CS 260: Foundations of Data Science

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Fall 2025

HAVERFORD COLLEGE

Materials by Sara Mathieson

Lab 7 notes

Logistic regression cost function:

$$J(\overrightarrow{w}) = -\sum_{i=1}^{n}[y_i \log(h_{\overrightarrow{w}}(\overrightarrow{x_i})) + (1 - y_i)\log(1 - h_{\overrightarrow{w}}(\overrightarrow{x_i}))]$$

if $h_{\overrightarrow{w}}(\overrightarrow{x_i}) = 0$ or $1 - h_{\overrightarrow{w}}(\overrightarrow{x_i}) = 0 \rightarrow$ skip log(0) or add 0

Outline for today

- Dimensionality reduction
- PCA for data visualization

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Principal Component Analysis (PCA)

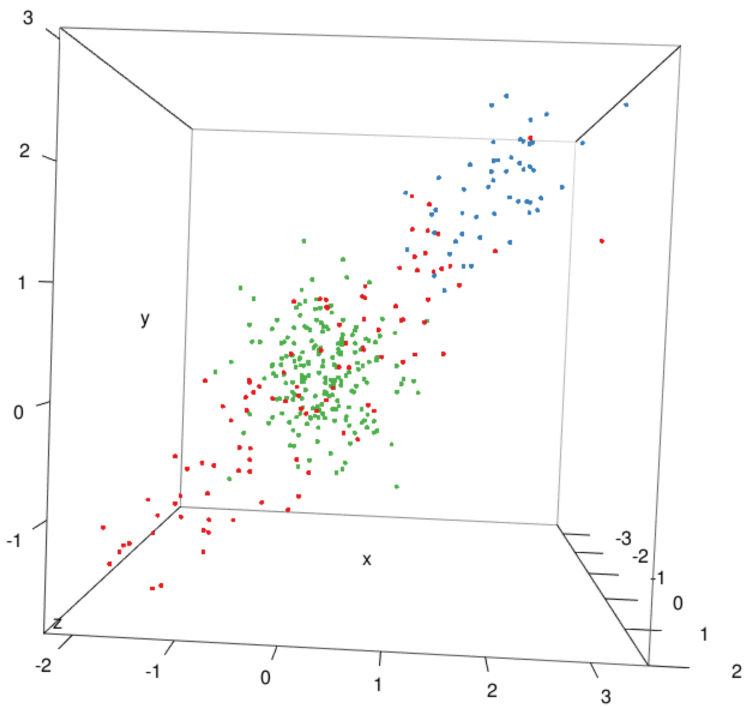
- Transforms *p*-dimensional data so that the new first dimension explains as much of the variation as possible, the new second explains as much of the remaining variation as possible, and so on

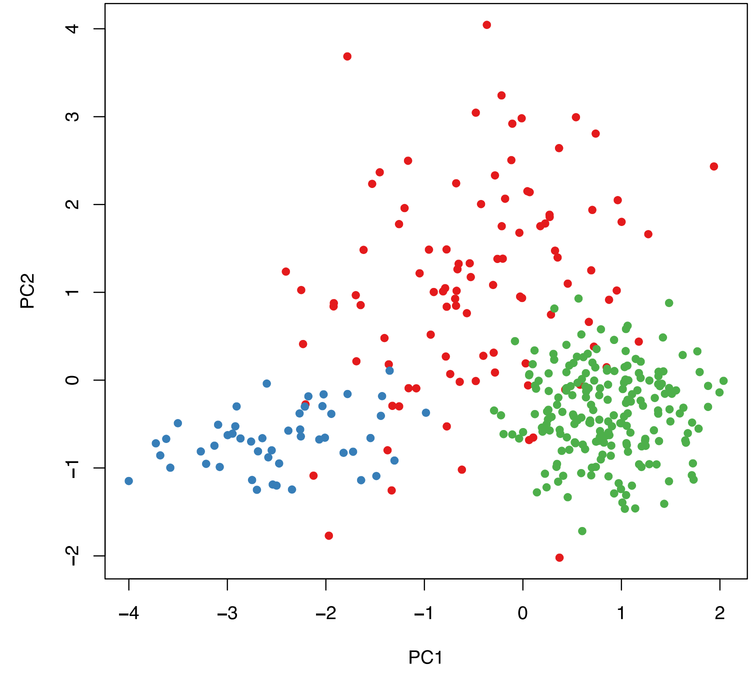
- PCA is a linear transformation

- Typically, we look at the first few dimensions of the transformed data as a means of dimensionality reduction and visualization

- PCA is often used for:
  - Data visualization
  - Infer qualitative relationships between groups

PCA Example





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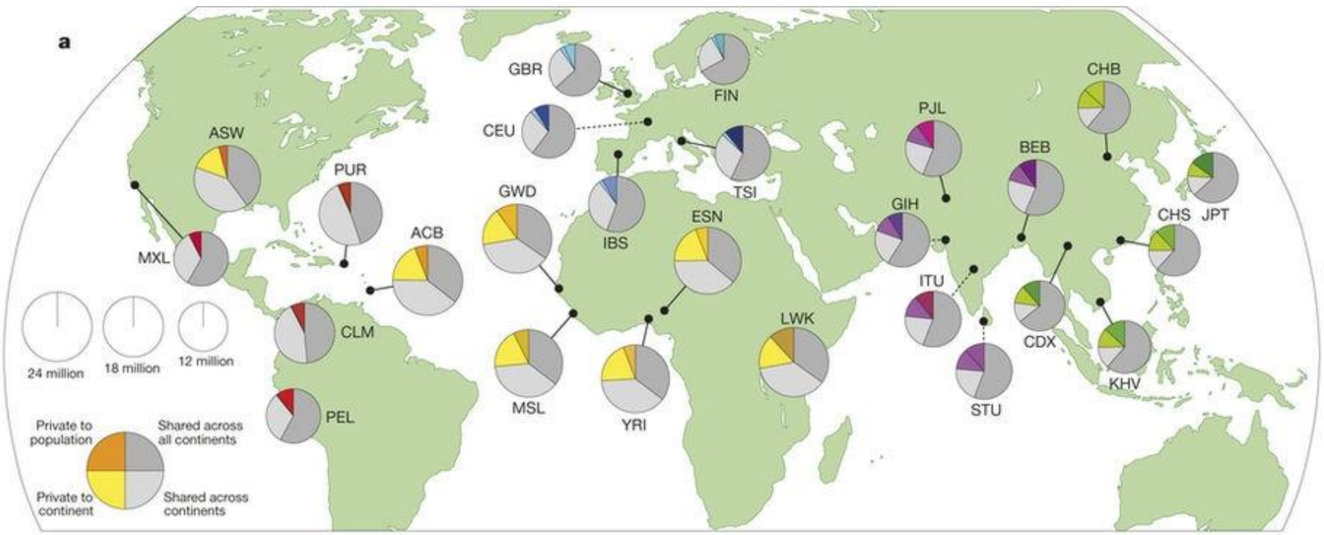
The 1000 Genomes project

- Whole-genome sequence data from 2504 individuals from 26 populations
- A catalog of human genetic variation, useful as a reference or imputation panel
- Completely public. Download from ftp://ftp-trace.ncbi.nih.gov/1000genomes/



Slide: Iain Mathieson

The 1000 Genomes Project Consortium, 2015; https://www.nature.com/articles/nature15393

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#CHROM	POS	ID	REF	ALT	QUAL	FILTER	INFO	FORMAT	HG00096	HG00097	HG00099	HG00100	HG00101	HG00102	HG00103	HG00105	HG00106	HG00107	HG00108	HG00109	HG00110	HG00111
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20	60579	.	G	A	100	PASS	.	GT	0|0	0|0	0|0	0|0	0|0	0|0	0|0	0|0	0|0	0|0	0|0	0|0	0|0	0|0
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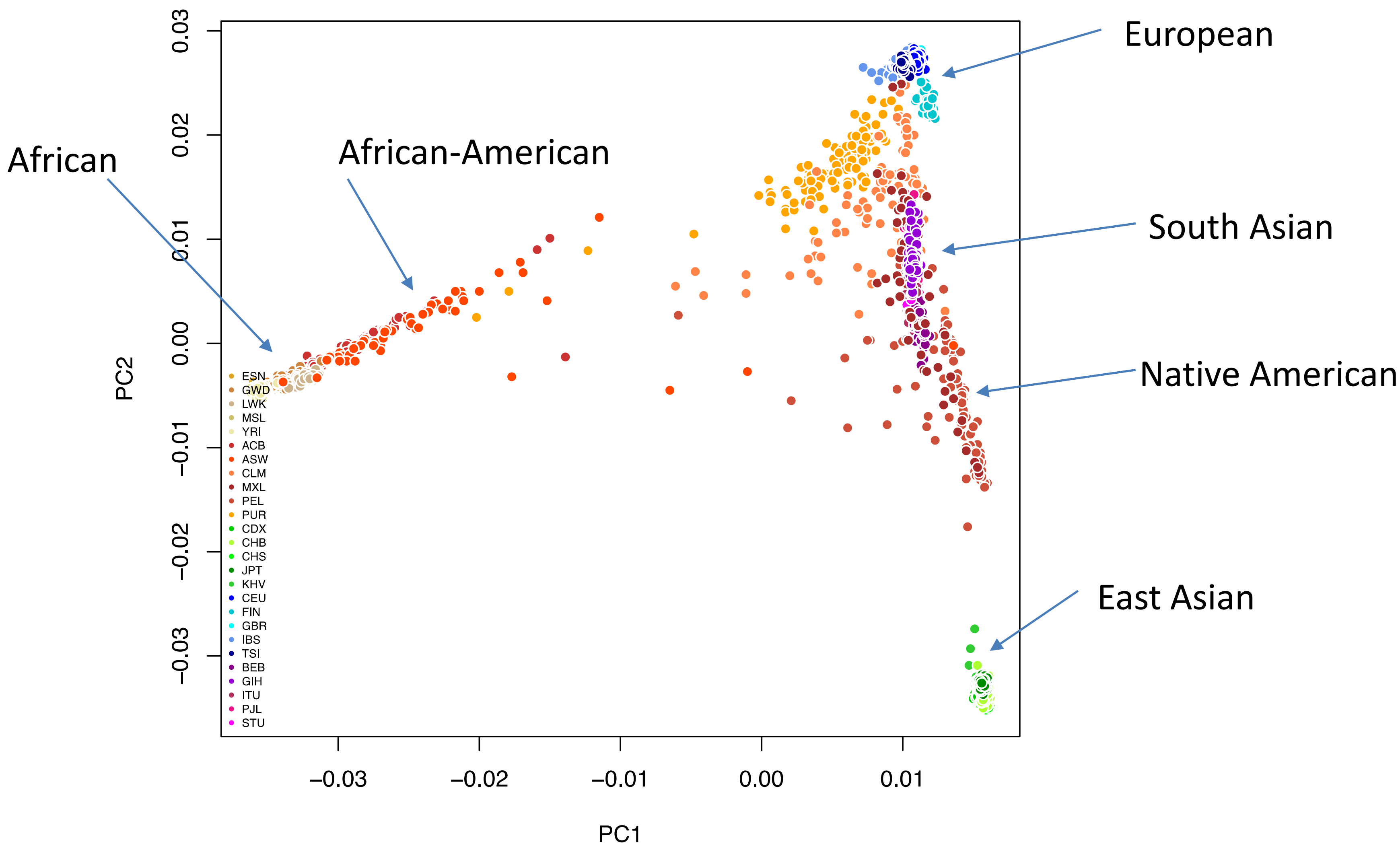
```

Global population structure

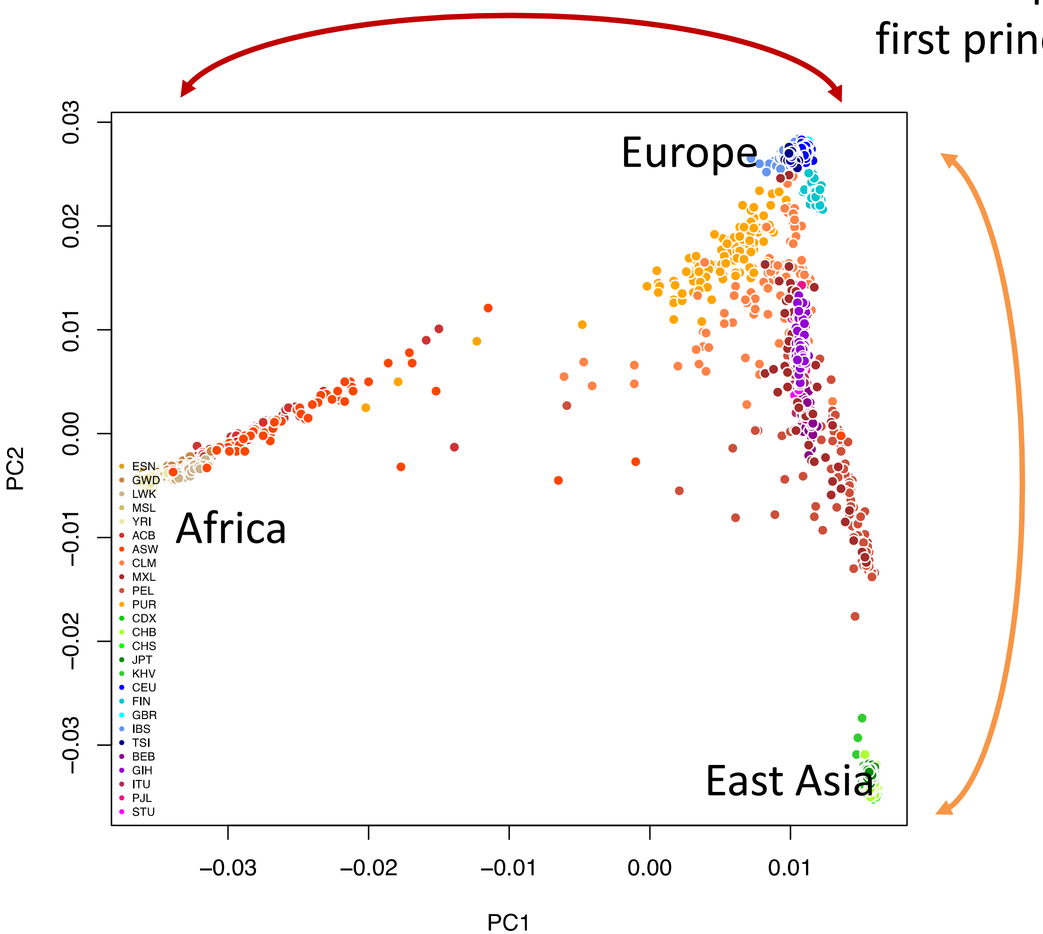


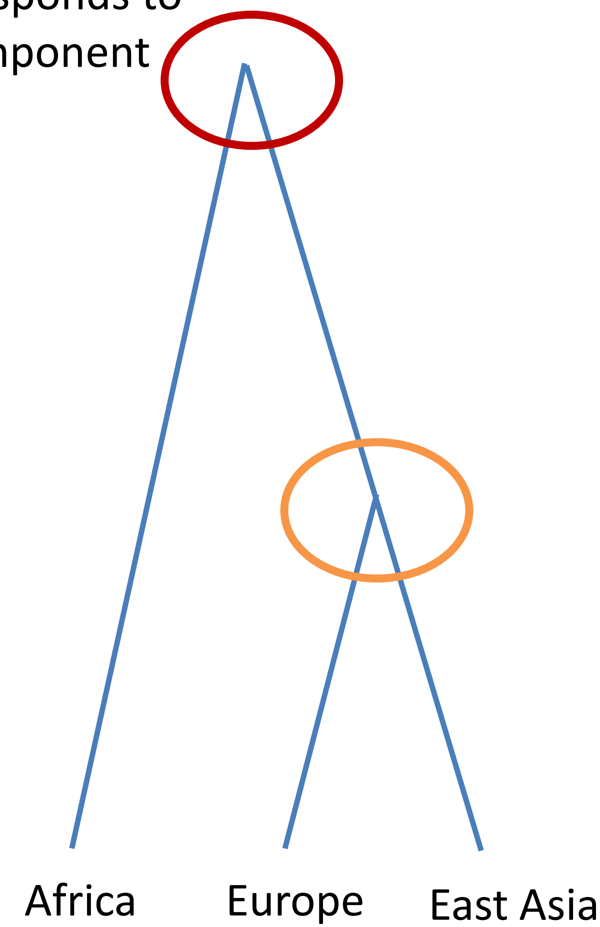
Slide: Iain Mathieson

What causes these patterns?

1. Populations splits separate populations

Oldest split corresponds to first principal component



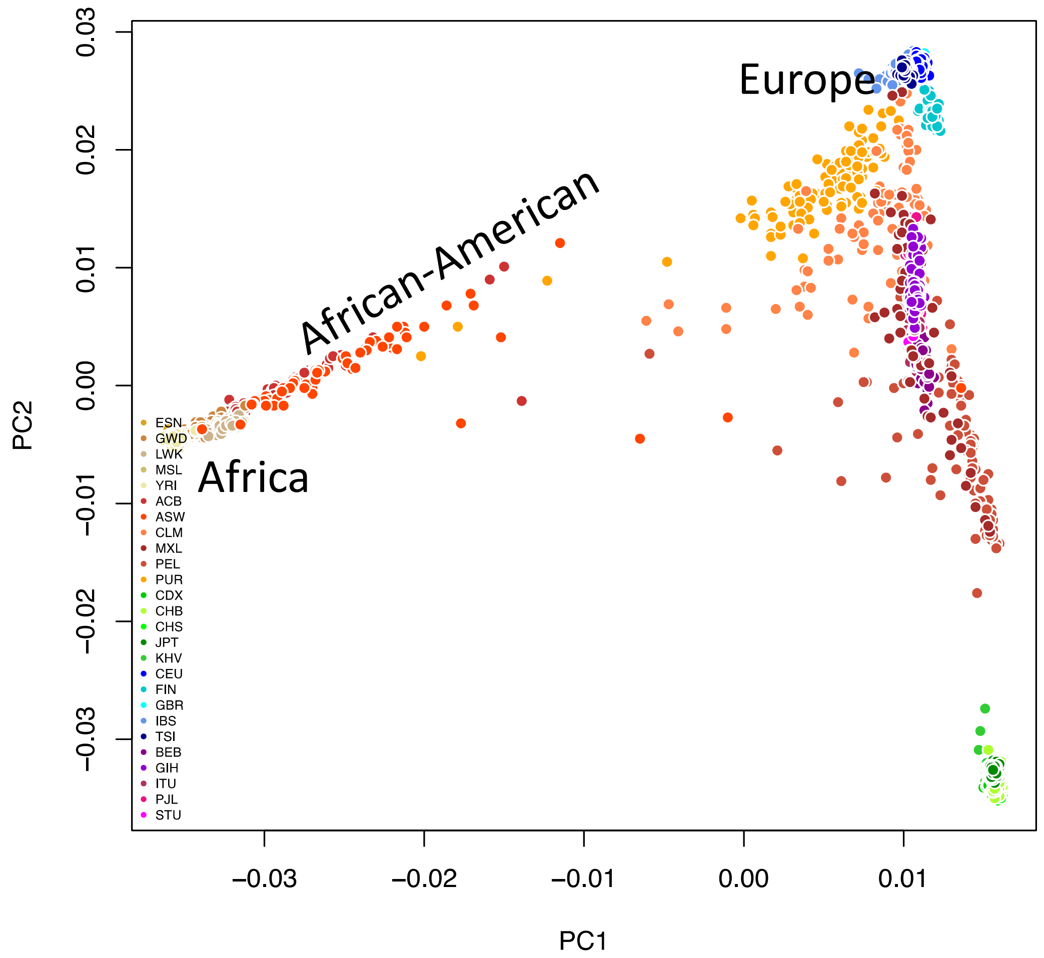


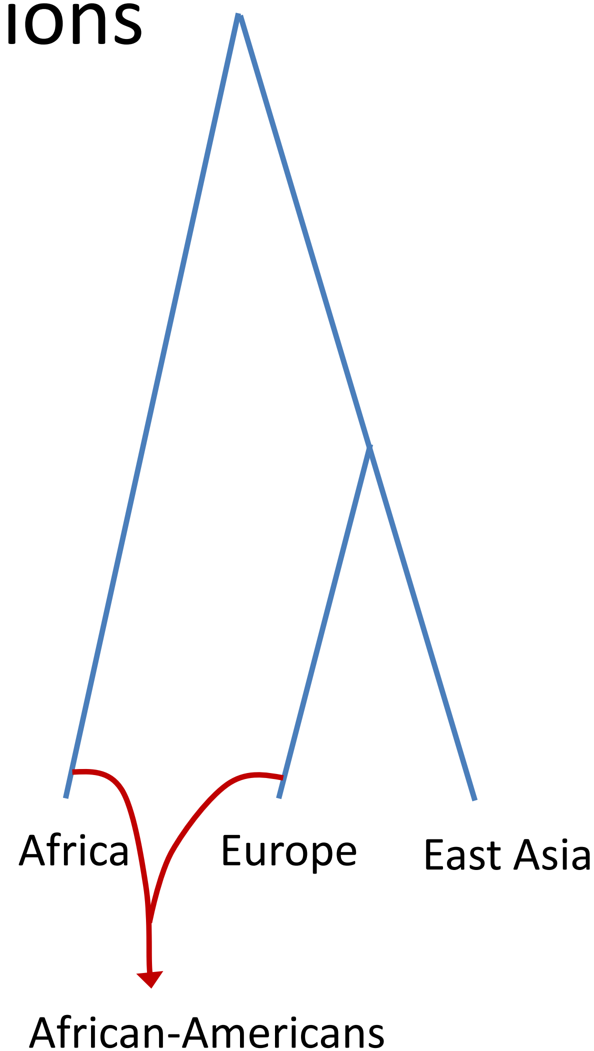
Slide: Iain Mathieson

McVean 2009: http://journals.plos.org/plosgenetics/article?id=10.1371/journal.pgen.1000686

What causes these patterns?

2. Admixture merges populations





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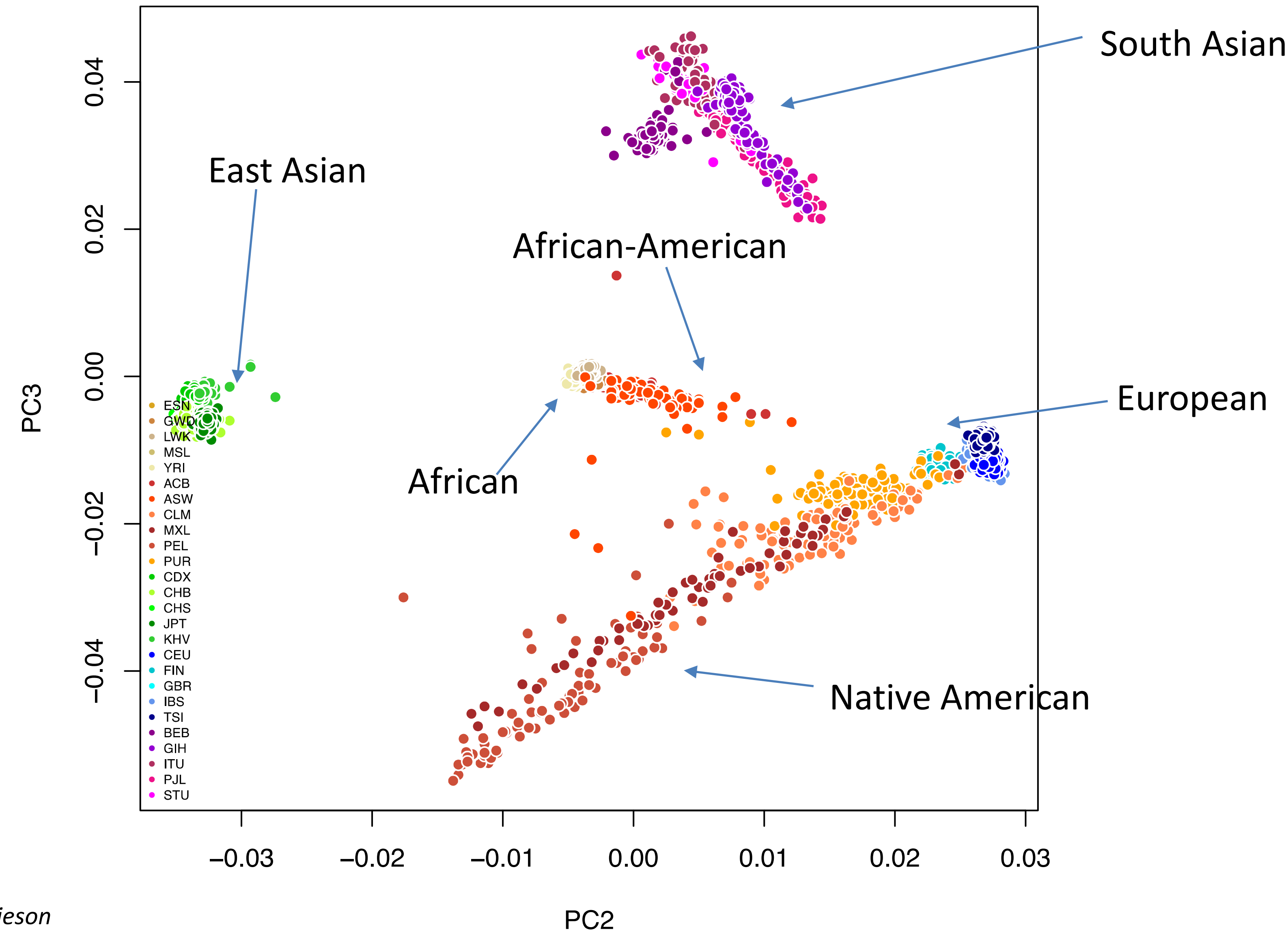
Global population structure

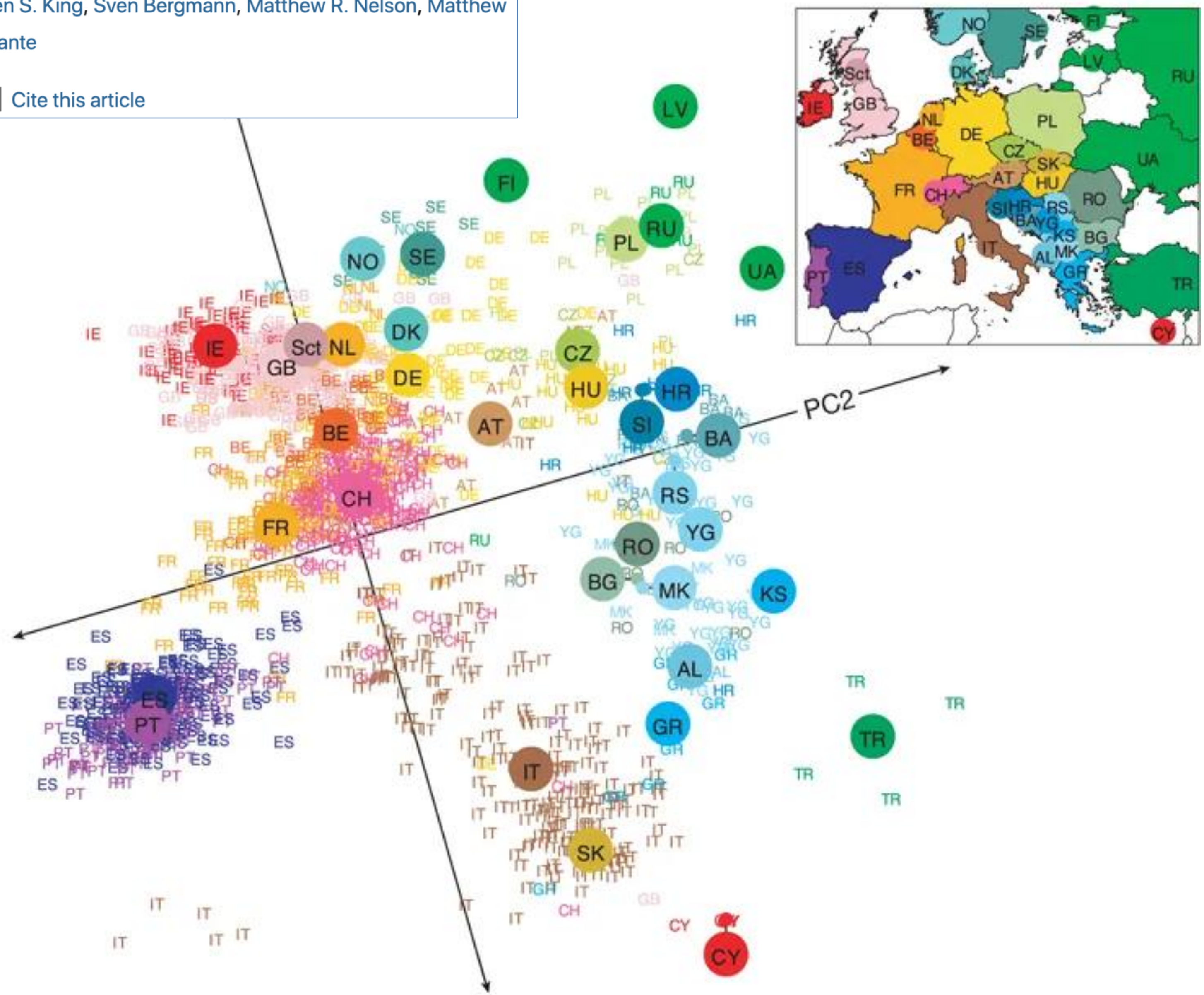


Slide: Iain Mathieson

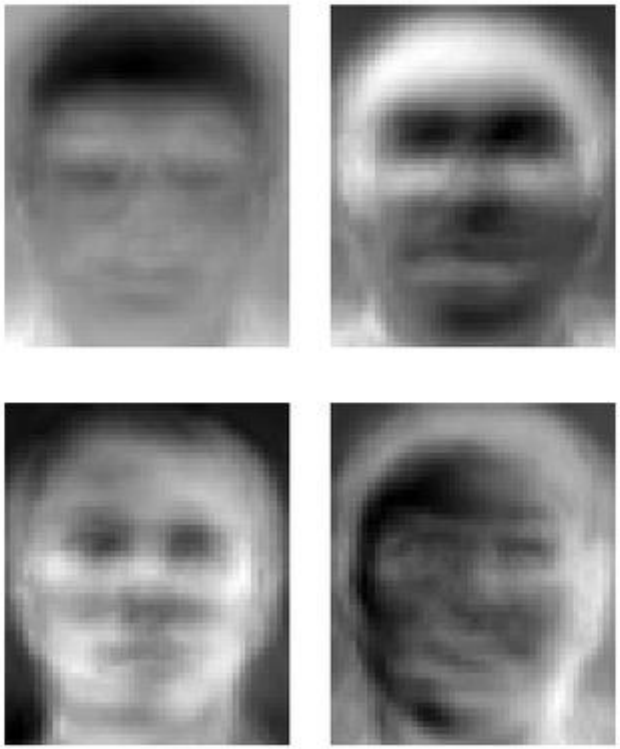
Genes mirror geography within Europe

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(2008) | Cite this article



PCA application: Eigenfaces



Wikipedia

- Low-dimensional representation of face images
- Used for face recognition/classification

Outline for today

- Dimensionality reduction
- PCA for data visualization

PCA Algorithm

<u>Step 1:</u>

$$X_{orig} = \left.\underbrace{\begin{bmatrix} \quad & \quad & \quad & \quad \\ \quad & \quad & \quad & \quad \\ \quad & \quad & \quad & \quad \end{bmatrix}}_{\text{p features}}\right\} n$$

p >> n

Goal: Create nx2 matrix for visualization

PCA Algorithm

<u>Step 2:</u> Subtract off column-wise mean

$$X_{orig} = \begin{bmatrix} 2 & 1 \\ 3 & 3 \end{bmatrix}$$

$$\overline{x_1} = 2.5 \qquad \overline{x_2} = 2$$

$$X = \begin{bmatrix} -0.5 & -1 \\ 0.5 & 1 \end{bmatrix}$$

PCA Algorithm

<u>Step 3:</u> Compute covariance matrix A

$$A = \begin{bmatrix} cov(f,f) & cov(f,g) \\ cov(g,f) & cov(g,g) \end{bmatrix}$$ 2 features f, g

square & symmetric

Runtime $O(np^2)$

$$cov(f,g) = \frac{1}{n-1}\sum_{i=1}^{n}(f_i - \bar{f})(g_i - \bar{g})$$

$$cov(f,f) = var(f) = \frac{1}{n-1}\sum_{i=1}^{n}(f_i - \bar{f})^2$$

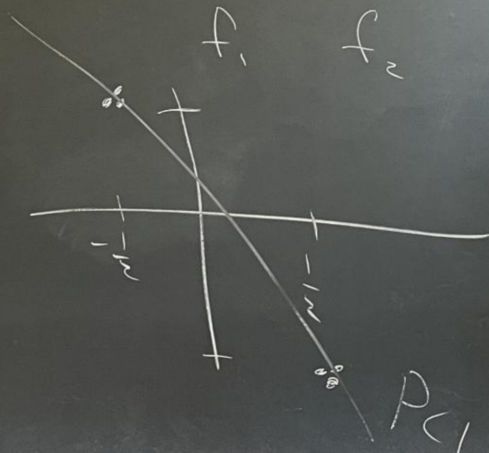
Handout 15, page 1

Handout 16

$\boxed{\text{Step 1 \& 2}}$

$$X = \begin{array}{cc} \begin{bmatrix} -1/2 & 1/2 \\ -1/2 & 1/2 \\ -1/2 & 1/2 \\ 1/2 & -1/2 \\ 1/2 & -1/2 \\ 1/2 & -1/2 \end{bmatrix} \\ f_1 \quad\quad f_2 \end{array}$$

orig $\begin{cases} \bar{f}_1 = \frac{1}{2} \\ \bar{f}_2 = \frac{1}{2} \end{cases}$



$\boxed{\text{Step 3}}$

$$A = \begin{bmatrix} var(f_1) & cov(f_1, f_2) \\ cov(f_2, f_1) & var(f_2) \end{bmatrix}$$

$\bar{f}_1 = 0$

$\bar{f}_2 = 0$

$$cov(f_1, f_2) = \frac{1}{6-1}\left(-\frac{1}{2}\cdot\frac{1}{2}\right)\cdot 6$$

$$= -\frac{3}{10}$$

$$\Rightarrow A = \begin{bmatrix} 3/10 & -3/10 \\ -3/10 & 3/10 \end{bmatrix}$$

PCA Algorithm

Step 4: Compute eigenvalues and eigenvectors of A

eigenvalue

$$A\vec{v} = \lambda\vec{v}$$

eigenvector

$$\det(A - \lambda I) = 0$$

Solve for λ and plug into first equation to solve for $\vec{v}$

PCA Algorithm

<u>Step 5:</u> Sort eigenvectors by eigenvalues (high->low)

$$W = \begin{array}{c} \begin{array}{cccc} \lambda_1 & \lambda_2 & & \end{array} \\ \begin{bmatrix} \vdots & \vdots & & \vdots \\ \overrightarrow{v_1} & \overrightarrow{v_2} & \cdots & \overrightarrow{v_r} \\ \vdots & \vdots & & \vdots \end{bmatrix} \end{array} \qquad pxr$$

usually $r = 2$

first eigenvector

And compute the transformed data:

$$T_{nxr} = X_{nxp} W_{pxr}$$

Handout 15, page 2

Step 4

$$\det(A - \lambda I) = 0$$

$$\left(\begin{bmatrix} 3/10 & -3/10 \\ -3/10 & 3/10 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) = 0$$

6

$$\det \left(\begin{bmatrix} 3/10 - \lambda & -3/10 \\ -3/10 & 3/10 - \lambda \end{bmatrix} \right) = 0$$

$$\left(\frac{3}{10} - \lambda \right)^2 - (3/10)^2 = 0$$

$$\cancel{\left(\frac{3}{10} \right)^2} - 2 \cdot \frac{3}{10} \lambda + \lambda^2 - \cancel{\left(\frac{3}{10} \right)^2} = 0$$

$$\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc$$

$$\Rightarrow \boxed{\lambda^2 - \frac{3}{5} \lambda = 0}$$

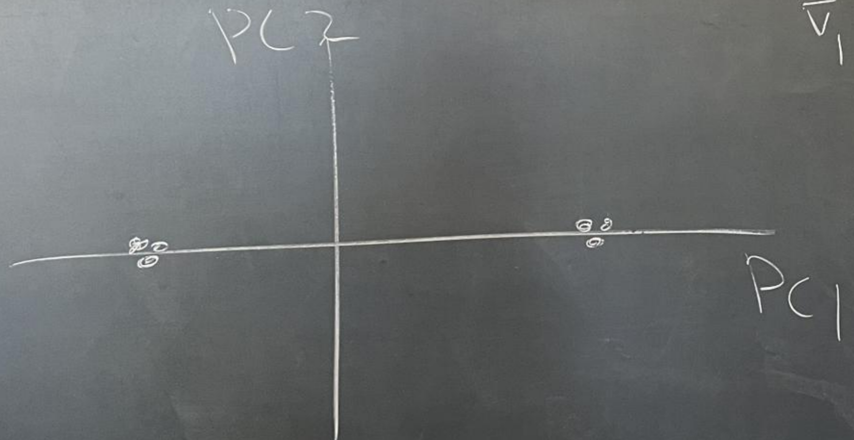
$$\lambda \left(\lambda - \frac{3}{5} \right) = 0 \Rightarrow \boxed{\begin{aligned} \lambda_1 &= \frac{3}{5} \\ \lambda_2 &= 0 \end{aligned}}$$

$$A \vec{v} = \lambda \vec{v}$$

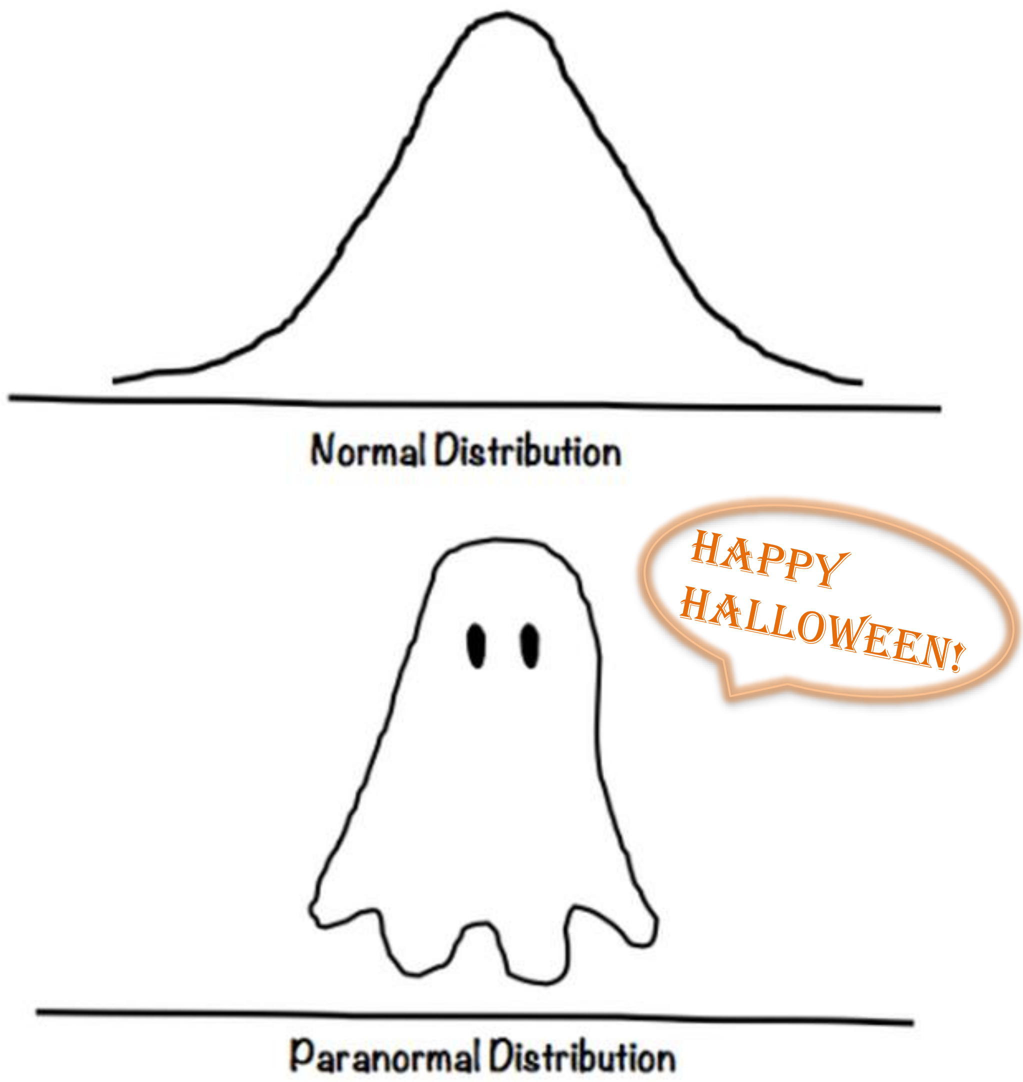
$\lambda_1 = 3/5 \qquad \lambda_2 = 0$

$$T_2 = XW_2 = \begin{bmatrix} -1/2 & 1/2 \\ -1/2 & 1/2 \\ -1/2 & 1/2 \\ 1/2 & -1/2 \\ 1/2 & -1/2 \\ 1/2 & -1/2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ -1 & 0 \\ -1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix}$$

$\vec{v}_1 \qquad \vec{v}_2$



Looking ahead: Statistics next week!



Pinterest