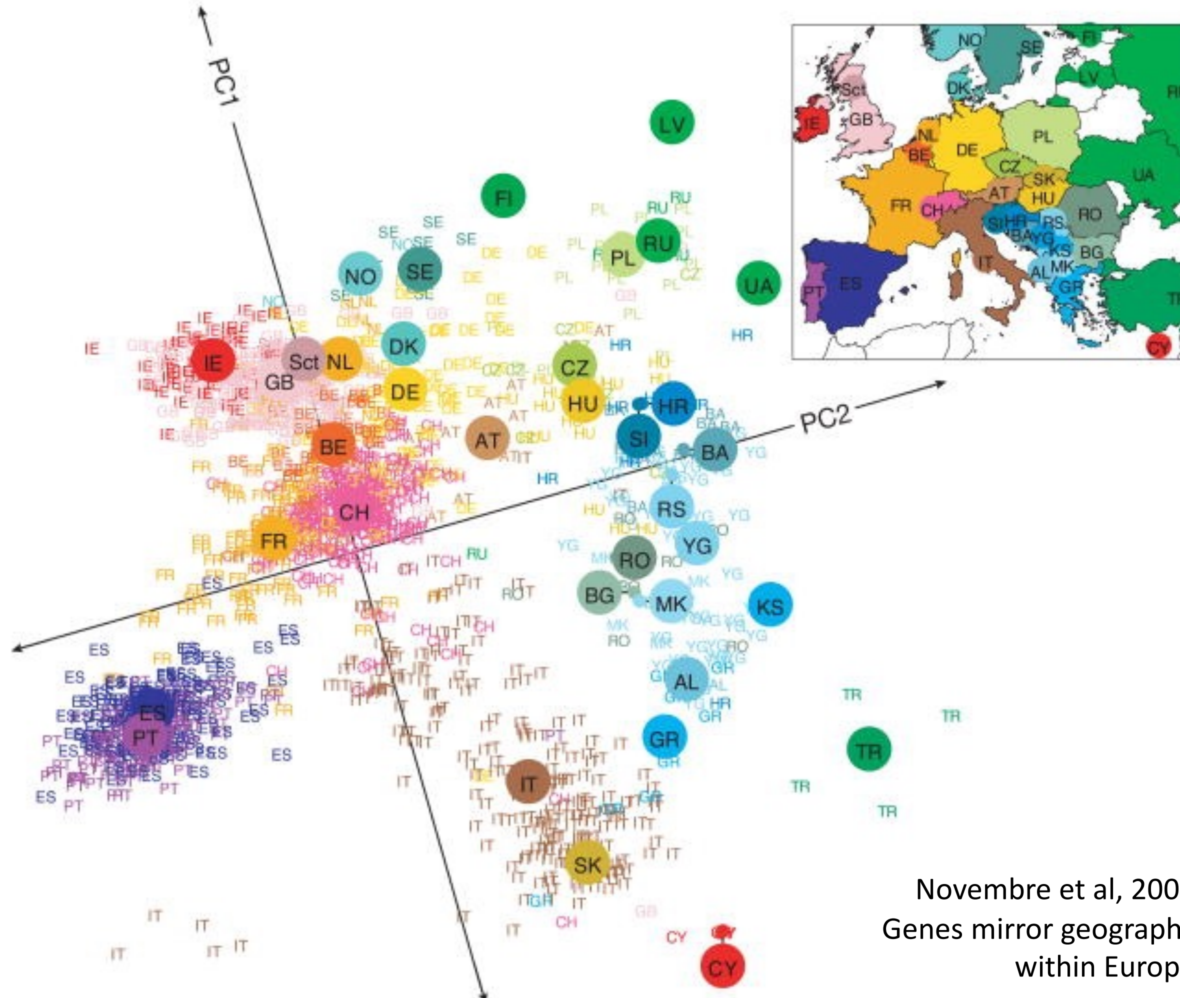



- Reorder rows and columns to put similar rows next to each other?
- Libraries to make exactly this sort of eye-candy are mature. This one is `sanborn.clustermap`
- Organizing data like this is deeply satisfying—it makes us think we have discovered truth.
- What if I told you linear algebra could do this?

# Why Reduce dimensions?


- Reducing the number of dimensions can make ML easier
- May reduce noise.
- Can exploit unlabeled data to make nicer inputs for ML
- We need dimension reduction and categorization to understand high-dimensional data
- Useful for making visualizations of high-dimensional data.

# Example: Genes mirror geography within Europe




m x n = 200k genetic loci x 1400 individuals

Novembre et al, 2008
Genes mirror geography
within Europe

10.1038/nature07331

# How many dimensions again?

n x m can be large (compared to our computers and our displays):

Twitter (500M tweets / day, May 2020)

Youtube (2.5 billion views / day)

Natural Language processing ($10^4$-$10^6$ words)

Netflix prize was 500K users x 20K movies

Biochemical or genetic assays ($10^4$-$10^7$ features of interest)

Image processing ($10^7$ pixels easy)

# Definition of eigenvectors and eigenvalues

There exists a set of vectors $\{e_i\}$

That has the following nice property

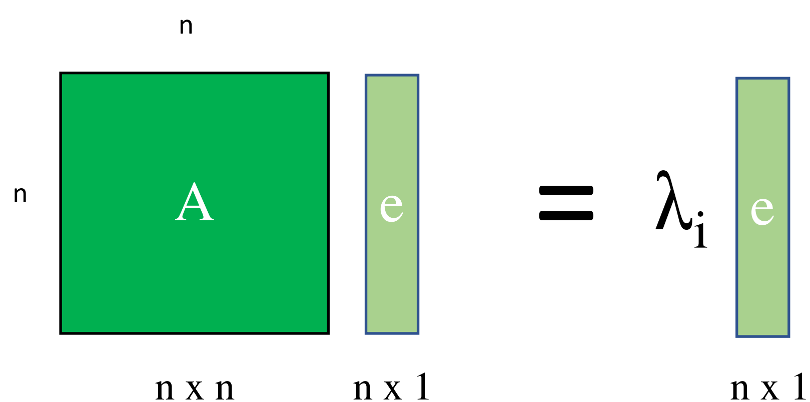
square matrix
n x n

ith eigenvalue

ith eigenvector
n x 1

$$\mathbf{A}\,\mathbf{e}_i = \lambda_i\,\mathbf{e}_i$$

square matrix

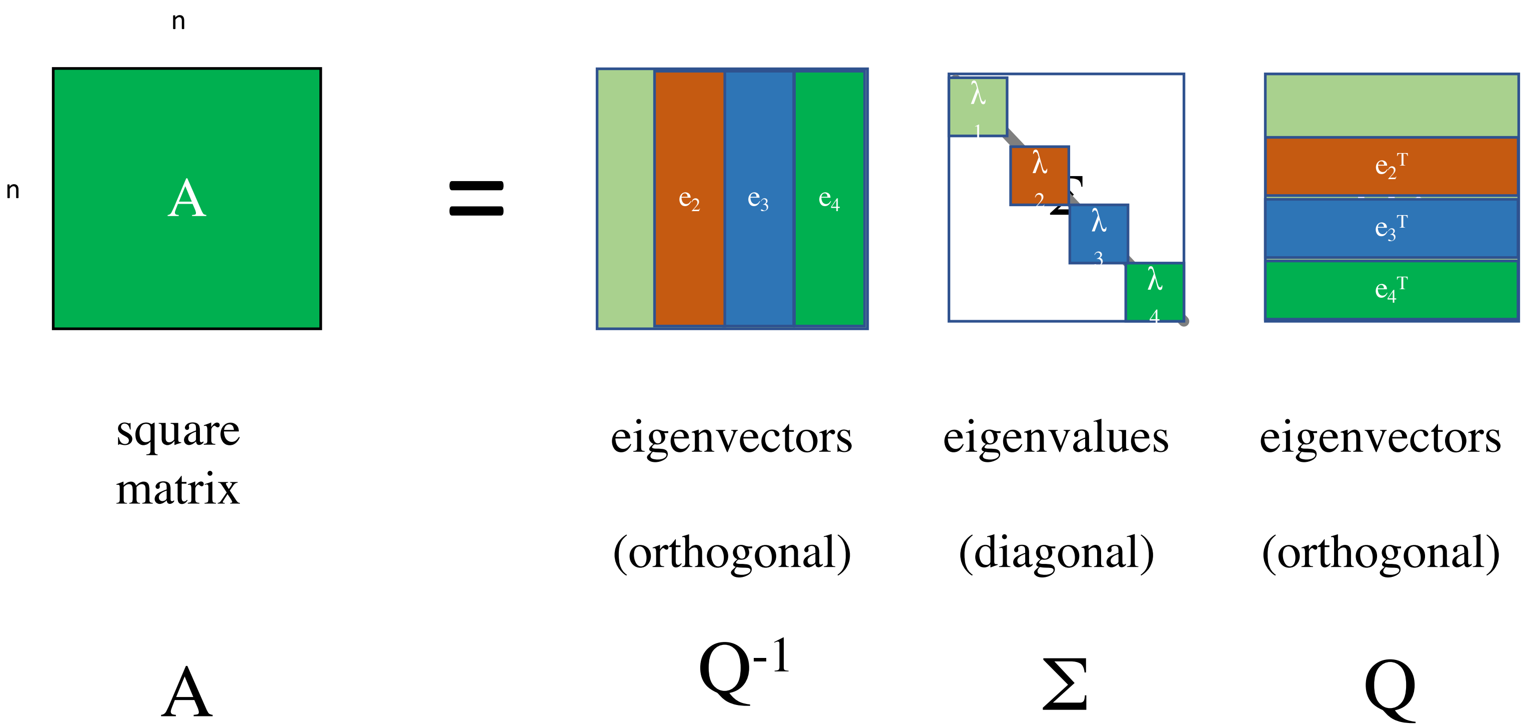


# Eigenvalue decomposition

These vectors can be constructed orthogonal (zero inner products)

and normal ( x dot x = 1 )

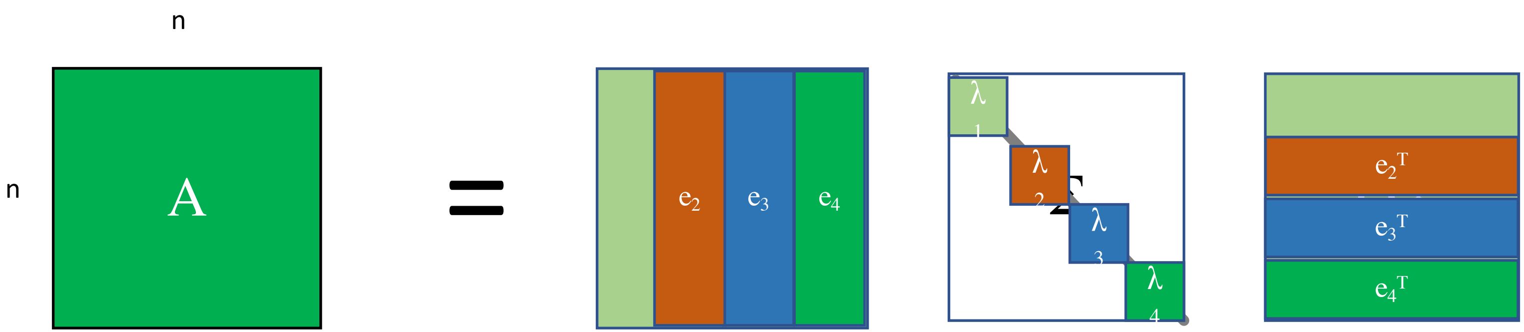
$$\mathbf{A} = \mathrm{Sum}_i\ \mathbf{e}_i^T \lambda_i \mathbf{e}_i$$



# Eigenvalue decomposition

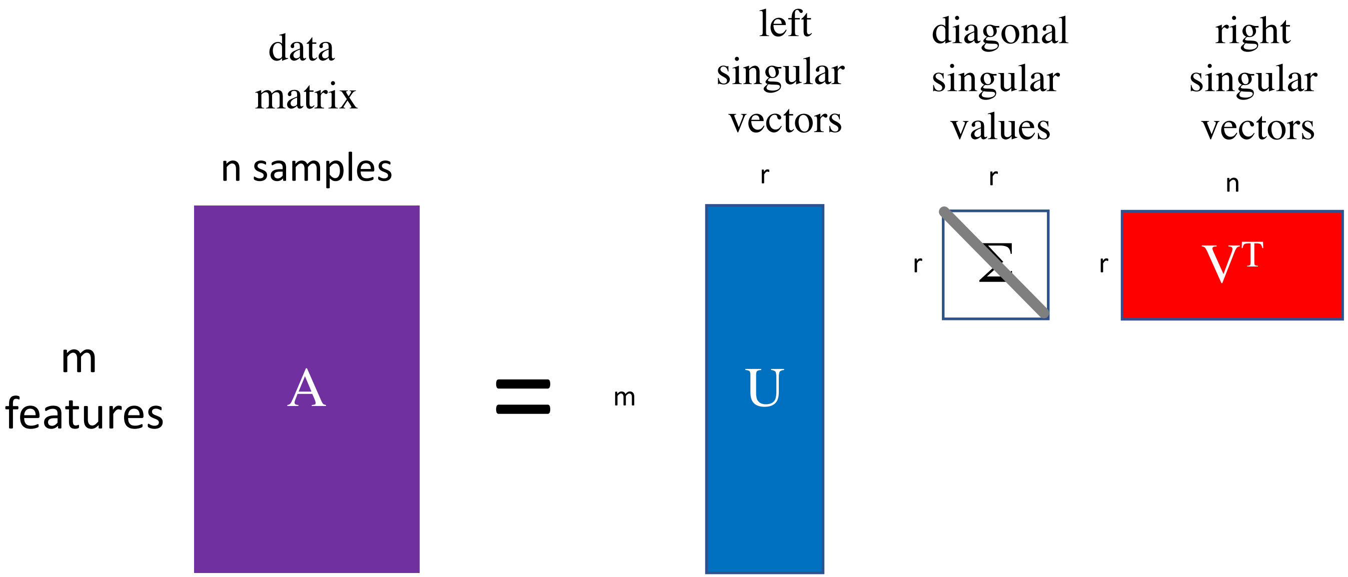
```
import numpy as np
from numpy import linalg as LA

# A library function will take a square matrix and give
# back a vector of eigenvalues and a matrix of eigenvectors.

A=np.array( [ [16, 2, 3, 13 ],[5, 11, 10, 8], [9, 7, 6, 12],
[4, 14, 15, 1] ])
evalues, evectors = LA.eig(A)
print(evalues)
print(evectors)
B=np.dot(np.dot(evectors , evalues * np.eye(4)) ,
LA.inv(evectors))
```

# Singular Value Decomposition (SVD)




- Eigenvalue decomposition is very nice, but only applies to square data matrices.
- Singular Value Decomposition (SVD) is a generalization for rectangular matrices

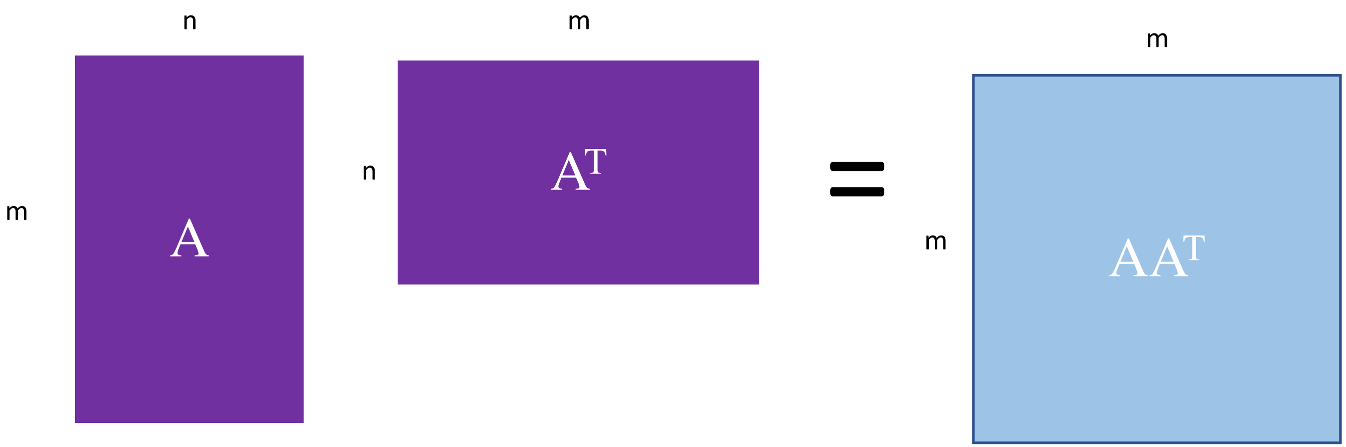
# Singular Value Decomposition (SVD)




- Eigenvalue decomposition is very nice, but only applies to square data matrices.
- Singular Value Decomposition (SVD) is a generalization for rectangular matrices

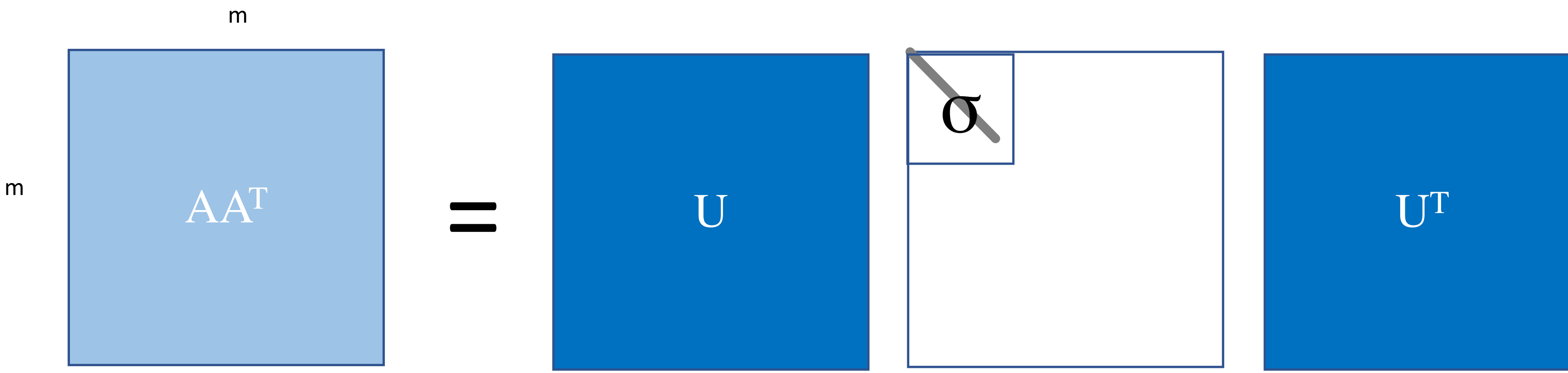
# Constructing SVD - rows

- Recipe for building SVD:



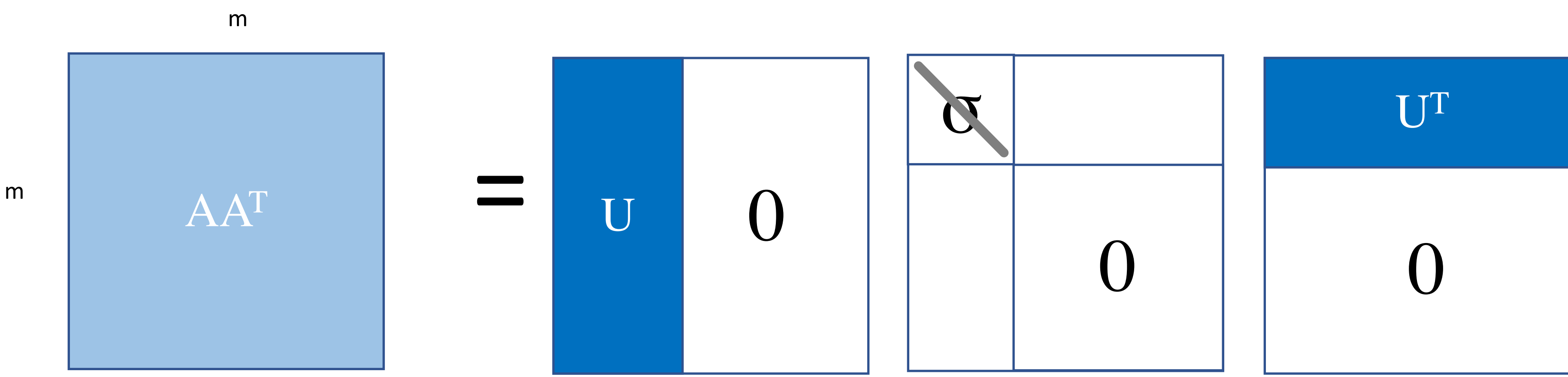

This is the matrix of inner products between rows;
summed over all the samples

# Constructing SVD - rows



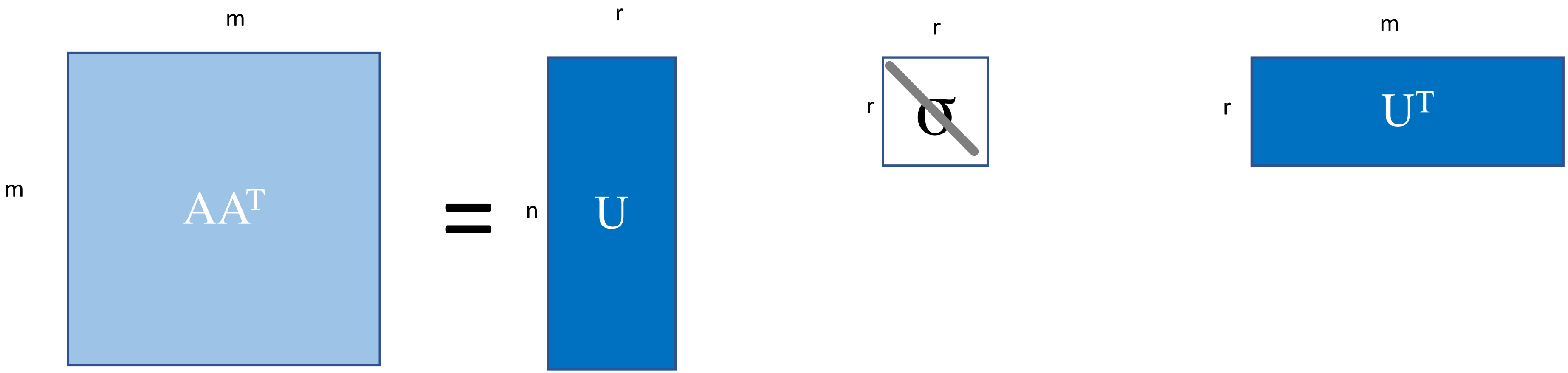

- Now take the eigenvalue decomposition of $AA^T$

# Constructing SVD - rows



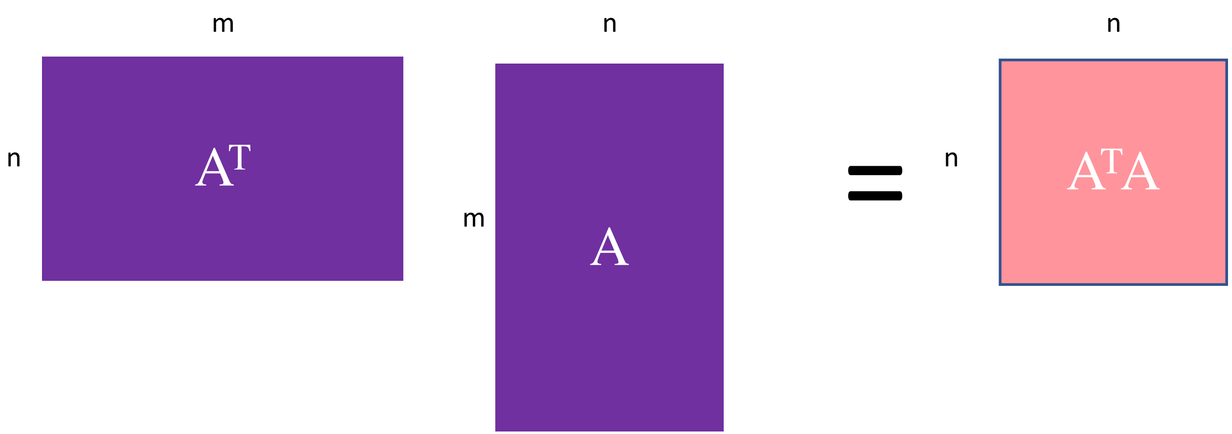

- Now take the eigenvalue decomposition of $AA^T$
- I have a bunch of zero eigenvalues, so I have a bunch of eigenvectors that can't contribute to the sum

# Constructing SVD - rows




- Now take the eigenvalue decomposition of $AA^T$
- $U$ (n x r) , $\sigma$ (r), $U^T$ (r x n)

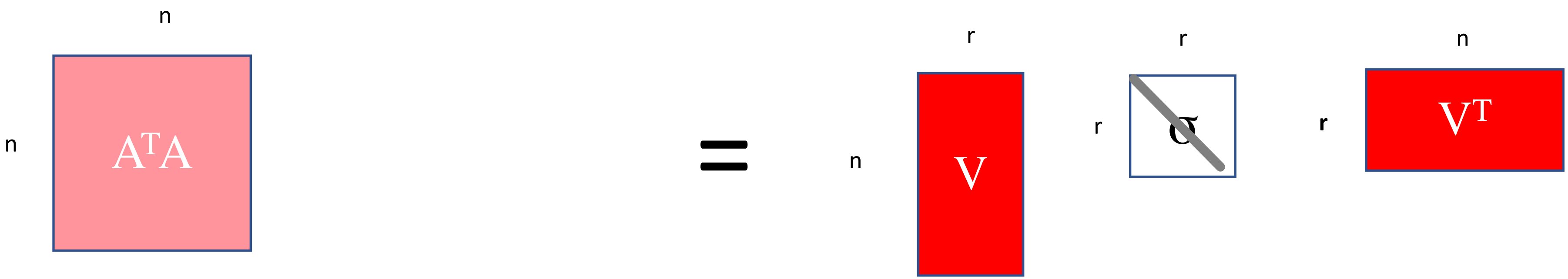
# Constructing SVD - columns




- This matrix has dimensions n_samples x n_samples.

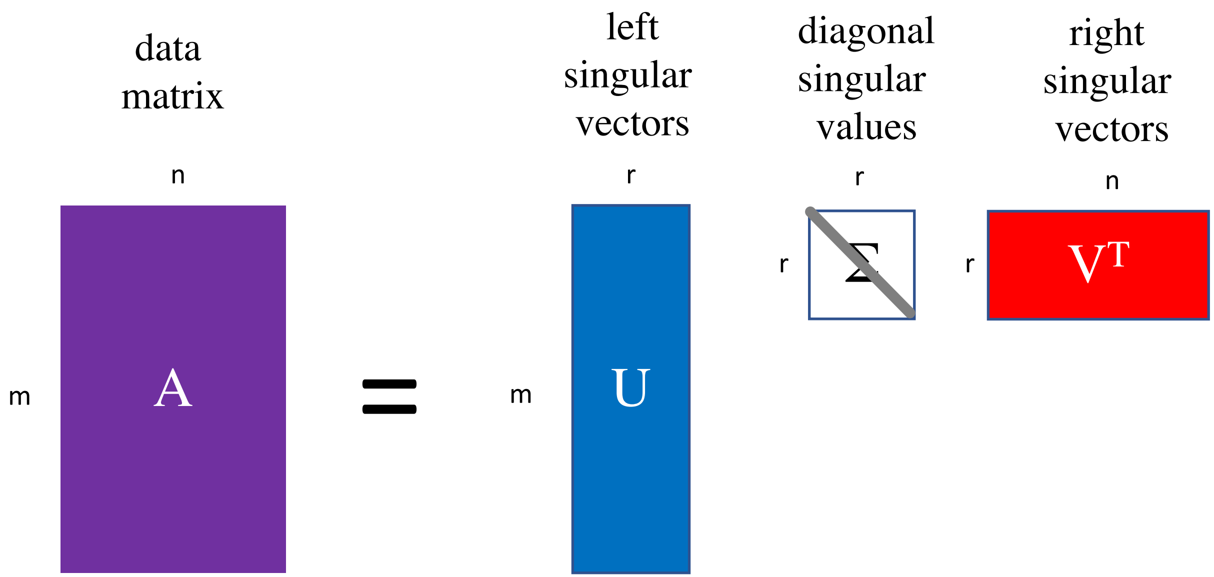
# Constructing SVD - columns

Eigenvalue decomposition again



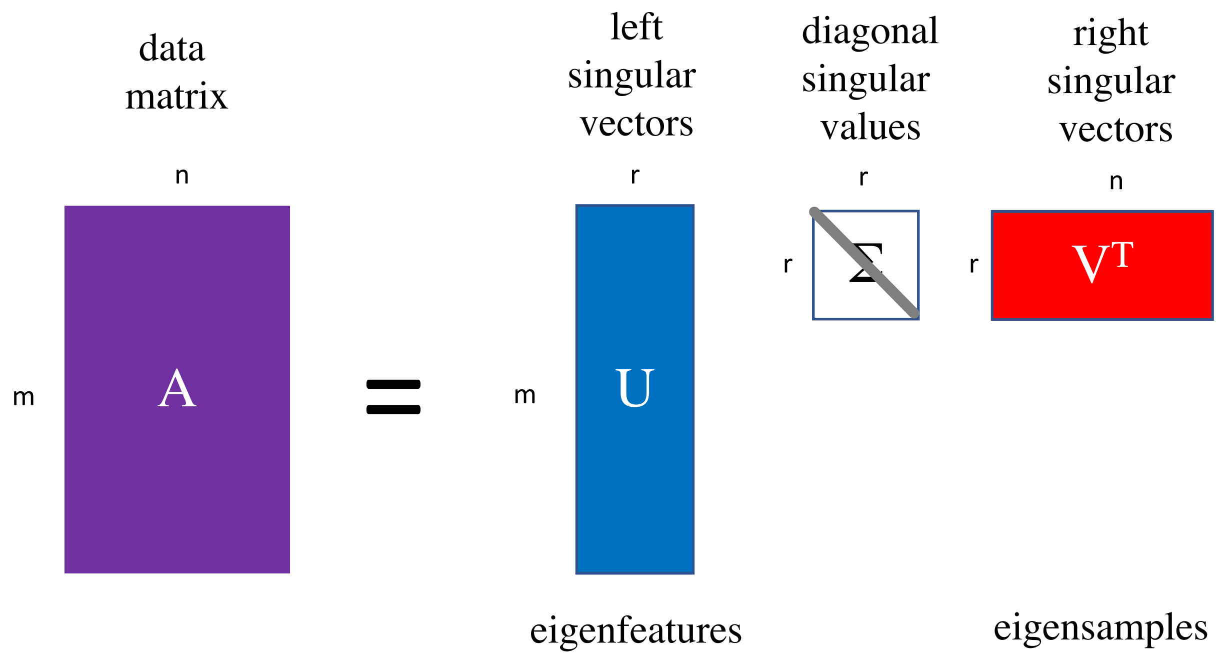

- Because of the relationship between $A^TA$ and $AA^T$ these two matrices have the same eigenvalues.
- Some of the eigenvalues have to be zero in the larger matrix

# Singular Value Decomposition (SVD)




- I have two sets of basis vectors and one set of r singular values.
- Two powers of A -> elements of $\Sigma$ are square roots of eigenvalues

# Singular Value Decomposition (SVD)




- I have two sets of basis vectors and one set of r singular values.
- Two powers of A -> elements of $\Sigma$ are square roots of eigenvalues

# SVD

```
import numpy as np
from numpy import linalg as LA

# 
https://numpy.org/doc/stable/refe
rence/generated/numpy.linalg.svd.
html

U, SIGMA, VT = LA.svd(A)
```

We could calculate SVD ourselves in two lines –

but we shouldn't

# Approximate, truncated SVD

```
import numpy as np
from numpy import linalg as LA
from sklearn.utils.extmath import randomized_svd

# https://scikit-learn.org/stable/modules/generated/sklearn.utils.extmath.randomized_svd.html


U, SIGMA, VT = randomized_svd(A, n_components=50)
```

The library functions use convergence or optimization to find approximate matrix factorizations.

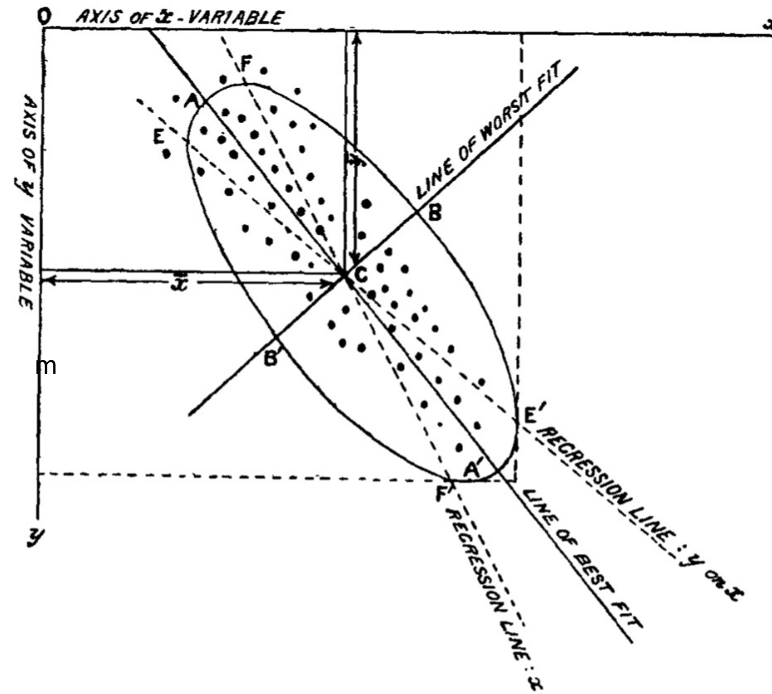
Does not actually build or store $A^T A$

Approximate and truncated decompositions are cheaper to compute.

# Principal Component analysis

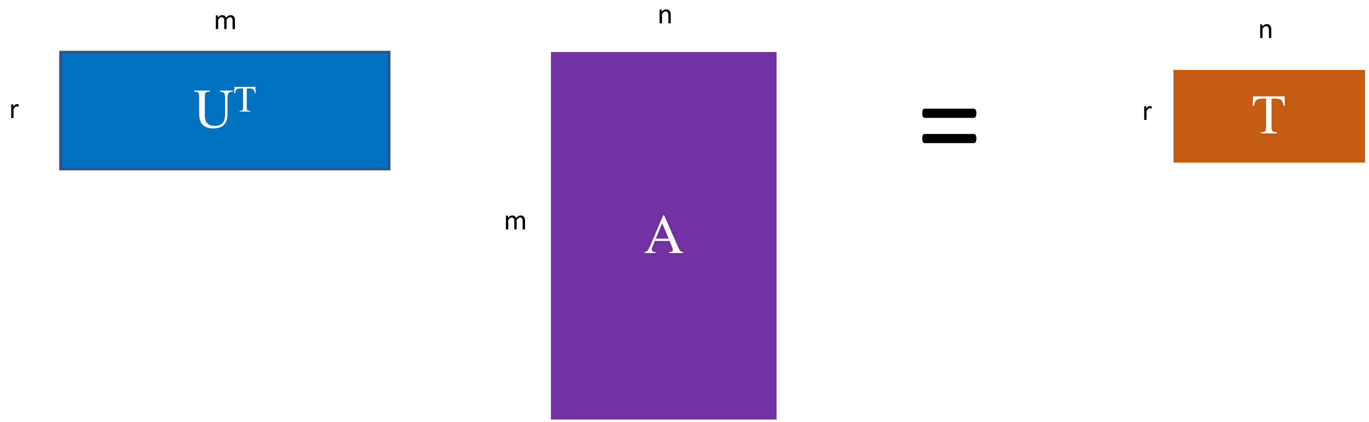
- SVD is a just linear algebra + geometry interpretation of the columnwise & rowwise inner products.
- PCA is the doctrine of using vectors derived from SVD to interpret data.
- The data points are rotated onto the singular vectors, renamed PCA coordinates
- AV = T (new coordinates)
- Can make pretty pictures

r




Pearson, 1901
doi: 10.1080/14786440109462720

# Principal Component analysis




This is the dimension reduction we might have asked for

Table 1

*Principal Components Analysis of BIS-11 Items (Oblique Rotation)*

| BIS-11 items | First-order factors 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 11. I "squirm" at plays or lectures. | **.84** | .17 | –.08 | –.03 | .03 | .02 |
| 32. I am restless at the theater or lectures. | **.84** | .19 | –.12 | –.06 | –.00 | –.03 |
| 5. I don't "pay attention." | **.57** | .04 | .16 | –.02 | .27 | .02 |
| 17. I act "on impulse." | .15 | **.74** | .08 | –.02 | –.20 | .06 |
| 20. I act on the spur of the moment. | .12 | **.72** | .19 | –.10 | –.19 | .01 |
| 23. I buy things on impulse. | –.08 | **.59** | –.04 | .28 | .10 | .11 |
| 12. I am a careful thinker.[a] | .17 | –.13 | **.64** | .17 | –.18 | .05 |
| 1. I plan tasks carefully.[a] | –.05 | .16 | **.64** | –.04 | .11 | –.10 |
| 8. I am self-controlled.[a] | .10 | .00 | **.63** | –.24 | .08 | –.17 |

Patton et al. 1995 Factor structure of the Barratt Impulsiveness Scale

doi: 10.1002/1097-4679(199511)51:6<768::AID-JCLP2270510607>3.0.CO;2-1

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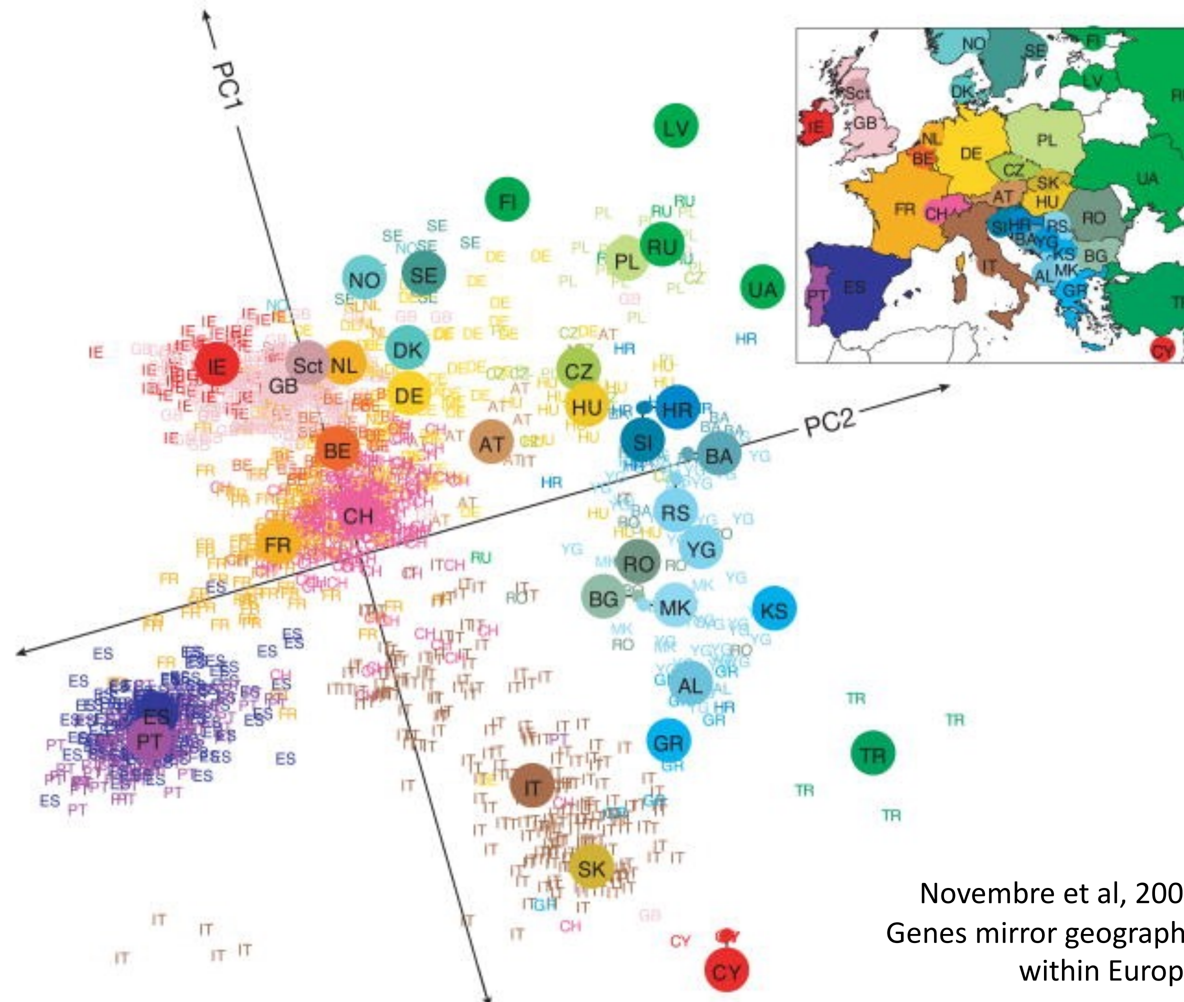
Data correlations here used to inform reduction of dimension from 35-question survey to 6 scores.

# Genes mirror geography within Europe




m x n = 200k genetic loci x 1400 individuals

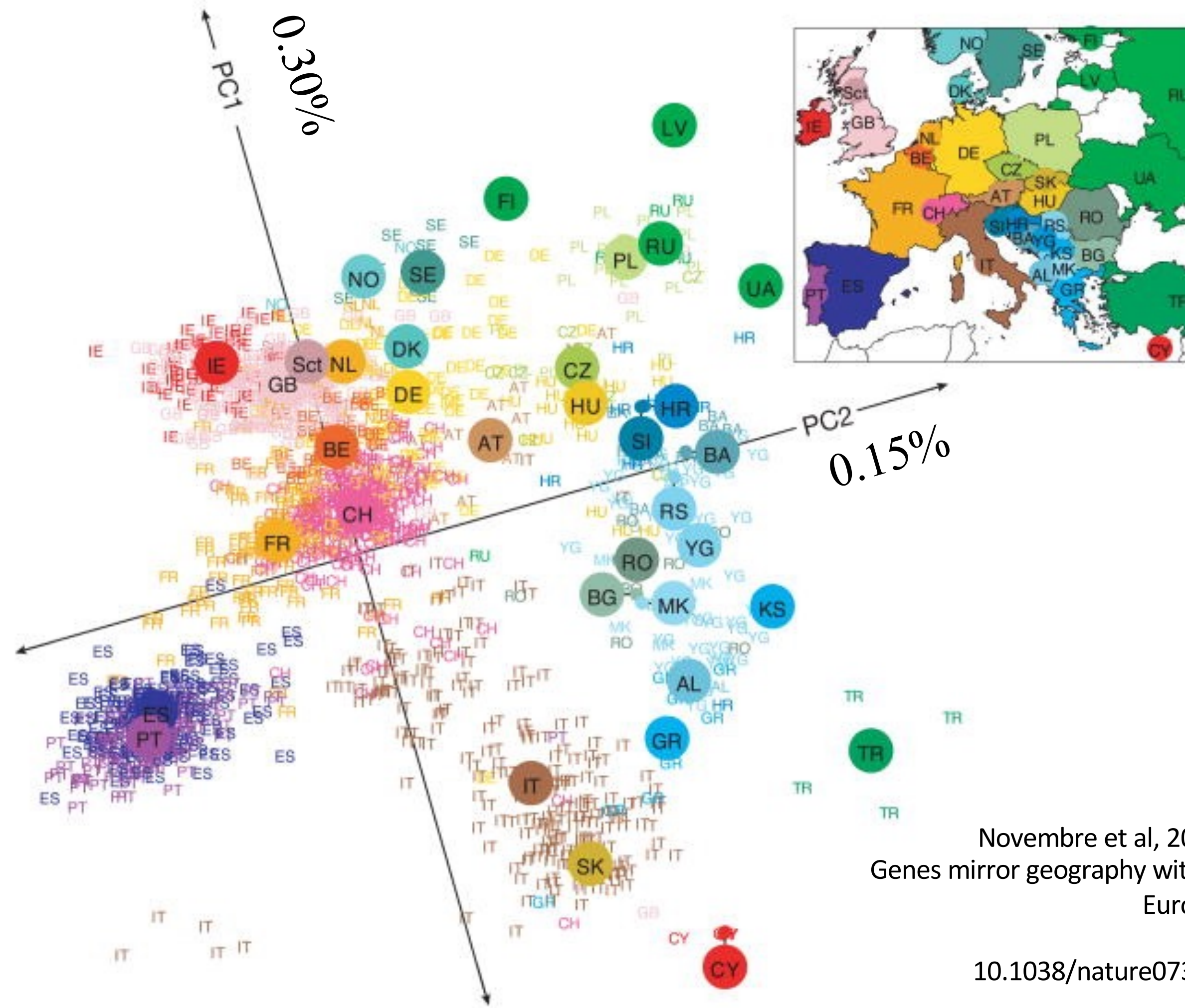
Novembre et al, 2008
Genes mirror geography
within Europe

10.1038/nature07331

# Genes mirror geography within Europe

Principal components and eigenvalues come back from largest to smallest magnitude.

It is conventional to report principal components along with the fraction of variance explained by each

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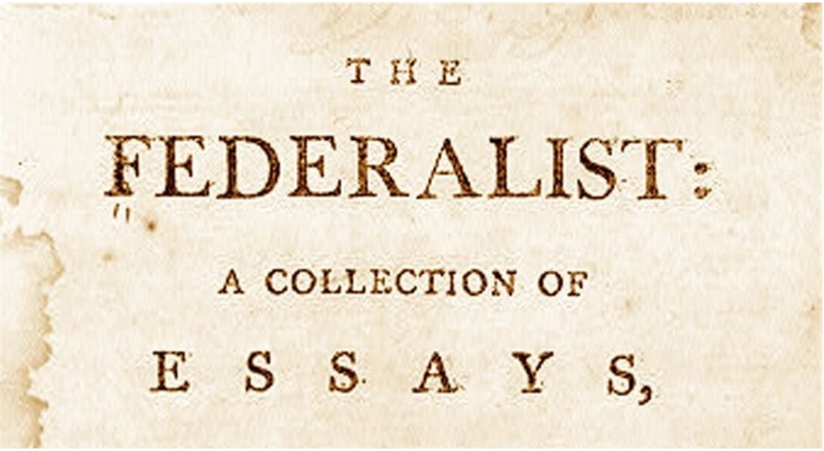
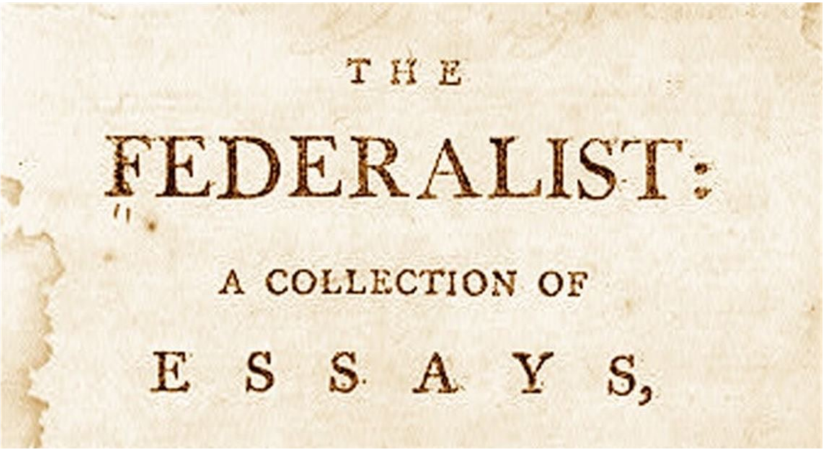



- 85 documents, initially published anonymously 1787-1788
- Authors' reminiscences disagree about authorship of some of the essays
- 85 documents parsed into vocabulary of ~10000 "words"

## What if your data looks like this?

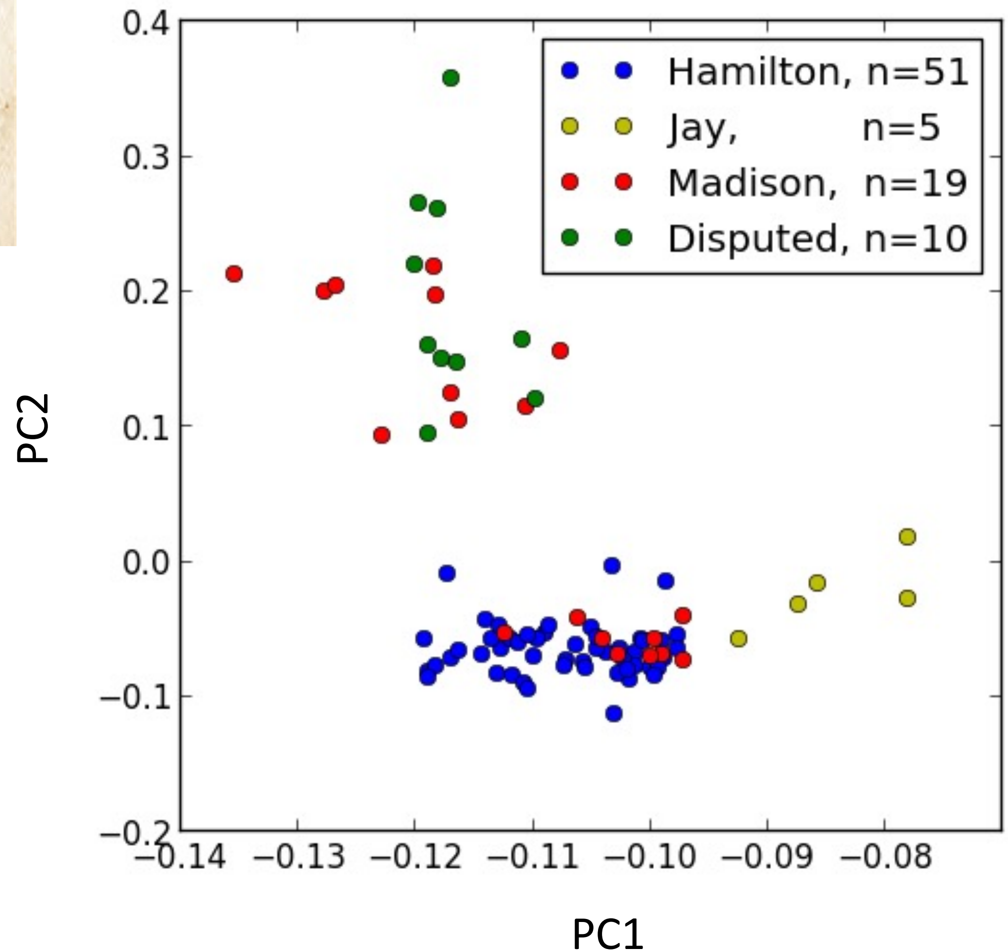
| | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| NEW | 7 | 3 | 2 | 1 | 1 | 2 | 11 | 3 | 7 | 2 | 2 | 4 | 4 | 6 | 3 | 2 | 1 | 3 | 2 | 2 |
| SO | 3 | 4 | 4 | 5 | 3 | 4 | 4 | 5 | 5 | 4 | 4 | 6 | 3 | 6 | 2 | 3 | 4 | 2 | 4 | 2 |
| THEY | 6 | 22 | 5 | 17 | 11 | 11 | 7 | 13 | 20 | 11 | 9 | 8 | 3 | 17 | 15 | 14 | 7 | 12 | 9 | 7 |
| AGAINST | 2 | 1 | 3 | 6 | 5 | 4 | 1 | 5 | 5 | 6 | 1 | 3 | 1 | 4 | 4 | 6 | 2 | 4 | 6 | 0 |
| ANY | 6 | 1 | 4 | 5 | 3 | 0 | 6 | 2 | 4 | 4 | 4 | 7 | 3 | 2 | 3 | 11 | 2 | 2 | 6 | 0 |
| EITHER | 2 | 0 | 5 | 4 | 1 | 5 | 3 | 1 | 3 | 1 | 3 | 0 | 0 | 1 | 1 | 3 | 1 | 0 | 1 | 0 |
| FOR | 13 | 14 | 11 | 12 | 8 | 14 | 15 | 9 | 11 | 18 | 19 | 8 | 2 | 19 | 18 | 9 | 12 | 8 | 8 | 17 |
| GOVERNMENT | 5 | 4 | 5 | 11 | 2 | 1 | 1 | 1 | 8 | 4 | 2 | 6 | 7 | 7 | 4 | 10 | 4 | 3 | 1 | 2 |
| GUARANTY | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| NATIONAL | 1 | 3 | 14 | 7 | 0 | 4 | 2 | 2 | 2 | 2 | 4 | 4 | 4 | 2 | 9 | 9 | 8 | 0 | 2 | 0 |
| NATURE | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 2 | 1 | 2 | 0 | 2 | 2 | 1 | 3 | 0 | 1 | 2 |
| ON | 9 | 8 | 6 | 11 | 5 | 2 | 13 | 11 | 9 | 18 | 5 | 12 | 3 | 17 | 10 | 4 | 2 | 16 | 17 | 7 |
| OTHER | 3 | 3 | 7 | 10 | 2 | 5 | 4 | 4 | 4 | 16 | 6 | 11 | 1 | 6 | 3 | 2 | 7 | 2 | 5 | 4 |
| OWN | 4 | 1 | 0 | 4 | 0 | 0 | 4 | 0 | 2 | 3 | 4 | 1 | 1 | 4 | 2 | 2 | 0 | 2 | 3 | 1 |
| STATES, | 0 | 0 | 6 | 0 | 1 | 3 | 4 | 4 | 4 | 1 | 5 | 1 | 3 | 3 | 1 | 2 | 1 | 1 | 1 | 2 |
| UPON | 6 | 1 | 0 | 0 | 0 | 4 | 11 | 3 | 4 | 0 | 6 | 7 | 2 | 0 | 10 | 6 | 6 | 1 | 0 | 1 |
| COULD | 1 | 1 | 1 | 2 | 0 | 0 | 2 | 3 | 3 | 2 | 3 | 2 | 0 | 1 | 3 | 12 | 1 | 2 | 2 | 1 |
| KIND | 0 | 2 | 1 | 0 | 1 | 0 | 0 | 0 | 3 | 0 | 1 | 1 | 0 | 0 | 5 | 4 | 1 | 0 | 0 | 0 |
| SHALL | 7 | 1 | 0 | 6 | 1 | 1 | 1 | 0 | 4 | 2 | 3 | 1 | 3 | 0 | 1 | 1 | 1 | 0 | 2 | 0 |
| SHOULD | 1 | 3 | 4 | 1 | 4 | 2 | 7 | 4 | 4 | 0 | 3 | 4 | 0 | 2 | 6 | 6 | 2 | 1 | 0 | 0 |
| STATES | 2 | 1 | 4 | 1 | 0 | 4 | 25 | 7 | 5 | 1 | 7 | 8 | 5 | 8 | 8 | 6 | 2 | 0 | 2 | 0 |
| TOTAL | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| VALUE | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 |
| WANT | 0 | 0 | 2 | 1 | 0 | 1 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 1 |
| WHO | 8 | 7 | 1 | 3 | 3 | 7 | 2 | 0 | 3 | 9 | 4 | 1 | 3 | 1 | 6 | 5 | 2 | 8 | 5 | 3 |
| AT | 8 | 9 | 1 | 2 | 4 | 6 | 11 | 11 | 10 | 8 | 11 | 13 | 1 | 7 | 24 | 11 | 7 | 4 | 5 | 8 |
| BETWEEN | 0 | 0 | 0 | 2 | 3 | 8 | 9 | 3 | 3 | 3 | 4 | 5 | 1 | 4 | 2 | 3 | 4 | 2 | 4 | 1 |
| DUTIES | 0 | 0 | 0 | 1 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 2 |
| EACH | 0 | 5 | 0 | 2 | 6 | 4 | 4 | 2 | 0 | 4 | 7 | 4 | 4 | 0 | 5 | 1 | 2 | 2 | 2 | 4 |
| LANDS | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |




- Sometimes $\sum(x-\bar{x})(y-\bar{y})$

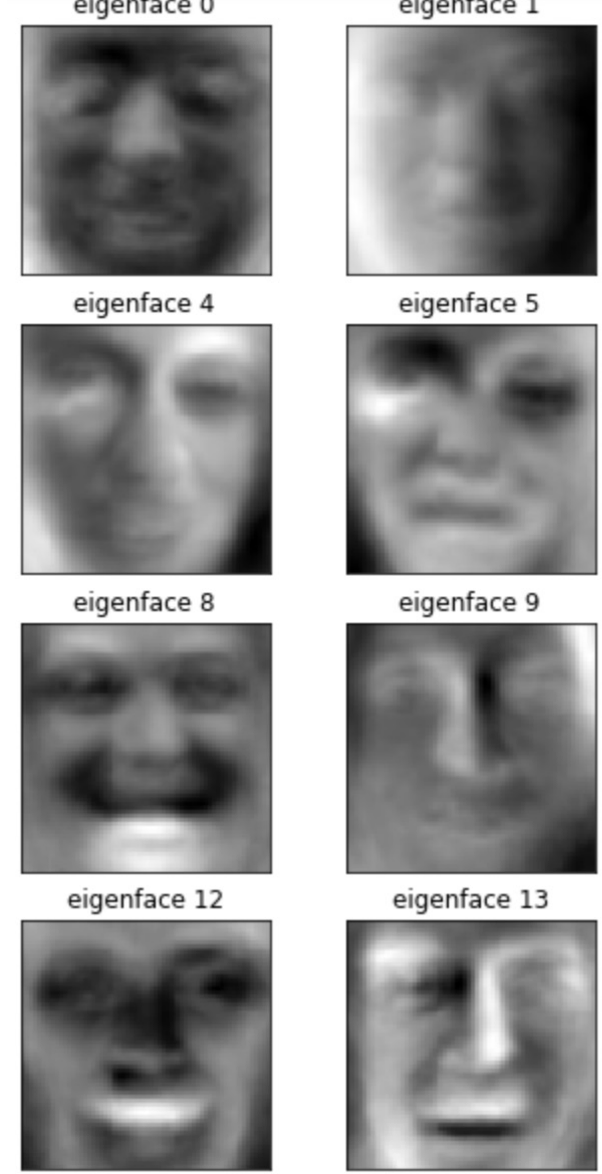
is not an appropriate distance score for your data.

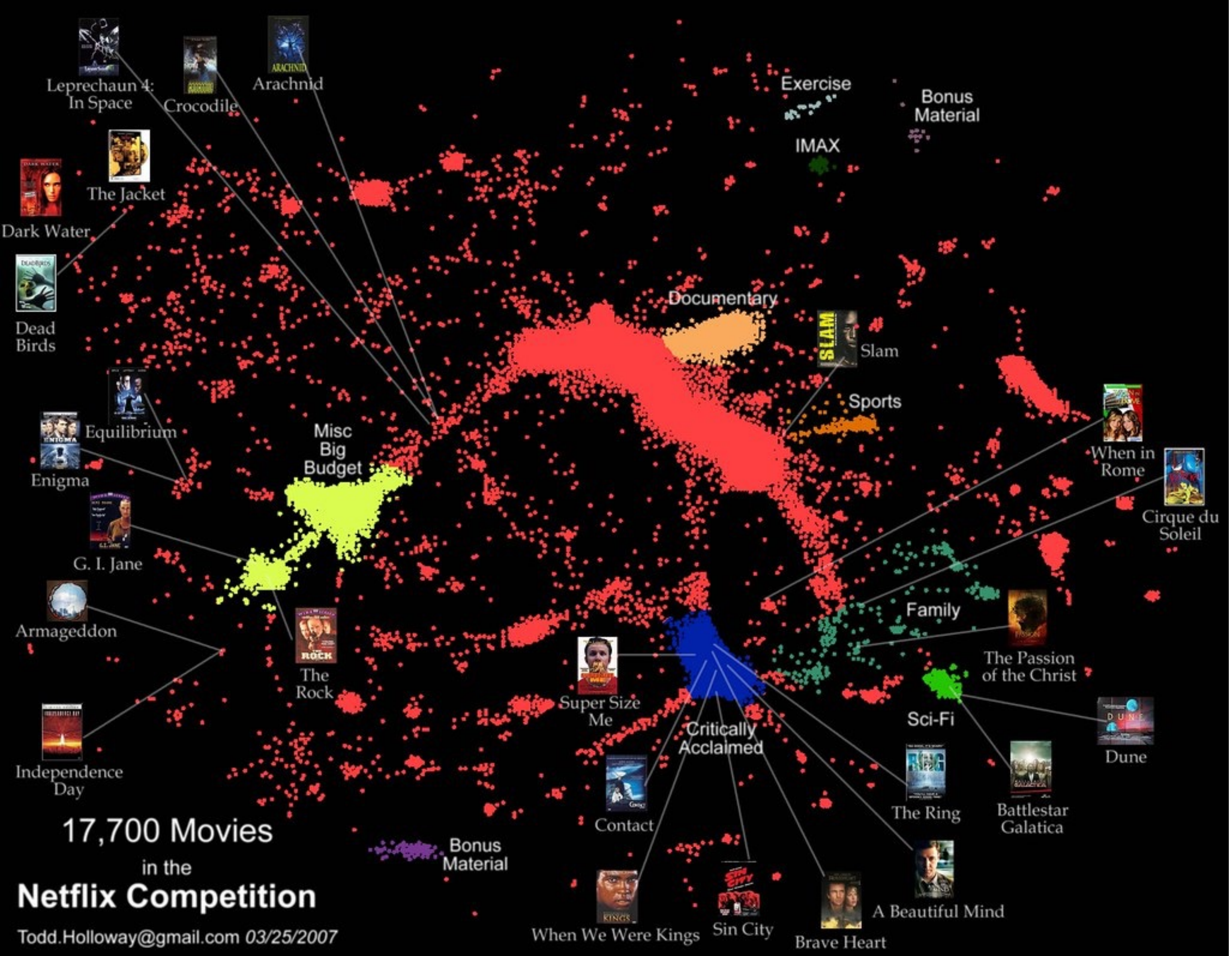
- You can run PCA on an n x n distance matrix evaluated using a domain-specific columnwise comparison.
- Resulting low-dimensional coordinates visualize vocabulary/style relationships



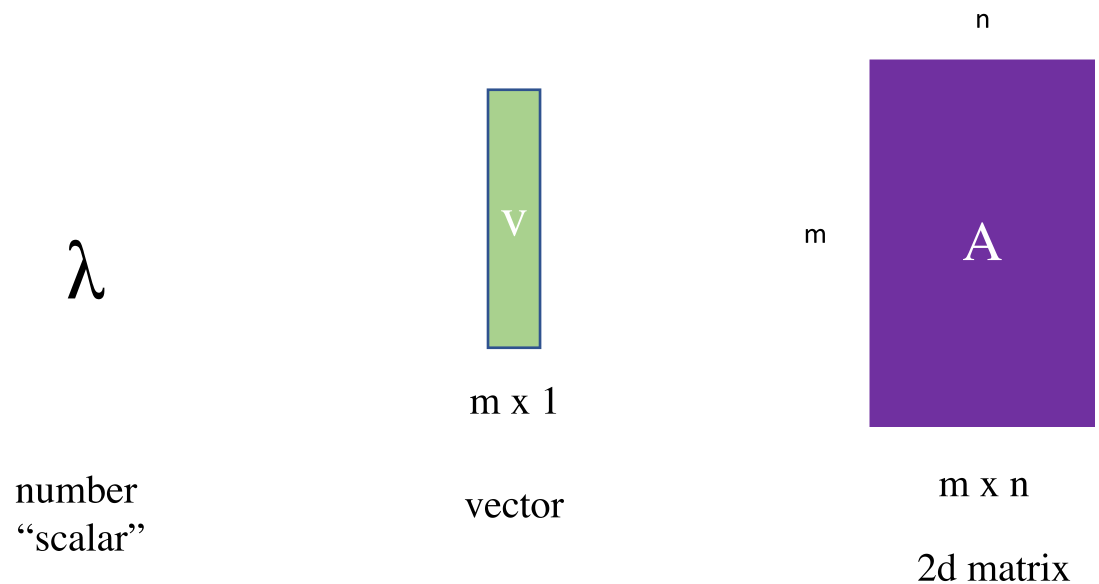
# Caveats

- SVD/PCA don't know anything but the cloud of points and its correlations.
- Each new sample builds a different set of basis vectors
- Hard to interpret: positive and negative values in the eigenvectors
- Does not handle non-numerical values—have to change the objective function for that (Netflix)

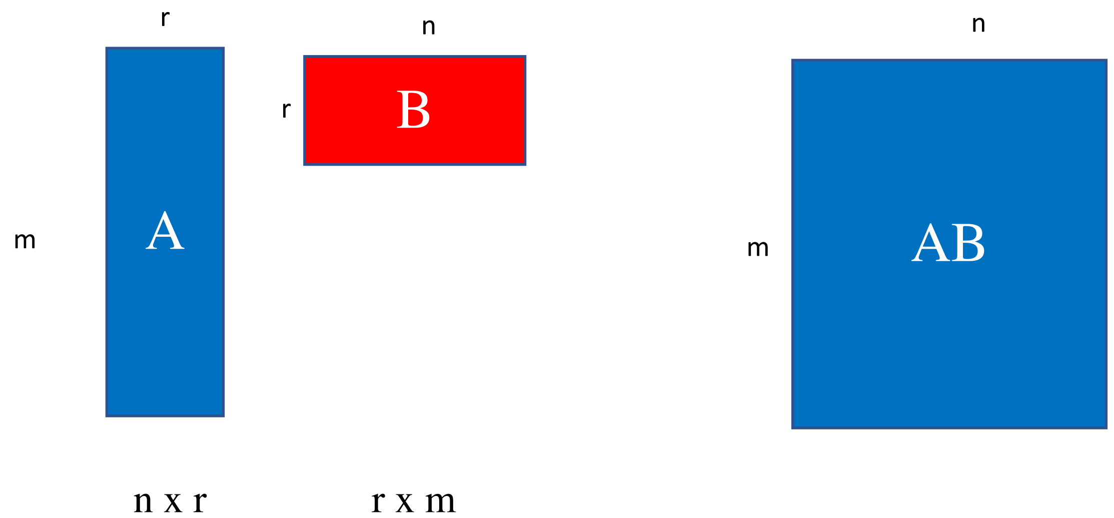



Leprechaun 4: In Space
Crocodile
Arachnid
Exercise
Bonus Material
IMAX
The Jacket
Dark Water
Dead Birds
Documentary
Slam
Sports
Equilibrium
Enigma
Misc Big Budget
When in Rome
Cirque du Soleil
G. I. Jane
Armageddon
The Rock
Family
The Passion of the Christ
Super Size Me
Critically Acclaimed
Sci-Fi
Dune
Independence Day
Contact
The Ring
Battlestar Galatica
17,700 Movies
in the
Netflix Competition
Bonus Material
A Beautiful Mind
When We Were Kings
Sin City
Brave Heart
Todd.Holloway@gmail.com 03/25/2007

# Linear algebra objects

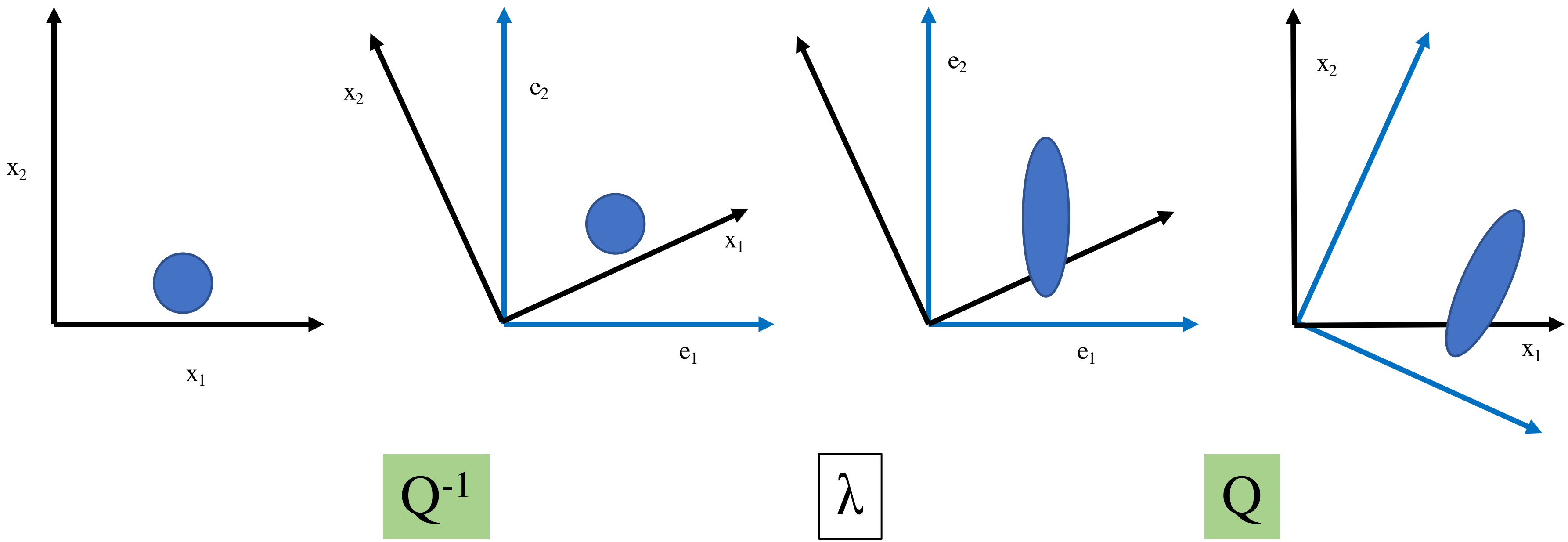


# Matrix multiplication




2d matrix

# Transformation of x1, x2 using A



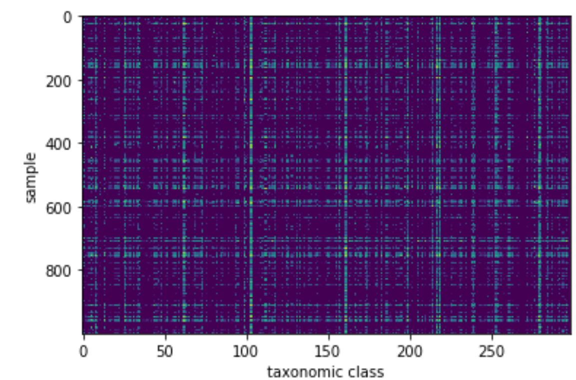
# Dimension reduction

For a general matrix representing n observations of m traits:

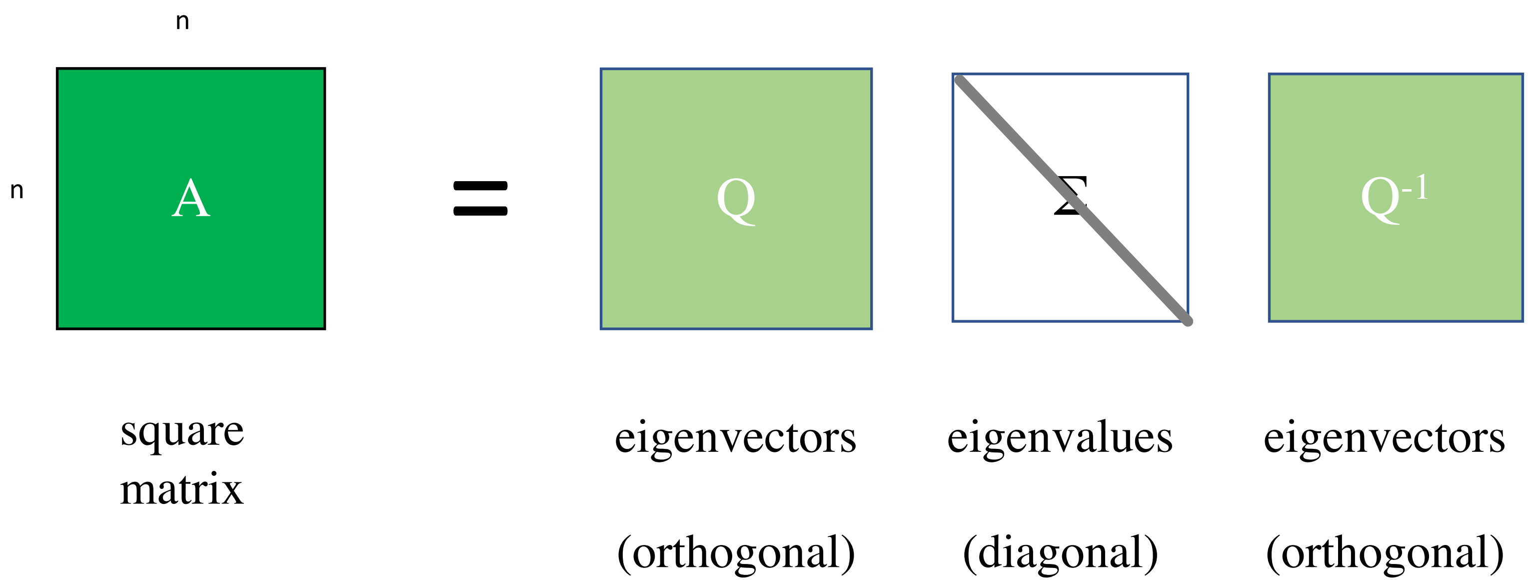
A ( m x n)

It is unlikely that all of the elements in this matrix are independent; there is likely some “structure”

If I could replace A with an approximation of A that has fewer than n x m numbers, A will be cheaper to store, faster to copy, can run on computers with less memory.



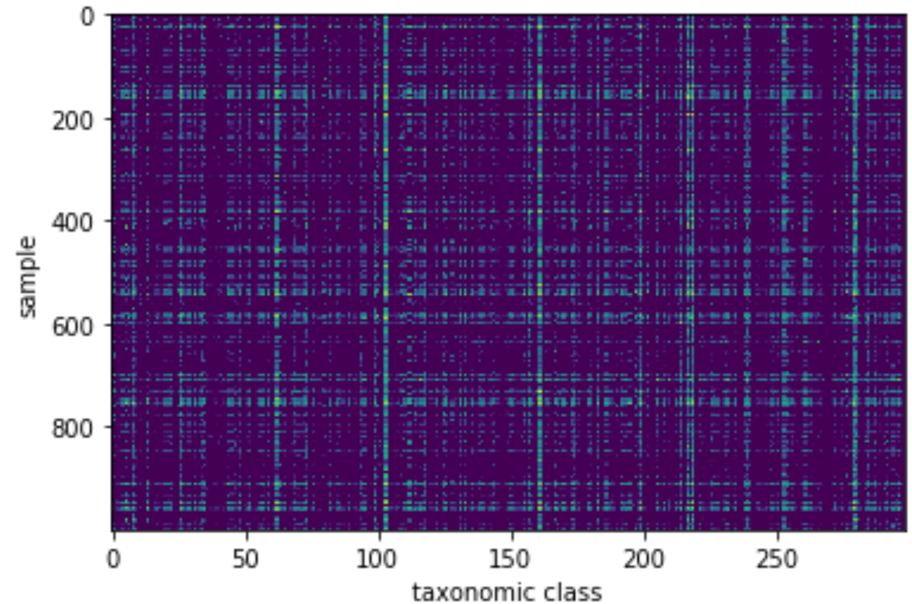
# Eigenvalue decomposition



# A (n x m)

(rows x columns)

(n “samples”  by m “features”)




| | Hydrozoa | Sphingobacteriia | Marattiopsida | Pedinophyceae | Chrysiogenetes (class) | Fusobacteria (class) | Amphibia |
|---|---|---|---|---|---|---|---|
| **(Index,)** | | | | | | | |
| **mgm4703051.3.mg** | 2 | 354 | 0 | 0 | 0 | 0 | 0 |
| **mgm4755207.3.mg** | 3430 | 0 | 25 | 14 | 33111 | 101765 | 5094 |
| **mgm4473196.3.mg** | 150 | 0 | 0 | 10 | 1265 | 487614 | 11598 |
| **mgm4679127.3.mg** | 0 | 245 | 0 | 0 | 0 | 0 | 0 |
| **mgm4529798.3.mg** | 2 | 4588 | 0 | 0 | 25 | 0 | 56 |

# Now this looks like “structure”

Organizing data like this is deeply satisfying—it makes us think we have discovered truth.

Mature libraries to make exactly this sort of eye-candy graphs. This one is `sanborn.clustermap`

What if I told you linear algebra could do this?