LECTURE 22

Last class: · A $n\times n$ symmetric $\Rightarrow$ spectral decomposition $A=\sum_i \lambda_i u_i u_i^T = U\Lambda U^T$

· A $m\times n$ general $\Rightarrow$ SVD $A=\sum \sigma_i u_i v_i^T = U\Sigma V^T$

· Optimization meaning:

$\lambda_1 = \max_v v^TAv$, $u_1 = \arg\max$ $\qquad$ $\sigma_1 = \max_v \|Av\|_2$, $v_1 = \arg\max \ldots$

$\lambda_2 = \max_{v\perp v_1} v^TAv$, $u_2 = \arg\max$ $\qquad$ $\ldots$

· Matrix norms: $\|A\|_F^2 = \sum_{ij} A_{ij}^2 = \sum_i \sigma_i(A)^2$

MATRIX NORMS CTD.

Def The operator (a.k.a. spectral) norm:

$$\|A\| = \max_{\|x\|_2=1} \|Ax\|_2 = \sigma_1(A) = \max_x \frac{\|Ax\|_2}{\|x\|_2}$$

by optimizational meaning (prev. class)

FACTS

→ (a) $\|A\| \le \|A\|_F \le \sqrt{r}\,\|A\|$ where $r=\text{rank}(A)$

$$\left[\ \sigma_1(A)^2 \le \sum_{i=1}^{r} \sigma_i(A)^2 \le r\cdot\sigma_1(A)^2\ \right]$$

(b) (Diagonal) $A=\begin{bmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_n \end{bmatrix} \Rightarrow$ by SVD, $(\sigma_i(A)) = (d_i) \Rightarrow \boxed{\|A\| = \max_i |d_i|}$

(c) (Orthog. invariance) $\|UA\| = \|AV\| = \|A\|$ $\forall$ orthogonal U,V

$\left[\ \|UAx\|_2 = \|Ax\|_2\ \right]$

(d) (Quadratic form) If A is symmetric, $\boxed{\|A\| = \max_{x \text{ unit}} |x^TAx|}$

[DIY using spectral representation, orth. invariance, and (a)]

$\|A\| = \max|\lambda_i(A)|$

(e) $\|A+B\| \le \|A\| + \|B\|$ $\quad$ (Δ ineq.)

(f) $\|AB\| \le \|A\|\,\|B\|$ $\quad$ $\left[\ \|ABx\|_2 \le \|A\|\cdot\|Bx\|_2 \le \|A\|\cdot\|B\|\cdot\|x\|_2\ \right]$

(g) $\|A^T\| = \|A\|$

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RANDOM VECTORS

$X \in \mathbb{R}^d$

- <u>Mean</u> $\mathbb{E}X = \mu$
- Variance in 1D: $Var(X) = \mathbb{E}(X-\mu)^2 = \mathbb{E}X^2 - \mu^2$

  $\downarrow$

  <u>Covariance matrix</u> in KD: $\boxed{Cov(X) = \mathbb{E}(X-\mu)(X-\mu)^T = \mathbb{E}XX^T - \mu\mu^T.}$

- Entries:

  $Cov(X)_{ij} = \mathbb{E}(X-\mu)_i(X-\mu)_j = \mathbb{E}(X_i - \mathbb{E}X_i)(X_j - \mathbb{E}X_j) = Cov(X_i, X_j)$

  Diagonal entries:

  $Cov(X)_{ii} = Cov(X_i, X_i) = Var(X_i)$

- <u>Ex</u>: $X \in \mathbb{R}^2$ $\quad Cov(X) = \begin{bmatrix} Var(X_1) & Cov(X_1, X_2) \\ Cov(X_2, X_1) & Var(X_2) \end{bmatrix}$

- $Cov(X)$ is a $\underbrace{d \times d \text{ symmetric}}_{\text{Obvious}}$ $\underbrace{\text{PSD matrix}}_{\text{Proof}}$.

$\forall v \in \mathbb{R}^d$: $\quad v^T \Sigma v = v^T \mathbb{E}XX^T v = \mathbb{E}\underbrace{v^T X}_{\langle v, X\rangle}\underbrace{X^T v}_{\langle X, v\rangle} = \mathbb{E}\langle X, v\rangle^2 \geq 0. \quad (*)$

EXAMPLE: M.D. NORMAL DISTRIBUTION

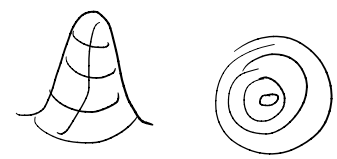
- **Def** | $Z=(Z_1,\dots,Z_d)\in\mathbb{R}^d$ is a standard normal r.vector if $Z_i\sim N(0,1)$ independent

- $\mathbb{E}Z=0$, $\mathrm{Cov}(Z)=\begin{bmatrix}1&&0\\&1&\\0&&\ddots\ 1\end{bmatrix}=I_d$ $\Rightarrow$ notation $\boxed{Z\sim N(0,I_n)}$

- pdf: $f(x)=f(x_1)\cdots f(x_d)=\frac{1}{\sqrt{2\pi}}e^{-x_1^2/2}\cdots\frac{1}{\sqrt{2\pi}}e^{-x_d^2/2}=\boxed{\frac{1}{(2\pi)^{d/2}}e^{-\|x\|_2^2/2}}$ $x\in\mathbb{R}^d$

- $f(x)$ is rotationally invariant: $f(x)=f(Ux)$ $\forall$ orth. U $\Rightarrow$

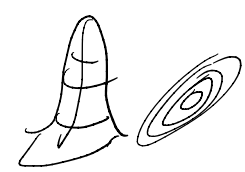
Prop (Rotation invariance) If $Z\sim N(0,I_n)$ then $UZ\sim N(0,I_n)$ $\forall$ orthogonal matrix U



Def (General normal)
$X=(X_1,\dots,X_d)\in\mathbb{R}^d$ is a normal r.vector if X is an affine transformation of a standard normal r.vector $Z\sim N(0,I_n)$, i.e.
$$X=AZ+\mu \qquad \text{for some invertible } A\in\mathbb{R}^{d\times d},\ \mu\in\mathbb{R}^d.$$

- $\mathbb{E}X=\mu$,
$$\mathrm{Cov}(X)=\mathbb{E}(AZ)(AZ)^T=\mathbb{E}\left[AZZ^TA^T\right]=A\cdot\underbrace{\mathbb{E}\left[ZZ^T\right]}_{=I_d}\cdot A^T=\boxed{AA^T=:\Sigma}$$

- **Ex**: pdf of X is
$$f(x)=\frac{1}{(2\pi)^{d/2}\sqrt{\det(\Sigma)}}\exp\left(-\frac{(x-\mu)^T\Sigma^{-1}(x-\mu)}{2}\right),\quad x\in\mathbb{R}^d$$

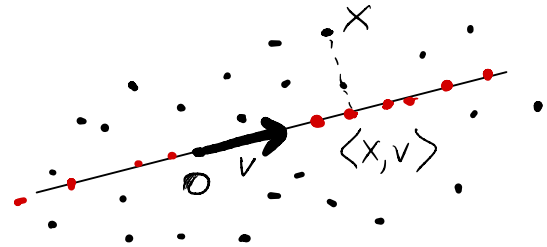


$\Rightarrow$ pdf is determined by μ,Σ. $\Rightarrow$ notation $\boxed{X\sim N(\mu,\Sigma)}$

Principal Component Analysis

- Let $X \in \mathbb{R}^d$ be a random vector with mean 0 (for simplicity - by translation) and $Cov(X) = \Sigma$.

- Reduce dimension? project X onto 1D line that "best explains" the variation in X.



$\Leftrightarrow$ find a unit vector v that maximizes

$$Var(\langle X, v\rangle) = \mathbb{E}\langle X, v\rangle^2 = v^T \Sigma v \qquad (* \text{ p. } 1)$$

$$\max_{v \text{ unit}} Var\langle X, v\rangle = \max_{v} v^T \Sigma v = \boxed{\lambda_1(\Sigma)}, \qquad \text{argmax} = \boxed{v_1(\Sigma)}$$

- Next best direction:

$$\max_{\substack{v \perp v_1 \\ \text{unit}}} Var(X, v) = \boxed{\lambda_2(\Sigma)}, \qquad \text{argmax} = \boxed{v_2(\Sigma)}$$

$\Rightarrow$ project X onto 2D plane spanned by v_1, v_2.

PCA

- In order to reduce dimension of X from d to k, project X onto the subspace spanned by the top k eigenvectors of $Cov(X)$. "Principal components" of X.
- This subspace explains the variability of X the best among all k-dimensional subspaces.

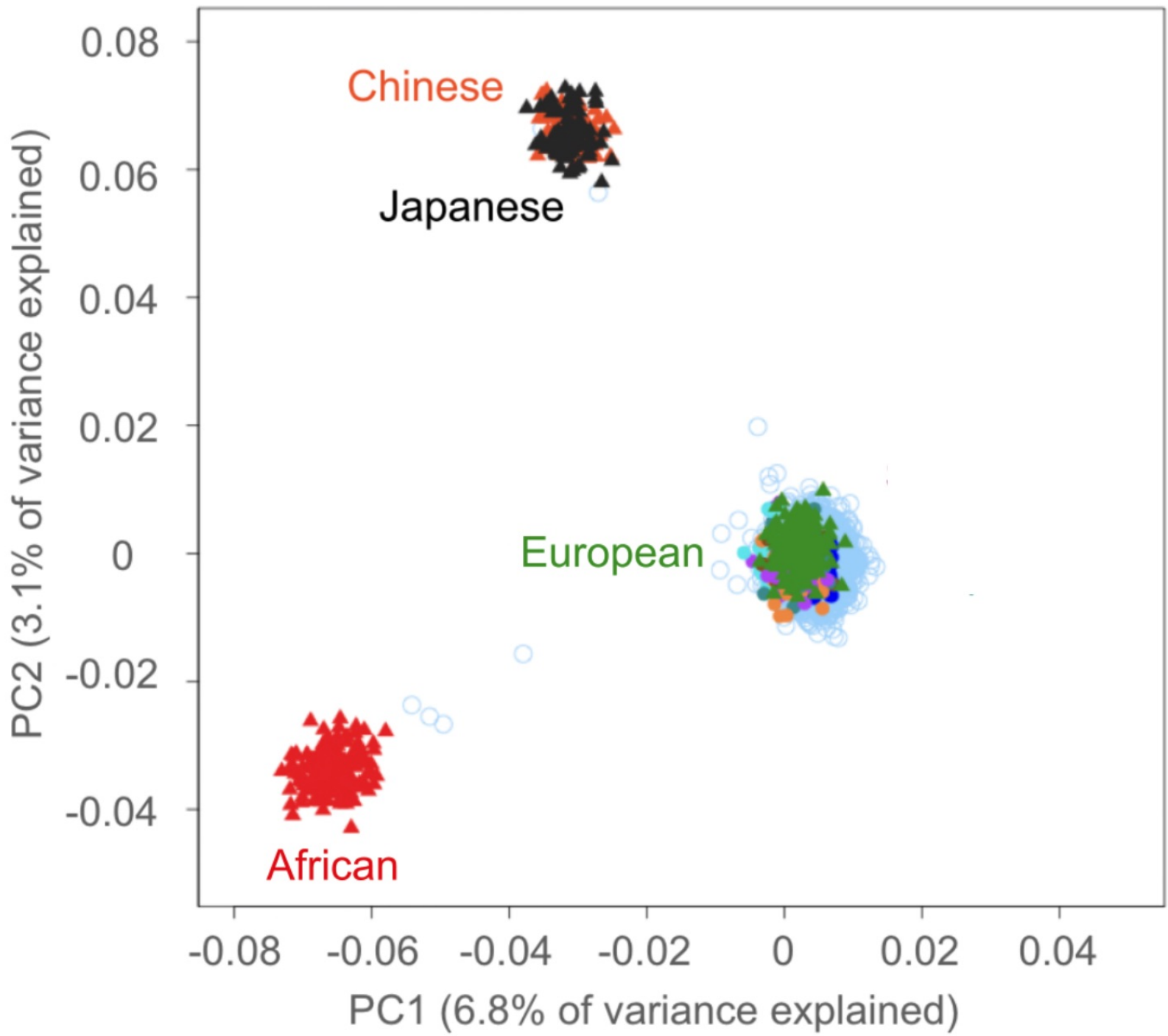
- Exploratory data analysis. Unsupervised learning.
- Advantages & disadvantages.

APPLICATION: GENETIC PCA

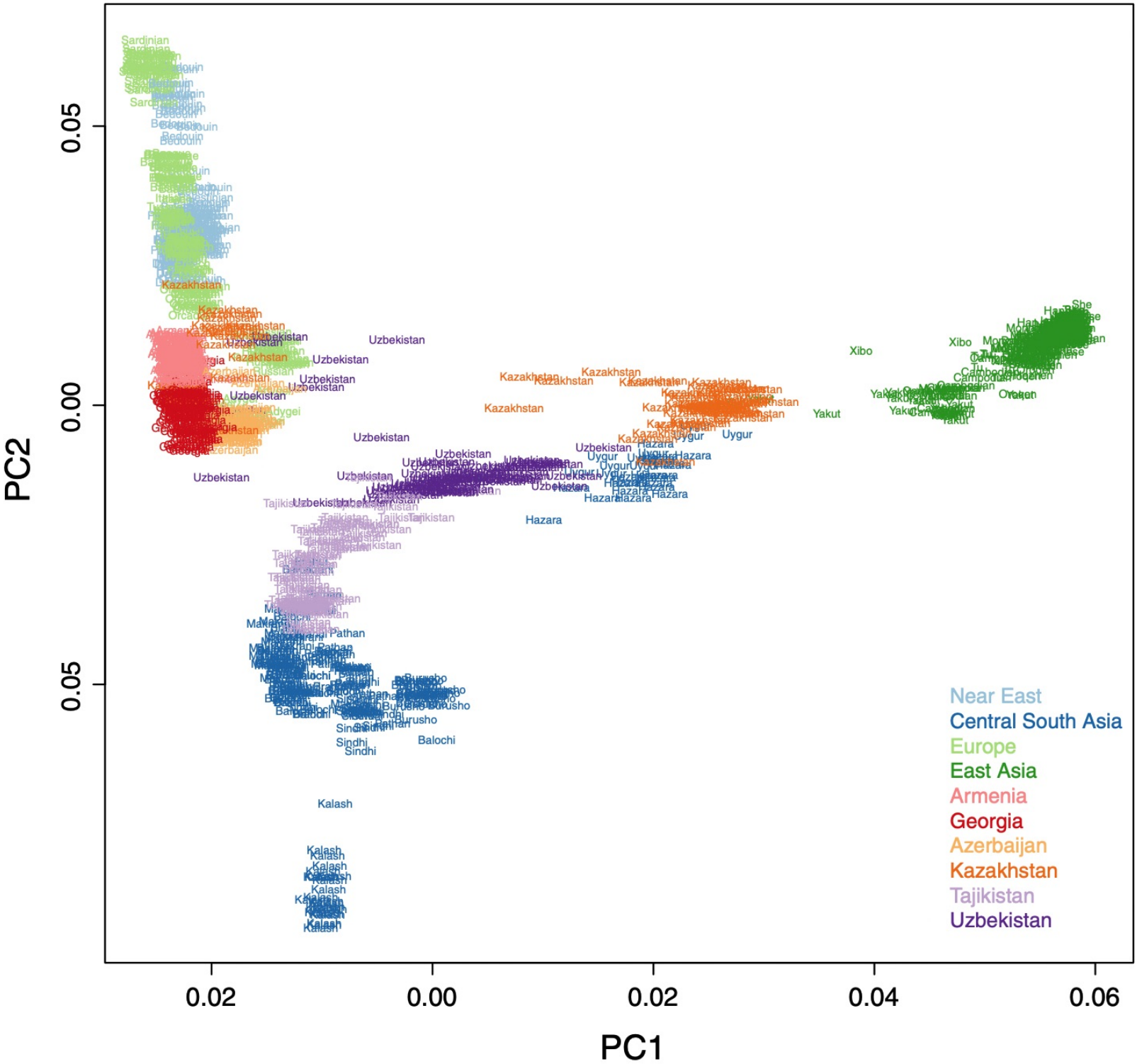
$X = (x_1, \dots, x_d)$ of a randomly chosen person

gene expressions

WORLD:



ASIA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PC1
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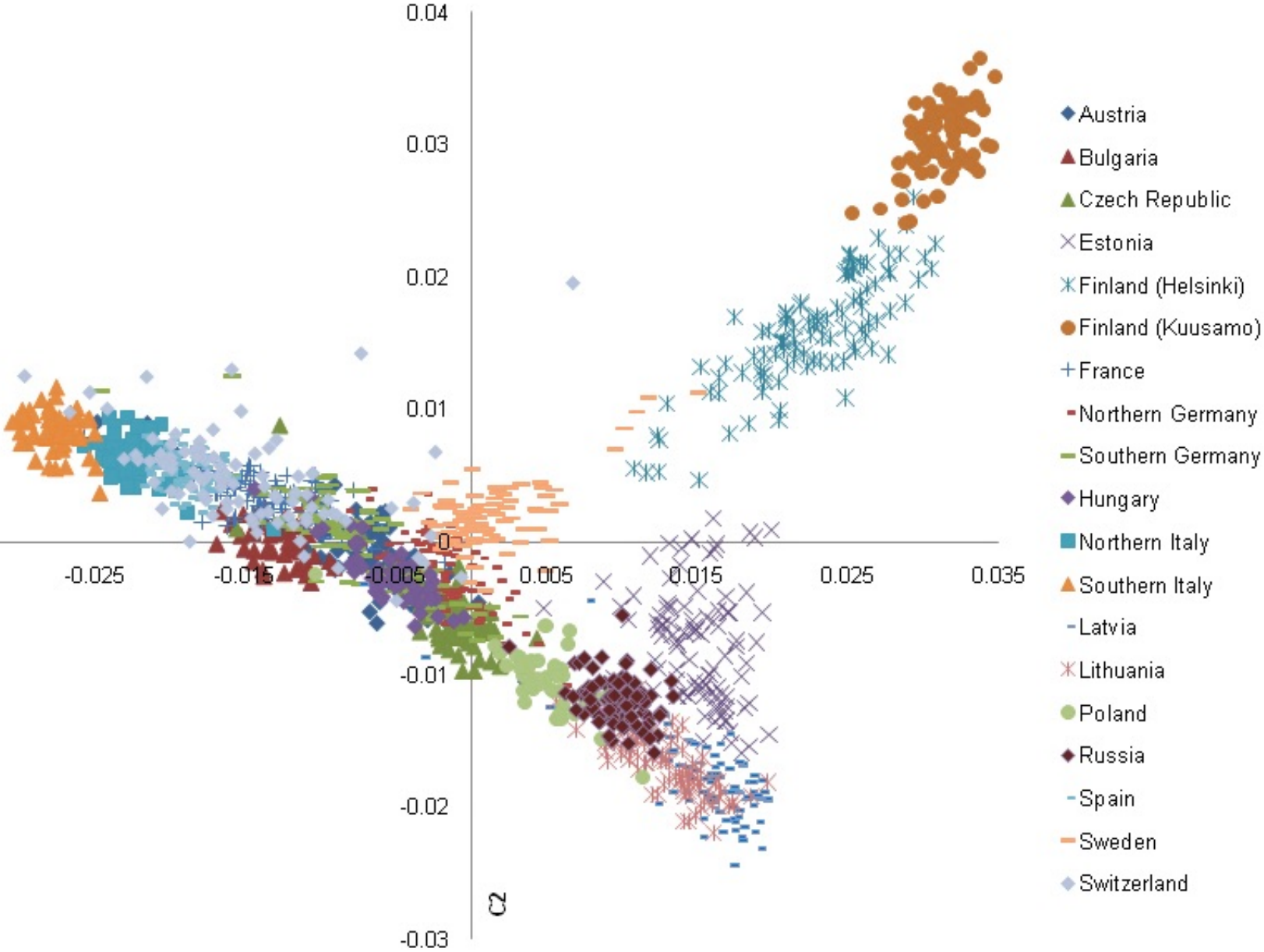
East Asia
Armenia
Georgia
Azerbaijan
Kazakhstan
Tajikistan
Uzbekistan

EUROPE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Estonia
Finland (Helsinki)
Finland (Kuusamo)
France
Northern Germany
Southern Germany
Hungary
Northern Italy
Southern Italy
Latvia
Lithuania
Poland
Russia
Spain
Sweden
Switzerland