Principal Component Analysis (PCA)

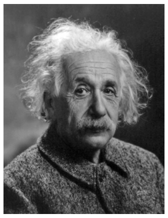
BCH394P/364C Systems Biology / Bioinformatics

Edward Marcotte, Univ of Texas at Austin

What is Principal Component Analysis? What does it do?

So, first let's build some intuition.

"You do not really understand something unless you can explain it to your grandmother", Albert Einstein



wikipedia

With thanks for many of these explanations to http://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues

What is Principal Component Analysis? What does it do?

A general (and imprecise) political example:

Suppose you conduct a political poll with 30 questions, each answered by 1 (*strongly disagree*) through 5 (*strongly agree*). Your data is the answers to these questions from many people, so it's 30-dimensional, and you want to understand what the major trends are.

You run PCA and discover 90% of your variance comes from one direction, corresponding not to a single question, but to a specific weighted combination of questions. This new hybrid axis corresponds to the political left-right spectrum, *i.e.* democrat/republican spectrum.

Now, you can study that, or factor it out & look at the remaining more subtle aspects of the data.

So, PCA is a method for discovering the major trends in data, simplifying the data to focus only on those trends, or removing those trends to focus on the remaining information.

Example: Christian Bueno, http://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues

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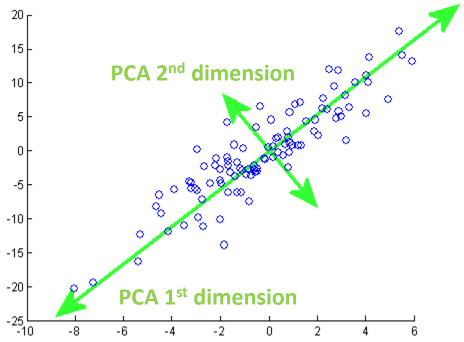
What is Principal Component Analysis? What does it do?

A more precise graphical example:

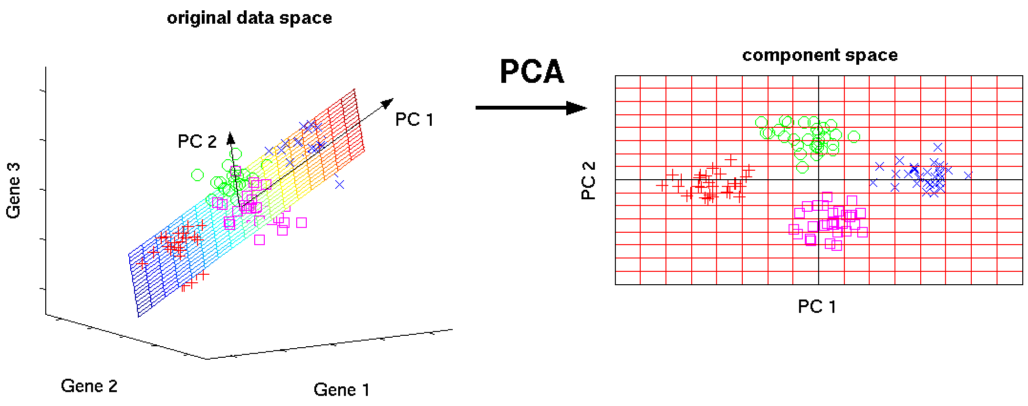
In a general sense,
PCA rotates your axes to "line up" better with your data.

Because rotation is a kind of linear transformation, your new dimensions will be weighted sums of the old ones, like $\langle 1\rangle=23\%\cdot[1]+46\%\cdot[2]+39\%\cdot[3]$



Quotes & image adapted from Isomorphismes, http://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues

PCA finds new variables which are linear combinations of the original variables such that in the new space, the data has fewer dimensions.



Imagine a data set consisting of points in 3D on the surface of a flat plate held up at an angle. In the original x, y, z axes you need 3 dimensions to represent the data, but with the correct linear transformation, you only need 2.

Quotes: Shlomo Argamon, from http://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues
Image: http://phdthesis-bioinformatics-maxplanckinstitute-molecularplantphys.matthias-scholz.de/

To summarize so far:

PCA is a technique to reduce dimension by:

1. Taking ***linear combinations*** of the original variables.
2. Each linear combination explains the ***most variance*** in the data it can.
3. Each linear combination is uncorrelated (***orthogonal***) with the others
4. Plot the data in terms of only the most important (***principal***) dimensions

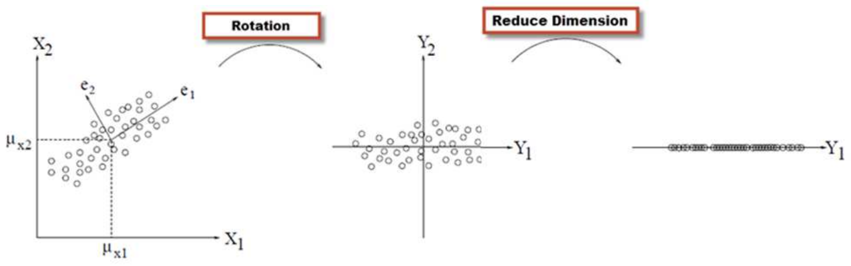
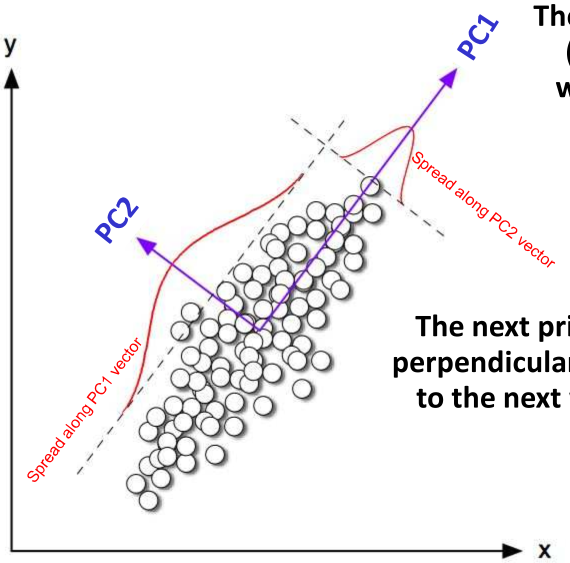


Image: http://blog.equametrics.com/2013/02/an-introduction-to-principal-component-analysis
Quote: http://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues



The first principal component (PC1) corresponds to the widest spread of the data.

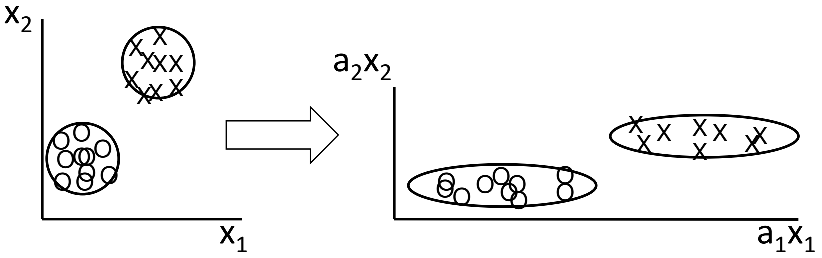
The next principal component (PC2) is perpendicular to the 1st, and corresponds to the next widest spread of the data.

& so on. There will be as many PCs as data dimensions, but ranked by diminishing importance.

http://web.media.mit.edu/~tristan/phd/dissertation/chapter5.html

Linear Transformations

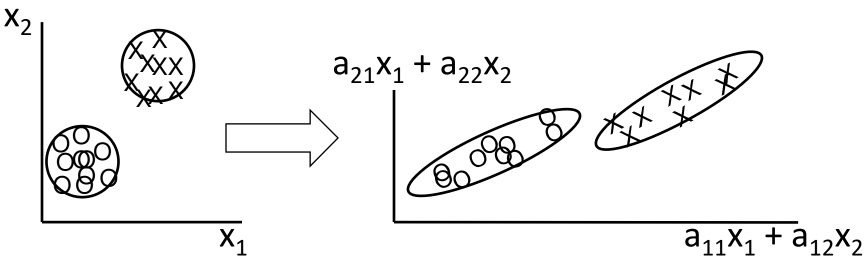
Scaling



Adapted from http://www.engr.sjsu.edu/~knapp/HCIRODPR/PR_Mahal/linear_tr.htm

Linear Transformations

Scaling & Rotating

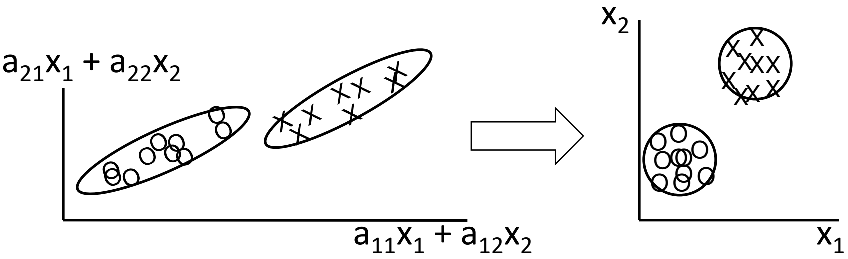


If we can stretch & rotate this way…

Adapted from http://www.engr.sjsu.edu/~knapp/HCIRODPR/PR_Mahal/linear_tr.htm

Linear Transformations

Scaling & Rotating

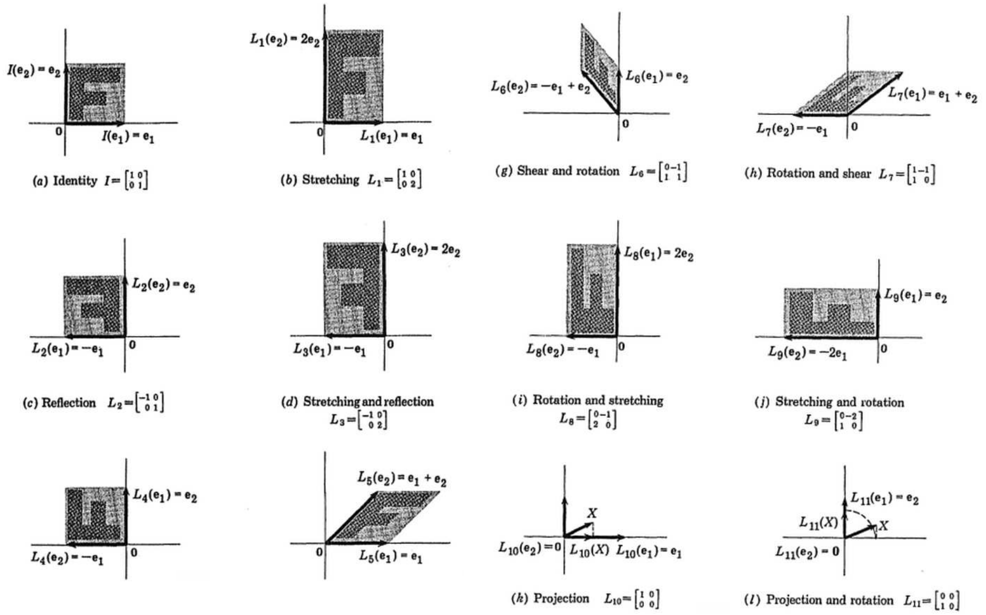


…then we can also go the other way.

To do this, we need to learn about covariance…

Adapted from http://www.engr.sjsu.edu/~knapp/HCIRODPR/PR_Mahal/linear_tr.htm

More examples of different linear transformations:



(*a*) Identity $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

(*b*) Stretching $L_1 = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$

(*g*) Shear and rotation $L_6 = \begin{bmatrix} 0 & -1 \\ 1 & 1 \end{bmatrix}$

(*h*) Rotation and shear $L_7 = \begin{bmatrix} 1 & -1 \\ 1 & 0 \end{bmatrix}$

(*c*) Reflection $L_2 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$

(*d*) Stretching and reflection $L_3 = \begin{bmatrix} -1 & 0 \\ 0 & 2 \end{bmatrix}$

(*i*) Rotation and stretching $L_8 = \begin{bmatrix} 0 & -1 \\ 2 & 0 \end{bmatrix}$

(*j*) Stretching and rotation $L_9 = \begin{bmatrix} 0 & -2 \\ 1 & 0 \end{bmatrix}$

(*k*) Projection $L_{10} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$

(*l*) Projection and rotation $L_{11} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$

http://isomorphismes.tumblr.com/post/11407834056/matrices-linear-algebra

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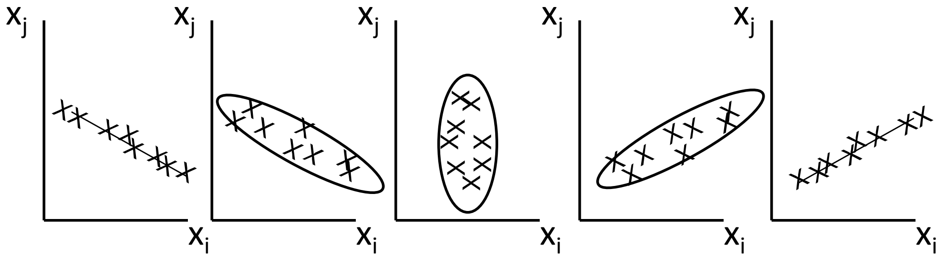
Covariance = measures tendency to vary together (to co-vary). Similar to correlation.



$c = -s_i s_j$ **$c = -0.5\ s_i s_j$**   **$c = 0$**   **$c = 0.5\ s_i s_j$**   **$c = s_i s_j$**

Anti-correlated   **Uncorrelated**   **Correlated**

Variance = average of the <u>squared</u> deviations of a feature from its mean
= μ^2 = (std deviation)^2 = covar(i,i)

Covariance = average of the <u>products</u> of the deviations of feature values from their means

$$\text{covar}(i,j) = \frac{[\,x(1,i) - m(i)\,]\,[\,x(1,j) - m(j)\,] + \ldots + [\,x(n,i) - m(i)\,]\,[\,x(n,j) - m(j)\,]}{n \quad \text{[or use (n-1) if sampling from a larger population]}}$$

Adapted from http://www.engr.sjsu.edu/~knapp/HCIRODPR/PR_Mahal/cov.htm

All of the **covariances** c(i,j) between features can be collected together into a **covariance matrix** C.

This summarizes all of the correlation structure among all pairs of features.

covariance between feature 1 and 2

covariance between feature 2 and n

$$\mathbf{C} = \begin{bmatrix} c(1,1) & c(1,2) & \cdots & c(1,n) \\ c(2,1) & c(2,2) & \cdots & c(2,n) \\ \vdots & \vdots & & \vdots \\ c(n,1) & c(n,2) & \cdots & c(n,n) \end{bmatrix}$$

etc.

We need one last concept: Eigenvectors and eigenvalues

An eigenvector v of a linear transformation *T* is a nonzero vector that, when *T* is applied to it, does not change direction. Applying *T* to the eigenvector only scales the eigenvector by the scalar value *λ*, called an eigenvalue.

That is:

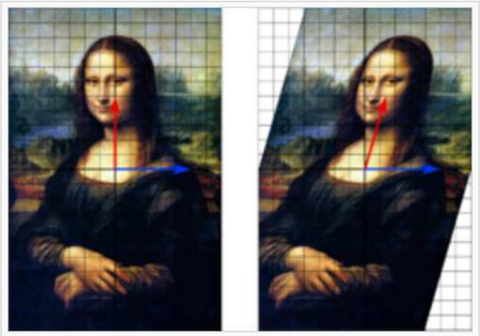
$$T(\mathbf{v}) = \lambda\mathbf{v}$$

eigenvalue (scalar)

square transformation matrix

eigenvector

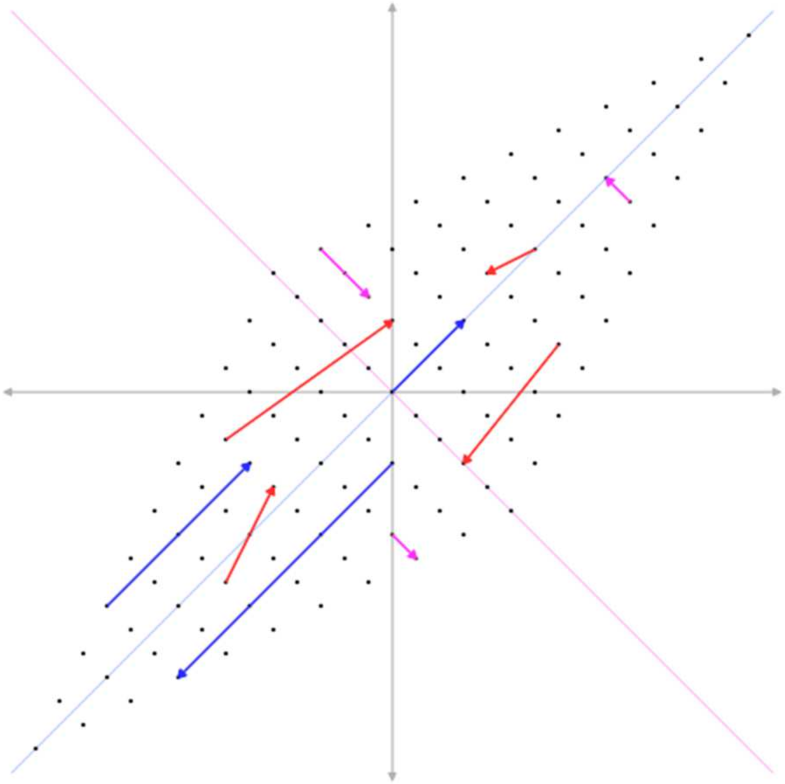
The eigenvector answers the question:
In which direction does my transformation matrix stretch?
& the eigenvalue indicates by how much



The blue arrow is an eigenvector of this linear transformation matrix, since it doesn't change direction.

Its scale is also unchanged, so its eigenvalue is 1.

Wikipedia



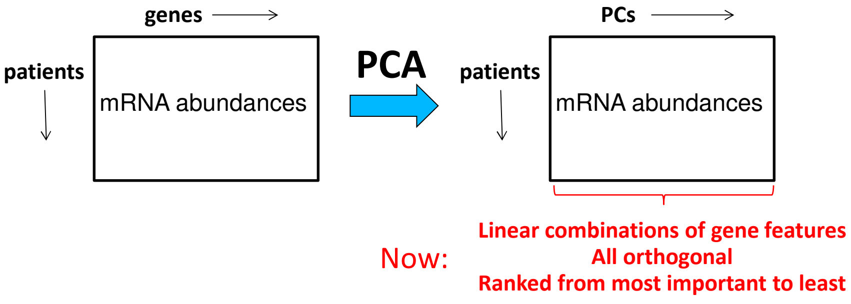
wikipedia

Calculating the PCA

1. Calculate the covariation matrix *C* between features of the data
2. Calculate the eigenvectors and eigenvalues of *C*
3. Order the eigenvectors according to the eigenvalues

PC1 is the eigenvector corresponding to the largest eigenvalue,
PC2 is the eigenvector corresponding to the next largest, etc.

The data can be plotted as projections along the PCs of interest.



genes →

patients ↓

mRNA abundances

PCA

PCs →

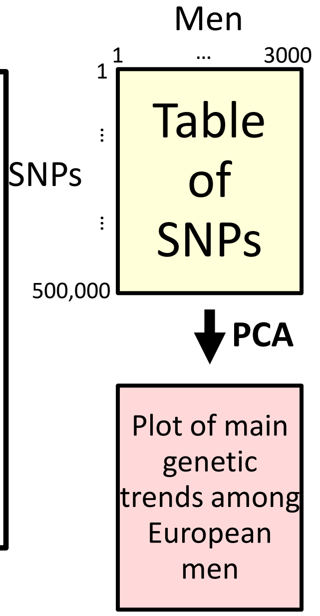
patients ↓

mRNA abundances

Now:

Linear combinations of gene features
All orthogonal
Ranked from most important to least

Here's a beautiful application of PCA that illustrates how it can simplify complicated datasets:



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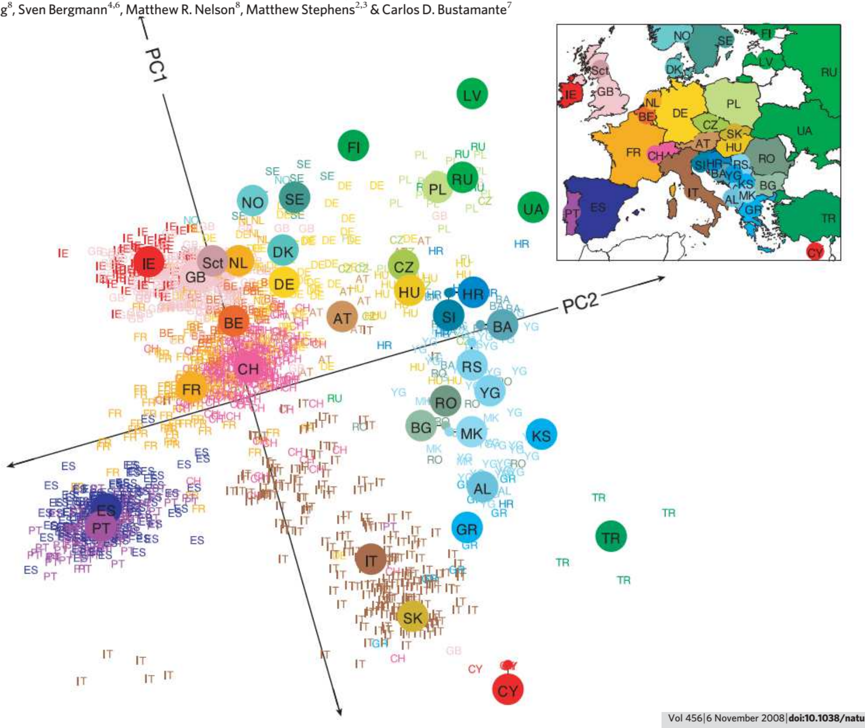
What do you think are the most important genetic trends among European men?

What might this picture → look like?

Vol 456|6 November 2008|doi:10.1038/nature07331

Genes mirror geography within Europe

John Novembre[1,2], Toby Johnson[4,5,6], Katarzyna Bryc[7], Zoltán Kutalik[4,6], Adam R. Boyko[7], Adam Auton[7], Amit Indap[7], Karen S. King[8], Sven Bergmann[4,6], Matthew R. Nelson[8], Matthew Stephens[2,3] & Carlos D. Bustamante[7]



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This is a map of their DNA. It recapitulates the map of Europe.

In other words, the strongest genetic trends across European men relate directly to their geographic locations (note: not nationality)

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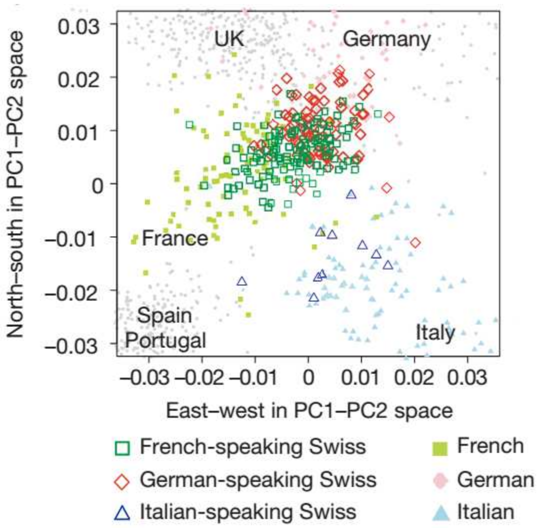
The trend even holds up within a country, e.g. Switzerland:



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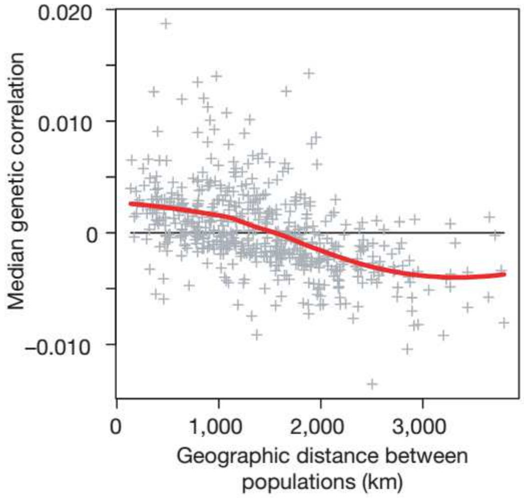
Why? Genetic similarity is strongly distance dependent in Europe, presumably because people tend to live near where they were born and tend to marry locally.



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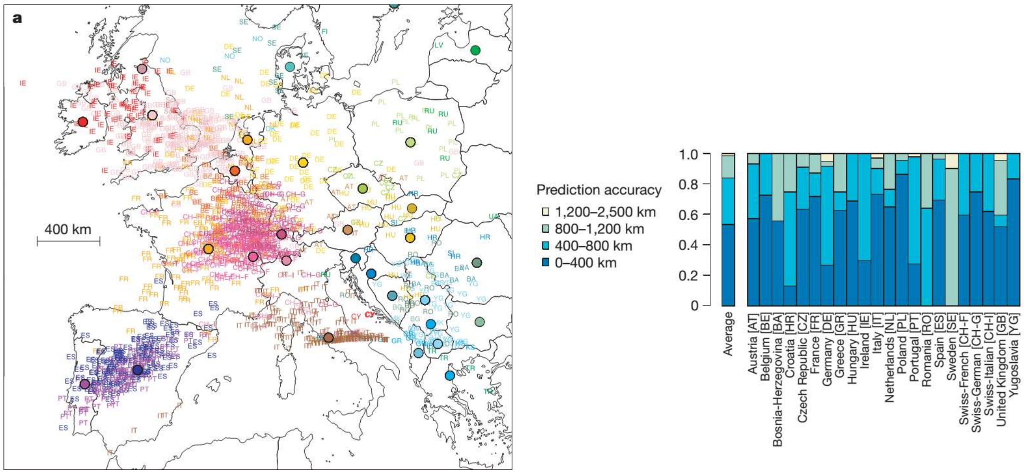
The trend is so strong that it can be used to *predict* where the men are from, e.g. shown here by leave-one-out cross-validation:



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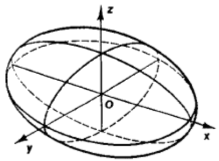
SUMMARY

In a sense, PCA fits a (multidimensional) ellipsoid to the data

- Described by directions and lengths of principal (semi-)axes, e.g. the axis of a cigar or egg or the plane of a pancake



encyclopedia2.thefreedictionary.com

- No matter how an ellipsoid is turned, the eigenvectors point in those principal directions. The eigenvalues give the lengths.
- The biggest eigenvalues correspond to the fattest directions (having the most data variance). The smallest eigenvalues correspond to the thinnest directions (least data variance).
- Ignoring the smallest directions (*i.e.*, collapsing them) loses relatively little information.

Adapted from whuber, http://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues