Principal Component Analysis (PCA)

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NYU / CUSP - GX 5006

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Eigenvectors and Eigenvalues

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$\mathbf{A}$ is a linear transformation $\mathbf{A} : \mathbb{R}^d \to \mathbb{R}^d$, so, for any $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{A}\mathbf{x}$ corresponds to scale, rotate, and/or reflect $\mathbf{x}$ in $\mathbb{R}^d$.

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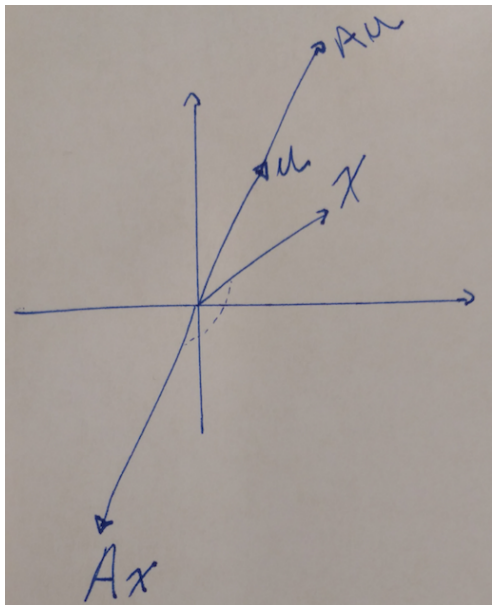
By definition, an eigenvector of $\mathbf{A}$ is never rotated by $\mathbf{A}$.



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- $\lambda \in \mathbb{R}$ and $\mathbf{u} \in \mathbb{R}^d$ (no complex numbers involved).
- The eigenvectors are orthogonal, that is, given eigenvectors $\mathbf{u}_i$ and $\mathbf{u}_j$ from $\mathbf{A}$

$$\mathbf{u}_i^\top \mathbf{u}_j = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{otherwise} \end{cases}$$

(assuming $\|\mathbf{u}_i\| = 1$)

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Spectral Decomposition of a Symmetric Matrix

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^\top$$

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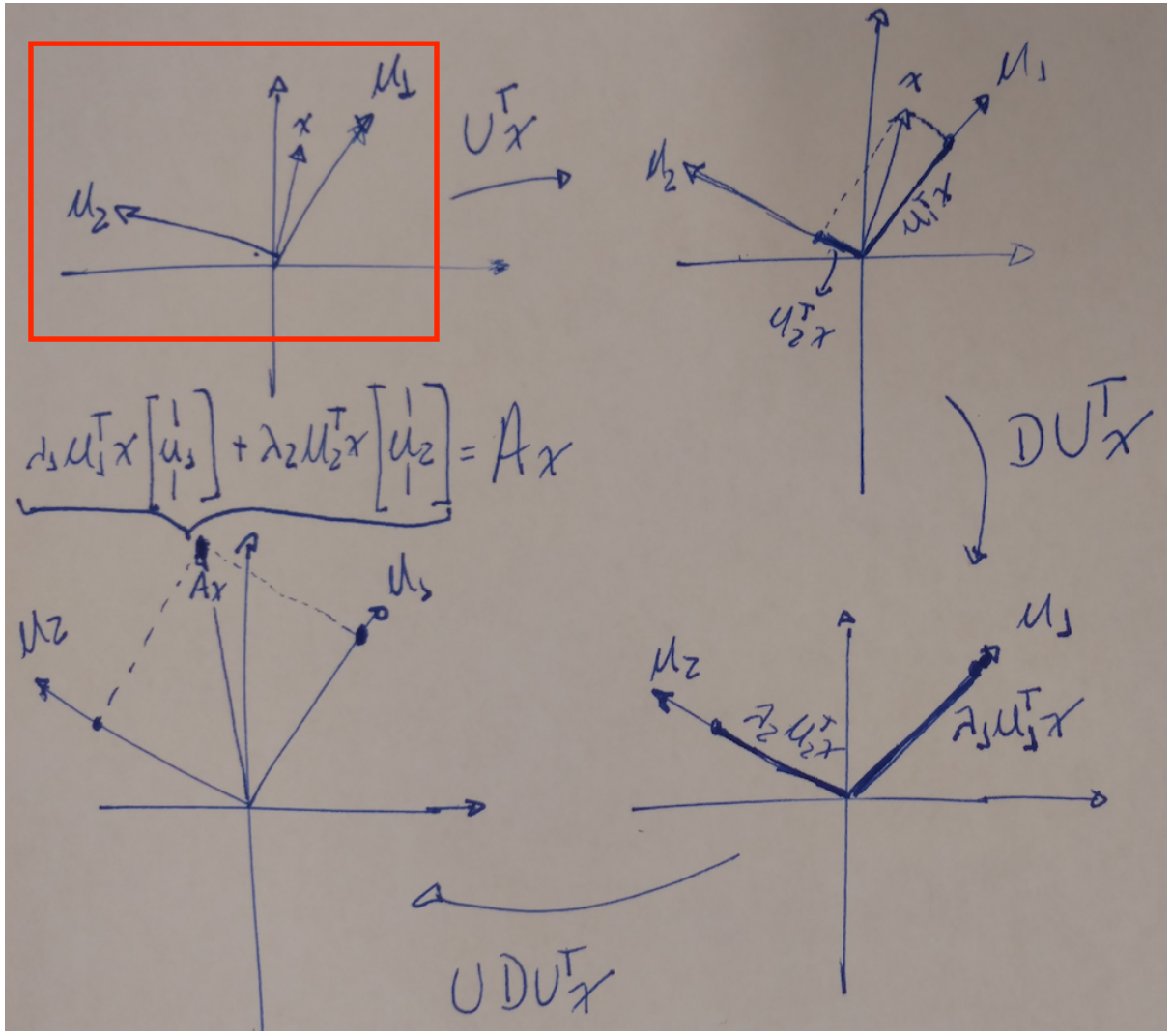

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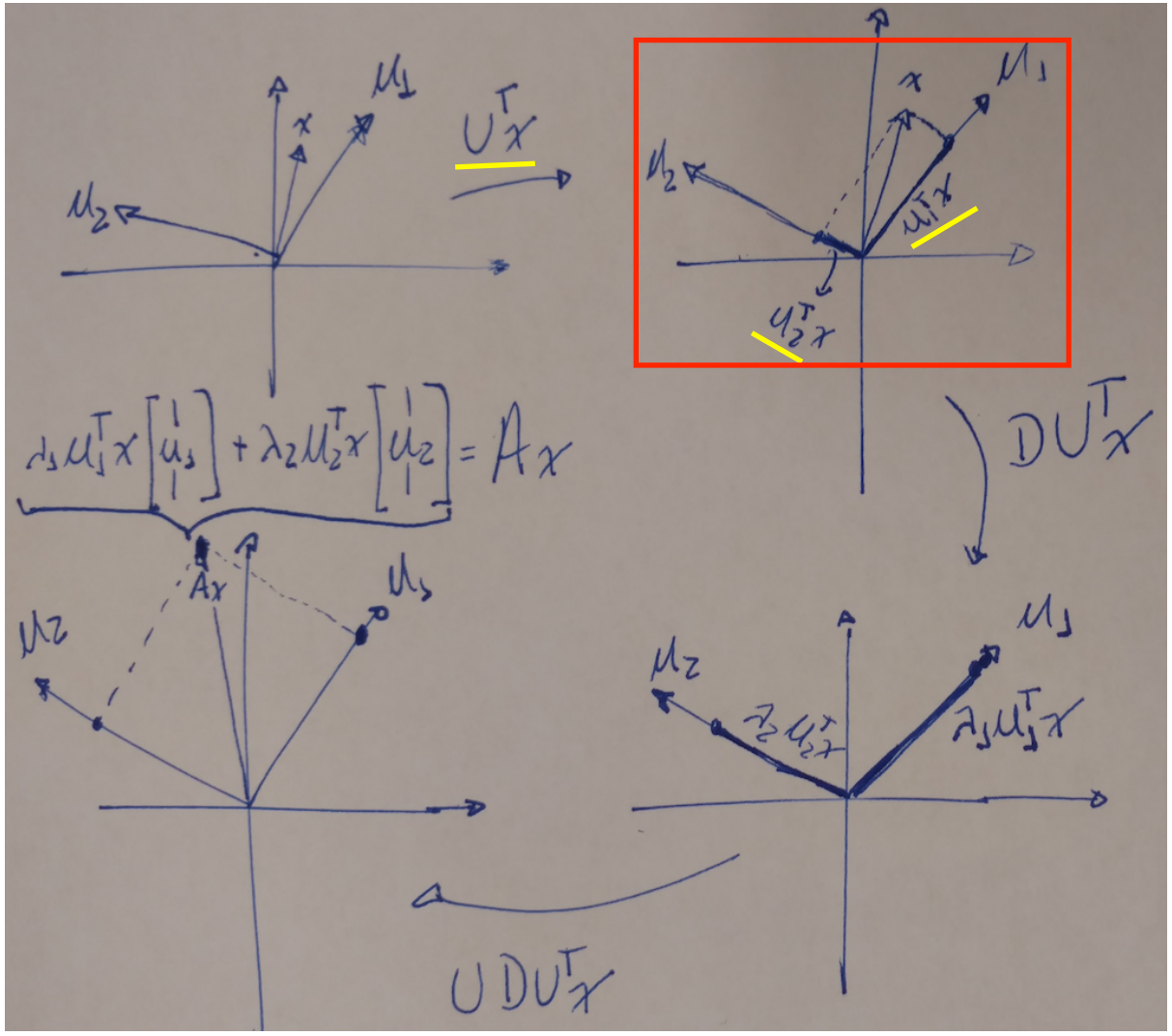

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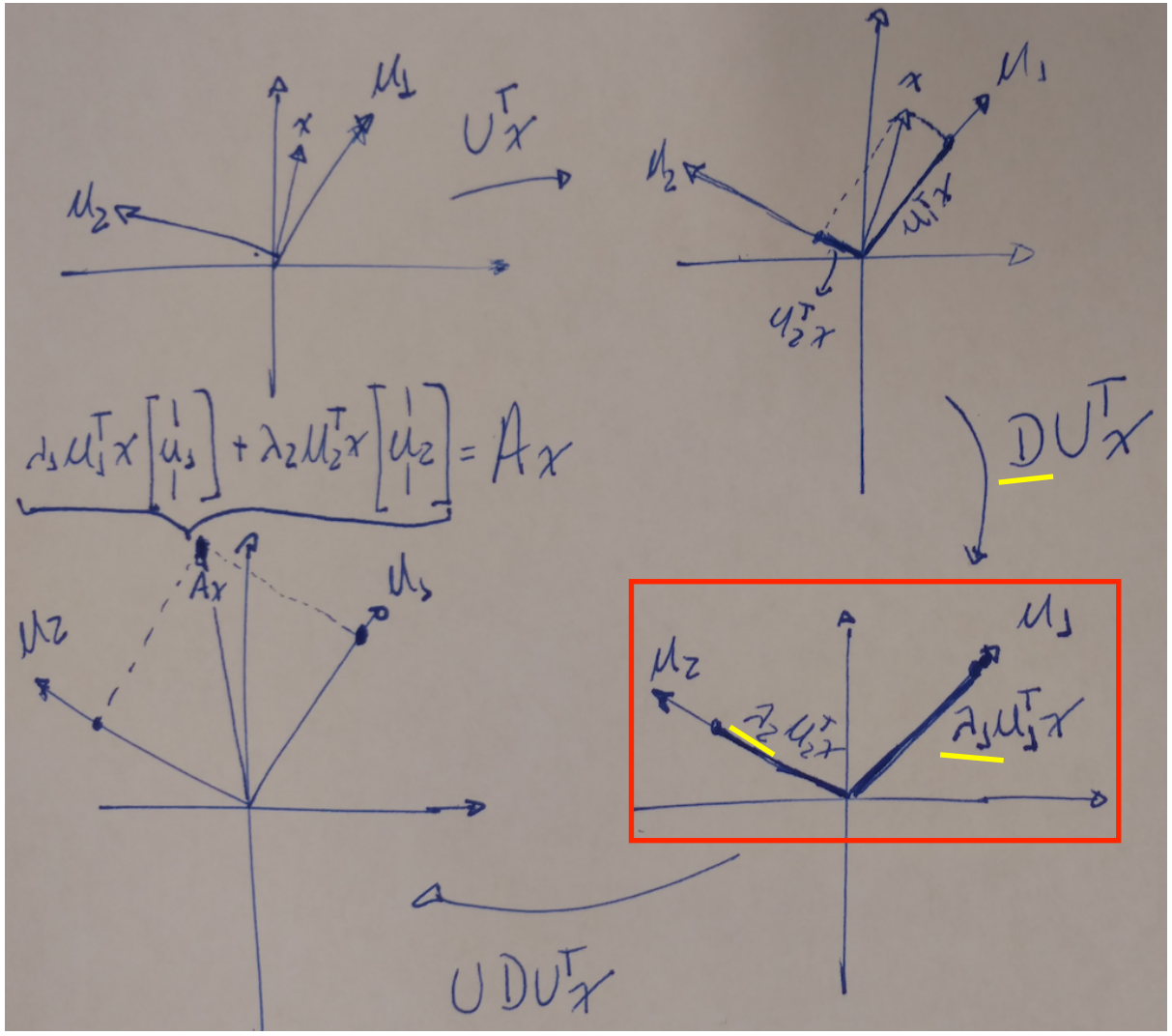

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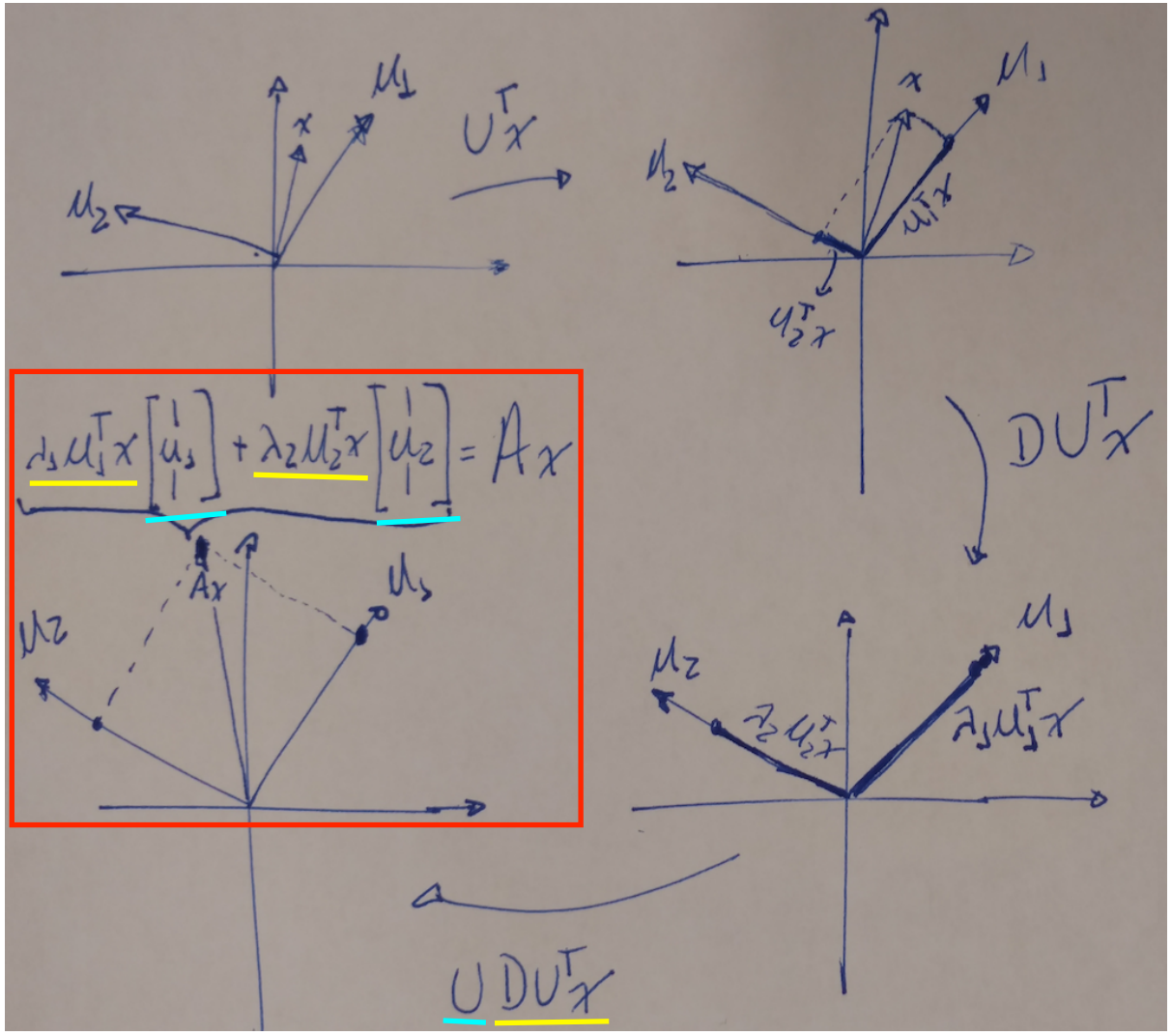

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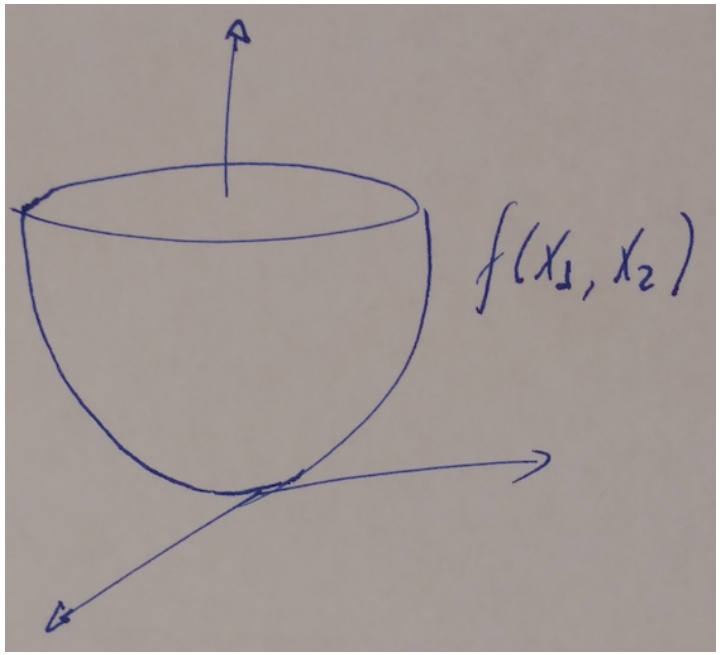

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$$f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}\mathbf{x}$$

$$\max_{\|\mathbf{x}\|=1} \{f(\mathbf{x})\} = \mathbf{u}_1^\top \mathbf{A}\mathbf{u}_1 = \lambda_1$$

$$\min_{\|\mathbf{x}\|=1} \{f(\mathbf{x})\} = \mathbf{u}_d^\top \mathbf{A}\mathbf{u}_d = \lambda_d$$

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$$f(x) \geq 0 \longrightarrow \lambda_1 \geq \lambda_2 \ldots \geq \lambda_d \geq 0$$

$$f(x) > 0 \longrightarrow \lambda_1 \geq \lambda_2 \ldots \geq \lambda_d > 0$$

Covariance Matrix

Let $\mathbf{x}_i = [x_{1i}, \ldots, x_{di}]^\top$, $\mathbf{x}_j = [x_{1j}, \ldots, x_{dj}]^\top$

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The covariance between $\mathbf{x}_i$ and $\mathbf{x}_j$ is given by

$$cov(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{d-1} \sum_{s=1}^{d} (x_{si} - \bar{x}_i)(x_{sj} - \bar{x}_j)$$

where $\bar{x}_i = \frac{1}{d} \sum_s x_{si}$ and $\bar{x}_j = \frac{1}{d} \sum_s x_{sj}$

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If we assume $\mathbf{x}_i$ and $\mathbf{x}_j$ centered, that is, $\bar{x}_i = 0$ and $\bar{x}_j = 0$

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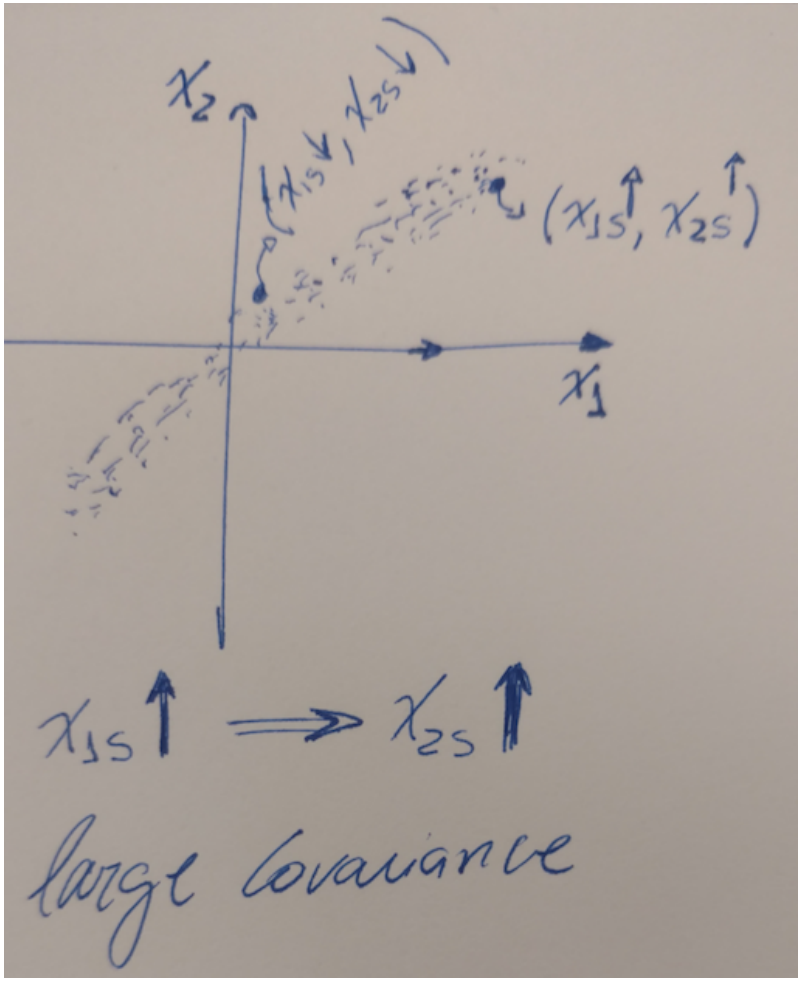

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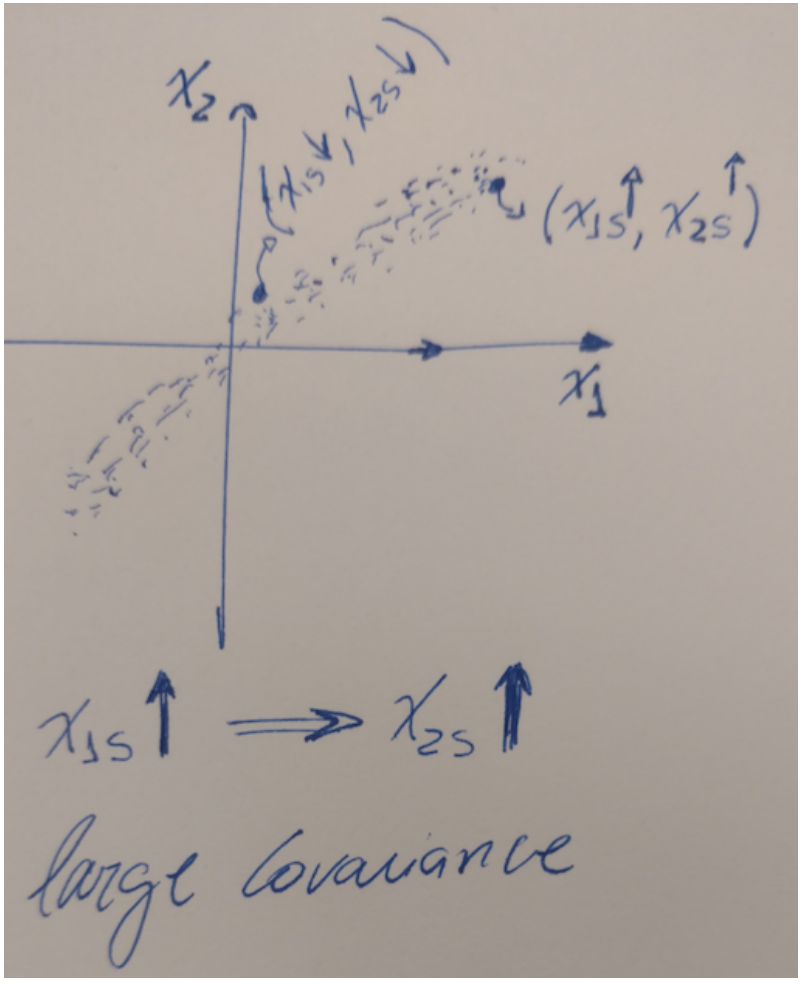

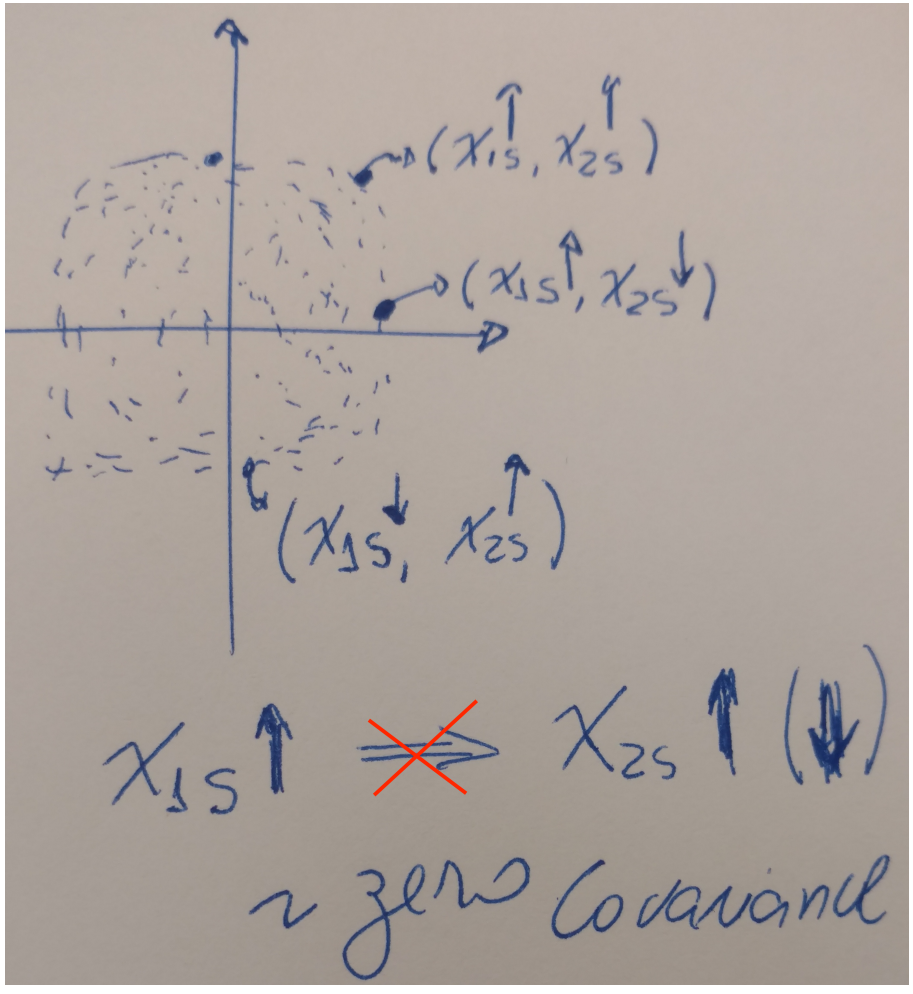

Covariance Matrix

Let $\mathbf{x}_i$, $i = 1, \ldots, n$ a set of data instances (points in $\mathbb{R}^d$) arranged as columns in a data matrix $\mathbf{X}$:

$$\mathbf{X} = \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \ldots & \mathbf{x}_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \ldots & x_{1n} \\ x_{21} & x_{22} & \ldots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{d1} & x_{d2} & \ldots & x_{dn} \end{bmatrix} \tag{1}$$

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Columns correspond to data instances

Rows correspond to a particular attribute.

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The covariance matrix of $\mathbf{X}$ is given by:

$$\frac{1}{n-1}\mathbf{X}\mathbf{X}^\top = \begin{bmatrix} cov(x_{1:}, x_{1:}) & cov(x_{1:}, x_{2:}) & \dots & cov(x_{1:}, x_{d:}) \\ cov(x_{2:}, x_{1:}) & cov(x_{2:}, x_{2:}) & \dots & cov(x_{2:}, x_{d:}) \\ \vdots & \vdots & \ddots & \vdots \\ cov(x_{d:}, x_{1:}) & cov(x_{d:}, x_{2:}) & \dots & cov(x_{d:}, x_{d:}) \end{bmatrix}$$

Variances are in the main diagonal

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Therefore, all the properties we saw before as to symmetric matrices and positive definite quadratic forms hold for the covariance matrix.

Principal Components: getting some intuition

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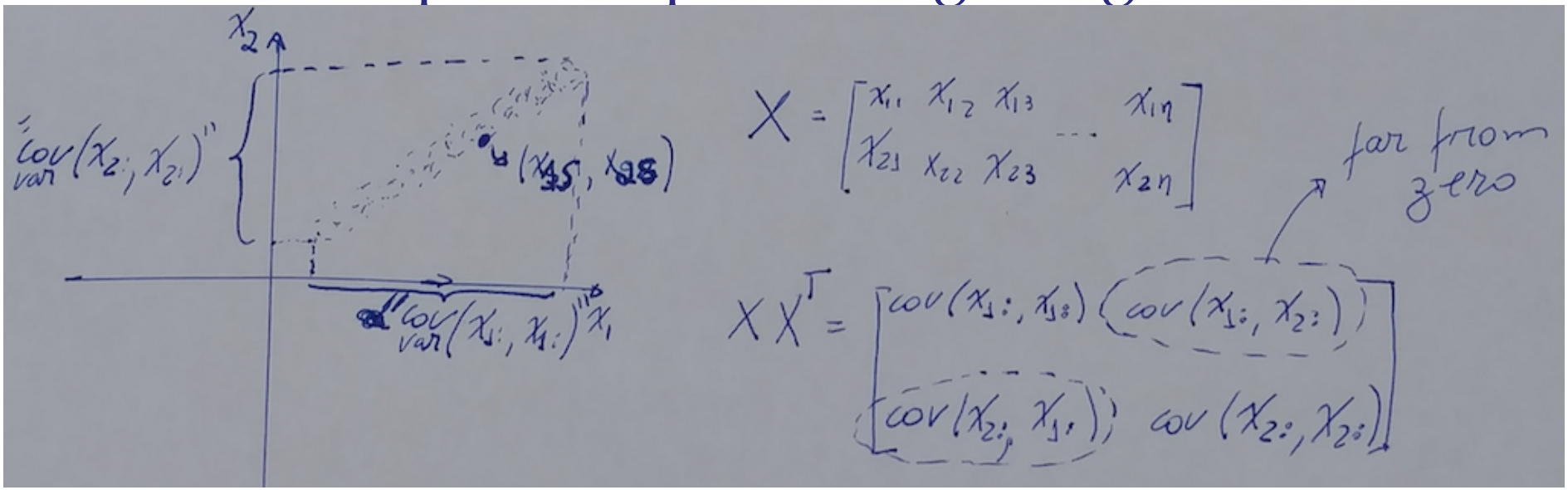

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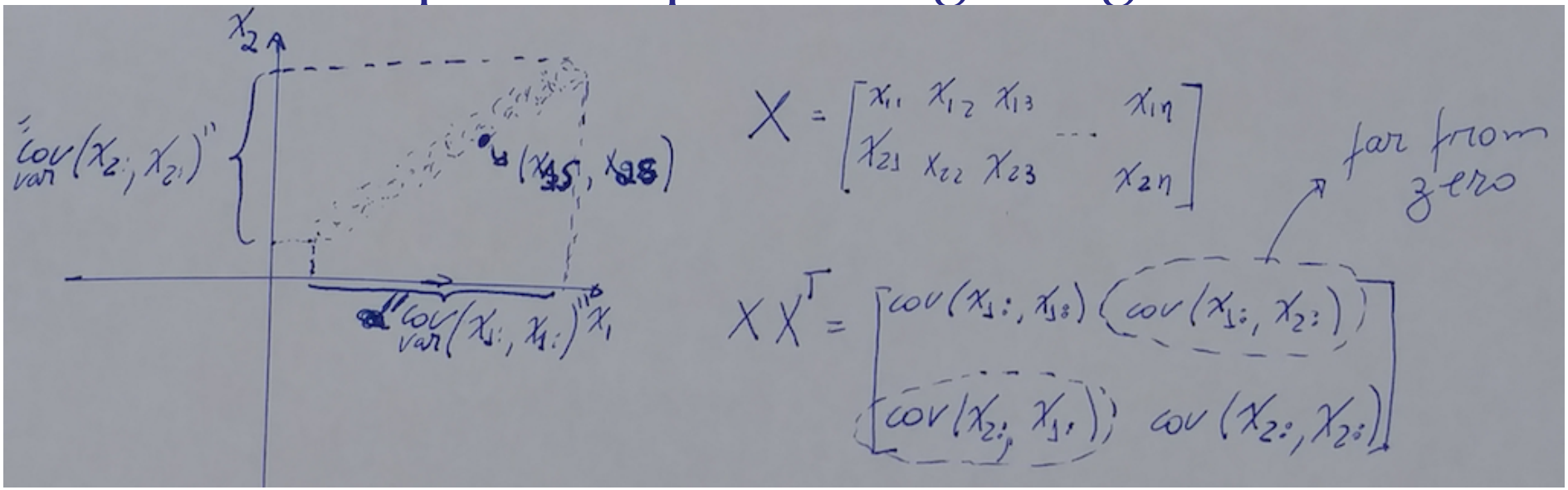

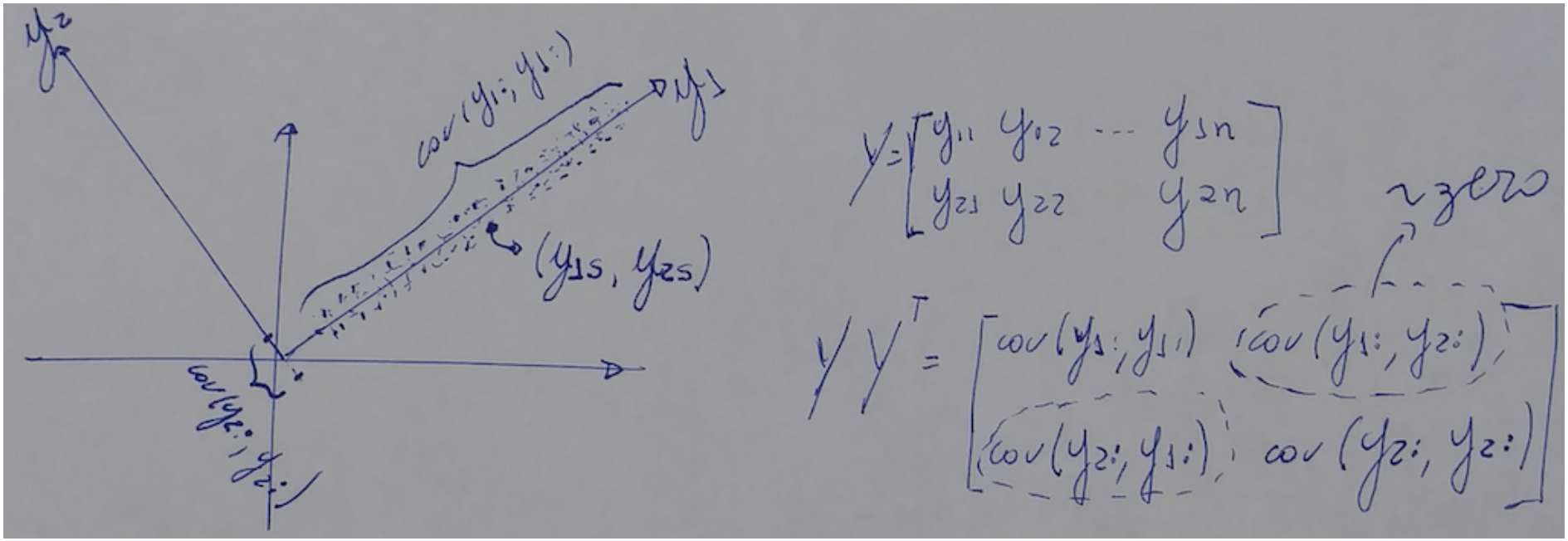

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Mathematically, we are looking for a change of basis matrix $\mathbf{P}$ such that

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where $\mathbf{D}$ is a diagonal matrix with diagonal elements corresponding to the variance of each coordinate/attribute.

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- we will be able to reduce the dimension of the data without loosing relevant information.

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Moreover,

$$\mathbf{u}_1^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}_1 = \lambda_1 \text{ (maximum of the quadratic form)}$$

$$\mathbf{u}_d^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}_d = \lambda_d \text{ (minimum of the quadratic form)}$$

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The coordinates of the data in the new basis is given by:

$$\mathbf{Y} = \mathbf{U}^\top \mathbf{X}$$

The diagonal matrix $\mathbf{D}$ in the decomposition $\mathbf{X}\mathbf{X}^\top = \mathbf{U}\mathbf{D}\mathbf{U}^\top$ contains the variances of each new coordinate.

Moreover,

$$\mathbf{u}_1^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}_1 = \lambda_1 \text{ (maximum of the quadratic form)}$$

$$\mathbf{u}_d^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}_d = \lambda_d \text{ (minimum of the quadratic form)}$$

$\mathbf{u}_1$ is the direction that maximizes the variance and $\mathbf{u}_d$ the direction that minimizes the variance.

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We can reconstruct "noise-free" data by $\hat{\mathbf{X}} = \mathbf{U}\hat{\mathbf{Y}}$

$$\hat{\mathbf{Y}} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1n} \\ & & \vdots & \\ y_{k1} & y_{k2} & \cdots & y_{kn} \\ 0 & 0 & \cdots & 0 \\ & & \vdots & \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

Principal Component Analysis

How to choose the ideal variance (singular value) cut off?

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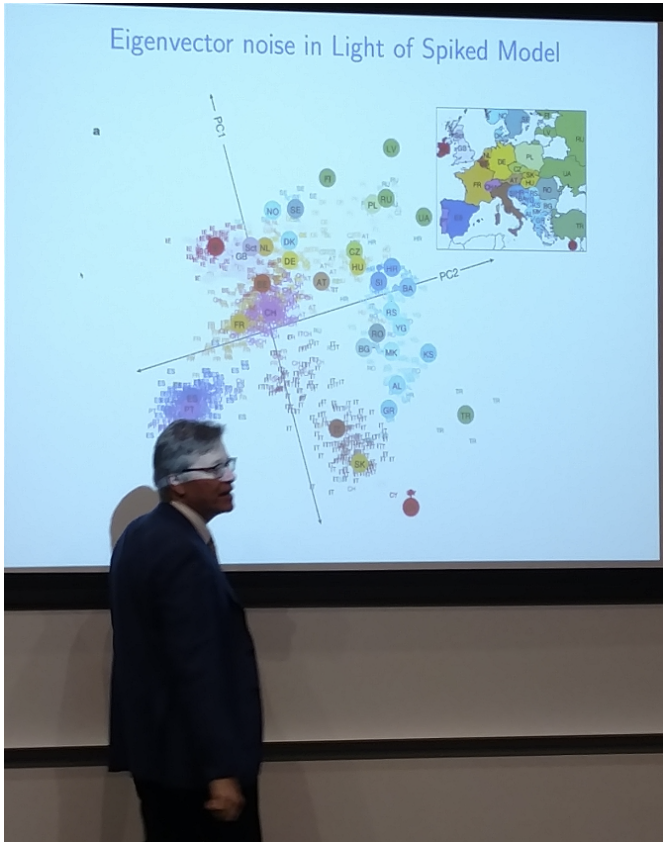

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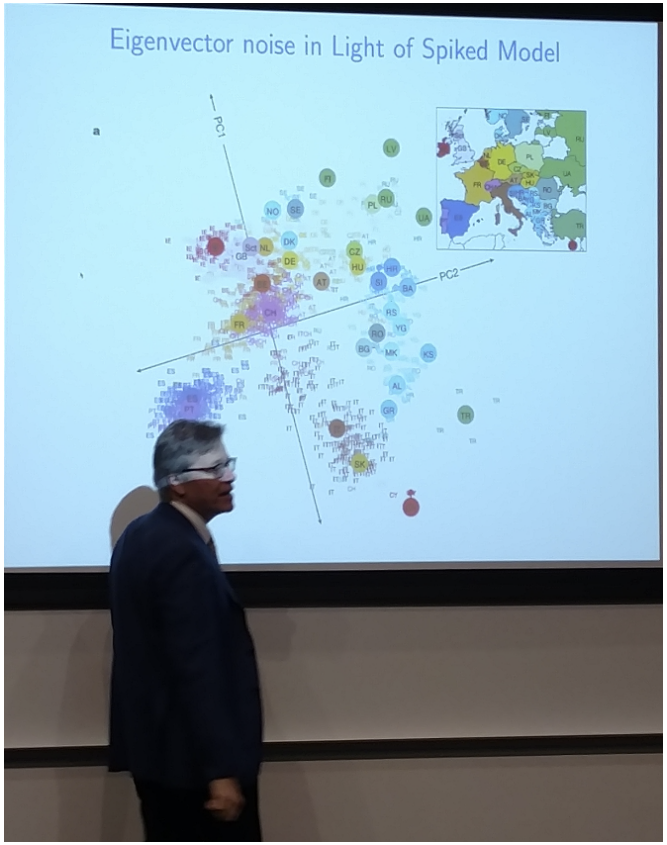

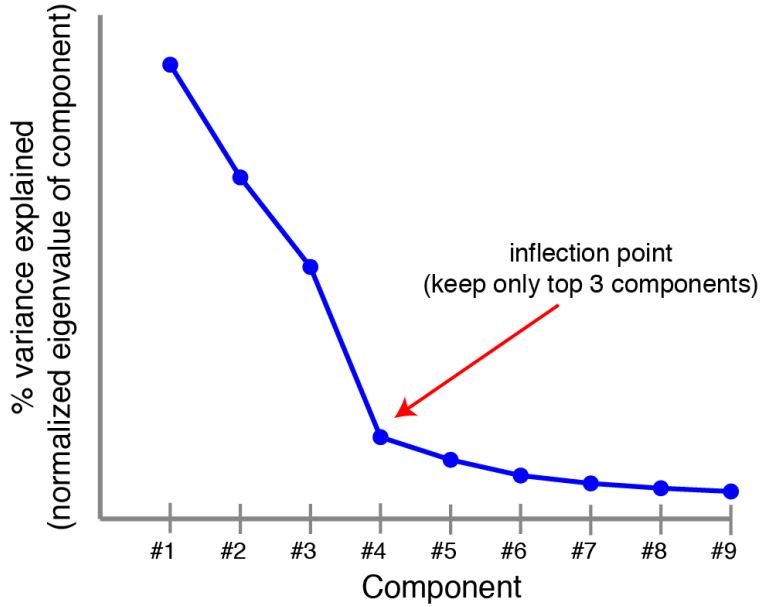

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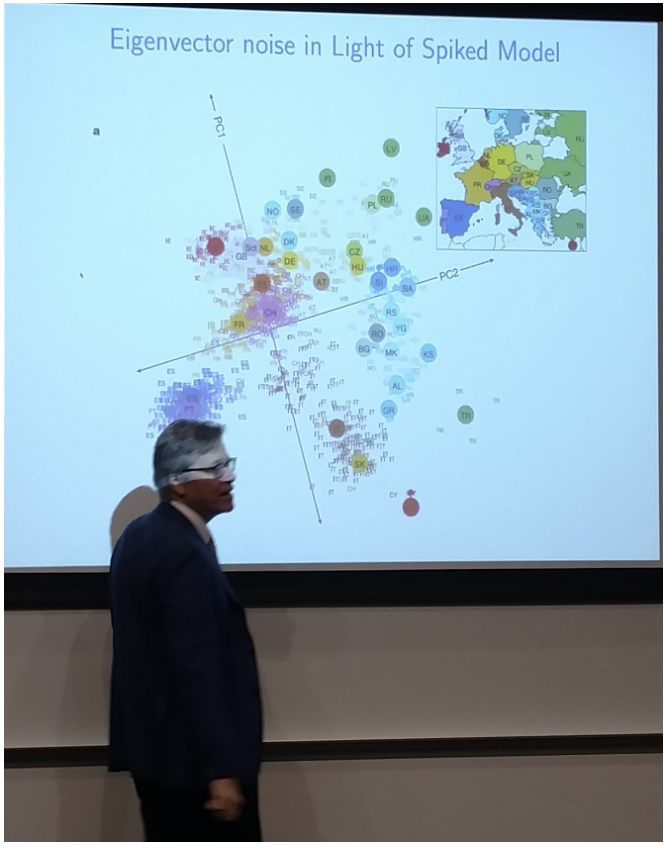

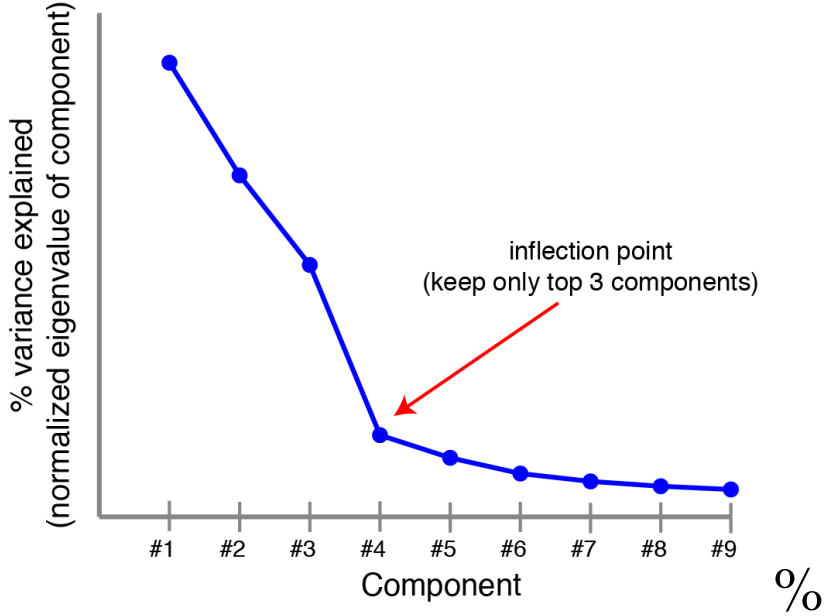

Variance Explained

$$T = \frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$$

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- The new coordinates have no semantic meaning
- PCA is sensitive to outliers

PCA via SVD

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Singular Value Decomposition (SVD)

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

where $\mathbf{\Sigma}$ is a diagonal matrix with non-zero entries $\sqrt{\lambda_i}$.

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Therefore,

$\mathbf{U}$: the principal directions

$\mathbf{\Sigma}\mathbf{V}^\top$: the coordinates of the data in the PCA space

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All the development so far assumes that $\mathbf{X}$ is centered (average of each row is zero).

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A centered version $\tilde{\mathbf{X}}$ of $\mathbf{X}$ is given by:

$$\tilde{\mathbf{X}} = \mathbf{X} - \overline{\mathbf{X}}$$

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