Linear Algebra in Neuroscience

Introduction to dimensionality reduction techniques

University of Helsinki
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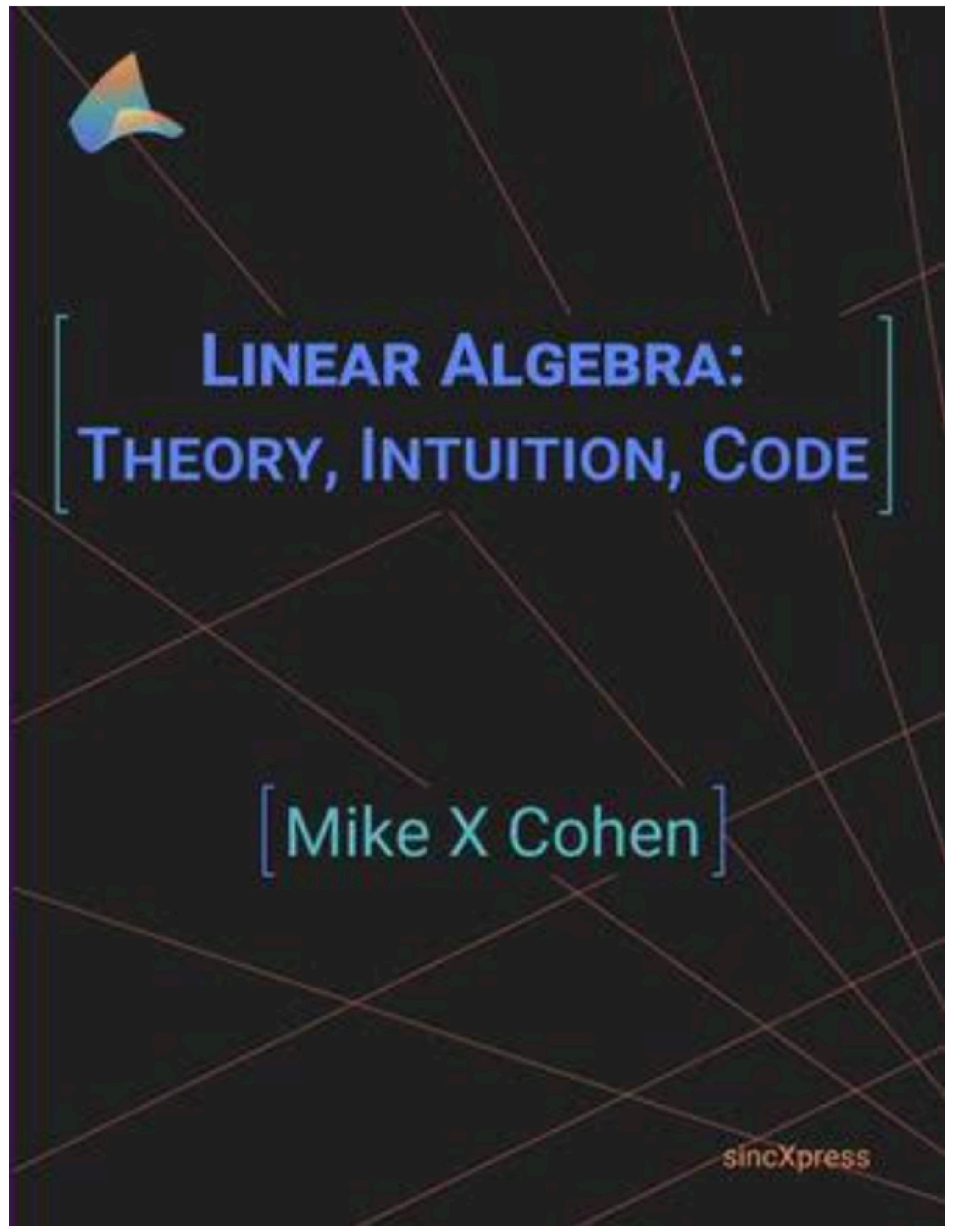
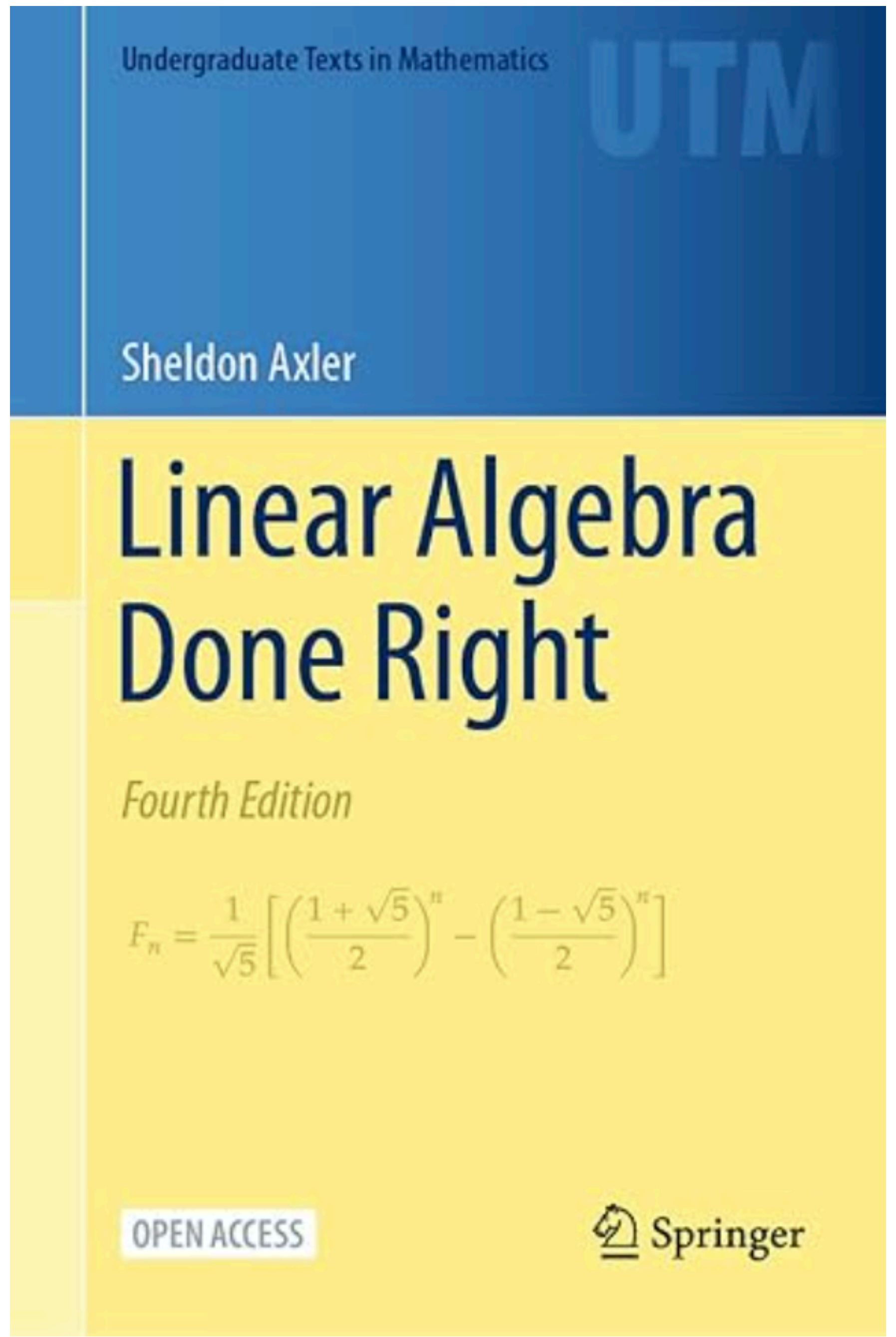
Outline

and resources

- Overview
- Eigendecomposition
- SVD
- PCA
- GED
- Hands-on

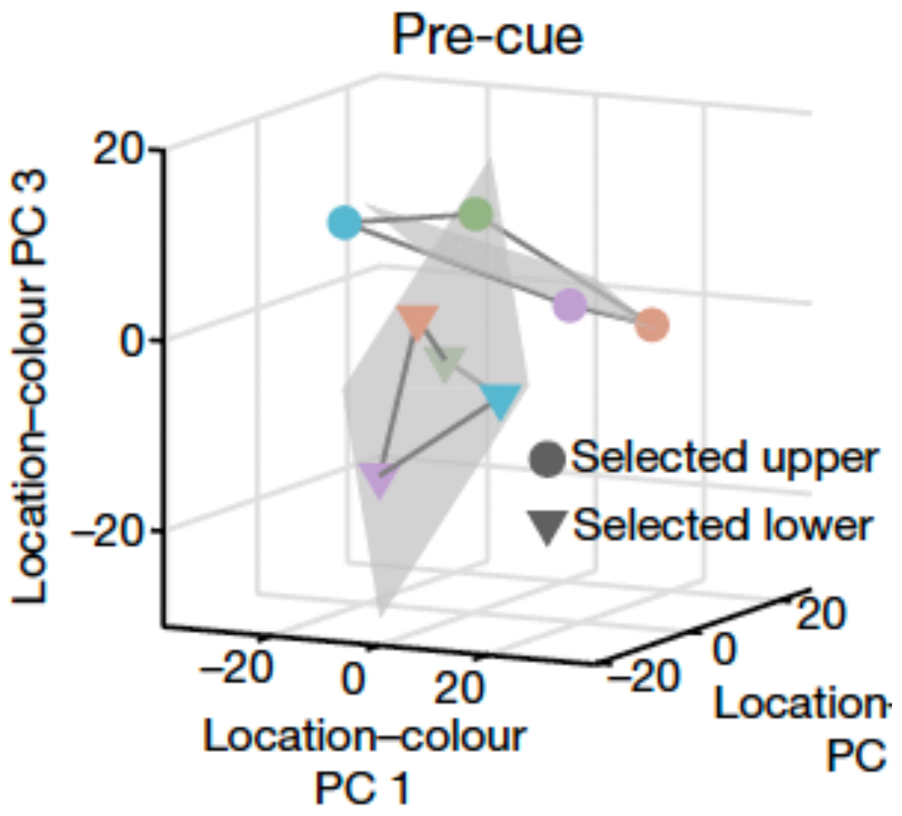




Overview

- Dimensionality reduction techniques allows to address the curse of dimensionality in large-scale neural recordings (Cunningham, 2014).
- High-dimensional neural activity is constrained to a lower-dimensional, structured subspace (neural manifold) where neural computations take place, enabling efficient information processing, generalization, and robustness to noise (Thibeault, 2023; Langdon, 2023;).

  - Neural subspaces encode multiple-item working memory contents (Xie, 2022; Panichello, 2021).



  - Head direction cells in mouse projects into a low dimensional ring structure (Duszkiewicz, 2024), consistent across sessions and subjects (Barbosa, 2024)

Linear algebra basics

Apologies in advance for the mathematicians!

* **vector space**: where the vectors live and move according to some rules (addition and scaling)

$$u = [2, 1] \quad \in \mathbb{R}^2$$

$$v = [1, 2, 3] \in \mathbb{R}^3$$

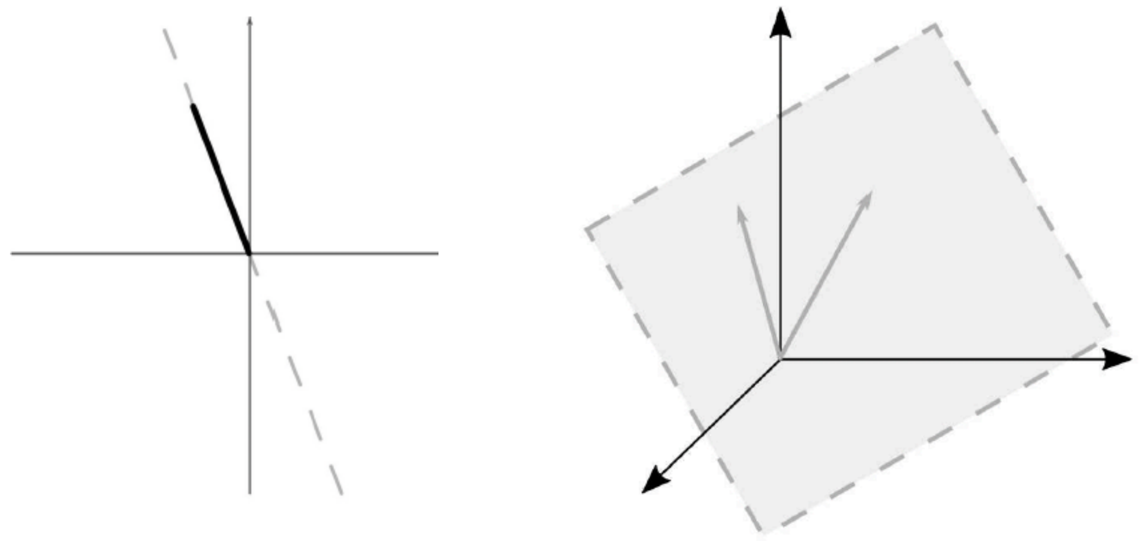
$$v = [1, 2, 3] \notin \mathbb{R}^2$$

* **basis of space**: set of independent vectors that **span** the vector space (ruler of the space) - simplest one are the cartesian basis vectors

$$\mathbb{R}^2 : \left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$$

* **Span**: all points you can reach by stretching and combining a collection of vectors

* **subspace**: the subset of a vector space, which is also a vector space.

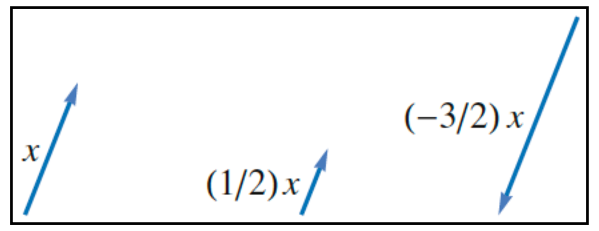


$$T = \{\, c\,[-1, 2] \mid c \in \mathbb{R} \,\} \quad \subset \mathbb{R}^2$$

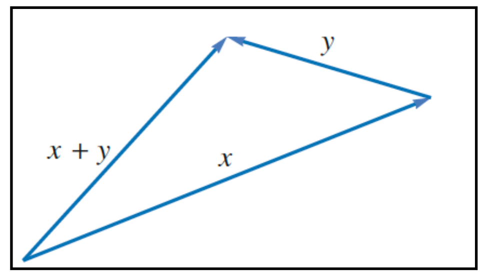
$$S = \{\, [x, y, 0] \mid x, y \in \mathbb{R} \,\} \subset \mathbb{R}^3$$

How vectors 'move' in vector spaces?

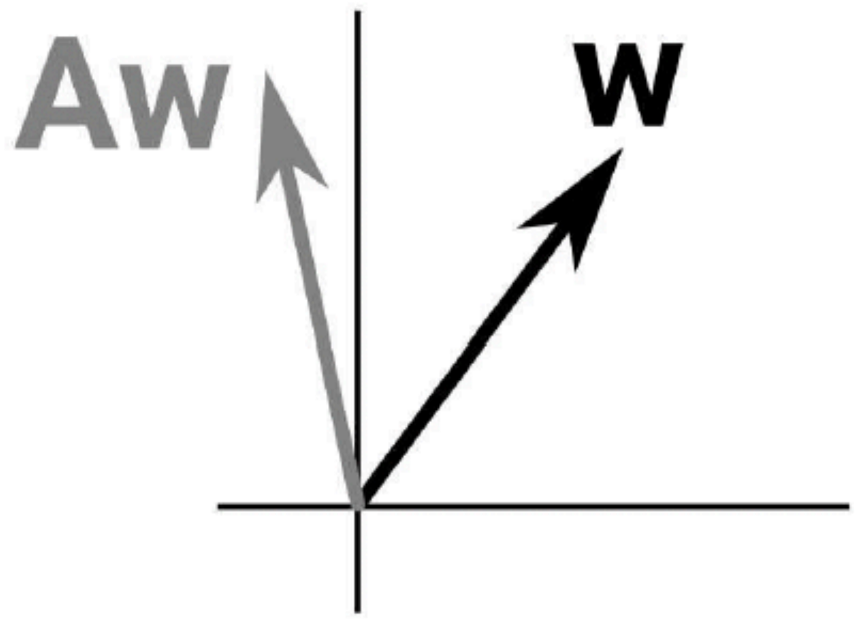
* **Scalar multiplication: λx**



* **Vector addition: x + y**



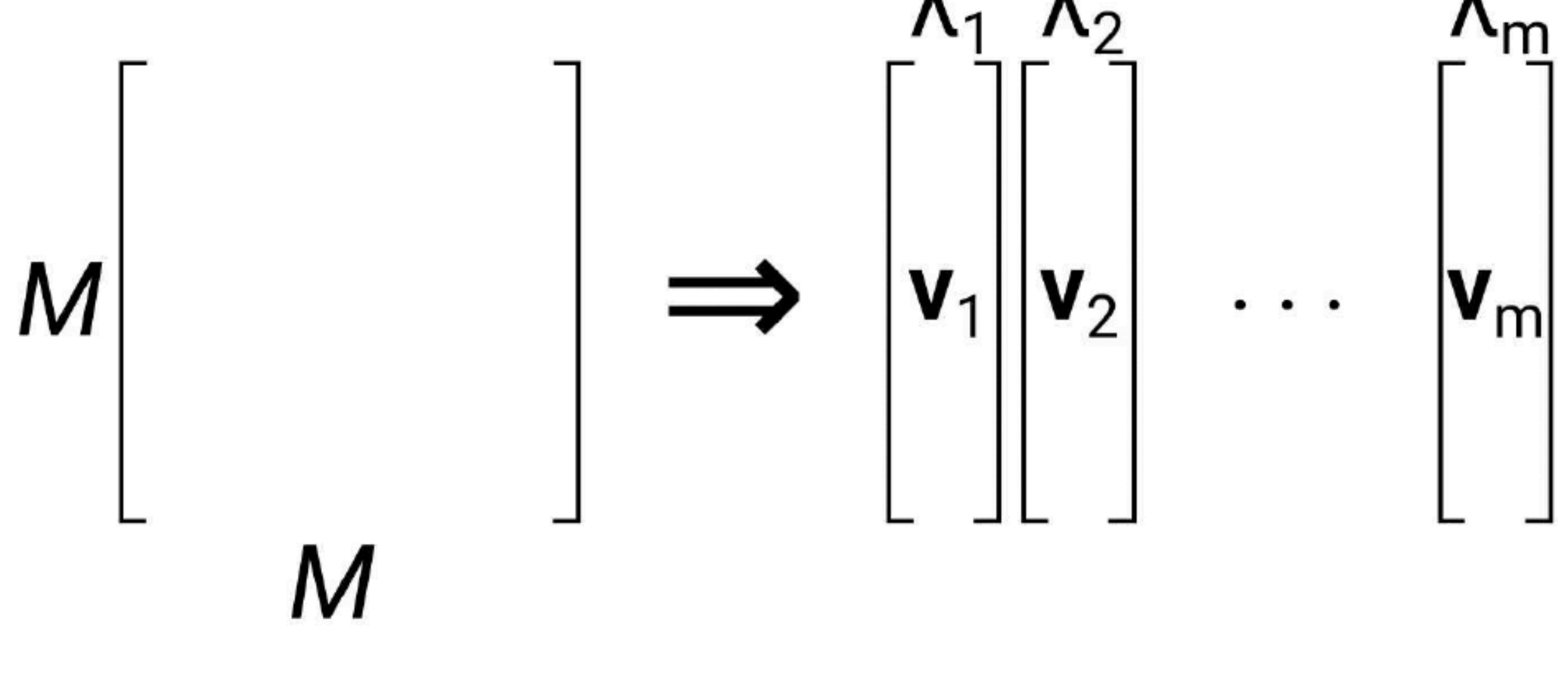
* **Matrix-vector multiplication: Aw**



Eigendecomposition

a.k.a. eigenvalue decomposition, eigenvector decomposition, diagonalization

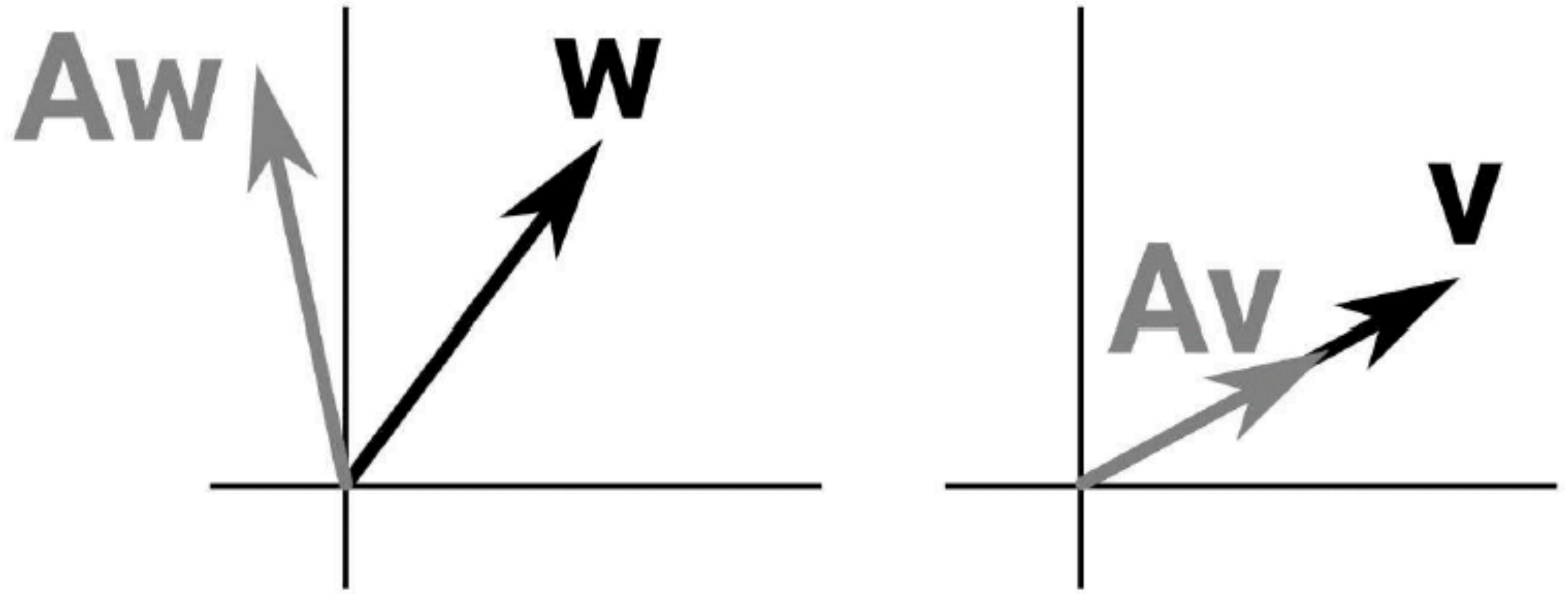
- Eigendecomposition applies only to square matrices
- Goal: extract 'features' called eigenvalues (λ, scalar) and eigenvectors (v, vector)



- Eigenvalue equation

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

- Effect of matrix is the same as the effect of scalar multiplication



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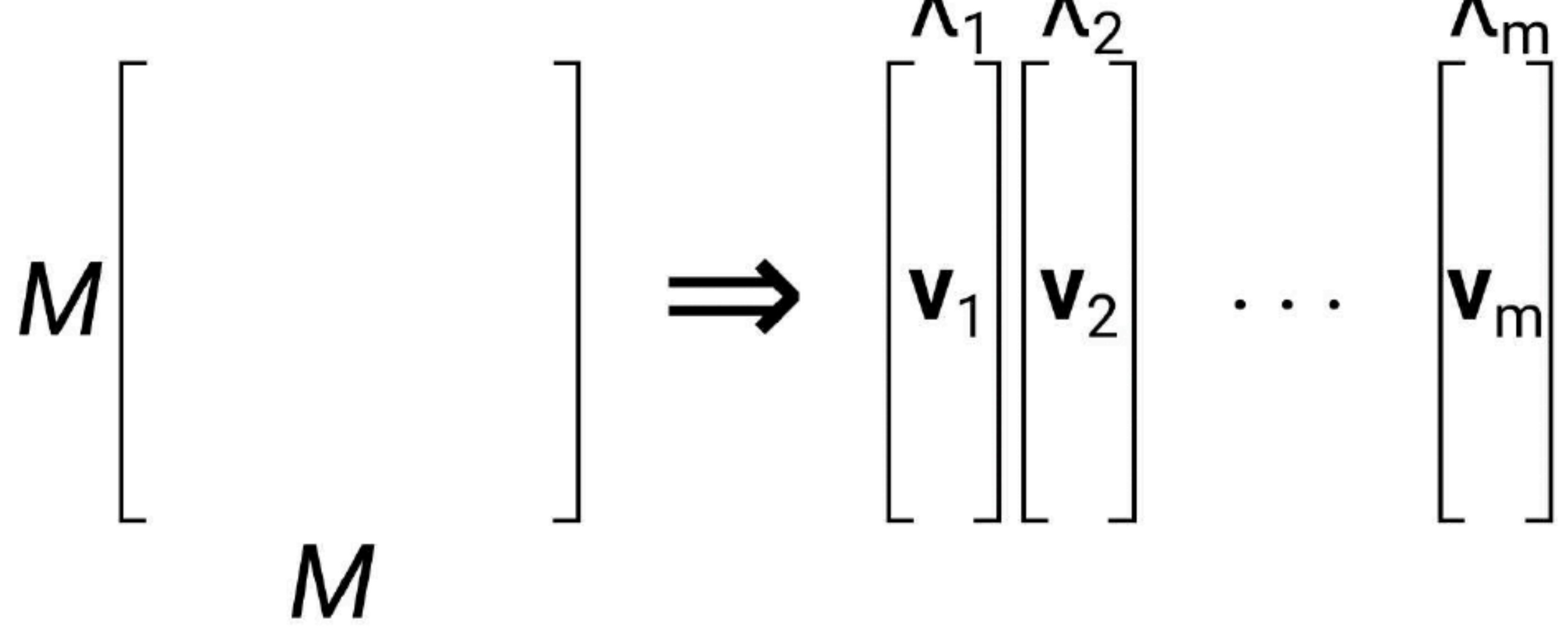
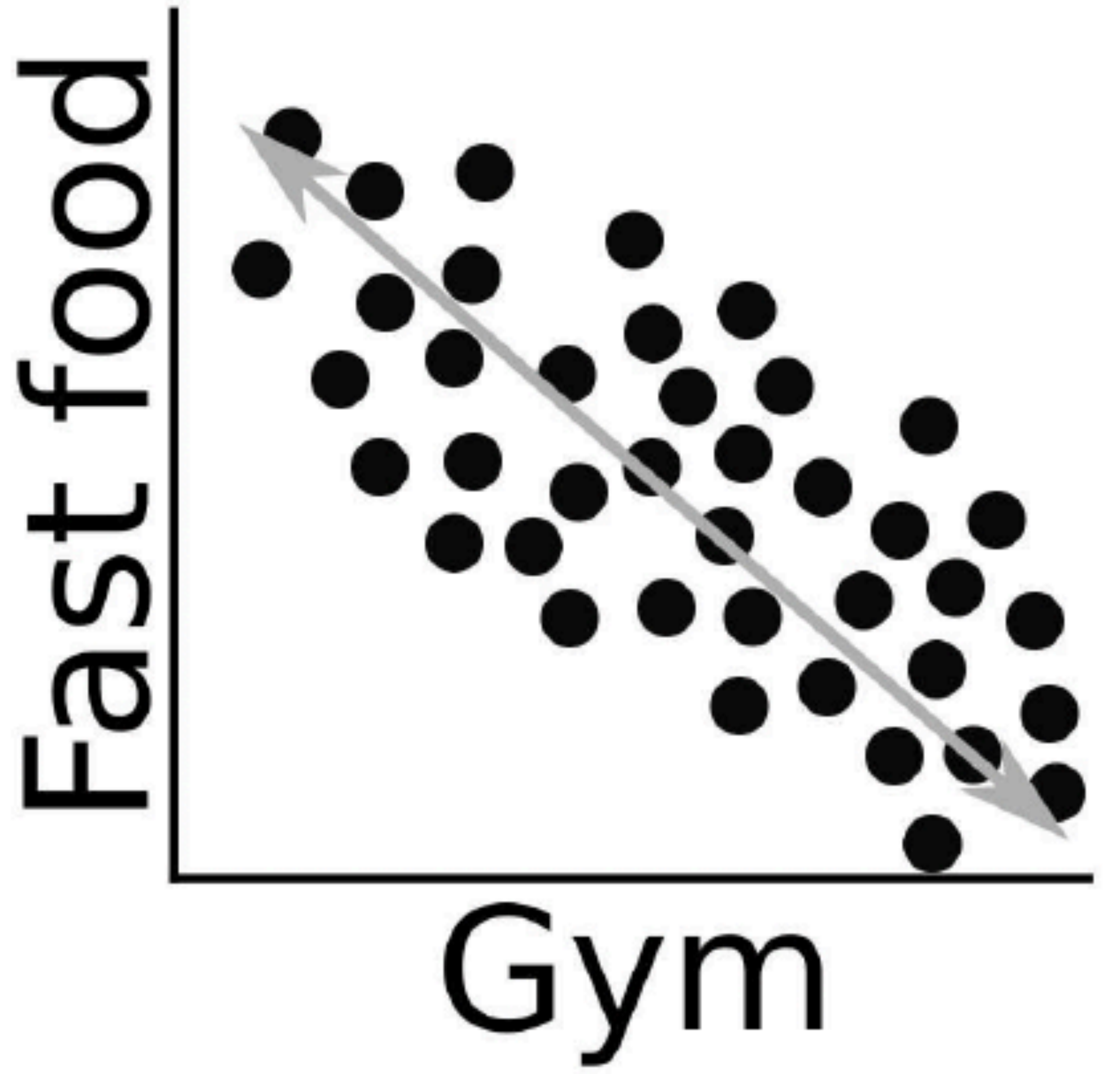


- Interpretation



Eigendecomposition

Finding eigenvalues and eigenvectors

* Find eigenvalues

$$Av = \lambda v$$

$$Av - \lambda v = 0$$

$$Av - \lambda I v = 0$$

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

* matrix A shifted by lambda, multiplied by a vector v, gives zeros vector = null space of matrix A

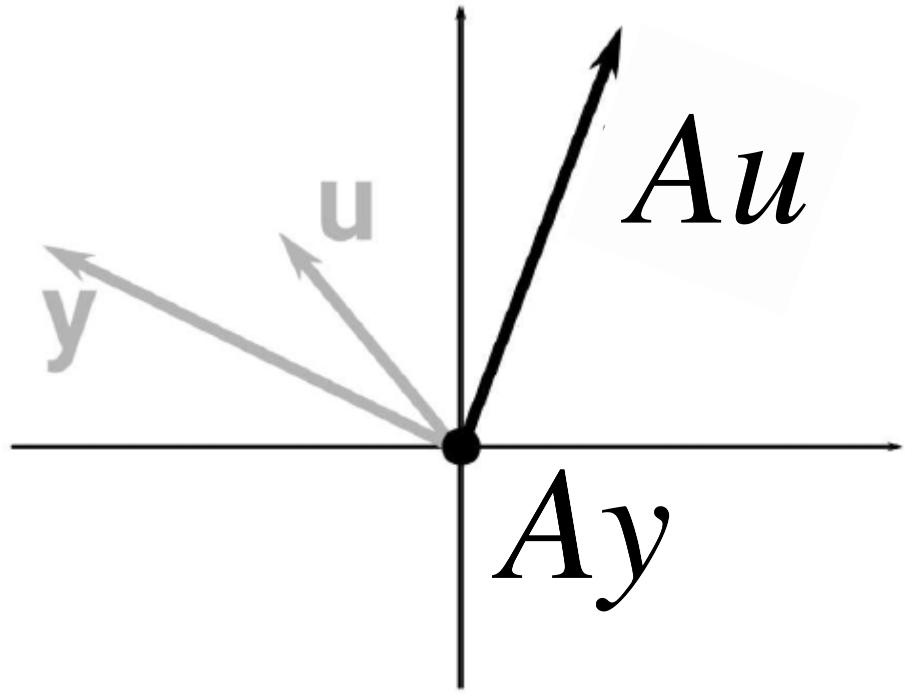
$$|A - \lambda I| = 0$$

* determinant of $A - \lambda I$ is zero

(Any square matrix with a non-trivial null space has determinant zero)

* **null space**: subspace containing all vectors (y) that satisfy (non-trivial)

$$Ay = 0$$



Eigendecomposition

Finding eigenvalues and eigenvectors

- Find eigenvalues

$$|A - \lambda I| = 0$$

$$\left| \begin{bmatrix} a & b \\ c & d \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right| = 0$$

$$\begin{vmatrix} a-\lambda & b \\ c & d-\lambda \end{vmatrix} = 0$$

$$(a-\lambda)(d-\lambda) - bc = 0$$

$$\lambda^2 - (a+d)\lambda + (ad-bc) = 0$$

$$\lambda = \frac{-b \pm \sqrt{b^2-4ac}}{2a}$$

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \quad \Rightarrow \quad \begin{vmatrix} 1-\lambda & 2 \\ 2 & 1-\lambda \end{vmatrix} = 0$$

$$(1-\lambda)(1-\lambda) - 4 = 0$$

$$\lambda^2 - 2\lambda - 3 = 0$$

$$(\lambda - 3)(\lambda + 1) = 0$$

$$\Rightarrow \lambda_1 = 3,\ \lambda_2 = -1$$

Eigendecomposition

Finding eigenvalues and eigenvectors

- Find eigenvectors

$$(A - \lambda_i I)v_i = 0$$

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \Rightarrow \lambda_1 = 3,\ \lambda_2 = -1$$

$$(A - \lambda_i I) \quad (A - \lambda_i I) \qquad (A - \lambda_i I)v_i = 0$$

$$\begin{bmatrix} 1-3 & 2 \\ 2 & 1-3 \end{bmatrix} = \begin{bmatrix} -2 & 2 \\ 2 & -2 \end{bmatrix} \Rightarrow \begin{bmatrix} -2 & 2 \\ 2 & -2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

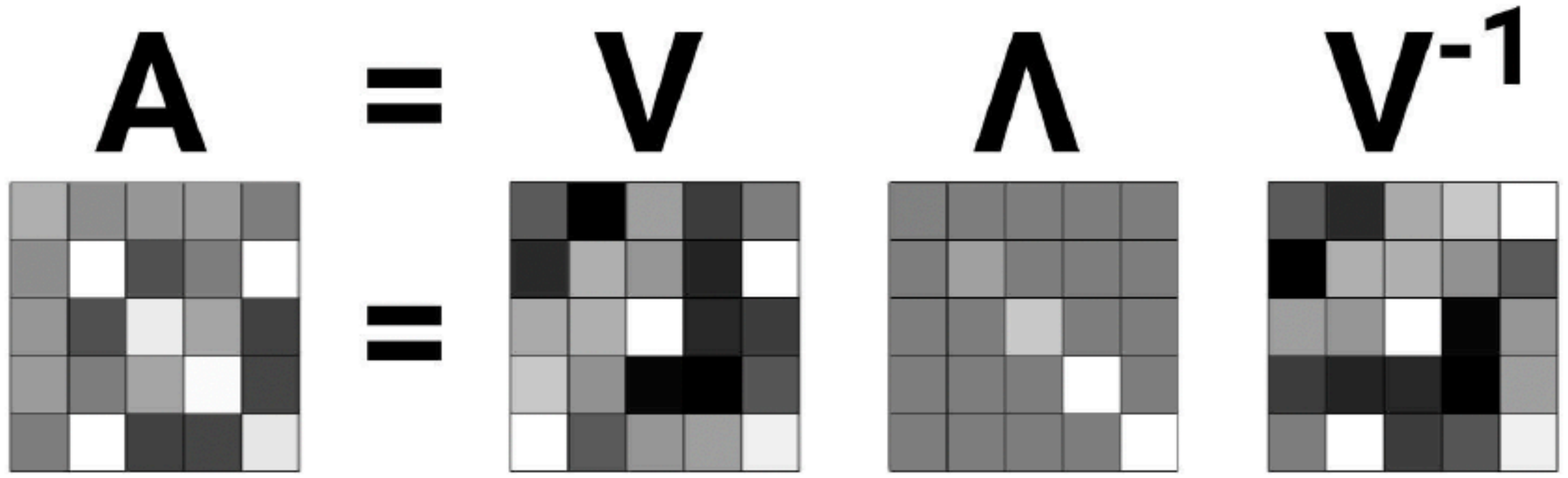
$$\begin{bmatrix} 1--1 & 2 \\ 2 & 1--1 \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \Rightarrow \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{cases} \lambda_1 = 3, & \mathbf{v}_1 = \alpha \begin{bmatrix} 1 & 1 \end{bmatrix}^{\mathrm{T}}, \quad \alpha \in \mathbb{R} \\ \lambda_2 = -1, & \mathbf{v}_2 = \beta \begin{bmatrix} -1 & 1 \end{bmatrix}^{\mathrm{T}}, \quad \beta \in \mathbb{R} \end{cases}$$

Eigendecomposition

Summary

- Only for squared matrices.
- Decomposition of a matrix into eigenvectors and eigenvalues.
- Eigenvectors indicate the direction of most variance in A
- Eigenvalues indicate the 'importance' of each eigenvector (variance explained)
- Eigenvectors are new basis vectors for A (if A is diagonalizable, which is the case for all symmetric matrices)



* matrix inverse:

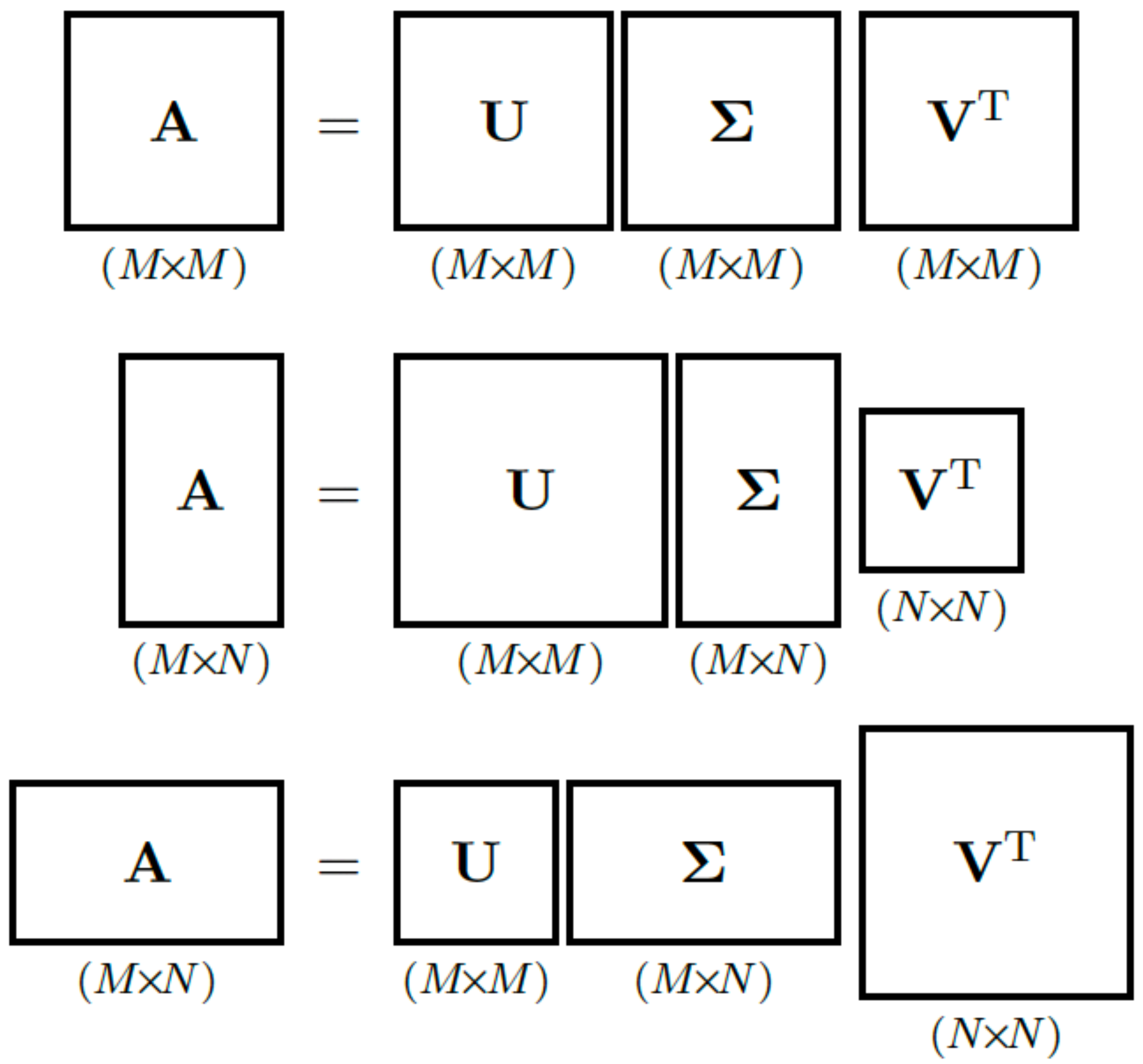
$$M^{-1}M = I$$

Singular Value Decomposition

SVD as generalization of eigendecomposition

- SVD applies also to non-square matrices
- Goal: extract ‘features’ called singular values (σ, scalar) and singular vectors (u v, vector)

$$A = U\Sigma V^T$$



- A is matrix (MxN)
- Σ is a diagonal matrix with **singular values σ** (all non-negative, all real-valued)
- U is the **left singular** vectors matrix with columns as orthonormal basis for R^M
- V is the **right singular** vectors matrix with columns as orthonormal basis for R^N

Singular Value Decomposition

Finding singular values and singular vectors

$$A = U\Sigma V^T$$

- Finding V and Σ matrices

$$A^T A = V\Sigma^2 V^T$$

(eigendecomposition of the transpose of A times A)

- Finding U matrix

$$AA^T = U\Sigma^2 U^T$$

(eigendecomposition of A times the transpose of A)

Singular Value Decomposition

SVD nice properties

- **Rank** of matrix A: number of non-zero elements in the diagonal of Σ

* **rank** of matrix: largest number of columns/rows that form a linearly independent set (full-rank vs reduced-rank or singular matrices)

Singular Value Decomposition

SVD nice properties

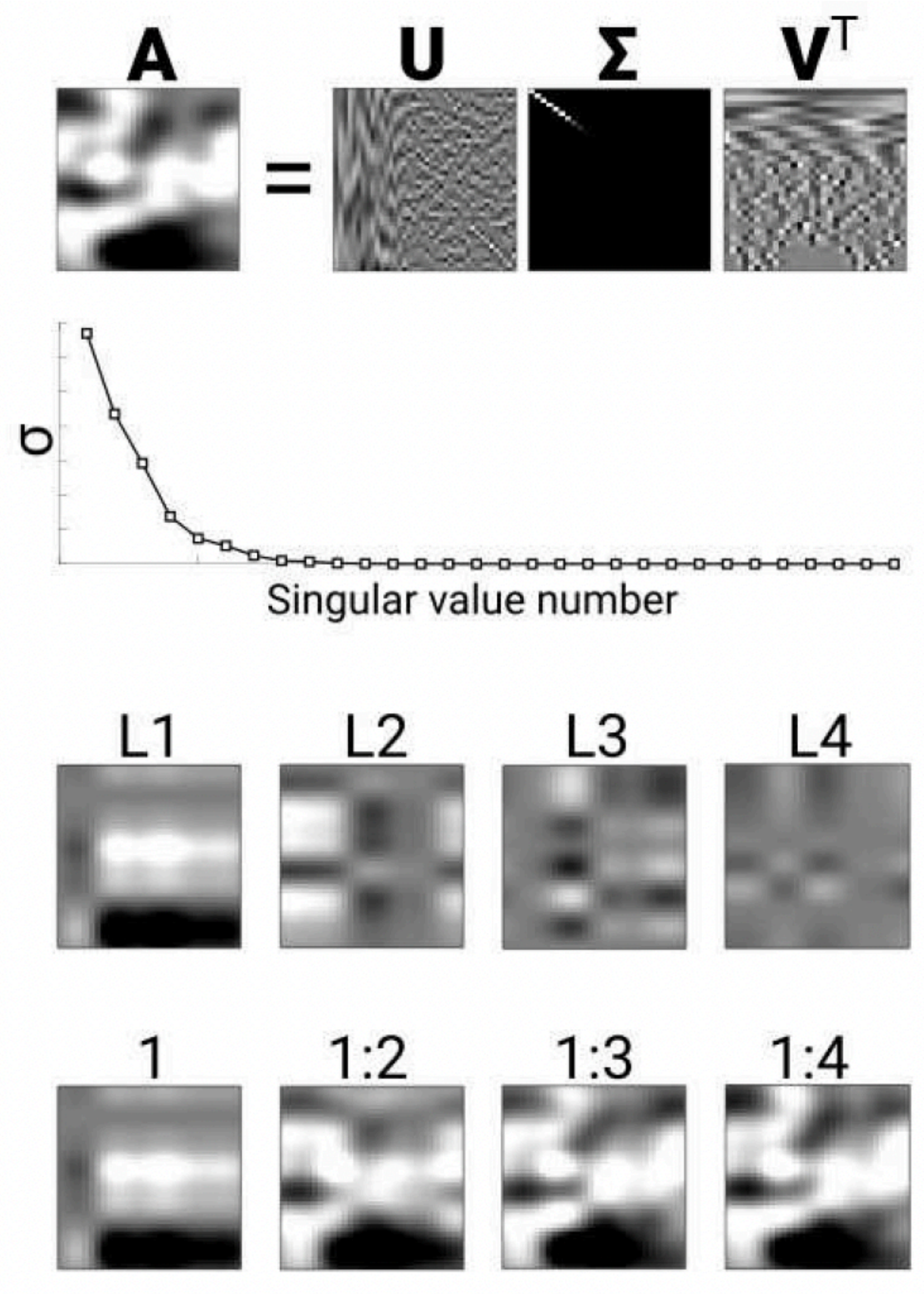
- **Low-rank approximation** of A:

$$\tilde{A} = \sum_{i=1}^{k} u_i \sigma_i v_i^T$$

- noise reduction

- ML classification

- data compression



Principal Component Analysis

Linear algebra aspects of PCA

- Multivariate dataset (X matrix) with observations (rows) and features (columns) - reduce dimensionality on features

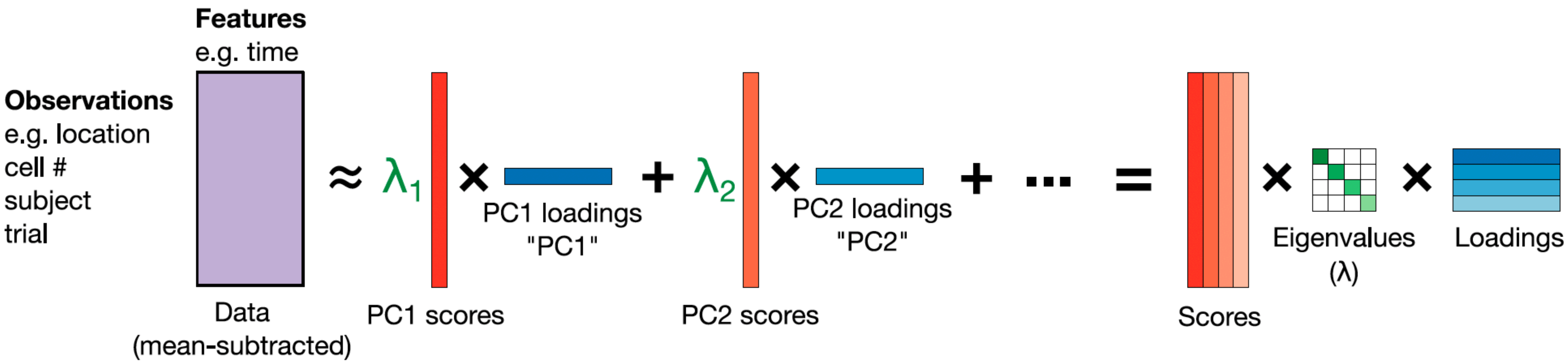
- Example 1:
  - Observations (rows): subjects
  - Columns (features): clinical scores

- Example 2:
  - Observations (rows): stimulus
  - Columns (features): neurons

Principal Component Analysis

Linear algebra aspects of PCA

- Goal PCA: decompose multivariate dataset into Principal Components (PCs), including scores and loadings.



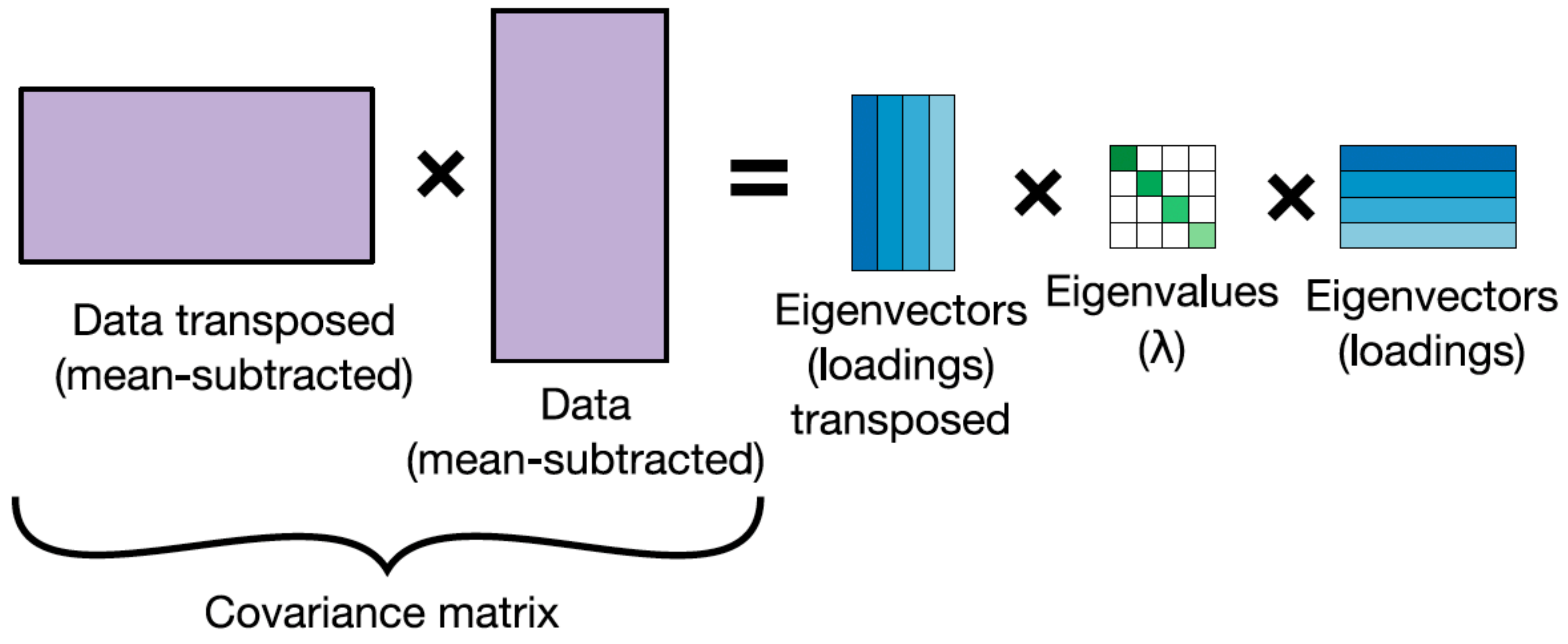
Shinn, 2023

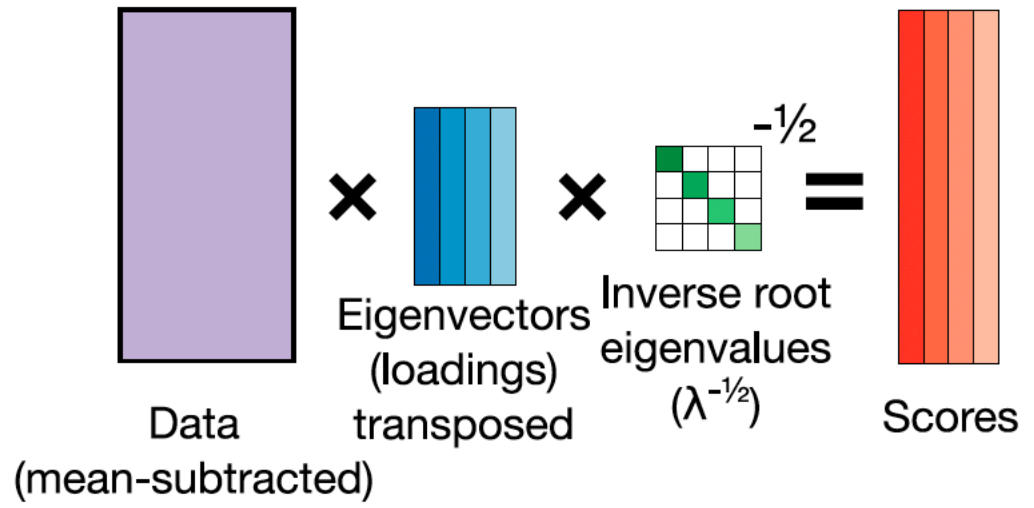
Principal Component Analysis

How to compute

1. Mean-center columns of X, then compute **covariance matrix** cov(X - mean(X)), dimension features by features.
2. **Eigendecomposition of cov(X - mean(X))**. Eigenvectors are **PC loadings**.
3. Compute 'components scores' (**PC scores**) as the weighted combination of all data features: $v_i^T X$ for component i.
4. Convert eigenvalues to **variance explained.**

- PCA in Matlab and Python is implemented with SVD, since works better for large datasets

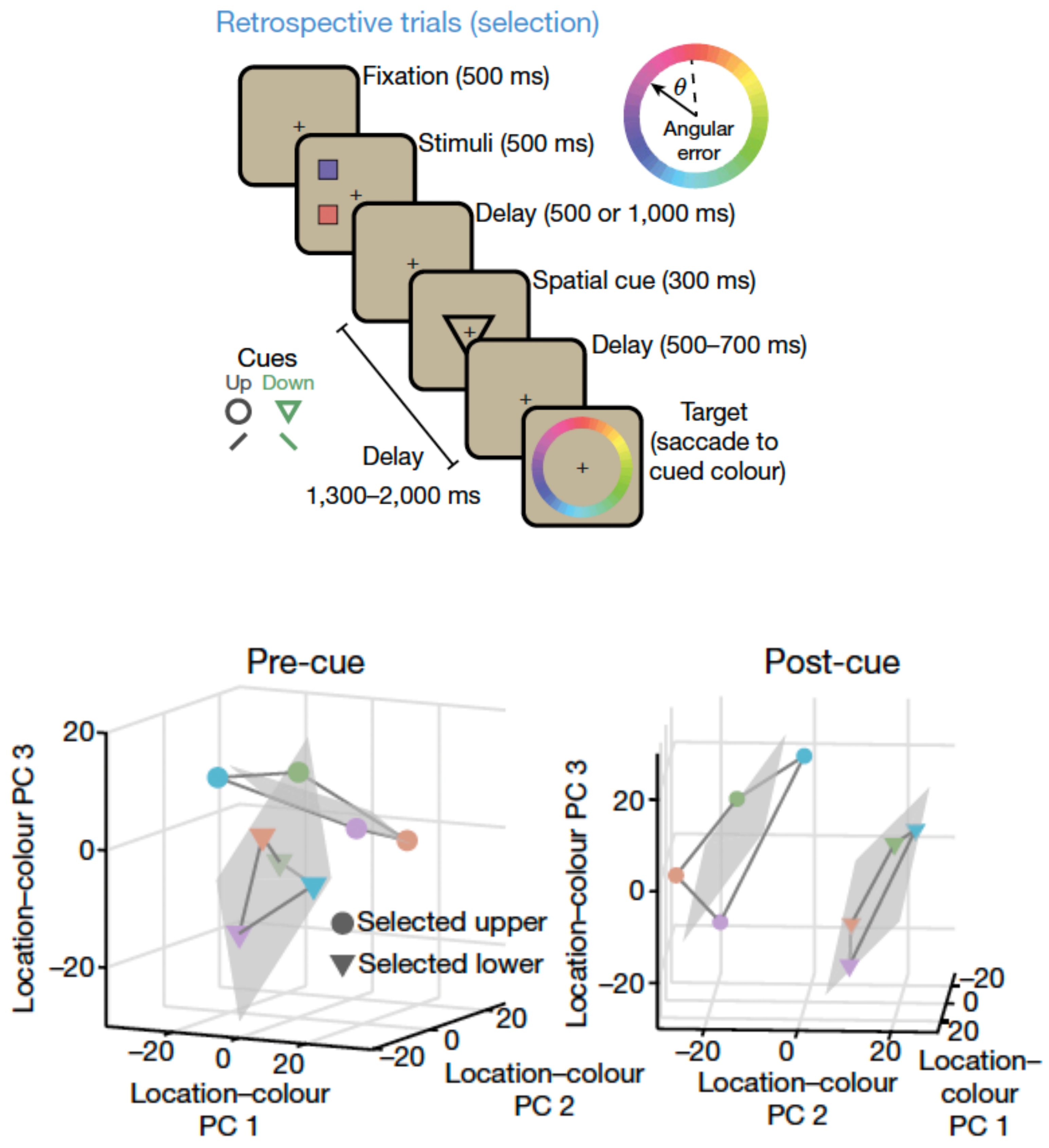




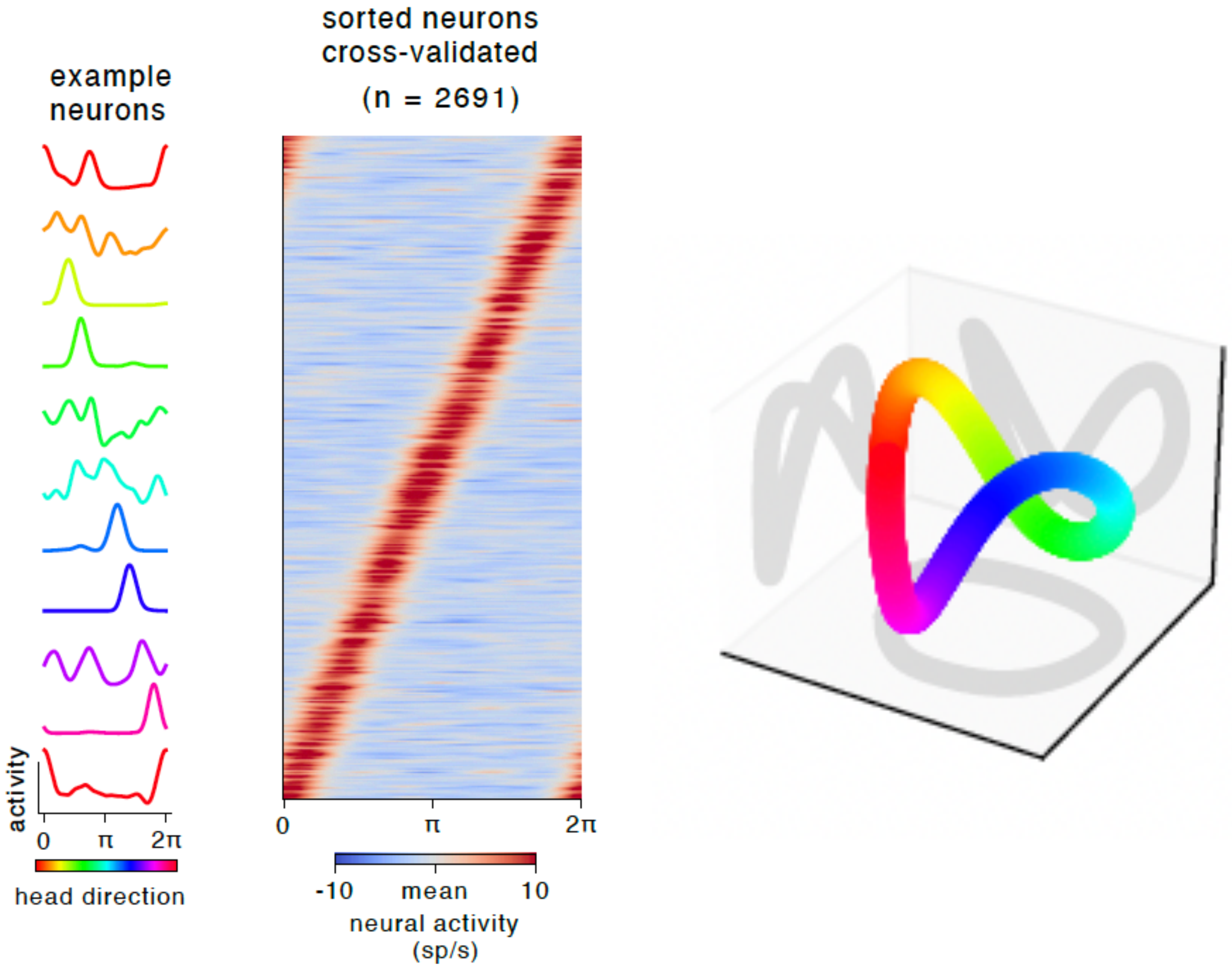
Shinn, 2023

Principal Component Analysis

Applications



Panichello (2021), see also Xie (2022), Tian (2024), Jahn (2024)



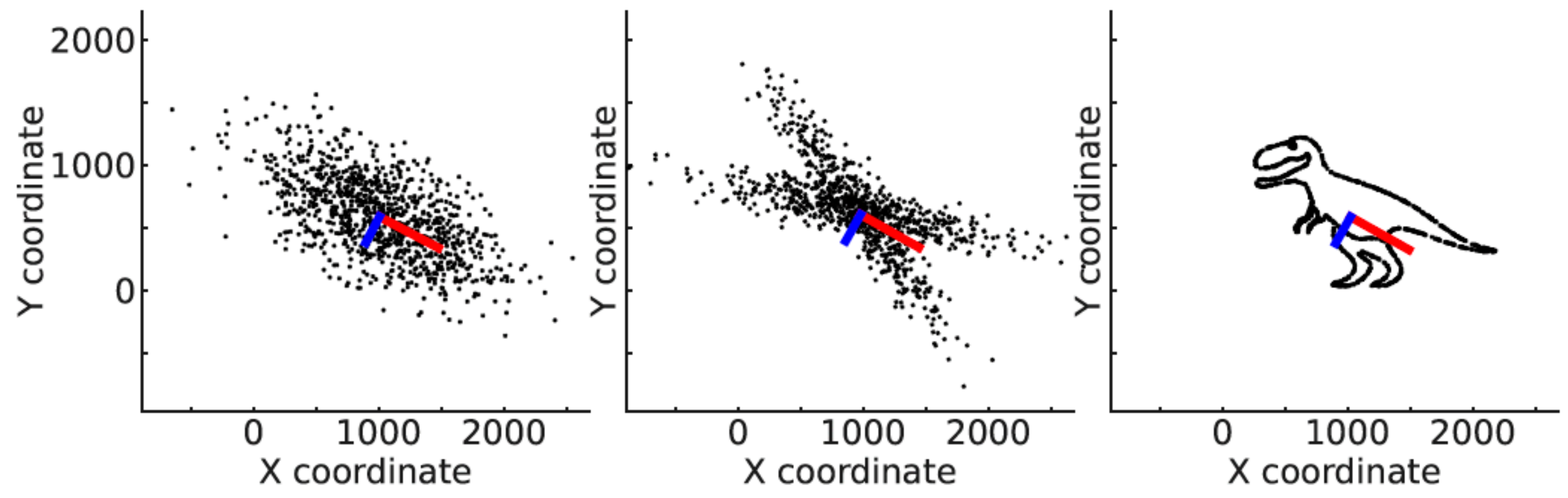
Duszkiewicz (2024), image from Barbosa (2024)

Principal Component Analysis

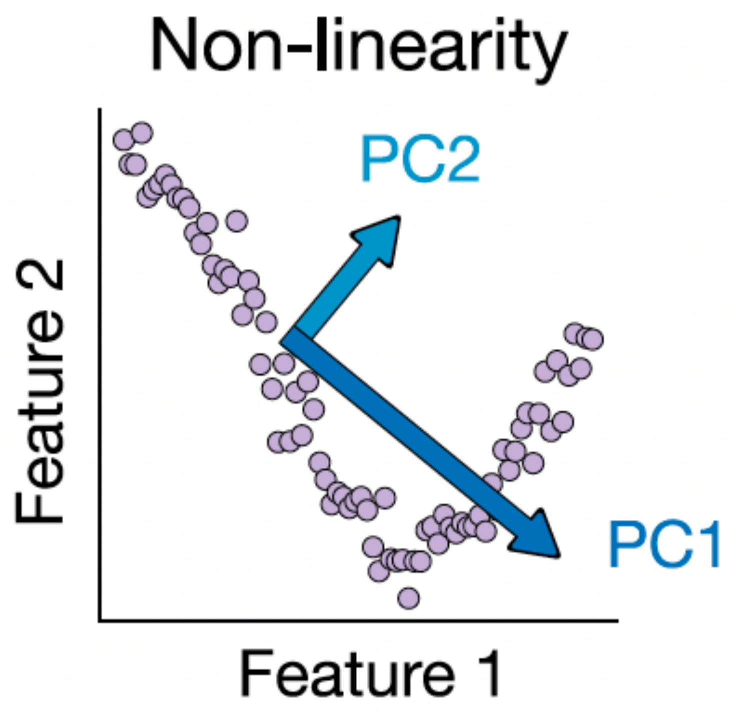
Limitations

- PCA assumes that directions of maximal variability are the most important (**variance-centric**):
  - unable to separate correlated sources.
  - maximal variance does not mean biologically meaningful

- PCA over data with smoothness and shifting in time or space (most of neuroscience data) produce '**phantom oscillations**' (Shinn, 2023)
- Blind to **non-linear** relationships.



Dyer and Kording, 2023



Shinn, 2023

Generalized eigendecomposition

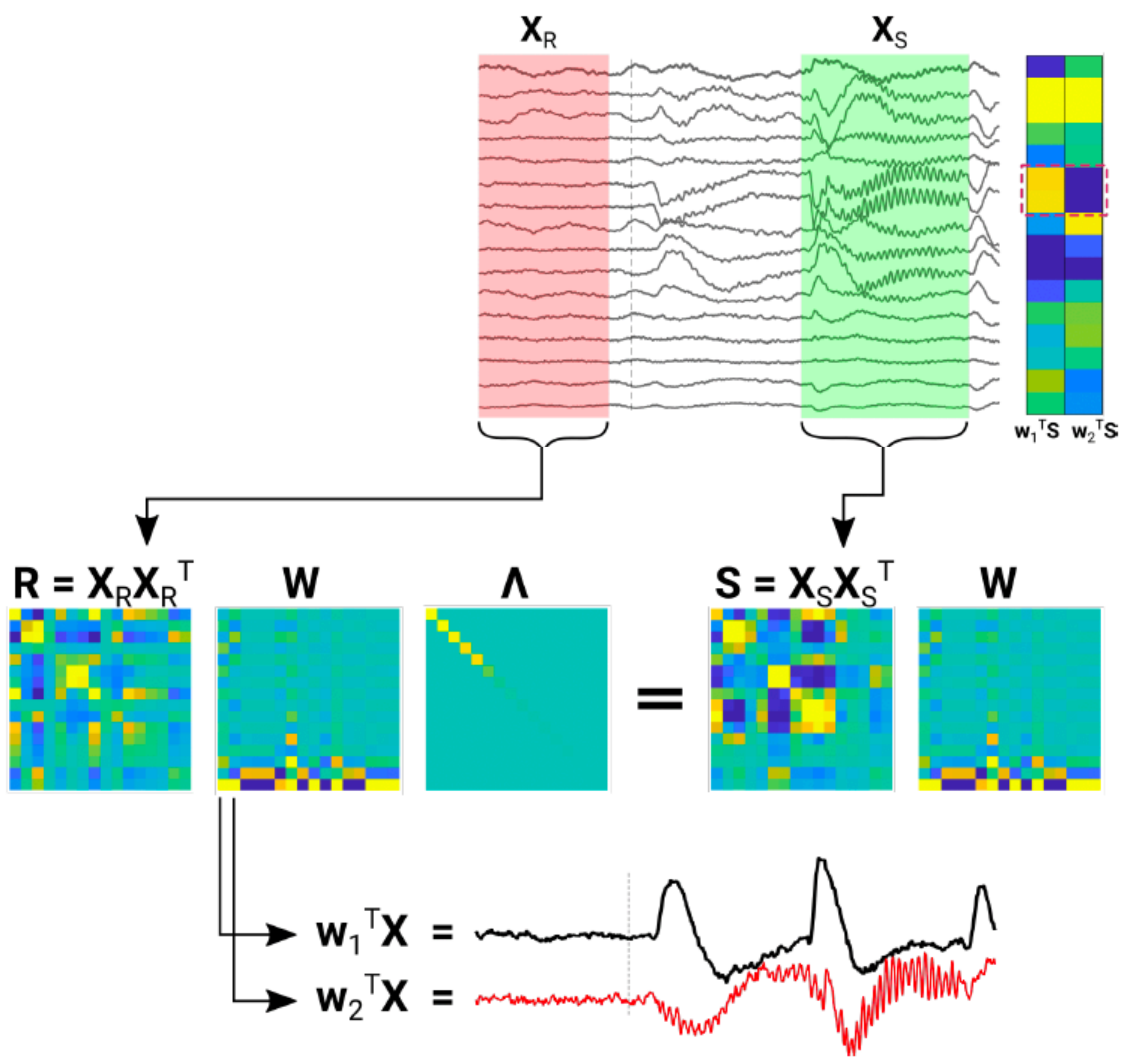
a.k.a. simultaneous diagonalization of two matrices

- Eigendecomposition: $A\mathbf{v} = \lambda \mathbf{v}$
- GED: $A\mathbf{v} = \lambda B\mathbf{v}$
- Interpretation: spatial filters created by GED are designed to maximize a contrast between two features of the data

$$(B^{-1}A)v = \lambda v$$

$$Cv = \lambda v$$

$$C = B^{-1}A$$



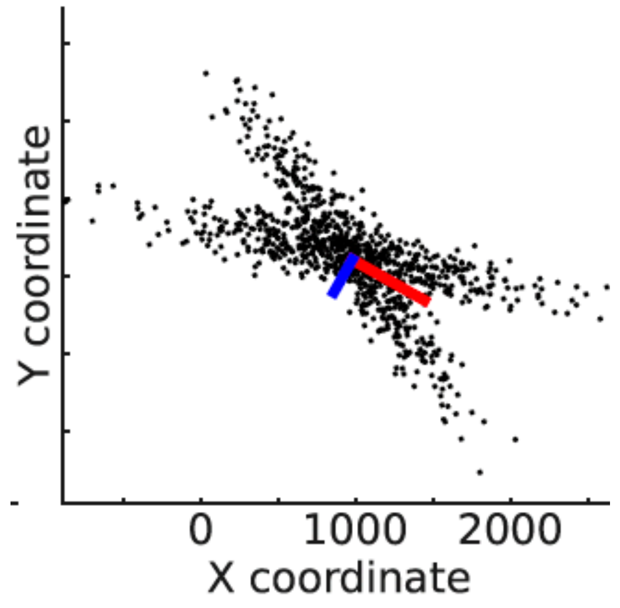
Cohen, 2021

Generalized eigendecomposition

advantages

- Based on specific hypotheses
  - experimental vs control condition,
  - pre stimulus vs post stimulus period,
  - trial-averaged vs single-trial,
  - narrowband vs broadband.
- Null hypothesis is that contrast ratio of 1 (no differences between S and R).
- Inferential statistics about the significance of components.

- Ability to separate correlated sources (more biologically plausible).



- Easy to apply as fast to compute.

Other dimensionality reduction techniques

Linear methods

- Independent Component Analysis
- Factor analysis
- Fourier transform
- Linear discriminant analysis
- Canonical correlation analysis (CCA)
- Partial Least Squares (PLS)
- **Complex PCA**

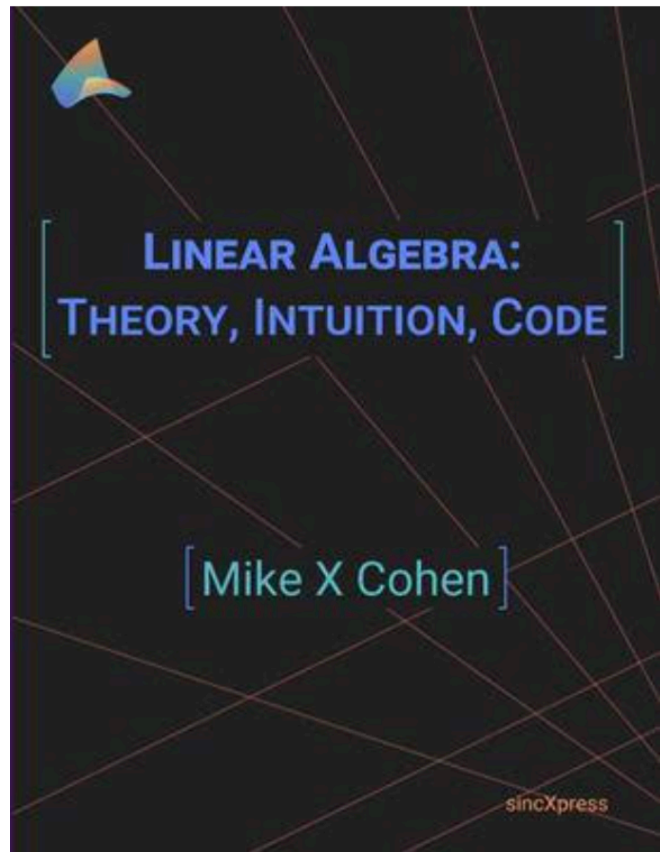
Non-linear methods

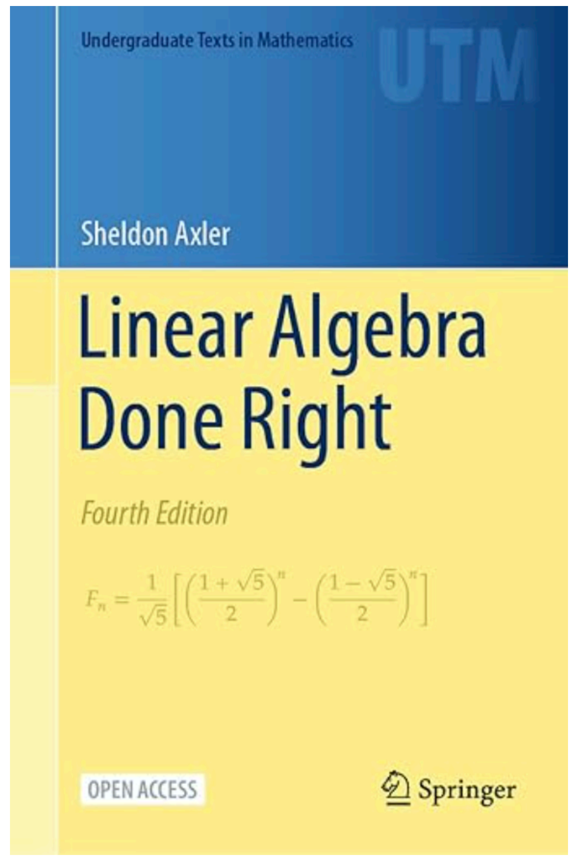
- **CEBRA (Consistent EmBeddings of high-dimensional Recordings using Auxiliary variables)**
- Kernel PCA
- Isomap
- Locally linear embedding (LLE)
- Hessian LLE
- Laplacian eigenmaps
- Generalized discriminant analysis (GDA)
- Autoencoders
- Nonnegative matrix factorization (NMF)
- t-SNE
- t-STE
- UMAP
- Poincaré
- GloVe
- Word2Vec

Roads, 2024

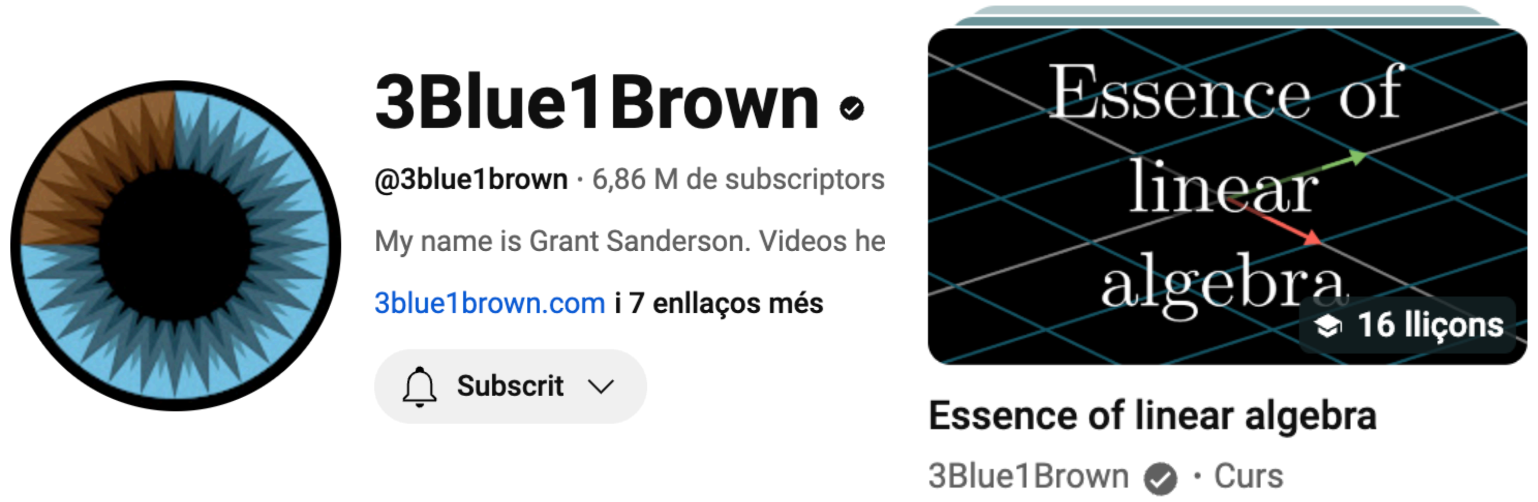
Resources

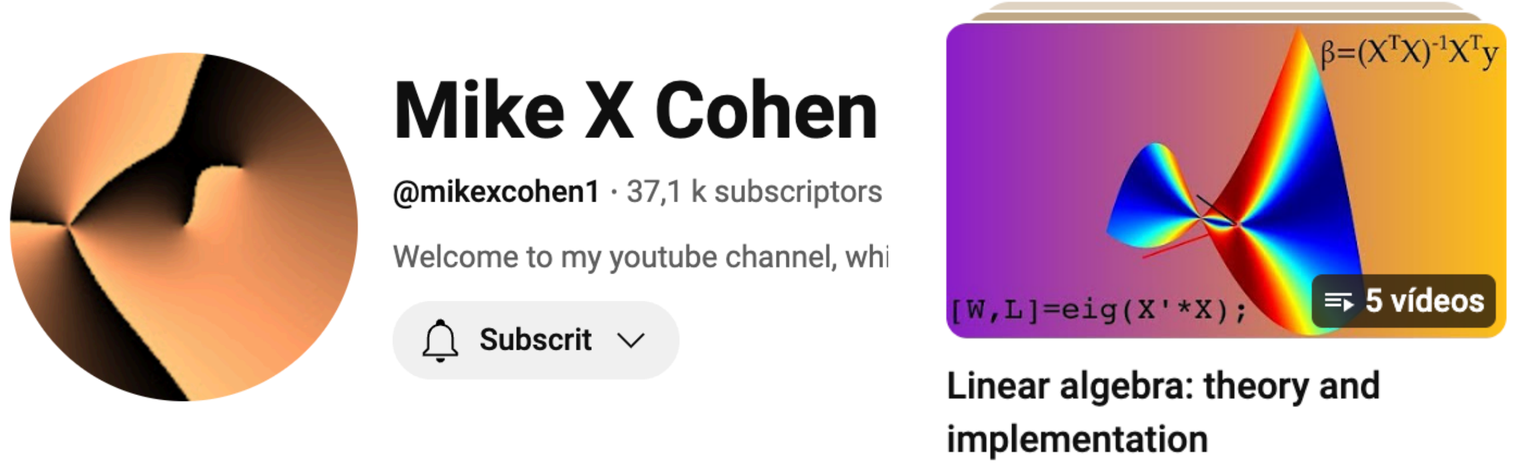
Books (open source)





Videos





Thanks!