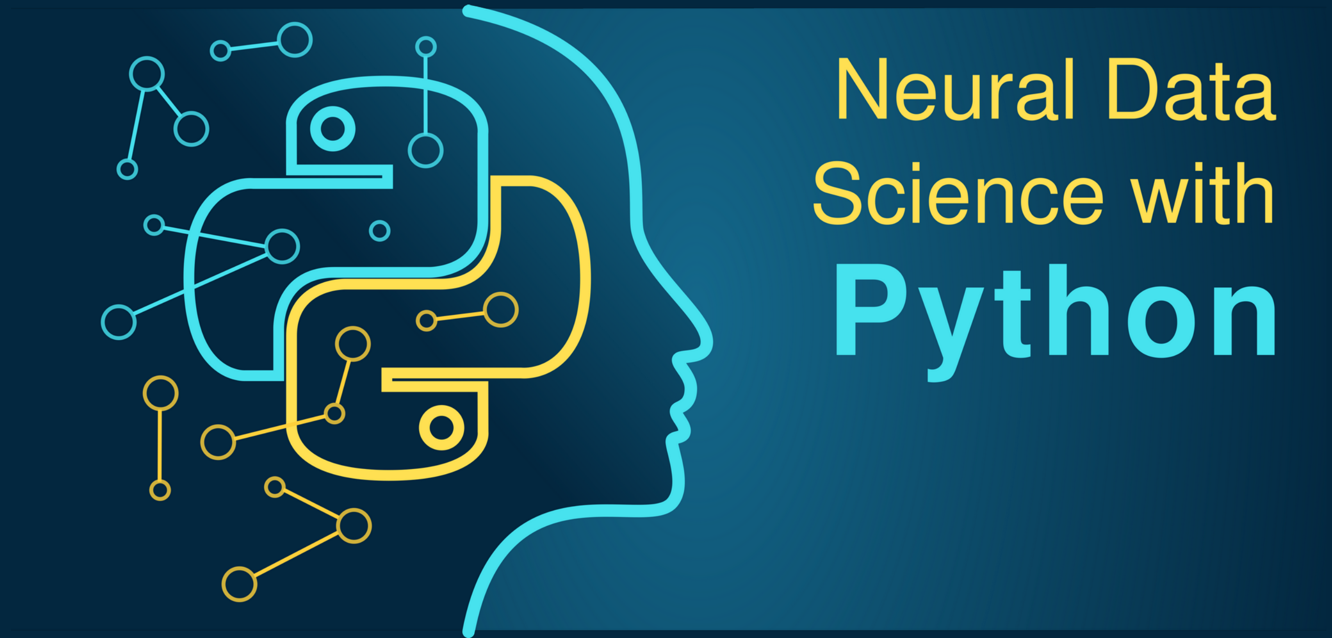


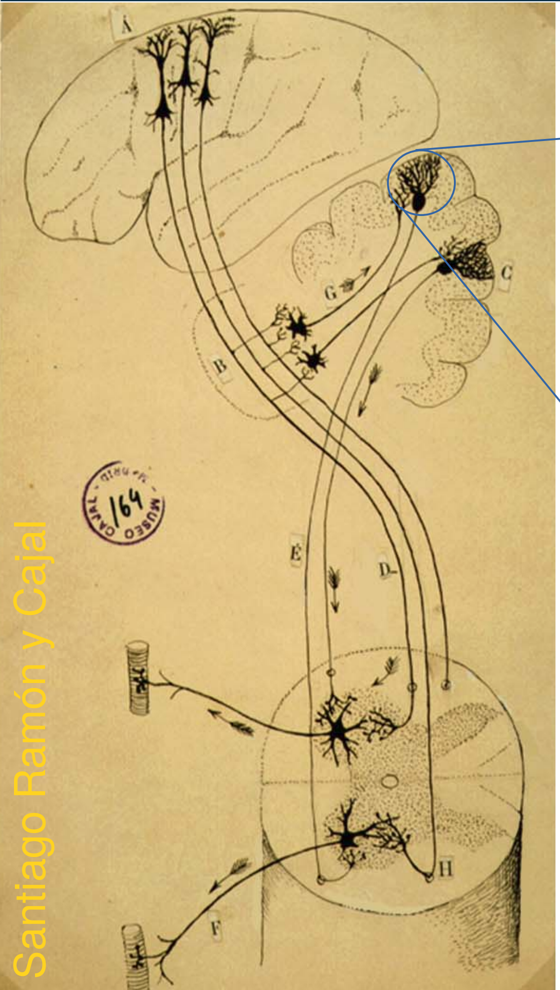
L8 : Dimensionality Reduction

Michael Graupner

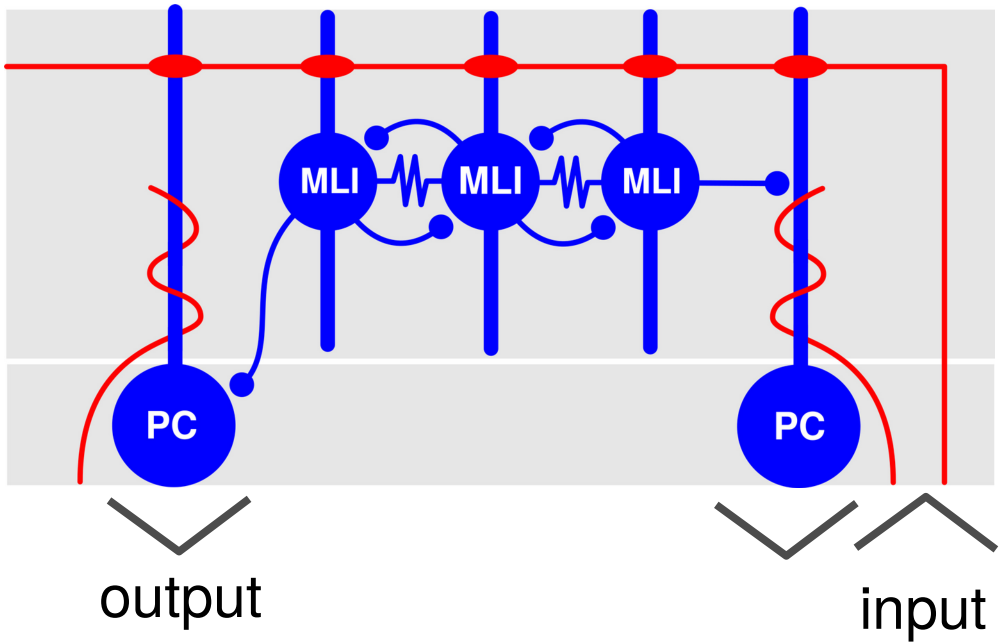
SPPIN – Saint-Pères Institute for the Neurosciences

Université de Paris, CNRS

Cerebellum and motor control



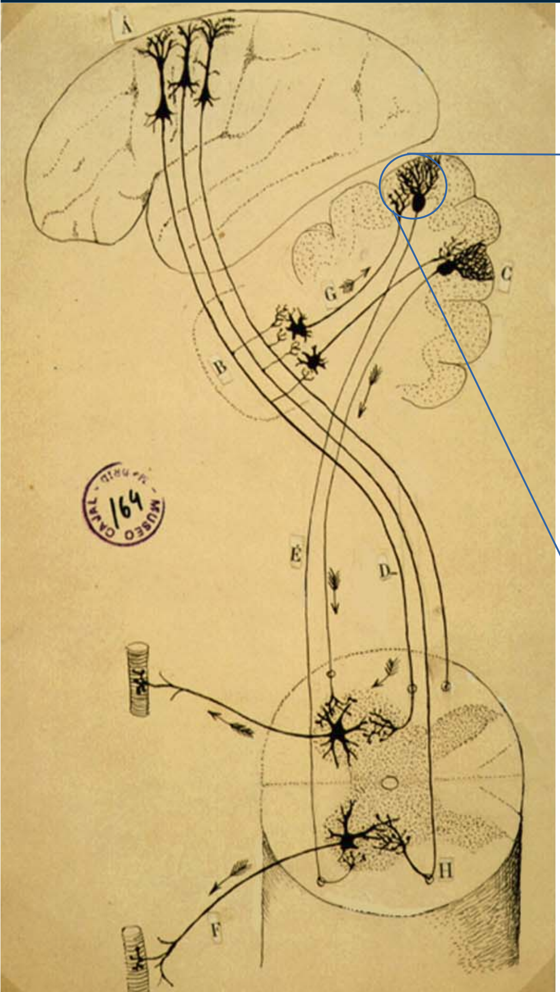
circuit of neurons in the cerebellum



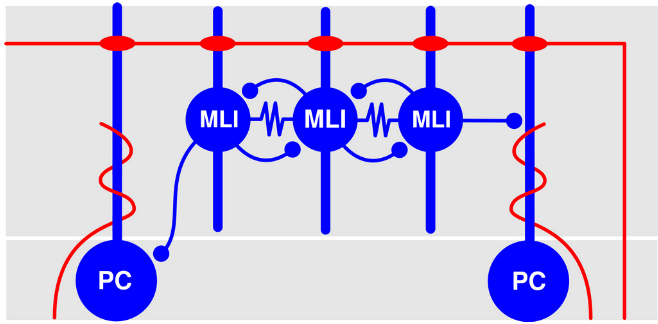
PC ... Purkinje cells

MLI ... molecular layer interneurons

Cerebellum and motor control

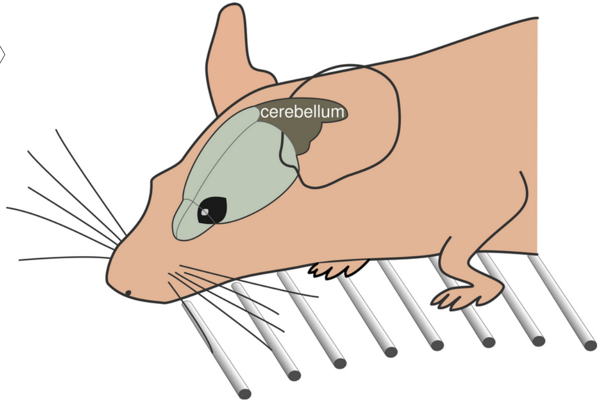


circuit of neurons in the cerebellum

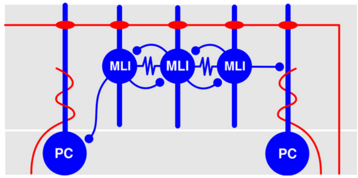


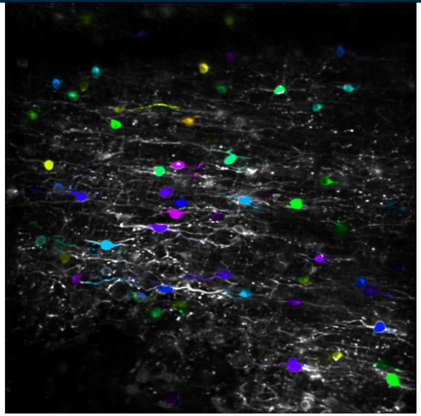
PC ... Purkinje cells
MLI ... molecular layer interneurons

animal walking on treadmill with rungs

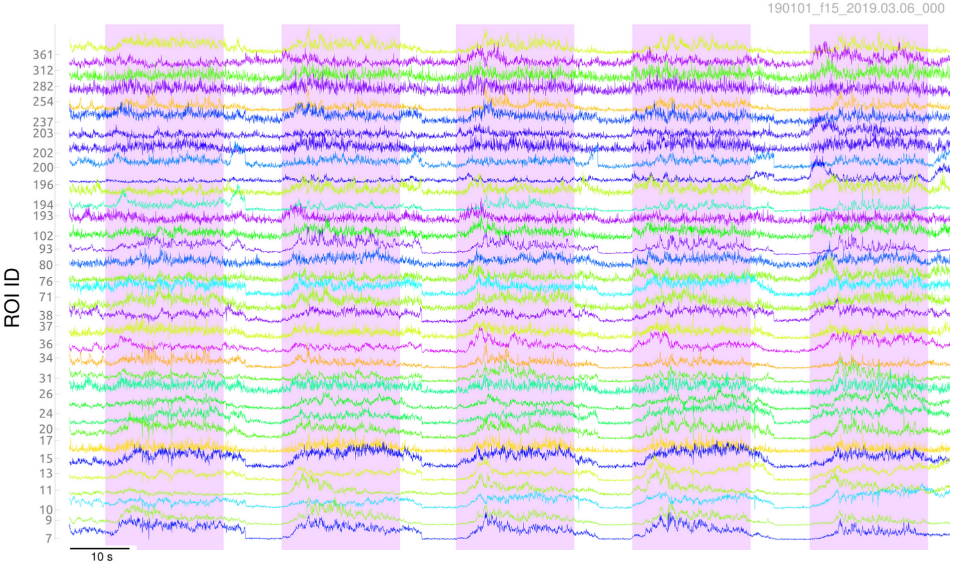


Investigating link between activities and walking



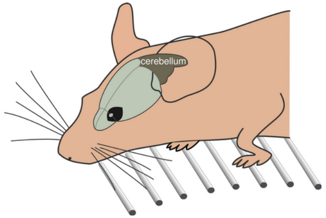


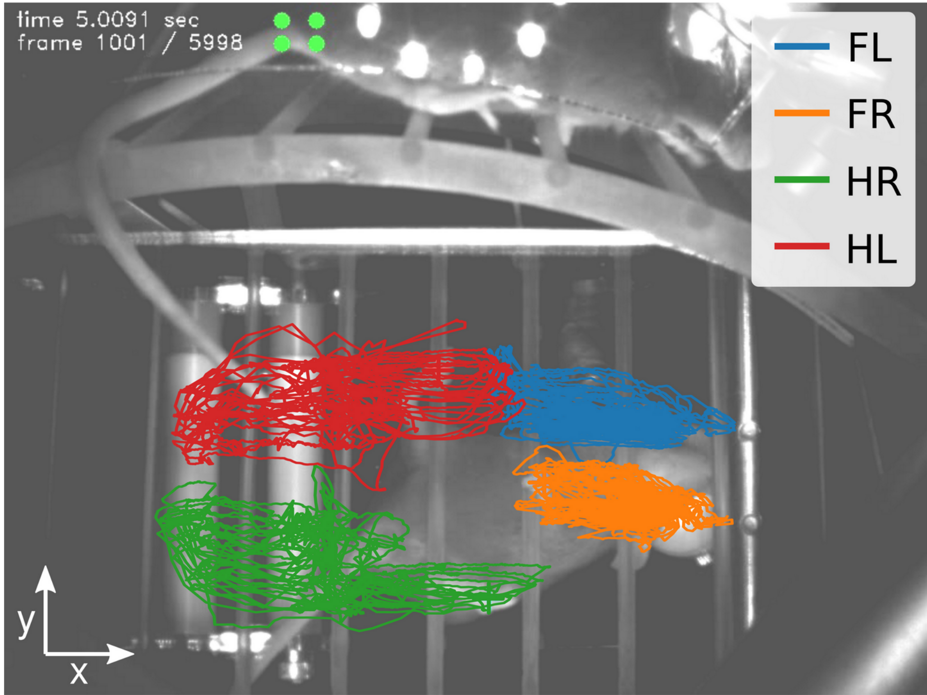
activity of neurons in the cerebellum



???

animal walking on treadmill with rungs

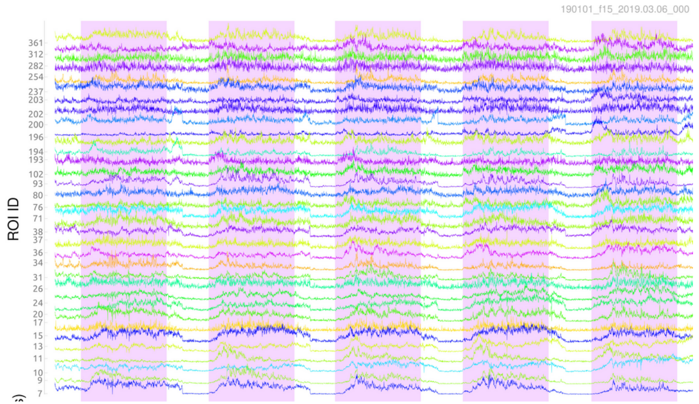




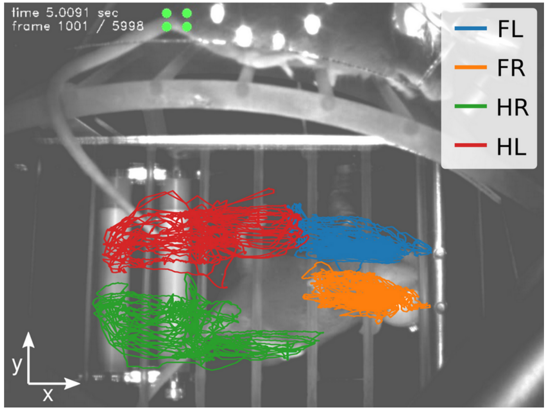
Intuition behind dimensionality reduction

Dimensionality reduction is applied in settings in which there are *D measured variables*, but one suspects that these variables *covary* according to a smaller number of *explanatory variables K,* where $K < D$.

D measured variables
(e.g. neural activities)



K explanatory variables
(e.g. walking state)

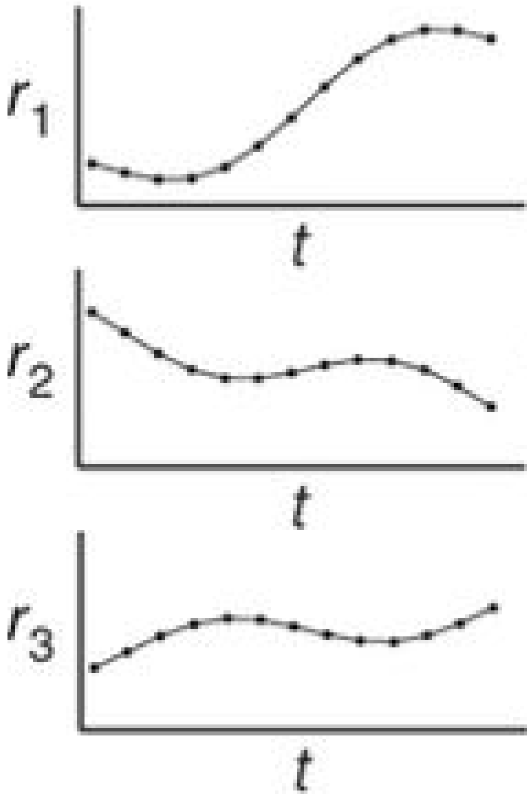


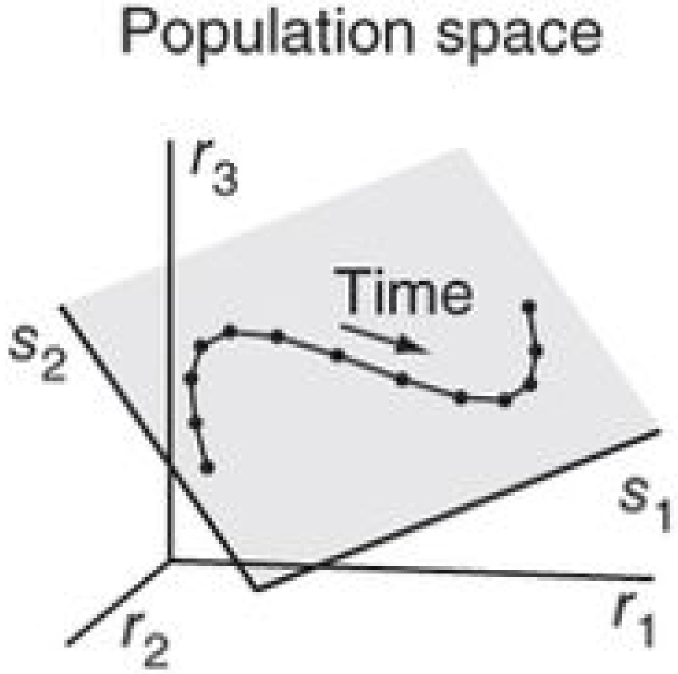
Dimensionality reduction

- Dimensionality reduction methods discover and extract these *K* explanatory variables
- explanatory variables are called *latent variables* because they are not directly observed
- any data variance not captured by the latent variables is considered to be noise
- *example* : neural population activity – recorded neurons belong to common network and are likely not independent of each other
  $\rightarrow$ fewer latent variables might be needed to explain population activity

Conceptual illustration of linear dim. reduction

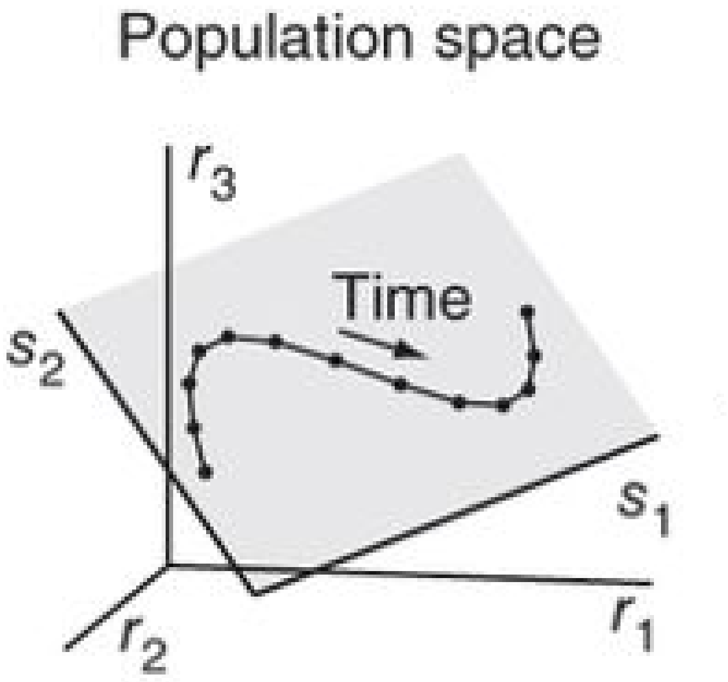
3 neurons (D=3)





population activity lies in a plane (shaded gray)

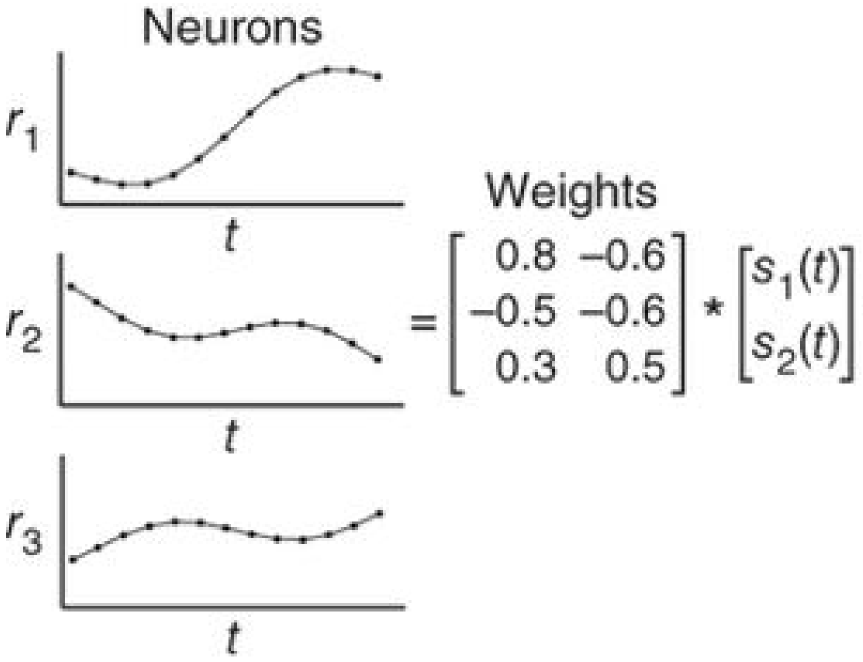
Conceptual illustration of linear dim. reduction



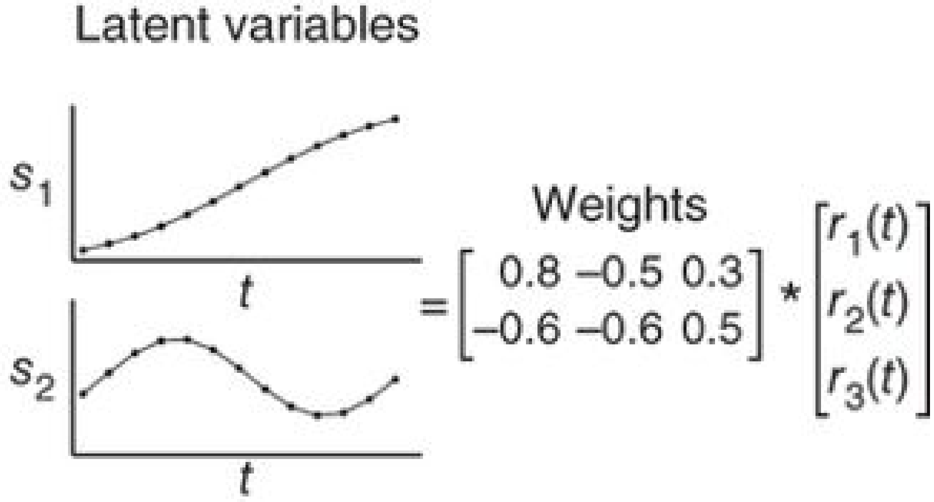
- population activity lies in a plane
- each point represents the population activity at a particular time
- each point can be equivalently referred to using the high-dimensional coordinates $[r_1,r_2,r_3]$ or
  the low-dimensional coordinates $[s_1,s_2]$
- the points trace out a trajectory over time, time is not plotted, time evolves implicitly along axis

Conceptual illustration of linear dim. reduction

neural activities can be reconstructed from weighted combination of the latent variables

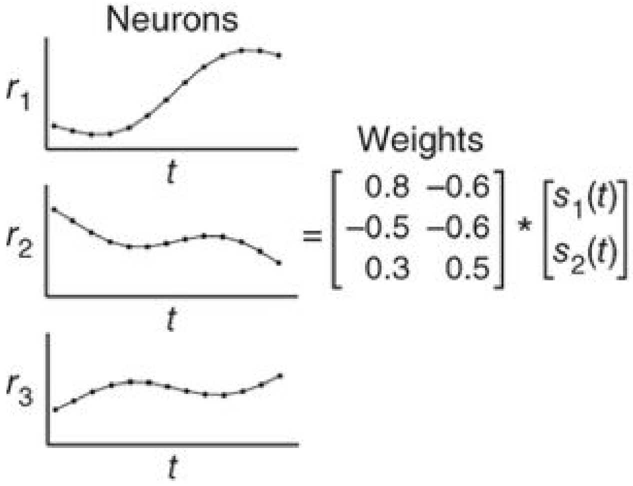


latent variables can be obtained by taking weighted combination population activity

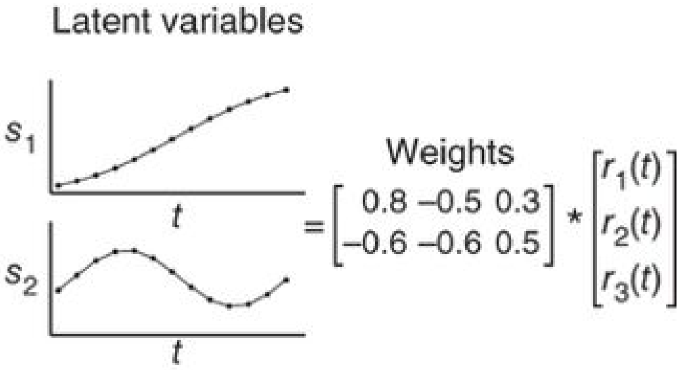


Conceptual illustration of linear dim. reduction

neural activities can be reconstructed from weighted combination of the latent variables

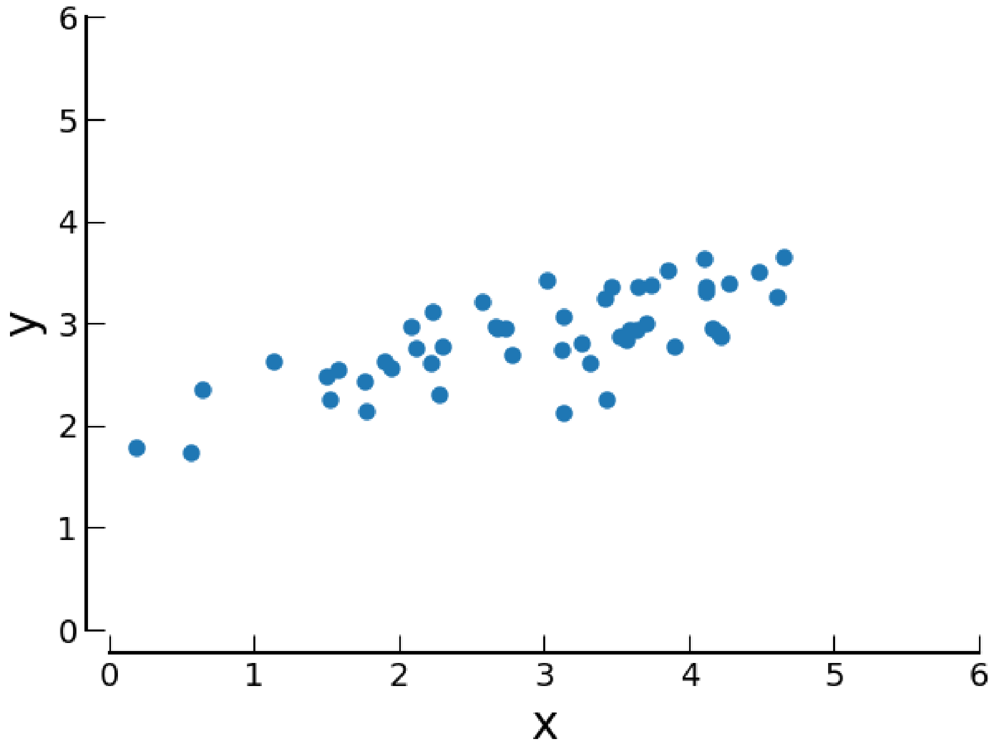


latent variables can be obtained by taking weighted combination of the population activity



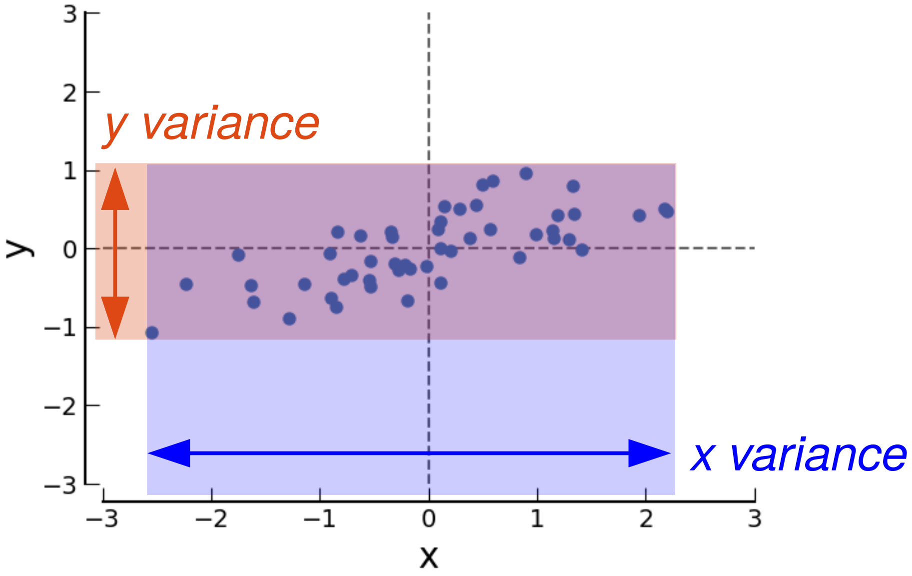
→ Weights and latent variables are determined by the dimensionality reduction method

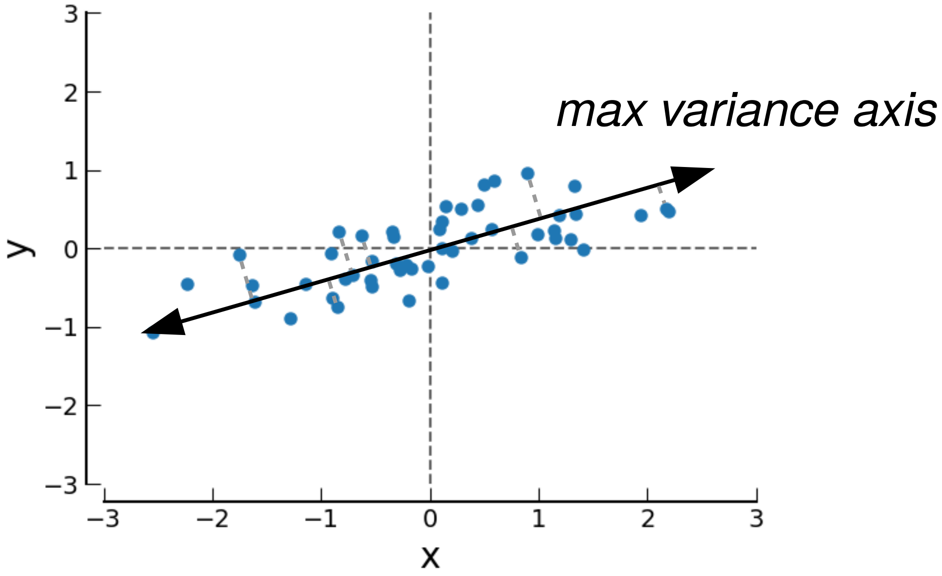
How does Principal Component Analysis work?



- **Principal Component Analysis (PCA)** is transformation method creating combinations of the original variable. PCA comes form the field of linear algebra.
- **Aim :** the new combination of variables will capture as much variance in the data as possible while eliminating correlations
- **Procedure :** PCA creates new variables by transforming the original observations to new dimensions using eigenvector and eigenvalues calculated from the covariance matrix of the original variables

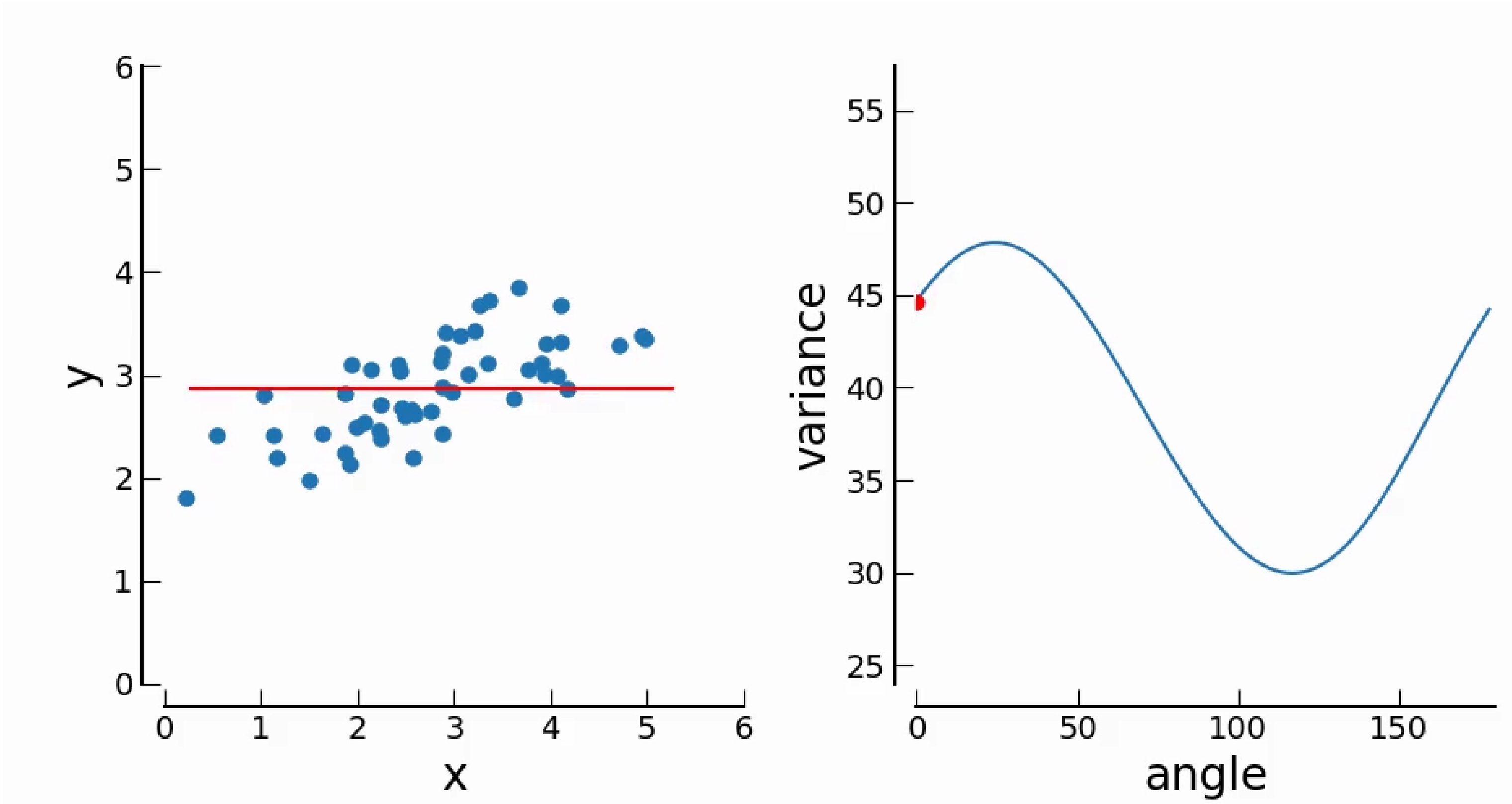
How does Principal Component Analysis work?





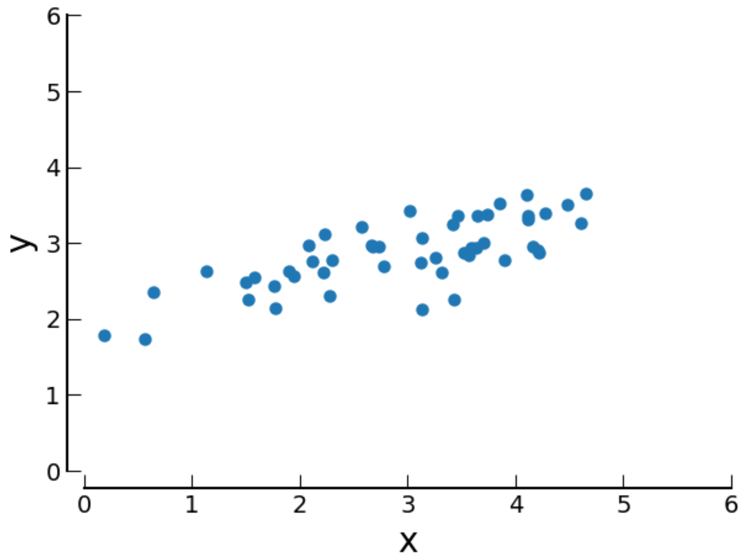
- **PCA** tries to find successively axes which account for the maximal variance in the data.
  - data is projected onto an axis and orientation varied to maximize variance

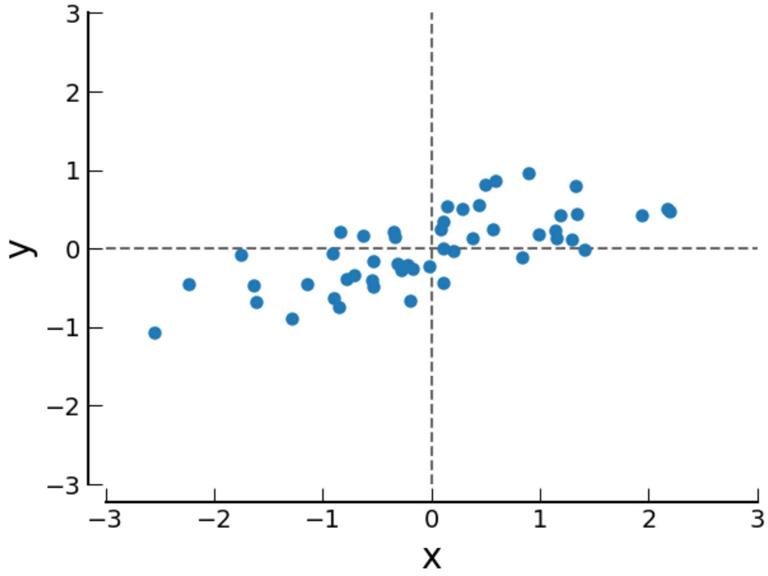
How does Principal Component Analysis work?



- **PCA** tries to find successively axes which account for the maximal variance in the data.

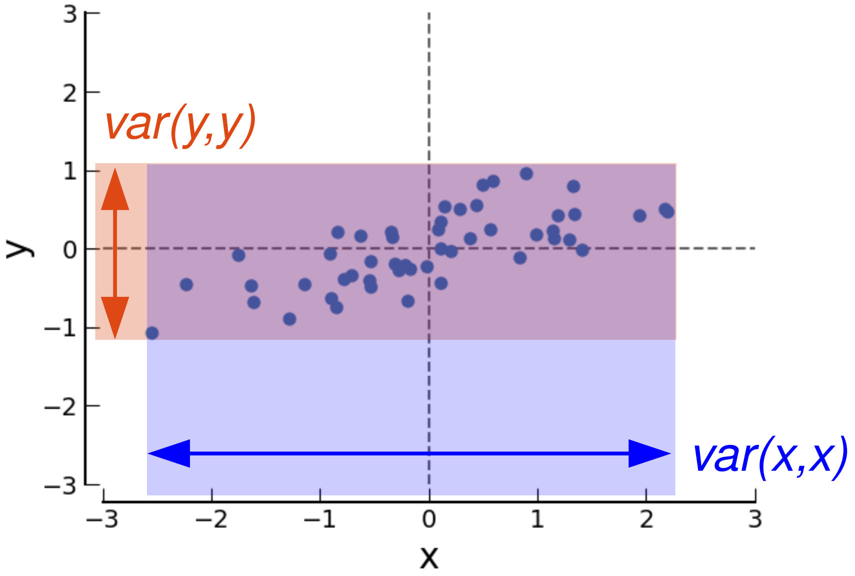
Steps to perform PCA





1) **Centering** the values of the input variables, i.e. substracting the mean (sometimes the data has to be **normalized** too if one considers variables of different units or scale)

Steps to perform PCA



covariance matrix

$$\begin{array}{cc} & \begin{array}{cc} x & y \end{array} \\ \begin{array}{c} x \\ y \end{array} & \begin{bmatrix} 1.16958234 & 0.36437495 \\ 0.36437495 & 0.22369298 \end{bmatrix} \end{array}$$

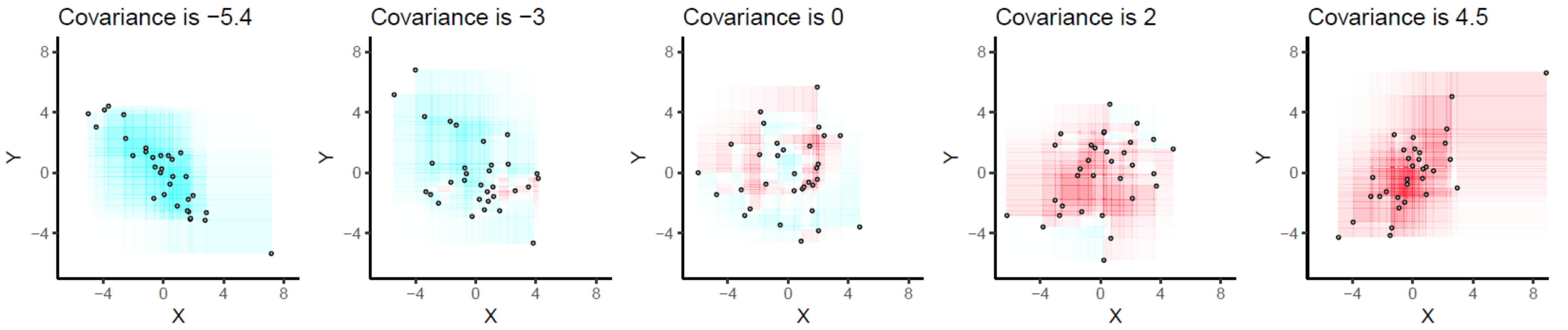
2) **Calculating the covariance matrix**

- symmetric matrix as covariance has no direction

Steps to perform PCA

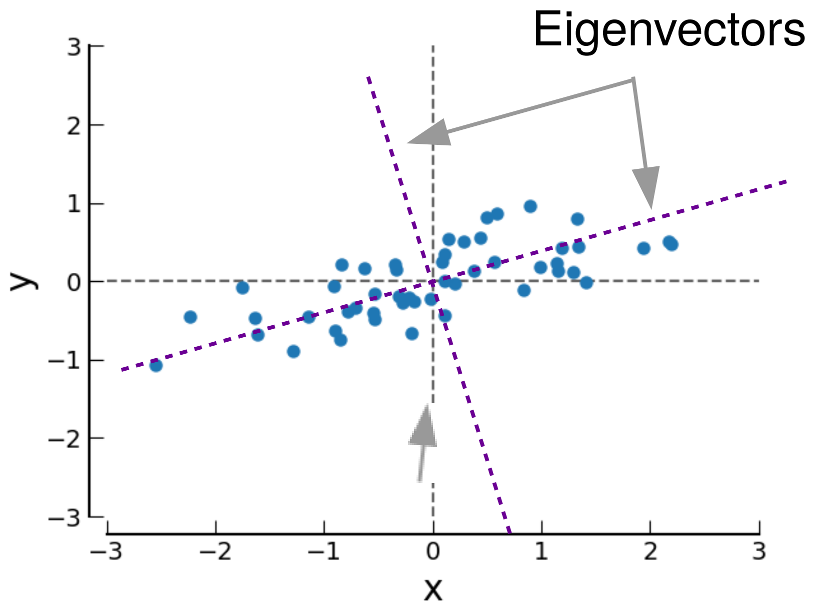
Covariance : measures *joint* variability of variables

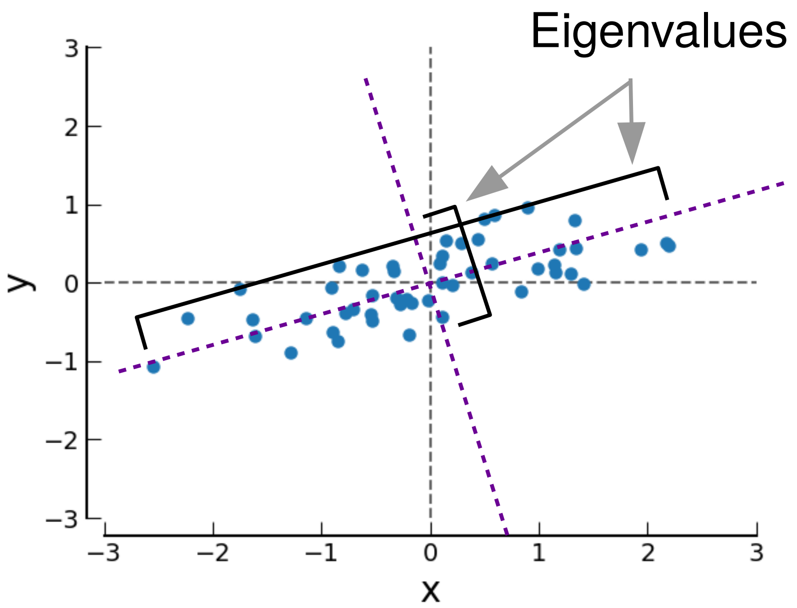
$$cov(x,y)=\frac{1}{n}\sum_{i=i}^{n}(x_i-\bar{x})(y_i-\bar{y})$$



- a large covariance (positive or negative) indicates a strong linear relationship btw. the variables
- covariance ~0 indicate weak or non-existing linear relationship

Steps to perform PCA





3) Perform eigendecomposition of the covariance matrix

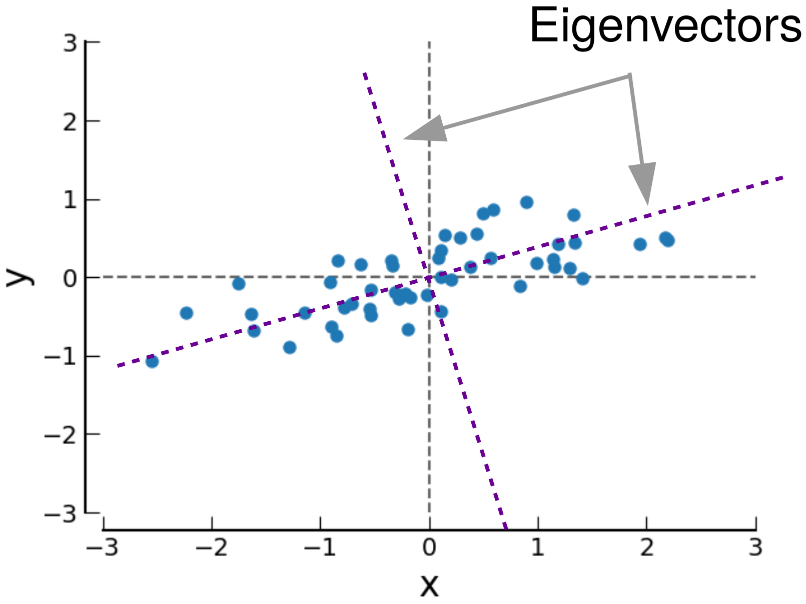
$$\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}$$

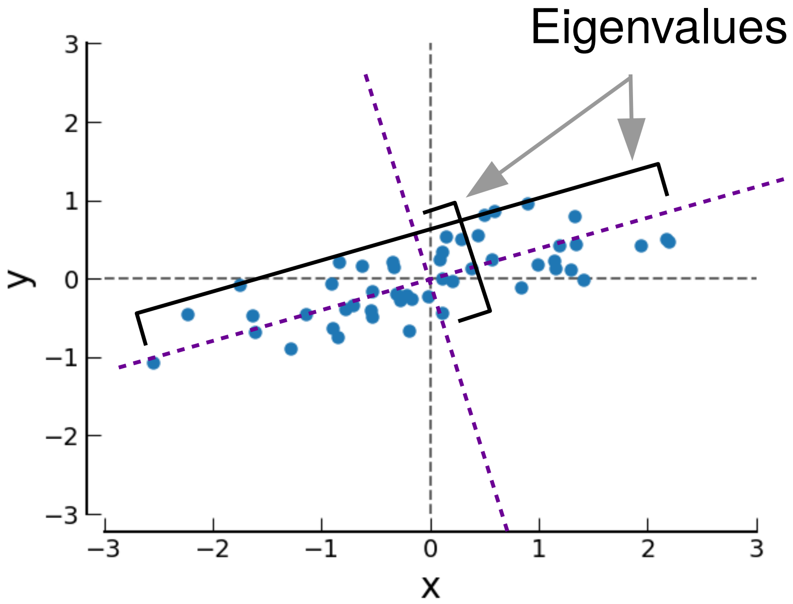
covariance matrix (symmetric)

eigenvector

eigenvalue (scalar)

Steps to perform PCA





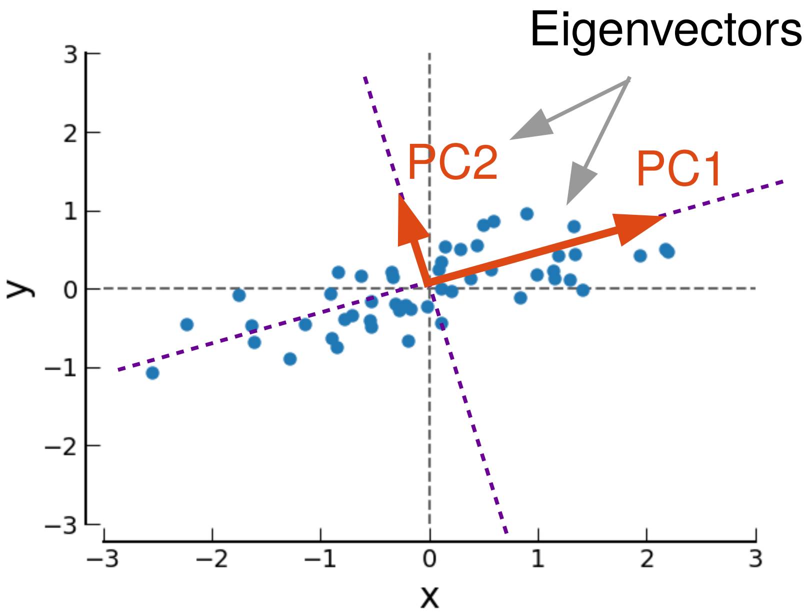
3) Perform eigendecomposition of the covariance matrix

this is where PCA find eigenvectors and eigenvalues of the data-set

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

- eigenvectors of the covariance matrix are the axes of the principal components
- eigenvalues describe the magnitude of the eigenvector (spread or the points)

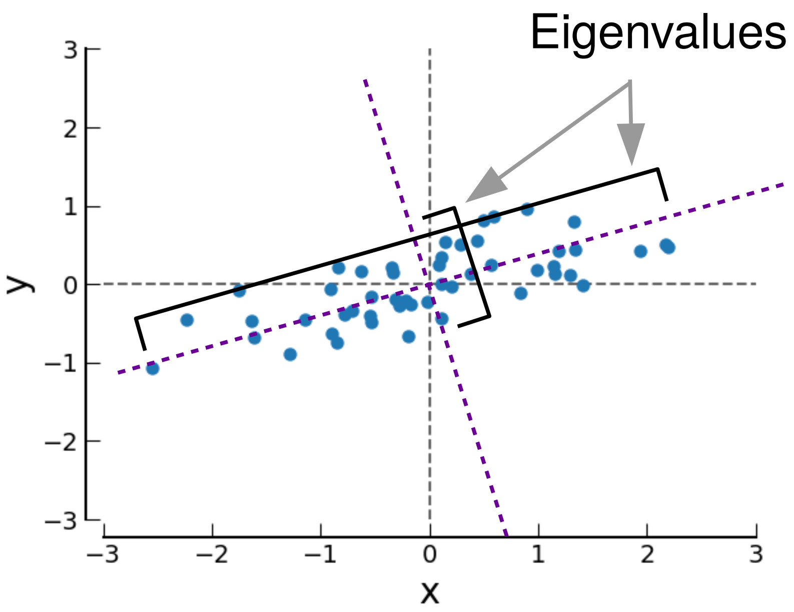
Steps to perform PCA

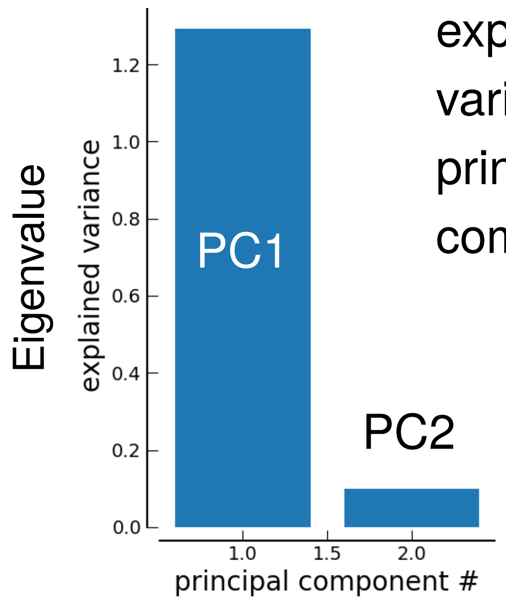


3) Eigendecomposition of the covariance matrix → Eigenvectors

- the first eigenvector will span the greatest variance found in the dataset
- all subsequent eigenvectors will be perpendicular (orthogonal), i.e., each of the principal components will be uncorrelated with each other

Steps to perform PCA





explained variance by the principal components

3) Eigendecomposition of the covariance matrix → Eigenvalues

- the first eigenvector spans the greatest variance
- principal components are sorted by descending eigenvalues
- principal components with the highest eigenvalues account for most variance in the data

Steps to perform PCA

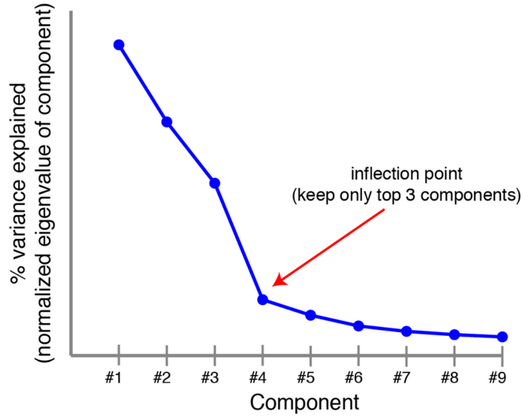
4) **Select number of principal components to keep**

- PCA returns as many principal components are there are variables

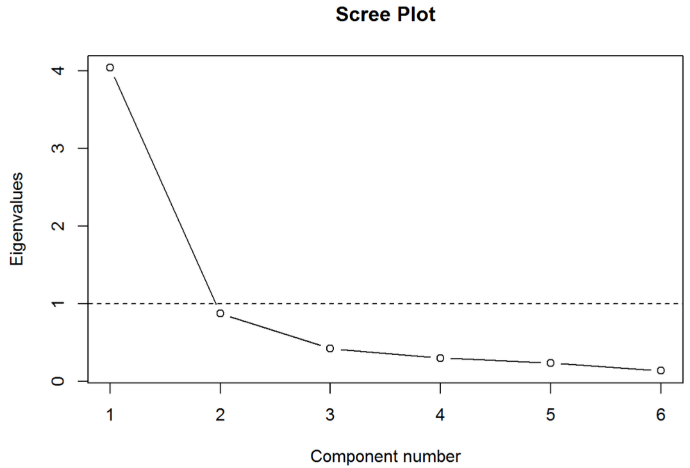
→ How do we know how many of these factors are essential ?

- most of the variance will be accounted for by top principal components
- various way to select principal components to keep

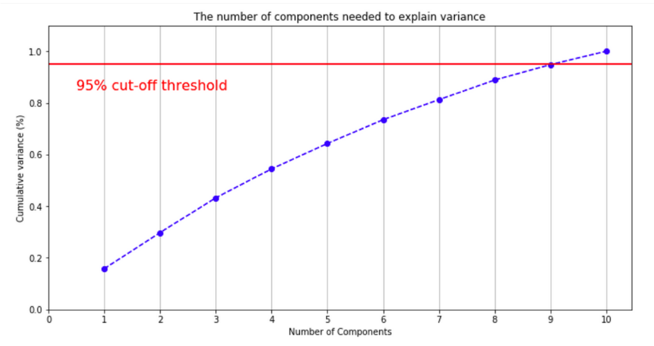
A) look for inflection point



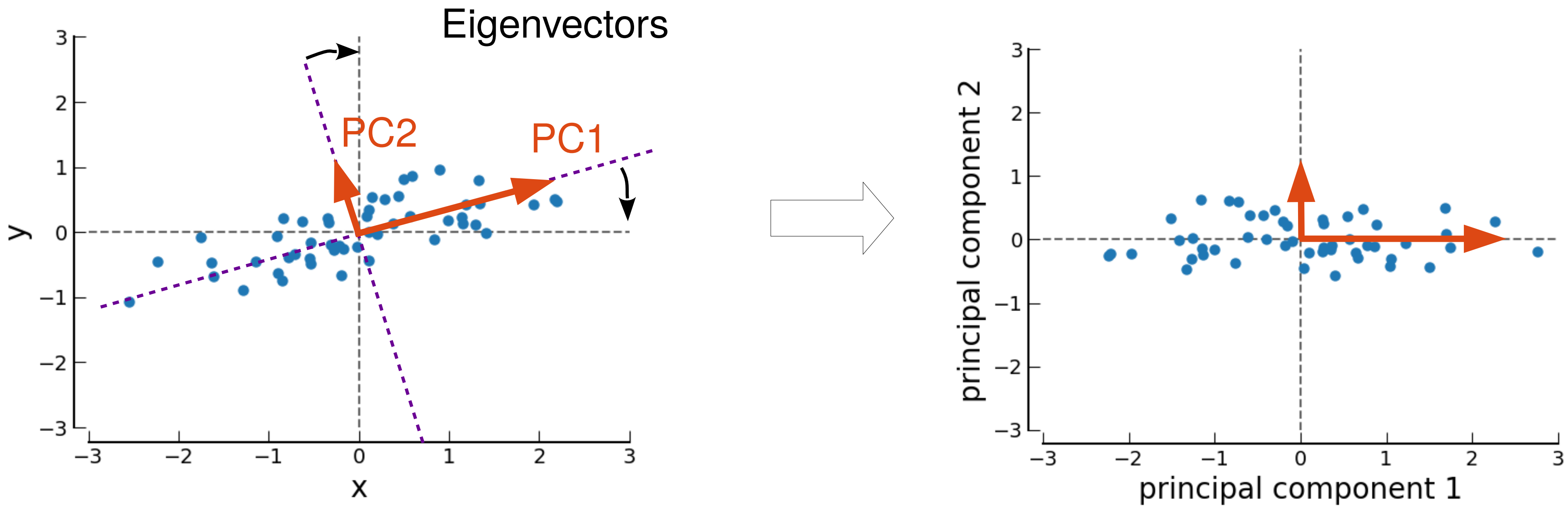
B) Kaiser criterion EV > *1*



C) threshold on variance explained



Steps to perform PCA



5) Original data is converted to the selected principal components

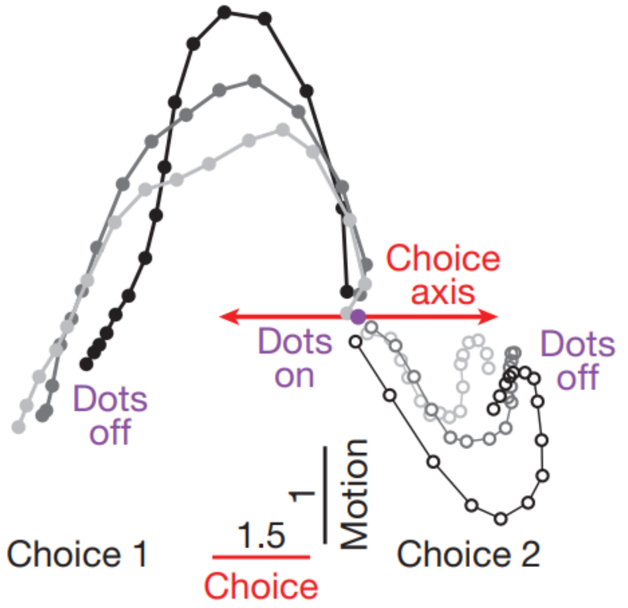
- projection matrix are simply selected eigenvectors concatenated to a matrix
matrix is multiplied with original observations

→ transformed dataset projected onto new space spanned by the principal components

Steps to perform PCA

6) Interpreting the meaning of the factors

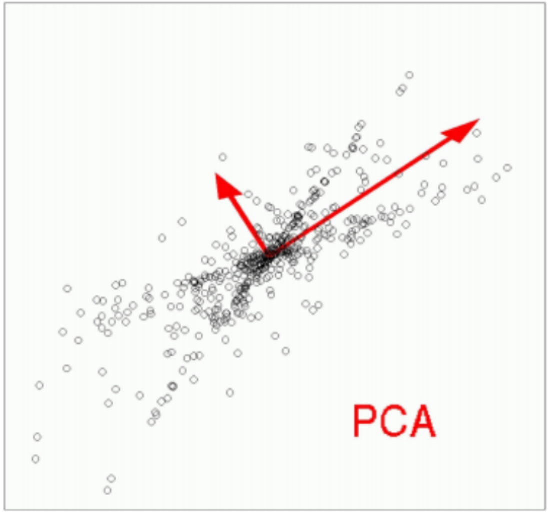
- visualizing temporal evolution of the first principal components
- using principal components to correlate with experimental observables
- classification and cluster analysis

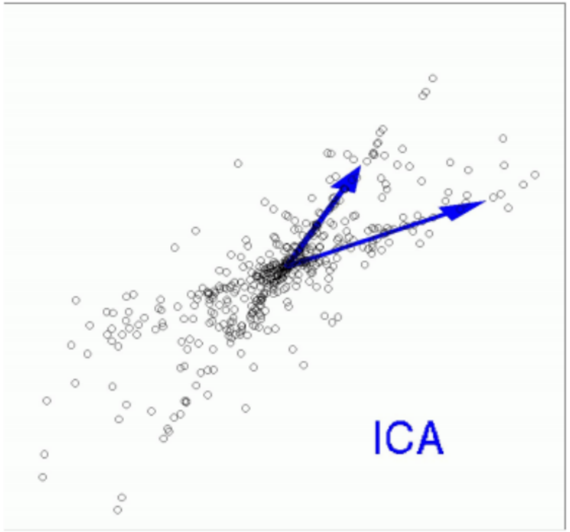


population activity recorded in PFC

[Mante et al. Nature 2013]

Other dimensionality reduction method : ICA





ICA – Independent Component Analysis

- tries to find independent components of data
- all components are equally important
- eigenvectors are not orthogonal