# Dimensionality reduction in Fluid Mechanics and Heat Transfer

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Master, 2022–2023, Poitiers

# Reduced-Order Modelling



- Ex. from Spalart et al. (1997): wing considered at cruising flight conditions *i.e.* $\mathrm{Re} = \mathcal{O}(10^7)$. Converged solution obtained for
  - about $10^{11}$ grid points, about $5 \times 10^6$ time steps.

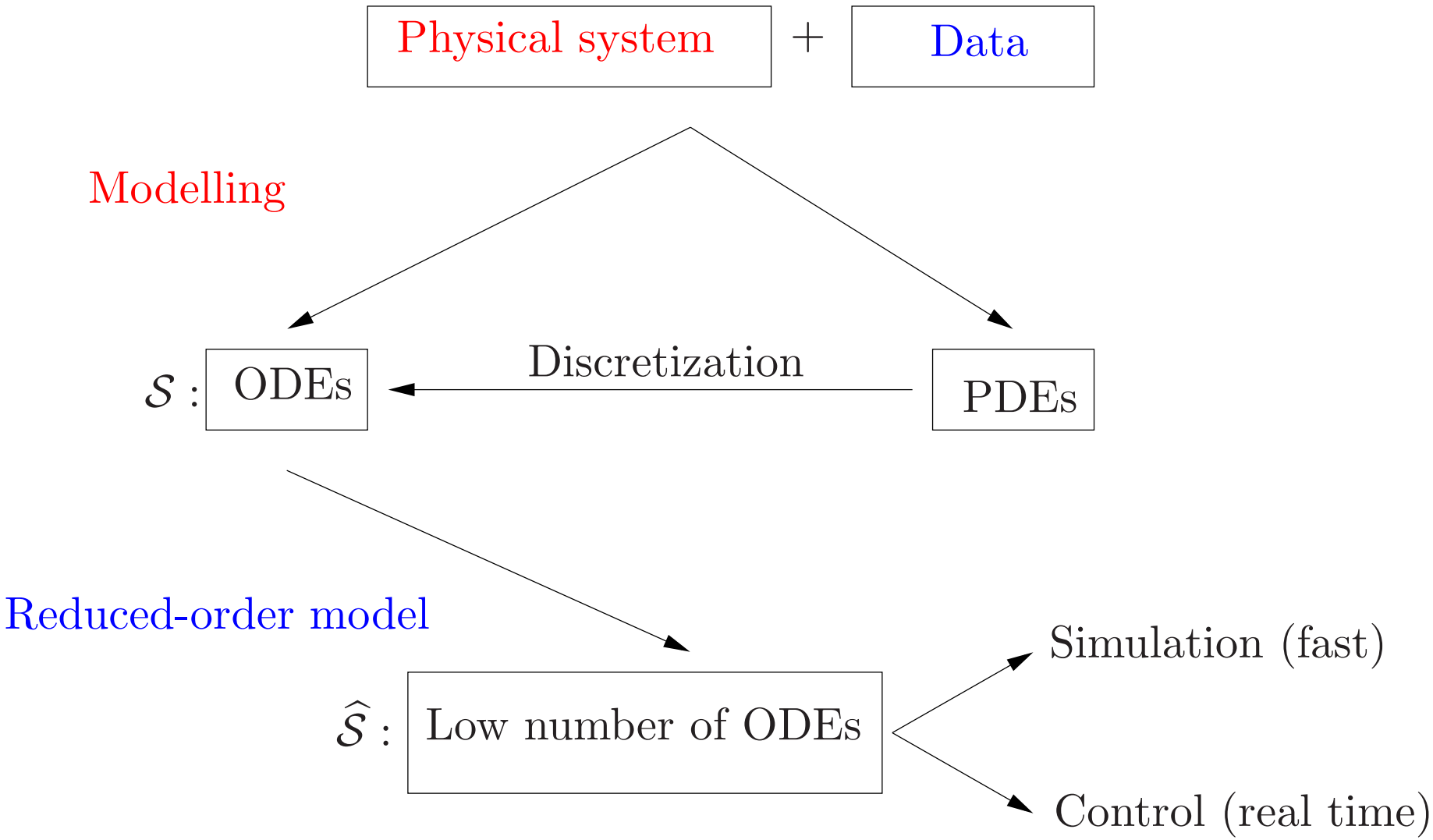
  **40 years for the first LES of a wing !!**
- Nearly impossible to solve numerically problems where
  - either, a great number of resolution of the state equations is necessary (continuation methods, parametric studies, optimization problems or optimal control,...),
  - either a solution in real time is searched (active control in closed-loop control for instance).
- Objective: reduce the number of degrees of freedom.

In fluid mechanics/turbulence :

- Prandtl boundary layer equations,
- RANS models ($k-\epsilon$, $k-\omega$),
- Large Eddy Simulation (LES),
- Low-order dynamical system based on *POD* (Lumley, 1967),
- Reduced-order models based on balanced, DMD and/or global modes.

# Reduced-Order Modelling





# Outline

1. Introduction
2. Preliminaries
   - Eigenvalue Decomposition
   - Singular Value Decomposition
   - Principal Component Analysis
   - Truncation
   - Data alignment
3. Data-based
   - Proper Orthogonal Decomposition
   - Dynamic Mode Decomposition
   - Cluster-based Reduced Order Model
4. Operator-based
   - Global stability analysis
   - Koopman analysis
   - Galerkin projection
5. Perspectives
6. Conclusion

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# Eigenvalue Decomposition

## Definition and application

- For $S \in \mathbb{C}^{n\times n}$, $\boldsymbol{v}_i \in \mathbb{C}^n$ and $\lambda_i \in \mathbb{C}$ are eigen-vectors/-values if:

$$S\,V = V\,\Lambda,$$

  with $V = (\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n) \in \mathbb{C}^{n\times n}$ and $\Lambda = \mathrm{diag}\,(\lambda_1, \lambda_2, \ldots, \lambda_n)$.
- If $S$ has $n$ linearly independent eigenvectors $\boldsymbol{v}_i$ then

$$S = V\,\Lambda\,V^{-1} \quad \text{eigendecomposition of } S$$

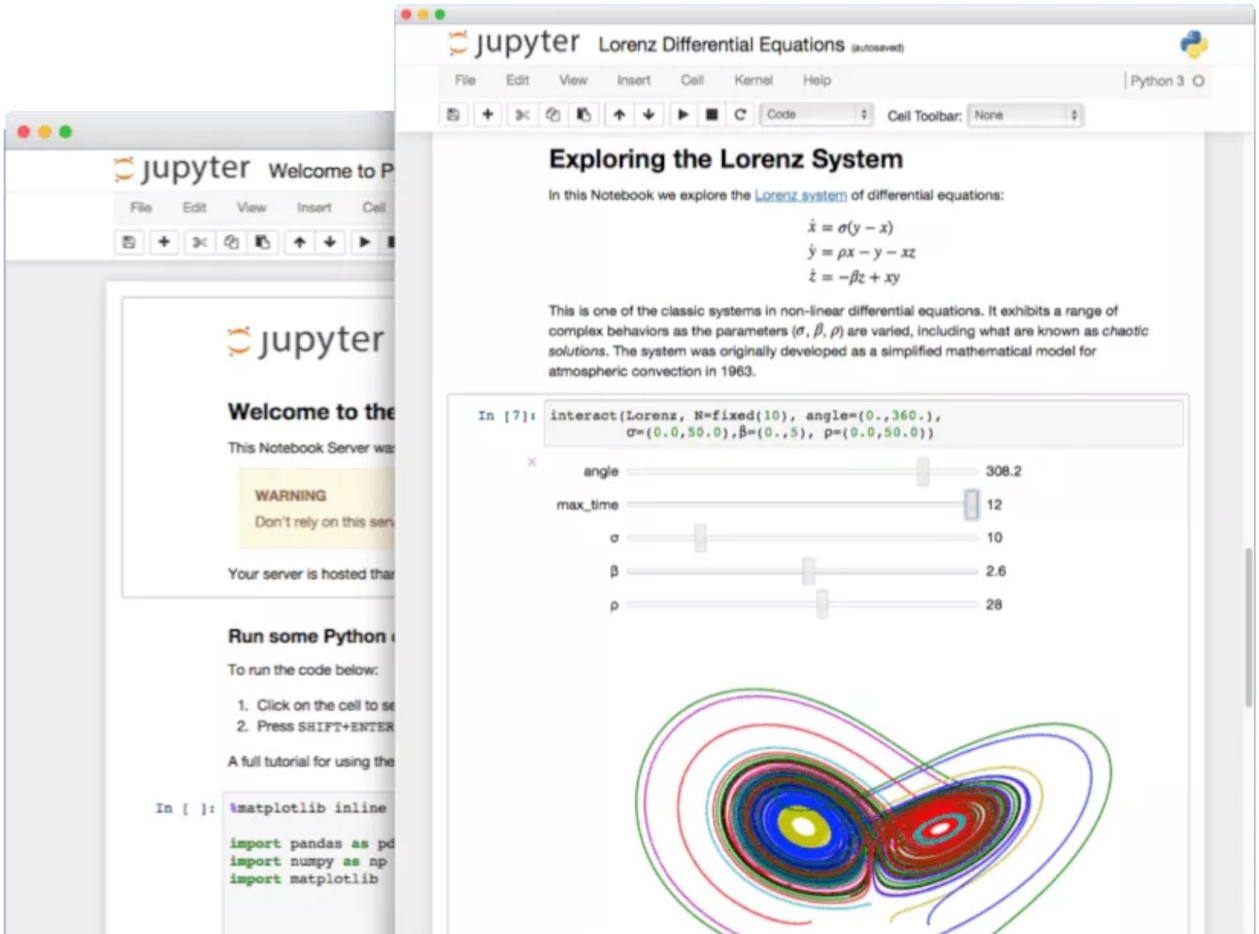
- Linear dynamical systems: $\dot{\boldsymbol{x}} = S\,\boldsymbol{x}$.

$$\begin{aligned}\boldsymbol{x}\,(t) &= \exp\,(S\,t)\;\boldsymbol{x}\,(t_0)\,,\\ &= V\;\exp\,(\Lambda\,t)\;V^{-1}\,\boldsymbol{x}\,(t_0)\\ &= \sum_{k=1}^{n} \boldsymbol{v}_k \exp\,(\lambda_k\,t)\,b_k.\end{aligned}$$

  - $\boldsymbol{b} = V^{-1}\,\boldsymbol{x}\,(t_0)\,$, *i.e.* $\boldsymbol{x}\,(t_0)$ in the eigenvector basis
  - $\mathrm{Re}(\lambda_k)$: growth rate $(>0)$ ; decay rate $(<0)$
  - $\mathrm{Im}(\lambda_k)$: frequency
  - System stable if $\mathrm{Re}(\lambda_k) < 0 \quad \forall k$

# Use of Jupyter Notebook

- Interactive computing
- Complete record of the user's sessions
- Include code, narrative text, equations and rich output.



# Eigenvalue Decomposition

## Matrices as linear transformations

- A **linear transformation** $T$ is a mapping between an input vector space ($\mathbb{R}^n$) and an output vector space ($\mathbb{R}^m$), *i.e.*

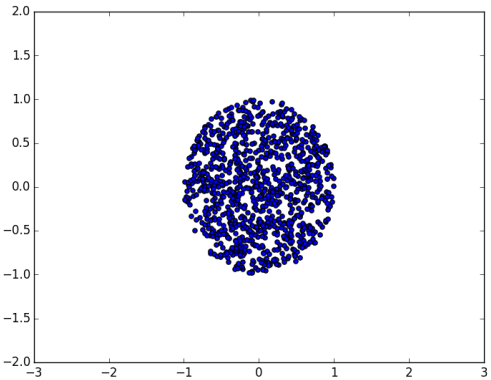
$$T(\boldsymbol{v}) = A\boldsymbol{v} \quad with \quad T : \mathbb{R}^n \longrightarrow \mathbb{R}^m$$

  where $A \in \mathbb{R}^{n \times m}$ is the matrix that defines the linear transformation.
- Different operations like **reflection**, **expansion/contraction**, **rotation** or **projection** are linear transformations.
- Every linear transformation can be thought as applying a matrix on an input vector.
- Graphical meaning by drawing the mapping of a set of unit vectors, see:

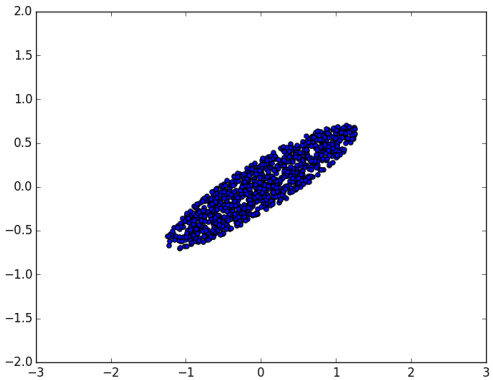
```
jupyter notebook Matrix_As_Linear_Transformations.ipynb
```

- Eigenvectors capture the directions in which vectors can grow or shrink.

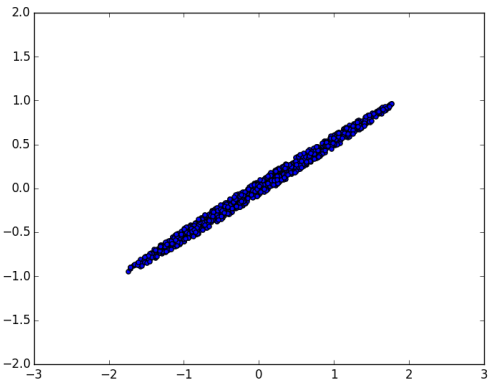
Let $\mathcal{C} = \{\boldsymbol{c}_i \mid \|\boldsymbol{c}_i\|_2 = 1\}$ and $S = \begin{pmatrix} 1.2 & 0.4 \\ 0.5 & 0.5 \end{pmatrix}$.



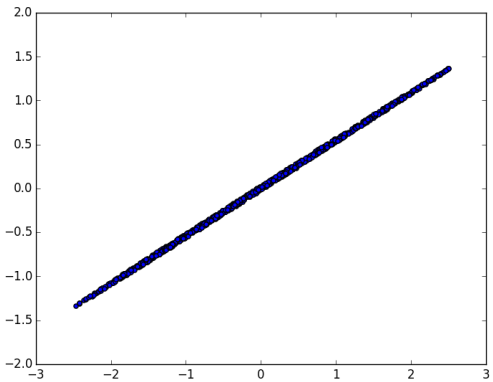
$\boldsymbol{c}$



$S\,\boldsymbol{c}$



$S^2\,\boldsymbol{c}$



$S^3\,\boldsymbol{c}$

Eigenvectors capture the directions in which vectors can grow or shrink.

# Rank of a Matrix

- The rank of a matrix is equal to the number of linearly independent rows (or columns) in it.
- Example

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

has rank 2: the first two columns are linearly independent, so the rank is at least 2, but since the third is a linear combination of the first two (the first column minus the second), the three columns are linearly dependent so the rank must be less than 3.

- See Introduction to Linear Algebra, G. Strang (2022).

# Singular Value Decomposition (SVD)



$$\boxed{S = U\Sigma V^{\mathrm{H}}} \in \mathbb{C}^{N_x \times N_t} \qquad \text{with}$$

- $U \in \mathbb{C}^{N_x \times N_x}$ unitary: $UU^{\mathrm{H}} = U^{\mathrm{H}}U = I_{N_x}$

  Left singular vectors: $U = (u_1, u_2, \cdots, u_{N_x})$
- $V \in \mathbb{C}^{N_t \times N_t}$ unitary: $VV^{\mathrm{H}} = V^{\mathrm{H}}V = I_{N_t}$

  Right singular vectors: $V = (v_1, v_2, \cdots, v_{N_t})$
- $\Sigma$ 'diagonal' matrix

Singular values: $\Sigma = \mathrm{diag}(\sigma_1, \cdots, \sigma_p, 0 \cdots, 0)$ with $p = \min(N_x, N_t)$

$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \sigma_{r+2} = \cdots = \sigma_p = 0$ where $r = \mathrm{rank}(S) \leq p$.

$$\Sigma = \begin{pmatrix} \Sigma_p & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \quad ; \quad \Sigma_p = \begin{pmatrix} \sigma_1 & 0 & 0 \\ \vdots & \ddots & 0 \\ 0 & \cdots & \sigma_p \end{pmatrix}$$

# SVD

Example for $N_x < N_t$ i.e. $p = N_x$

$S = U\Sigma V^{\mathrm{H}}$ where $S$ has more columns than rows.

$$S = \begin{pmatrix} \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_{N_x} \end{pmatrix} \left(\begin{array}{ccc|ccc} \sigma_1 & & & 0 & \cdots & 0 \\ & \ddots & & \vdots & & \vdots \\ & & \sigma_{N_x} & 0 & \cdots & 0 \end{array}\right) \left(\begin{array}{c} \boldsymbol{v}_1^{\mathrm{H}} \\ \vdots \\ \boldsymbol{v}_{N_x}^{\mathrm{H}} \\ \hline \boldsymbol{v}_{N_x+1}^{\mathrm{H}} \\ \vdots \\ \boldsymbol{v}_{N_t}^{\mathrm{H}} \end{array}\right)$$

# SVD

Example for $N_x > N_t$ i.e. $p = N_t$

$S = U\Sigma V^{\mathrm{H}}$ where $S$ has more rows than columns.

$$S = \begin{pmatrix} \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_{N_t} & \boldsymbol{u}_{N_t+1} & \cdots & \boldsymbol{u}_{N_x} \end{pmatrix} \left(\begin{array}{cccc} \sigma_1 & & & \\ & \ddots & & \\ & & & \sigma_{N_t} \\ \hline 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{array}\right) \begin{pmatrix} \boldsymbol{v}_1^{\mathrm{H}} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \boldsymbol{v}_{N_t}^{\mathrm{H}} \end{pmatrix}$$

# SVD

## Example

$$\boldsymbol{M} = \begin{bmatrix} 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \end{bmatrix}$$

$$\boldsymbol{U} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{5} & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{0} & 0 \end{bmatrix}$$

$$\boldsymbol{V}^{\mathrm{H}} = \begin{bmatrix} 0 & 0 & -1 & 0 & 0 \\ -\sqrt{0.2} & 0 & 0 & 0 & -\sqrt{0.8} \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -\sqrt{0.8} & 0 & 0 & 0 & \sqrt{0.2} \end{bmatrix}$$

# SVD

## Example

$$\boldsymbol{U}\boldsymbol{U}^{\mathrm{H}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \boldsymbol{I}_4$$

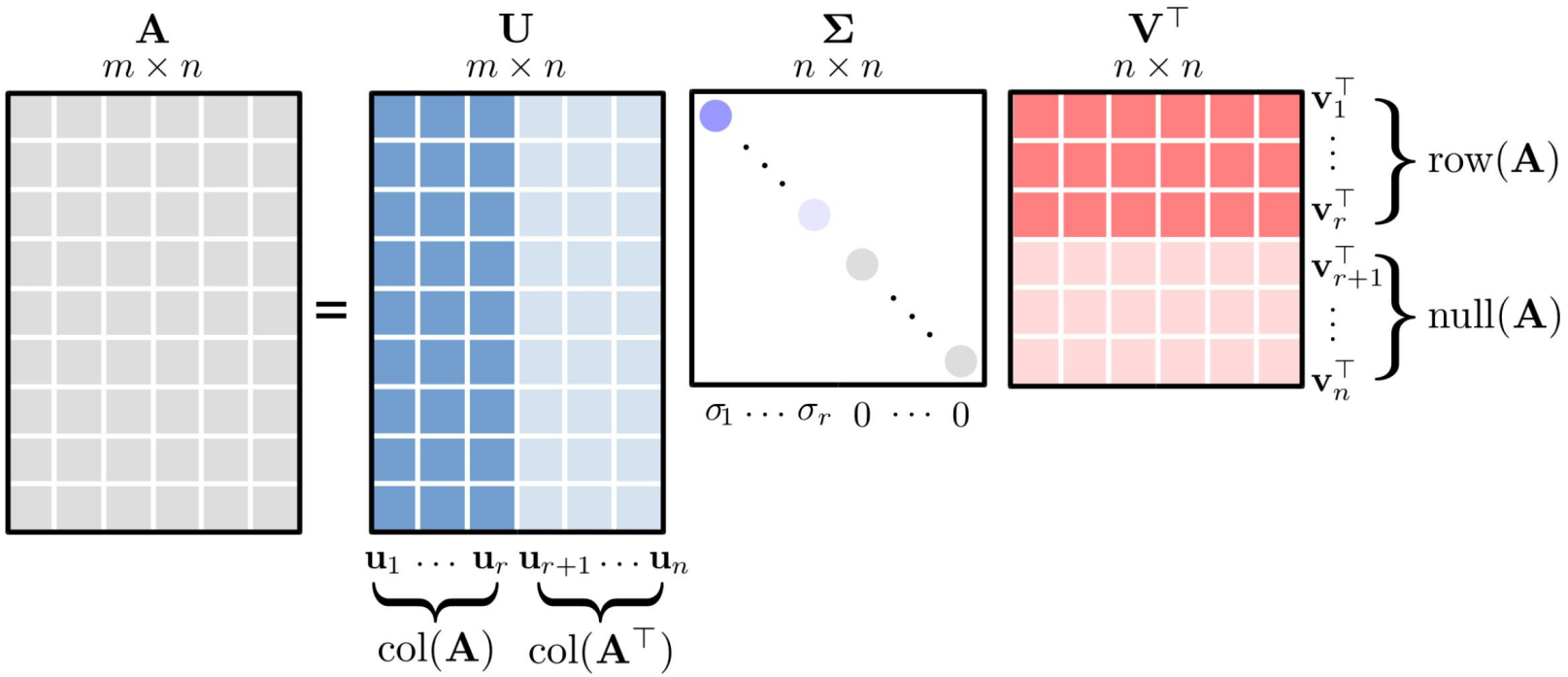
$$\boldsymbol{V}\boldsymbol{V}^{\mathrm{H}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} = \boldsymbol{I}_5$$

This particular singular value decomposition is not unique. Another valid expression of $\boldsymbol{V}$.

$$\boldsymbol{V}^{\mathrm{H}} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \sqrt{0.2} & 0 & 0 & 0 & \sqrt{0.8} \\ \sqrt{0.4} & 0 & 0 & \sqrt{0.5} & -\sqrt{0.1} \\ -\sqrt{0.4} & 0 & 0 & \sqrt{0.5} & \sqrt{0.1} \end{bmatrix}$$

# SVD

Schematic of the SVD for a rank-$r$ matrix, where $m \geq n$.




where

- col($\boldsymbol{A}$) is the column space, *i.e.* space spanned by any linear combination of the column vectors
- row($\boldsymbol{A}$) is the row space
- null($\boldsymbol{A}$) is the null space, *i.e.* $\{\boldsymbol{x} \mid \boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}\}$

# Truncated SVD approximations



⋆ If $r = \text{rank}(S)$, then the SVD of $S \in \mathbb{C}^{N_x \times N_t}$ can be written as

$$S = \begin{pmatrix} \underline{U}_{N_x \times r} & \overline{U}_{N_x \times (N_t - r)} \end{pmatrix} \begin{pmatrix} \underline{\Sigma}_{r \times r} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{V}_{N_t \times r} & \overline{V}_{N_t \times (N_t - r)} \end{pmatrix}^{\mathrm{H}}$$

$$S = \underline{U}_{N_x \times r} \underline{\Sigma}_{r \times r} \underline{V}^{\mathrm{H}}_{N_t \times r}$$

$$\boxed{S = \sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1^{\mathrm{H}} + \sigma_2 \boldsymbol{u}_2 \boldsymbol{v}_2^{\mathrm{H}} + \cdots + \sigma_r \boldsymbol{u}_r \boldsymbol{v}_r^{\mathrm{H}}.}$$

⋆ If we truncate to $k < r$ terms, then

$$S_k = U_k \Sigma_k V_k^{\mathrm{H}} = \sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1^{\mathrm{H}} + \sigma_2 \boldsymbol{u}_2 \boldsymbol{v}_2^{\mathrm{H}} + \cdots + \sigma_k \boldsymbol{u}_k \boldsymbol{v}_k^{\mathrm{H}}.$$

$S_k$ is an approximation of the matrix $S$. **How good is it?**

# SVD

## Reduced SVDs

1. **Full SVD**

2. **Thin**, or **economy-sized SVD**

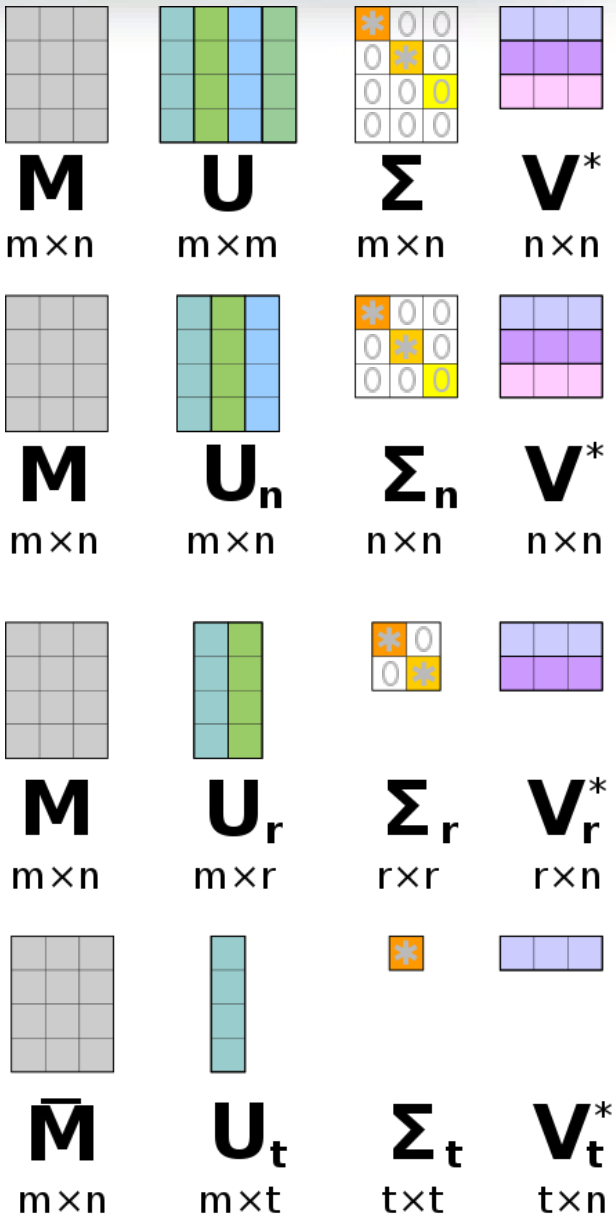
$$M = U_k \Sigma_k V_k^{\mathrm{H}}, \qquad k = \min(m, n)$$

3. **Compact SVD**

$$M = U_r \Sigma_r V_r^{\mathrm{H}}$$

4. **Truncated SVD** with $t \ll r$

$$\bar{M} = U_t \Sigma_t V_t^{\mathrm{H}}$$



# SVD

## Geometric interpretation

- The three transformations (2 rotations + 1 expansion/contraction) linked to the SVD, see:

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jupyter notebook SVD_Geometric.ipynb
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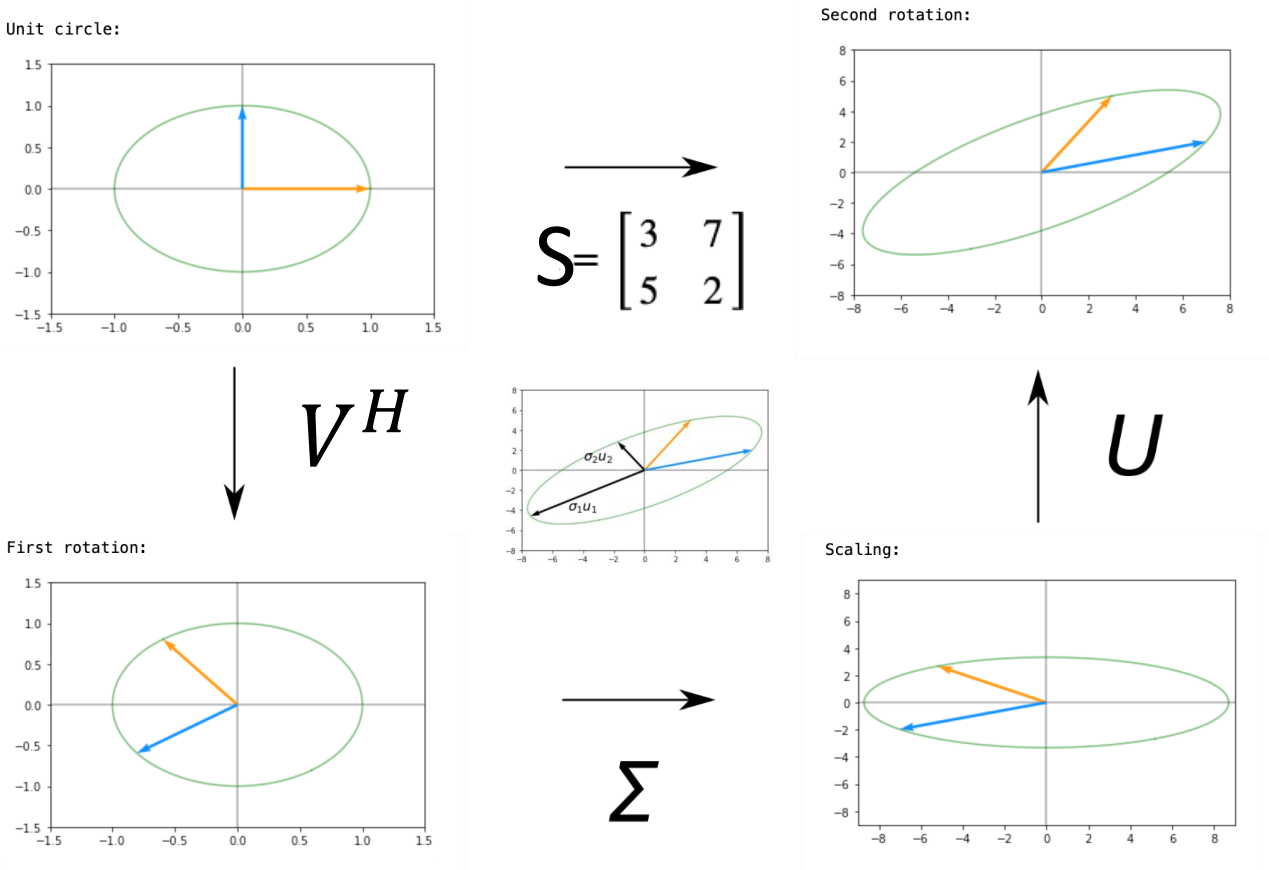
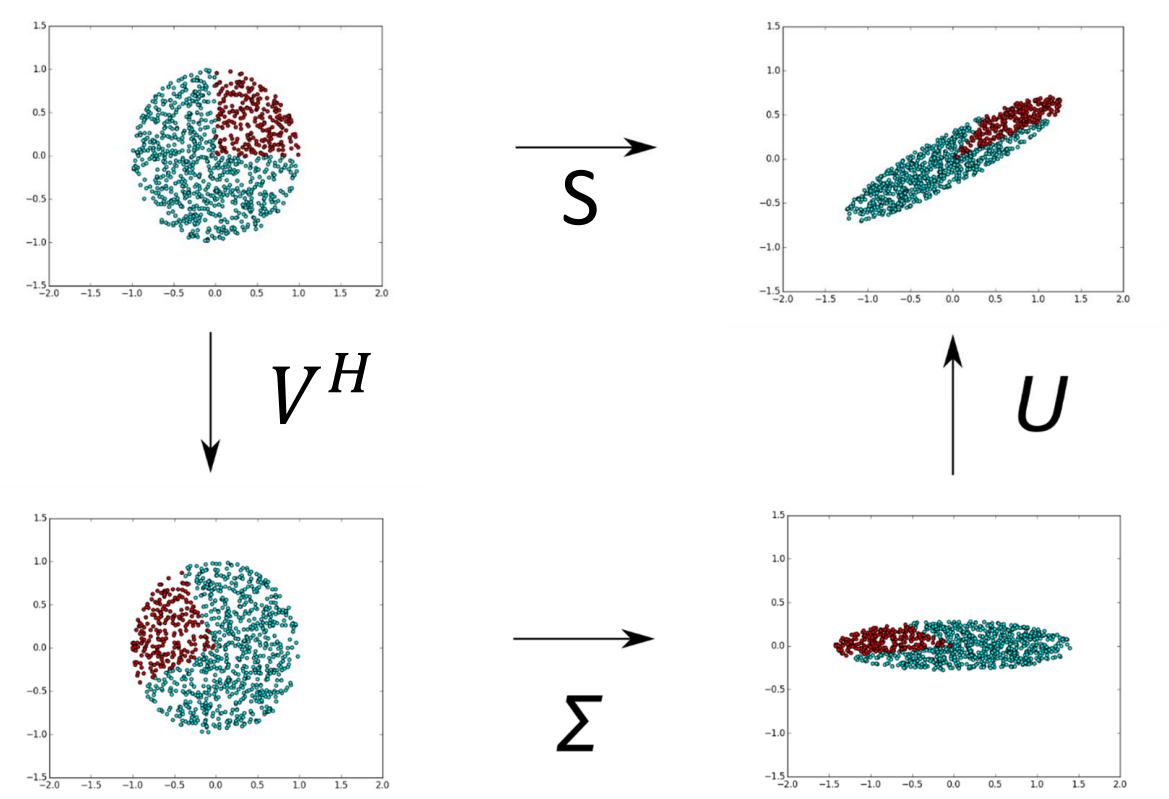


# SVD

## Geometric interpretation




- Columns $\boldsymbol{u}_i, i = 1, \cdots, r$ define an orthonormal basis of $S$
- Columns $\boldsymbol{v}_i, i = 1, \cdots, r$ define an orthonormal basis of $S^{\mathrm{H}}$
- Singular values $\sigma_i$ indicate amplification factors

$\Longrightarrow$ SVD: combination of rotations and dilatation.

# Adjoint and normal matrices

- Adjoint operator
  Each linear operator $A$ on a vector space $V$ defines an **adjoint** operator $A^*$ on $V$ according to the rule

$$\langle A\boldsymbol{x}, \boldsymbol{y}\rangle = \langle \boldsymbol{x}, A^*\boldsymbol{y}\rangle \quad \forall \boldsymbol{x}, \boldsymbol{y}$$

- Normal matrix
  A complex square matrix $A$ ($A \in \mathbb{C}^{n\times n}$) is **normal** if it commutes with its adjoint $A^*$, *i.e.*

$$A \text{ normal} \quad \Longleftrightarrow \quad A^*A = AA^*$$

- Hermitian inner product
  The inner product of two vectors $\boldsymbol{x}$ and $\boldsymbol{y} \in \mathbb{C}^n$ is given by

$$\langle \boldsymbol{x}, \boldsymbol{y}\rangle = \boldsymbol{y}^H\boldsymbol{x}$$

  where $\boldsymbol{y}^H$ is the conjugate transpose (Hermitian) of $\boldsymbol{y}$.

# Adjoint and normal matrices

- Adjoint matrix for the Hermitian inner product

$$\boxed{A^* = A^H}$$

Dem: By definition of the adjoint operator and Hermitian inner product, we have:

$$\langle A\boldsymbol{x}, \boldsymbol{y}\rangle = \langle \boldsymbol{x}, A^*\boldsymbol{y}\rangle$$

$$\boldsymbol{y}^H A\boldsymbol{x} = (A^*\boldsymbol{y})^H \boldsymbol{x} = \boldsymbol{y}^H (A^*)^H \boldsymbol{x} \quad \Longrightarrow A = (A^*)^H \text{ or } A^* = A^H$$

- Hermitian matrix: $A = A^H$ ; Skew Hermitian matrix: $A = -A^H$ ; Unitary matrix: $A^{-1} = A^H$ are special cases of normal matrices.
- Unitary diagonalization: A matrix $A \in \mathbb{C}^{n\times n}$ is normal if and only if it is unitarily similar to a diagonal matrix, *i.e.* $A$ has a complete orthonormal set of eigenvectors. There exist $U$ unitary and $D$ diagonal, such that

$$U^* A U = D$$

.

# SVD and eigenvalue problems



- Classical POD (Lumley, 1967)

$$SS^{\mathrm{H}} = \left(U\Sigma V^{\mathrm{H}}\right)\left(V\Sigma^{\mathrm{H}}U^{\mathrm{H}}\right) = U\Sigma\underbrace{V^{\mathrm{H}}V}_{I_{N_t}}\Sigma^{\mathrm{H}}U^{\mathrm{H}}$$

$$= U\Sigma^2U^{\mathrm{H}} = U\Lambda U^{\mathrm{H}}$$

$\Longrightarrow \left(SS^{\mathrm{H}}\right)U = U\Sigma^2 = U\Lambda$, *i.e.* columns of $U$ ev's of $SS^{\mathrm{H}} \in \mathbb{C}^{N_x\times N_x}$

- Snapshot POD (Sirovich, 1987)

$$S^{\mathrm{H}}S = \left(V\Sigma^{\mathrm{H}}U^{\mathrm{H}}\right)\left(U\Sigma V^{\mathrm{H}}\right) = V\Sigma^{\mathrm{H}}\underbrace{U^{\mathrm{H}}U}_{I_{N_x}}\Sigma V^{\mathrm{H}}$$

$$= V\Sigma^2V^{\mathrm{H}} = V\Lambda V^{\mathrm{H}}$$

$\Longrightarrow \left(S^{\mathrm{H}}S\right)V = V\Sigma^2 = V\Lambda$, *i.e.* columns of $V$ ev's of $S^{\mathrm{H}}S \in \mathbb{C}^{N_t\times N_t}$

- Singular values

$$\sigma_i = \sqrt{\lambda_i(S^{\mathrm{H}}S)} = \sqrt{\lambda_i(SS^{\mathrm{H}})} \quad i = 1, \cdots, r$$

# Low rank approximation of $S$

## Eckart-Young theorem

Let $S$ and $S_k \in \mathbb{C}^{N_x \times N_t}$.

$$\forall S, \text{ determine } S_k \text{ such that } \operatorname{rank}(S_k) = k < \operatorname{rank}(S)$$

Criterion:

minimization of the Frobenius norm of the error $S - S_k$.

Theorem: Eckart-Young

$$\min_{\operatorname{rank}(X) \leq k} \|S - X\|_F = \|S - S_k\|_F = \sqrt{\sum_{i=k+1}^{r} \sigma_i^2(S)}$$

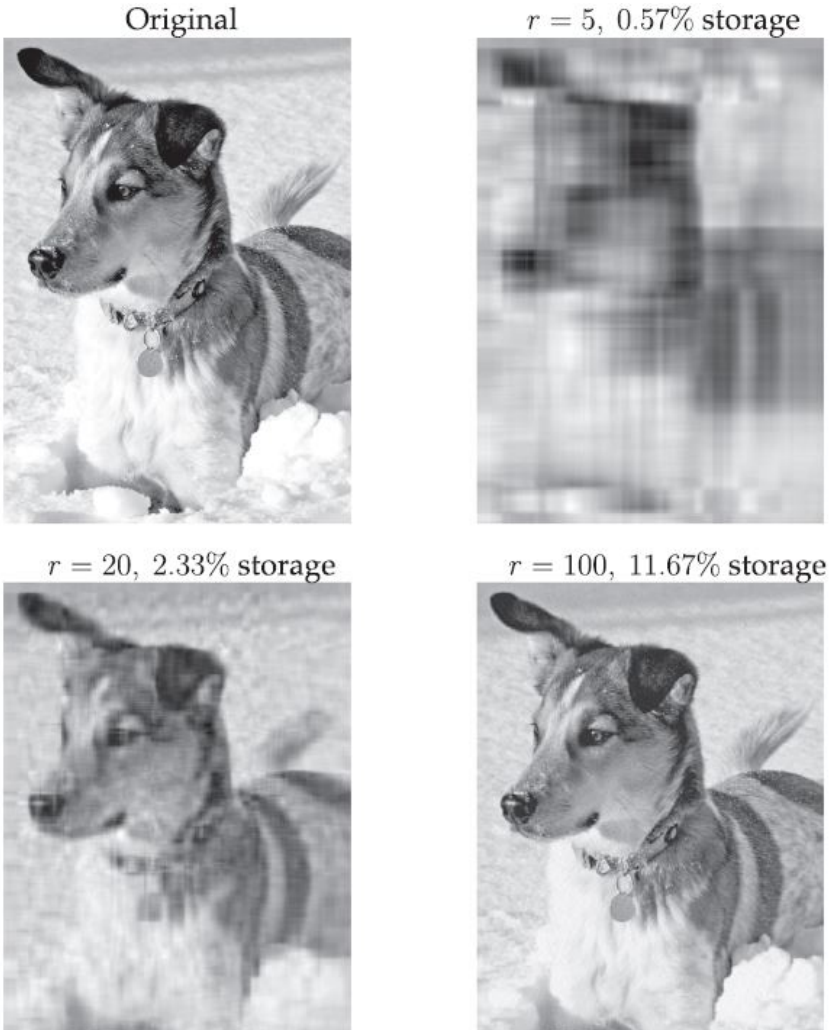
with $$S_k = U \begin{pmatrix} \Sigma_k & 0 \\ 0 & 0 \end{pmatrix} V^{\mathrm{H}} = \sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1^{\mathrm{H}} + \sigma_2 \boldsymbol{u}_2 \boldsymbol{v}_2^{\mathrm{H}} + \cdots + \sigma_k \boldsymbol{u}_k \boldsymbol{v}_k^{\mathrm{H}}$$

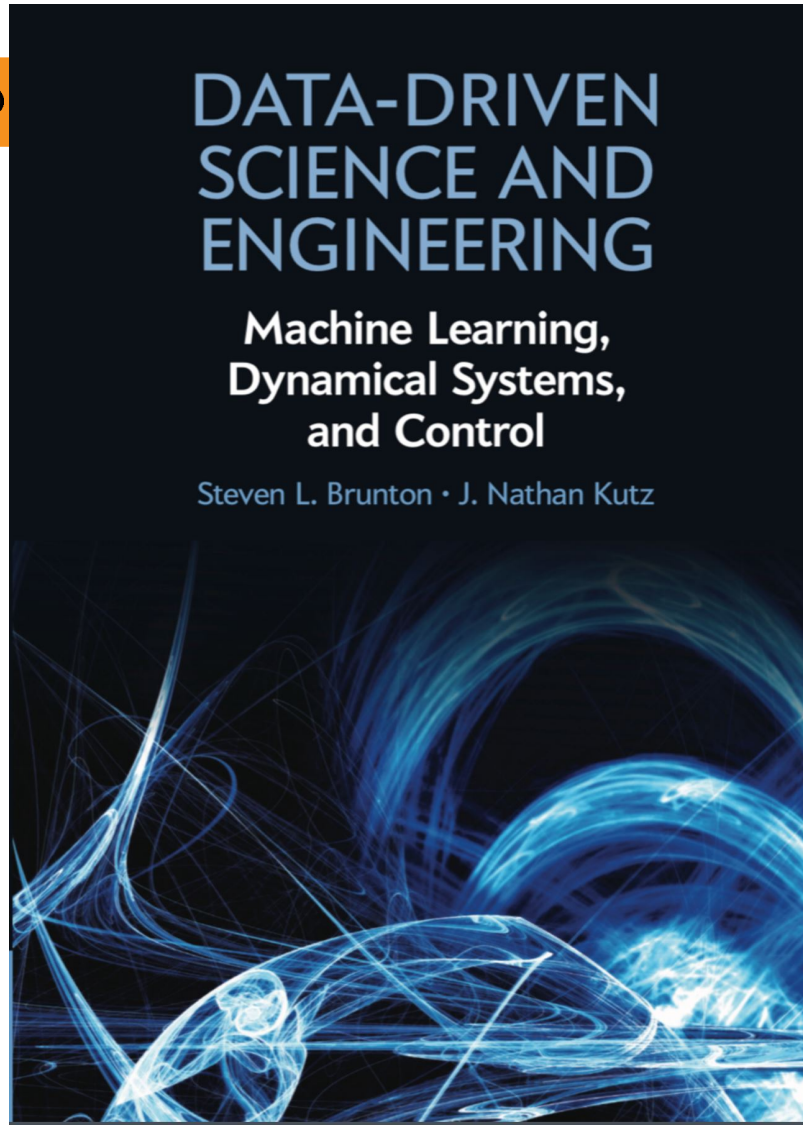
and $$||S||_F = \sqrt{\sum_{i=1}^{N_x} \sum_{j=1}^{N_t} s_{ij}^2} = \sqrt{\sum_{i=1}^{r} \sigma_i^2}.$$

Remark: This theorem establishes a relationship between the rank $k$ of the approximation, and the singular values of $S$.

# Image compression by SVD

- `jupyter notebook CH01_SEC02.ipynb`



# Least squares and pseudo inverse

- Consider $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ with $A \in \mathbb{C}^{n \times m}$.
- Assume $n \gg m$. There are more constraints than unknowns, the system is **overdetermined**. No solutions.We search for the least squares solution. Find $\boldsymbol{x}$ that minimizes

$$\begin{aligned} \|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|_2^2 &= (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x})^{\mathrm{H}} (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}) \\ &= \boldsymbol{b}^{\mathrm{H}}\boldsymbol{b} - \boldsymbol{b}^{\mathrm{H}}\boldsymbol{A}\boldsymbol{x} - \boldsymbol{x}^{\mathrm{H}}\boldsymbol{A}^{\mathrm{H}}\boldsymbol{b} + \boldsymbol{x}^{\mathrm{H}}\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A}\boldsymbol{x} \end{aligned}$$

Differentiating w.r.t $\boldsymbol{x}$ and setting the result equal to zero yields

$$-\left(\boldsymbol{b}^{\mathrm{H}}\boldsymbol{A}\right)^{\mathrm{H}} - \left(\boldsymbol{A}^{\mathrm{H}}\boldsymbol{b}\right)^{\mathrm{H}} + 2\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A}\boldsymbol{x} = 0$$

so

$$\boxed{\boldsymbol{x} = \left(\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{H}}\boldsymbol{b}}$$

# Least squares and pseudo inverse

- Using the SVD of $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{H}}$, we show that

$$\left(\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{H}} = \boxed{\boldsymbol{V}\boldsymbol{\Sigma}^{-1}\boldsymbol{U}^{\mathrm{H}} \triangleq \boldsymbol{A}^{\dagger}}$$

where $\boldsymbol{A}^{\dagger} \in \mathbb{C}^{m\times n}$ is the **Moore-Penrose left pseudo inverse** such that $\boldsymbol{A}^{\dagger}\boldsymbol{A} = \boldsymbol{I}_m$ and $\boldsymbol{A}\boldsymbol{A}^{\dagger} \neq \boldsymbol{I}_n$.

We have:

$$\boxed{\boldsymbol{x} = \boldsymbol{A}^{\dagger}\boldsymbol{b}}$$

Different applications of the Moore-Penrose Pseudoinverse:

- The Moore-Penrose Pseudoinverse (calculation)
- Using the pseudoinverse to solve a overdetermined system of linear equations
- Simple regression problem
- More realistic regression problem
- See: `jupyter notebook Moore_Penrose_Pseudo_Inverse.ipynb`

- Make a **linear regression model** of the **Boston Housing Data** to determine factors which best predict prices in the Boston housing market (13 features considered). The dataset contains a total of 506 cases. The attributes of each case are:
  1. CRIM - per capita crime rate by town
  2. ZN - proportion of residential land zoned for lots over 25,000 sq.ft.
  3. INDUS - proportion of non-retail business acres per town.
  4. CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise)
  5. NOX - nitric oxides concentration (parts per 10 million)
  6. RM - average number of rooms per dwelling
  7. AGE - proportion of owner-occupied units built prior to 1940
  8. DIS - weighted distances to five Boston employment centres
  9. RAD - index of accessibility to radial highways
  10. TAX - full-value property-tax rate per $10,000
  11. PTRATIO - pupil-teacher ratio by town
  12. B - $1000(Bk - 0.63)^2$ where Bk is the proportion of blacks by town
  13. LSTAT - % lower status of the population
  14. MEDV - Median value of owner-occupied homes in $1000's

`jupyter notebook CH01_SEC04_3_Housing.ipynb`

or see

`https://www.kaggle.com/prasadperera/the-boston-housing-dataset`

for a deeper analysis.

# Principal Component Analysis (PCA)



- We collect a number of $m$ measurements in a single experiment, and arrange the data into a row vector:

$$\boldsymbol{s} = (s_1, s_2, \cdots, s_m)$$

- We stay consistent with the PCA literature and arrange the data in rows, rather than in columns.
- The measurements may be features of an observable, or different physical quantities.
- A number of experiments are conducted, and each measurement vector $\boldsymbol{s}$ is arranged as a row in a large matrix $\boldsymbol{X}$.
- We compute the row-wise mean $\bar{\boldsymbol{x}}$ (the mean of all rows), and subtract it from $\boldsymbol{X}$.

$$\bar{x}_j = \frac{1}{n}\sum_{i=1}^{n} X_{ij} \quad ; \quad \bar{\boldsymbol{X}} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \bar{\boldsymbol{x}} \quad \text{(mean matrix)}$$

# Principal Component Analysis (PCA)



- Subtracting $\bar{\boldsymbol{X}}$ from $\boldsymbol{X}$ results in the mean-subtracted data $\boldsymbol{B}$:

$$\boldsymbol{B} = \boldsymbol{X} - \bar{\boldsymbol{X}}$$

- The covariance matrix of the rows of $\boldsymbol{B}$ is given by

$$\boldsymbol{C} = \frac{1}{n-1}\boldsymbol{B}^{\mathrm{H}}\boldsymbol{B} \quad \text{where } \boldsymbol{C} \text{ is Hermitian}$$

- The first principal component $\boldsymbol{u}_1$ is given as:

$$\boldsymbol{u}_1 = \arg\max_{\|\boldsymbol{u}_1\|=1} \boldsymbol{u}_1^{\mathrm{H}}\boldsymbol{B}^{\mathrm{H}}\boldsymbol{B}\boldsymbol{u}_1$$

i.e. the eigenvector of $\boldsymbol{B}^{\mathrm{H}}\boldsymbol{B}$ corresponding to the largest eigenvalue. It is clear from the SVD properties that it corresponds to the left singular vector of $\boldsymbol{B}$ corresponding to the largest singular value. It is possible to obtain the principal components by computing

$$\boldsymbol{C}\boldsymbol{V} = \boldsymbol{\Lambda}\boldsymbol{V}$$

# Principal Component Analysis (PCA)

## Noisy Gaussian Data

- PCA to Noisy Gaussian Data

```
jupyter notebook CH01_SEC05_1_PCAGaussian.ipynb
```

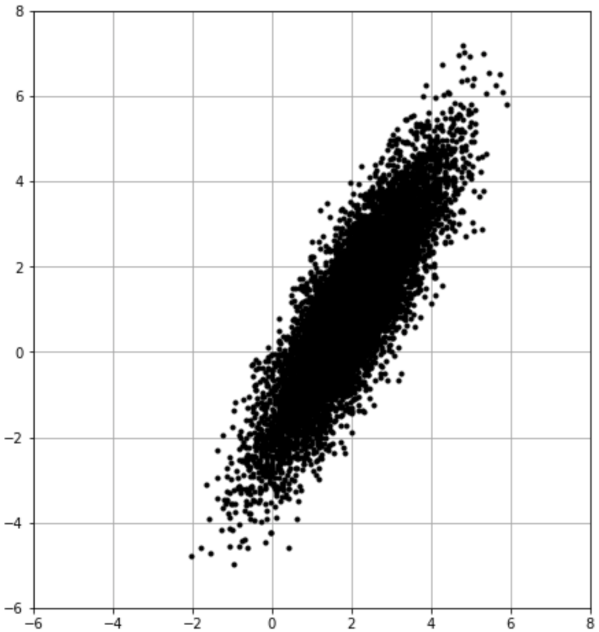
Data:

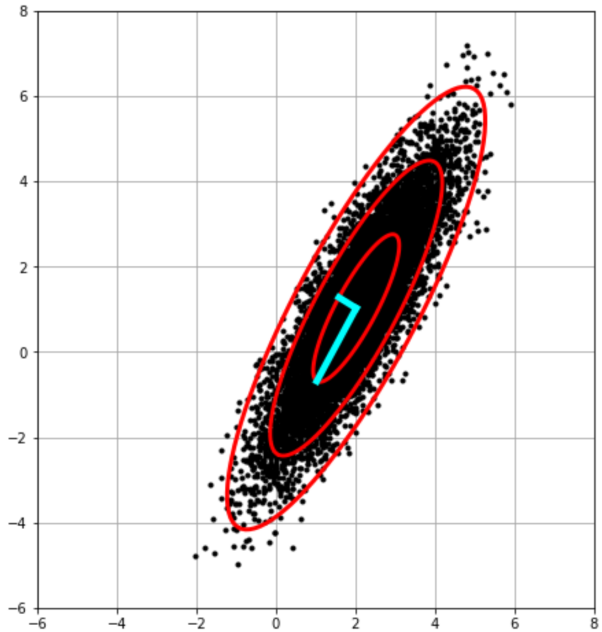
10, 000 vectors from a two-dimensional normal distribution with zero mean and unit variance.

Vectors scaled by 2 in the $x$ direction and 0.5 in the $y$ direction.

Vectors rotated by $\pi/3$.

Vectors translated to $\boldsymbol{x}_C = [2 \quad 1]^T$.



# Principal Component Analysis (PCA)



`jupyter notebook CH01_SEC06_1.ipynb`

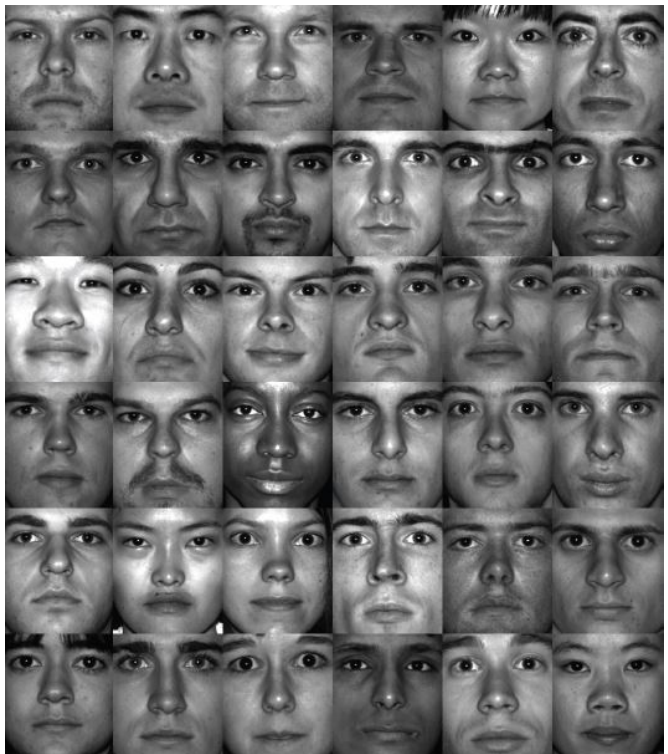
- Eigenfaces example.

  Data: Extended Yale Face Database B

  Cropped and aligned images of 38 individuals under 64 lighting conditions (not for all !!).

  Each image is 192 pixels tall and 168 pixels wide.

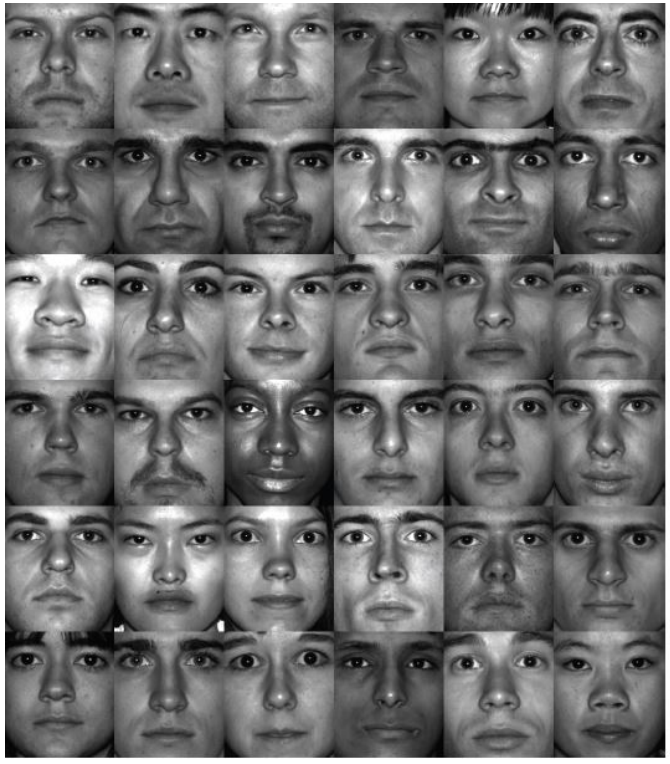
  Image reshaped into large column vector with $192 \times 168 = 32,256$ elements. First 36 people in the database for training, and last 2 for testing.



# Principal Component Analysis (PCA)

## Eigenfaces example

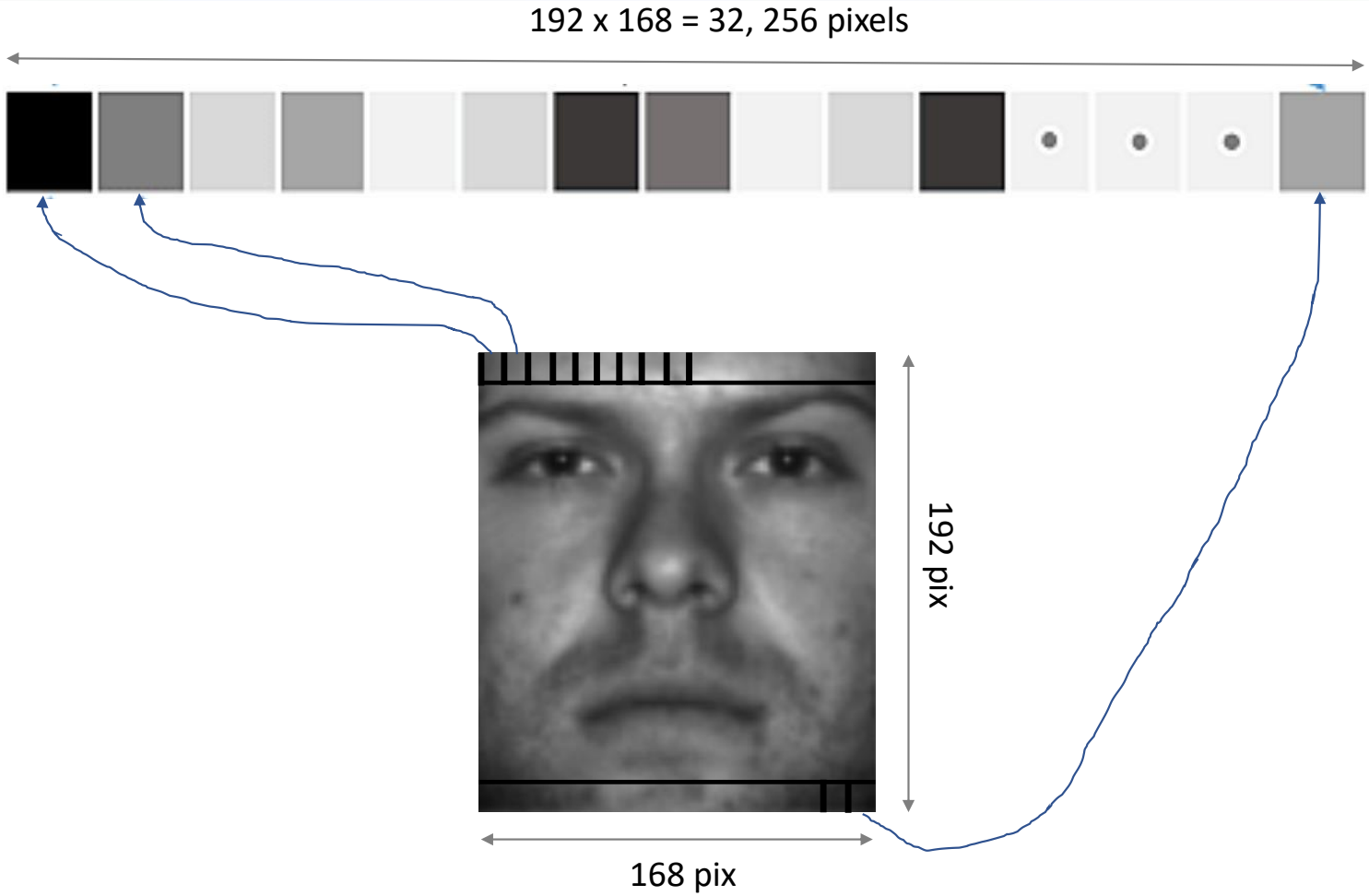
- `jupyter notebook CH01_SEC06_1.ipynb` (load images)



Left: Single image for each person used for training.
Right: All images for a specific person (64 lighting conditions at max)

# Principal Component Analysis (PCA)

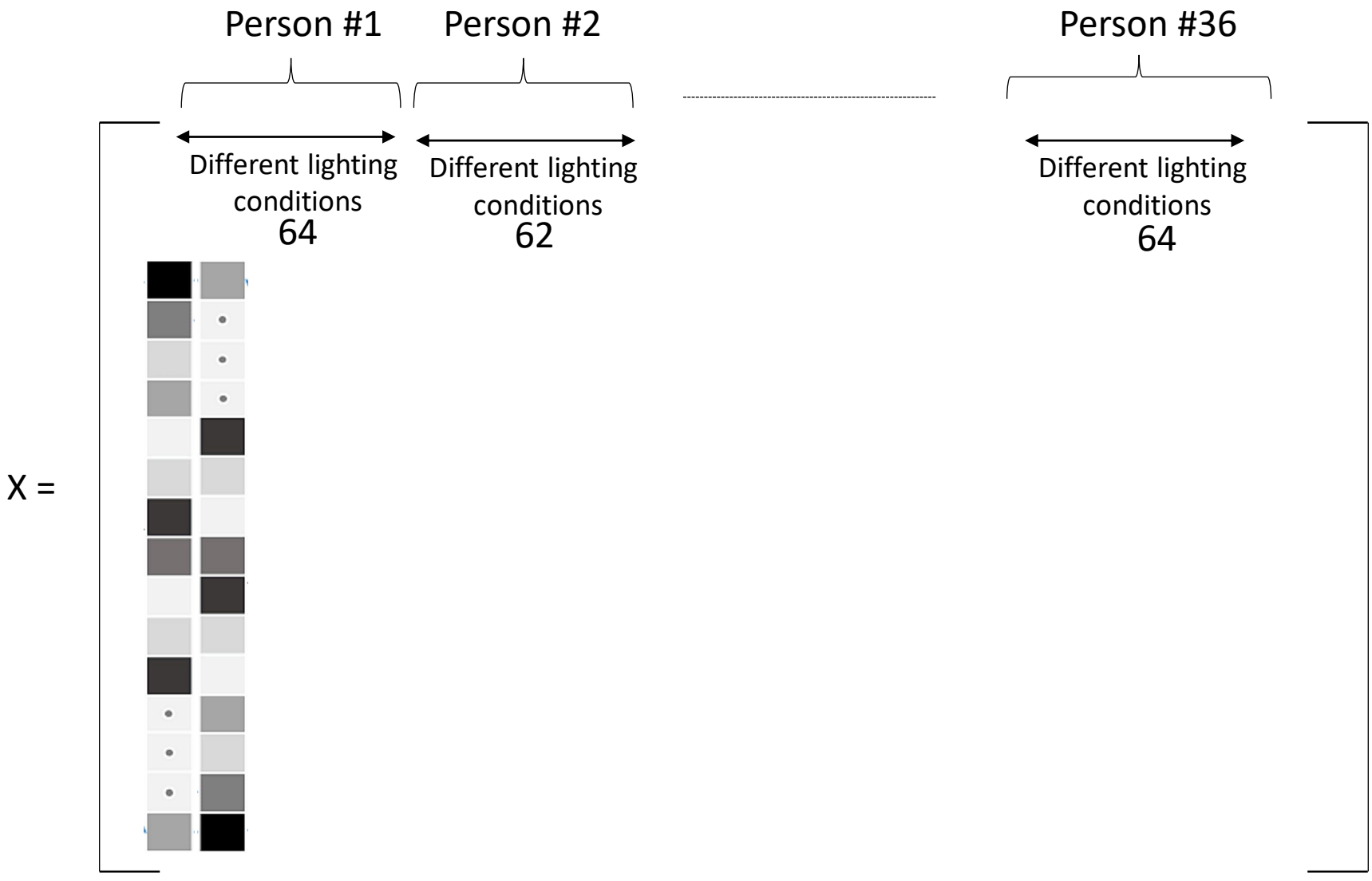
## Eigenfaces example




Example of image (192 x 168 pixels), it will result in a flattened array of length 32, 256 pixels.

# Principal Component Analysis (PCA)

## Eigenfaces example



# Orthogonal projections

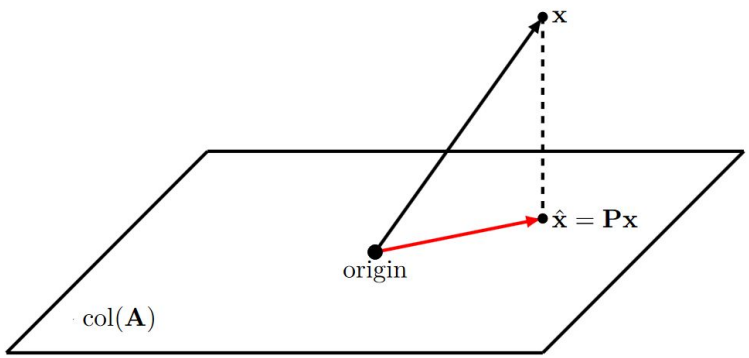
Let $V$ be a subspace of $\mathbb{R}^n$.

1. Find a basis $\boldsymbol{v}_1, \boldsymbol{v}_2, \cdots, \boldsymbol{v}_m$ for $V$
2. Let $\boldsymbol{A}$ be the matrix with columns $\boldsymbol{v}_i$. Then (see least squares approximation)

$$\boxed{\boldsymbol{P} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{H}}}$$

   is the matrix of the orthogonal projection onto $V$.

If $\boldsymbol{v}_i$ is a unitary basis ($\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A} = \boldsymbol{I}$), then $\boxed{\boldsymbol{P} = \boldsymbol{A}\boldsymbol{A}^{\mathrm{H}}}$.

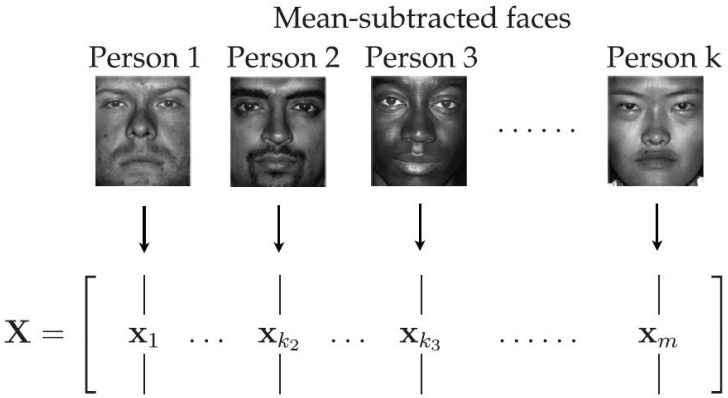



Geometric illustration of the orthogonal projection operator $\boldsymbol{P}$. A vector $\boldsymbol{x}$ is projected onto the column space of $\boldsymbol{A}$, *i.e.* $\boldsymbol{P}\boldsymbol{x} \in \mathrm{col}(\boldsymbol{A})$.

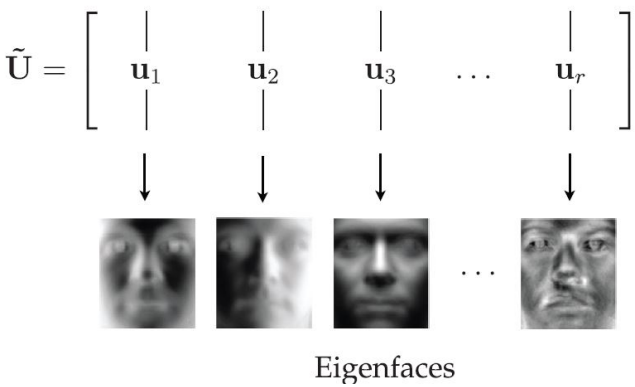
# Principal Component Analysis (PCA)

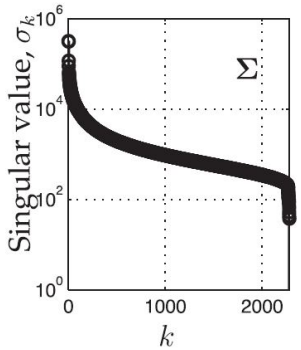
## Eigenfaces example

1. Compute the average face by averaging over the columns.
2. Compute eigenfaces on mean-subtracted data.








$\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^* \approx \tilde{\mathbf{U}}\tilde{\Sigma}\tilde{\mathbf{V}}^*$ (>>[U,S,V]=svd(X,'econ');)

3. Test how well a rank-$r$ SVD basis will approximate the image using the orthogonal projection on the space spanned by $U$:

$$\tilde{\boldsymbol{x}}_{\text{Test}} = \mathcal{P}_{\text{Eigenfaces}}(\boldsymbol{x}_{\text{Test}}) = \underbrace{\boldsymbol{U}\boldsymbol{U}^{\text{H}}}_{P_{\text{Eigenfaces}}} \boldsymbol{x}_{\text{Test}}$$

# Principal Component Analysis (PCA)

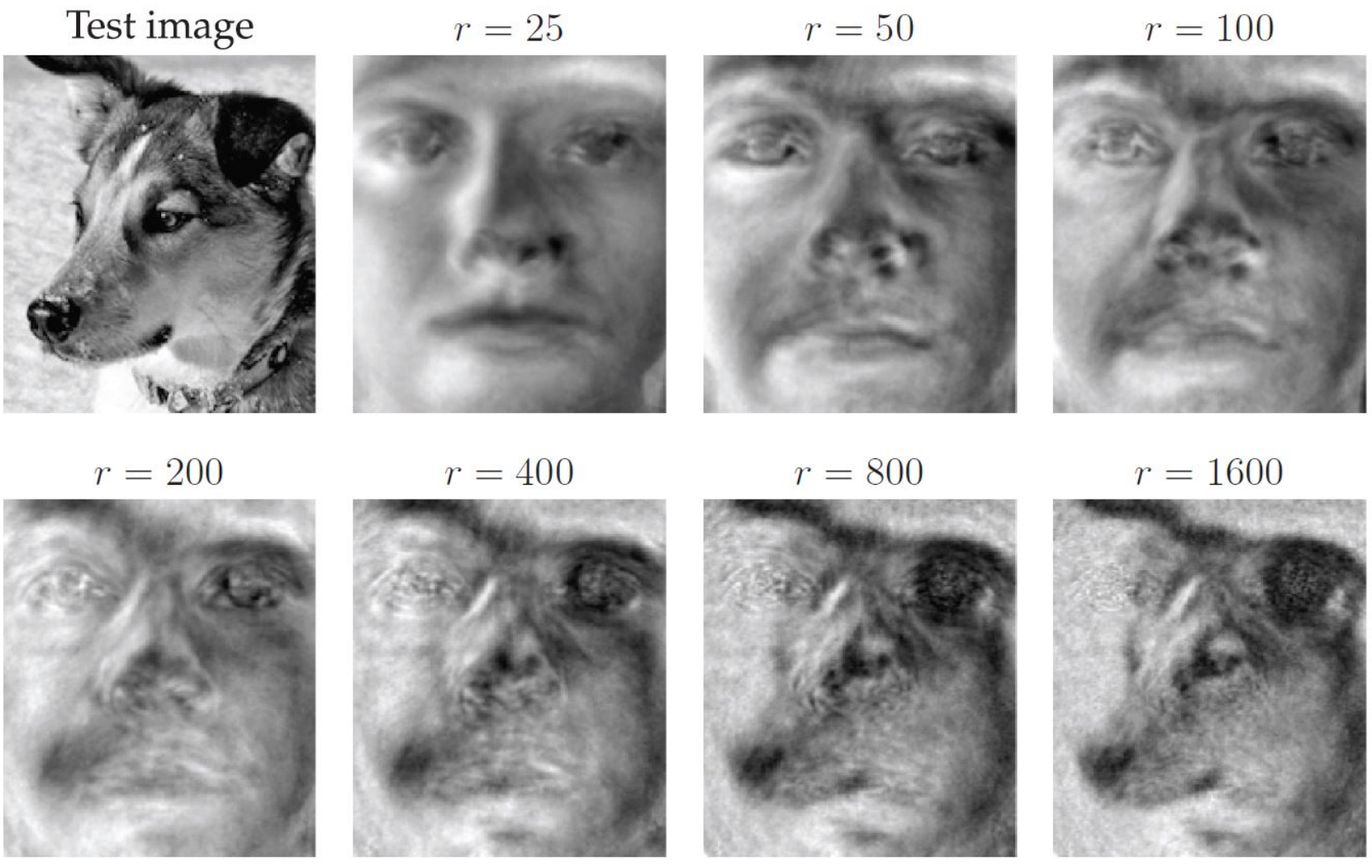
## Eigenfaces example

- `jupyter notebook CH01_SEC06_2_3_4.ipynb` (image approximations)

# Principal Component Analysis (PCA)

## Eigenfaces example

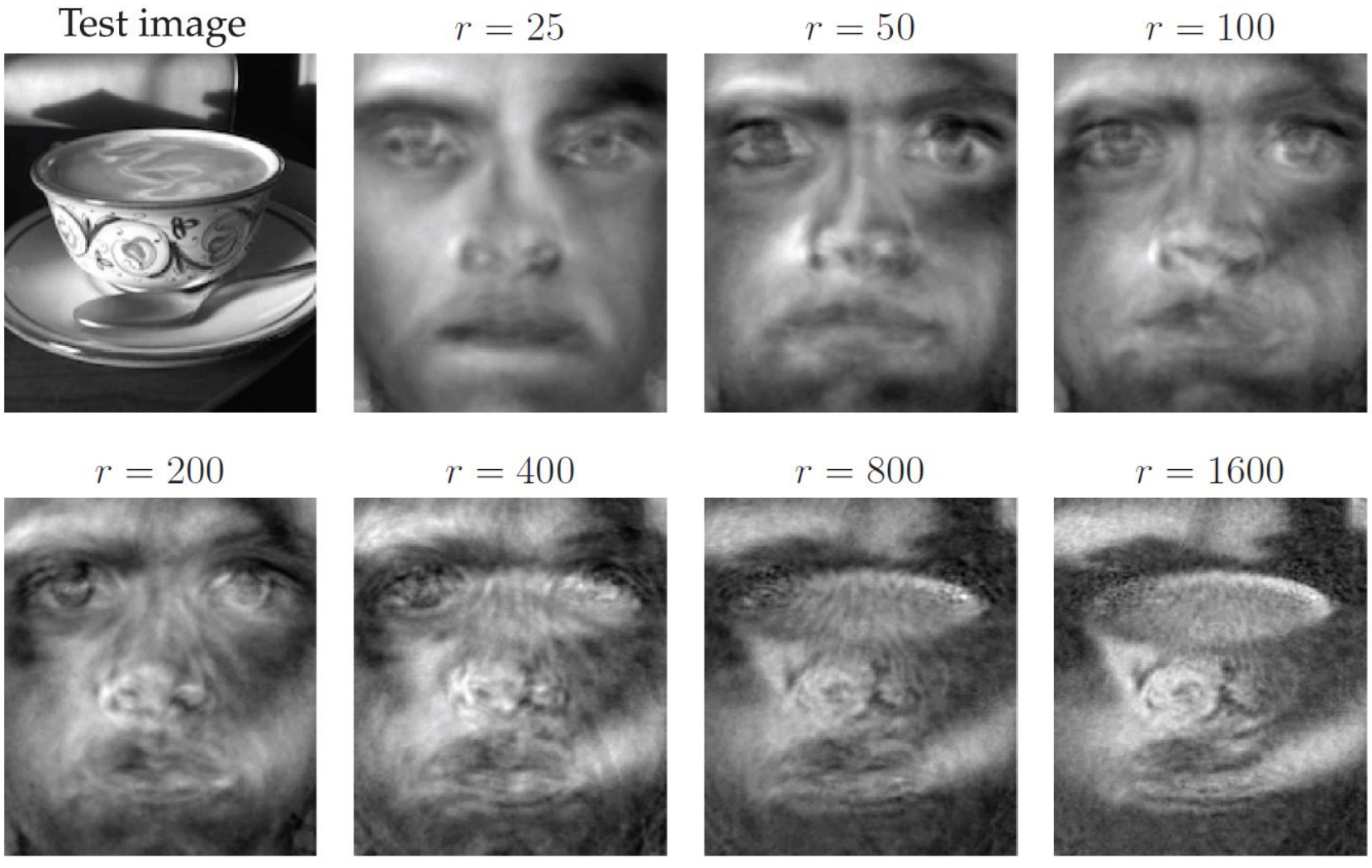
- Approximations of a dog



# Principal Component Analysis (PCA)

## Eigenfaces example

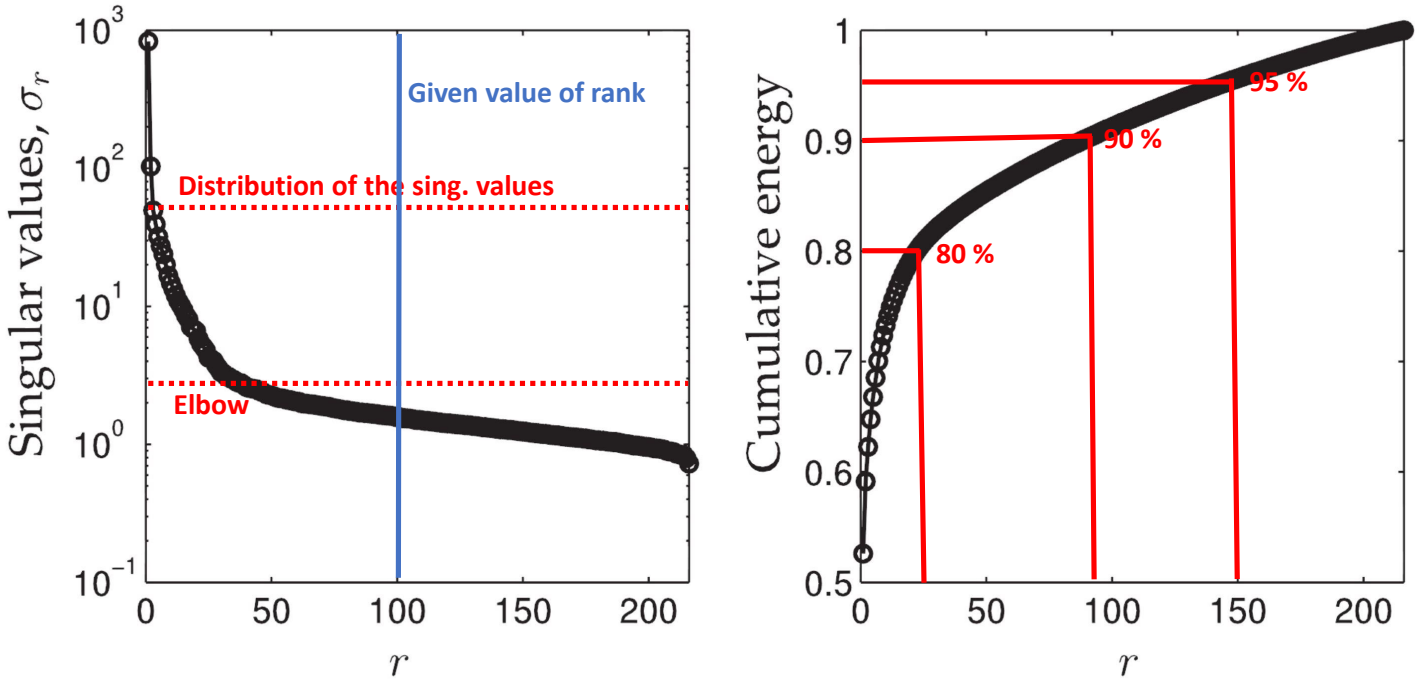
- Approximations of a cappucino



# SVD

## Truncation of the singular values

Singular values for the ovarian cancer data.




Where to truncate the singular values?

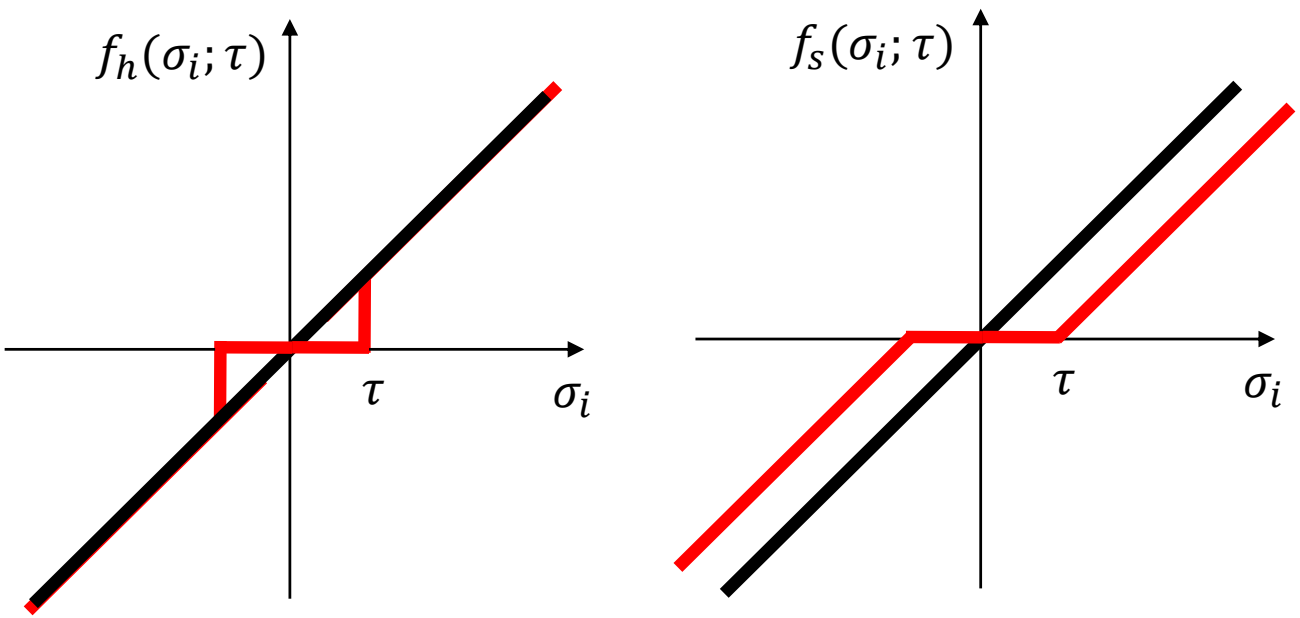
- Distribution of the singular values (ratio $\sigma_i/\sigma_{i+1}$)
- "Elbow" criterion
- Given value of rank
- Pre-determined amount of the variance or energy

Truncation may be viewed as a hard threshold on singular values.

# SVD

## Soft and Hard threshold

In many algorithms, a difference is made between *hard-thresholding* and *soft-thresholding* (see Murphy, 2012, p. 433).




(a) Hard thresholding. (b) Soft thresholding.

# SVD

## Soft and Hard threshold

In **hard-thresholding**, the filter function $f_h$ is defined as

$$f_h(\sigma_i;\tau) = \begin{cases} \sigma_i, & \text{if } \sigma_i > \tau \\ 0, & \text{otherwise} \end{cases},$$

whereas **in soft-thresholding**, the filter function $f_s$ is defined as

$$f_s(\sigma_i;\tau) = \begin{cases} \sigma_i - \tau, & \text{if } \sigma_i > \tau \\ 0, & \text{otherwise} \end{cases}.$$

We note $\mathbf{\Sigma}_+ = \text{Diag}((\sigma_i)_+)$, the matrix of filtered singular values, where $(\sigma_i)_+ = f_h(\sigma_i;\tau)$.

# SVD

## Optimal hard threshold

- Optimal Hard Threshold (Gavish and Donoho, 2014).

Hypothesis: $\boldsymbol{X}$ has a low-rank structure contaminated with Gaussian white noise.

$$\boldsymbol{X} = \boldsymbol{X}_{\text{True}} + \gamma \boldsymbol{X}_{\text{Noise}}$$

$\boldsymbol{X}_{\text{Noise}}$: i.i.d. Gaussian random variables with zero mean and unit variance. When $\gamma$ is known, we have:

1. If $\boldsymbol{X} \in \mathbb{R}^{n \times n}$, then

$$\tau = \frac{4}{\sqrt{3}} \sqrt{n} \gamma$$

2. If $\boldsymbol{X} \in \mathbb{R}^{n \times m}$ and $n \gg m$, then $\beta = \frac{m}{n}$ and

$$\tau = \lambda(\beta) \sqrt{n} \gamma \quad \text{with} \quad \lambda(\beta) = \left( 2(\beta + 1) + \frac{8\beta}{\beta + 1 + (\beta^2 + 14\beta + 1)^{1/2}} \right)^{1/2}$$

Note that when $\beta = 1$, $\lambda(\beta) = \frac{4}{\sqrt{3}}$. If $m \gg n$, then $\beta = \frac{n}{m}$.

# SVD

## Optimal hard threshold

3. For unknown parameter $\gamma$ and $\boldsymbol{X} \in \mathbb{R}^{n \times m}$

$$\tau = \frac{\lambda(\beta)}{\mu_\beta} \sigma_{\text{median}}$$

where

- $\sigma_{\text{median}}$ is the *median* singular value, and
- $\mu_\beta$ is solution to

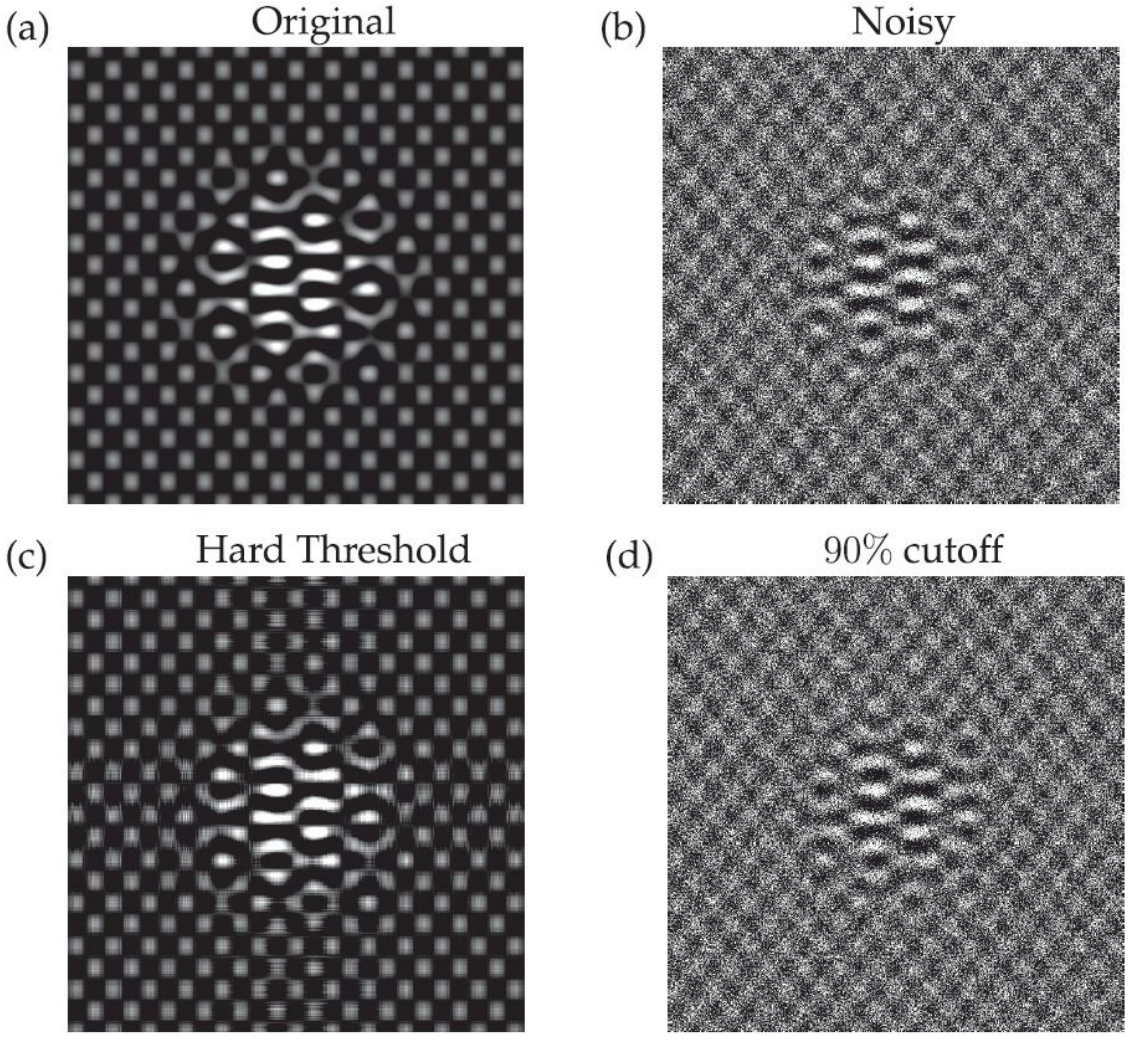
$$\int_{(1-\beta)^2}^{\mu_\beta} \frac{\left[\left((1+\sqrt{\beta})^2 - t\right)\left(t - (1-\sqrt{\beta})^2\right)\right]^{1/2}}{2\pi t} \, \mathrm{d}t = \frac{1}{2}$$

Numerical approximation is provided in Gavish and Donoho (2014) (Matlab code).

# Optimal hard threshold



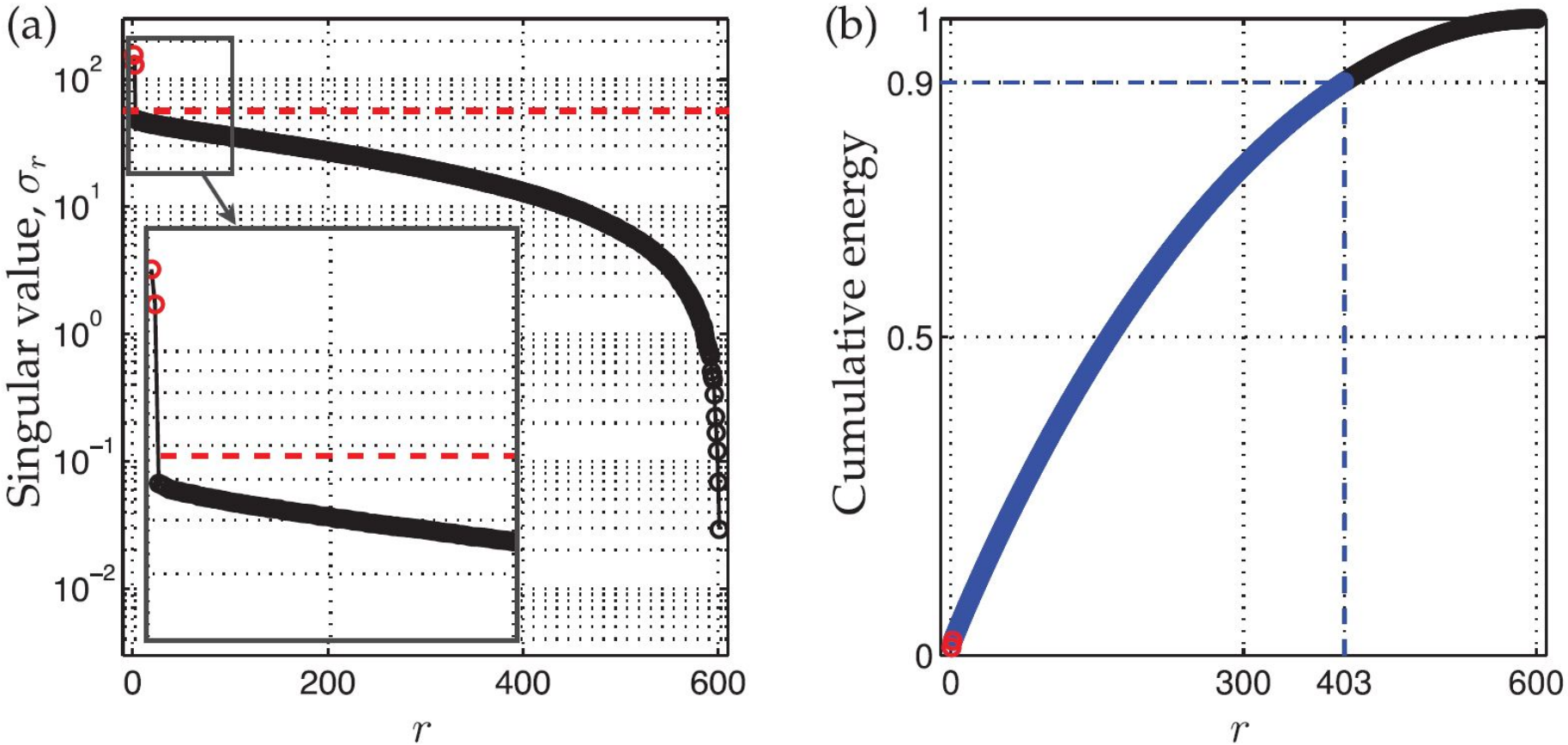
- `jupyter notebook CH01_SEC07_1.ipynb`




Optimal hard threshold is able to filter the noise more effectively.

# Optimal hard threshold

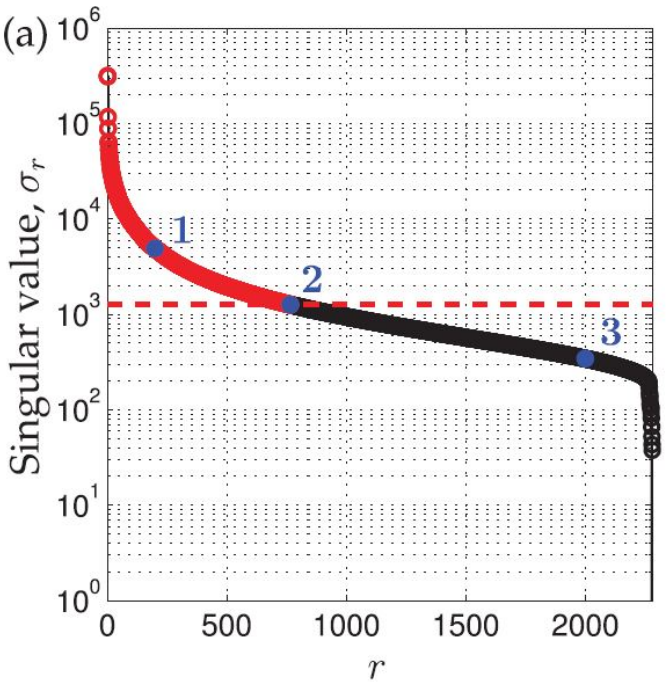


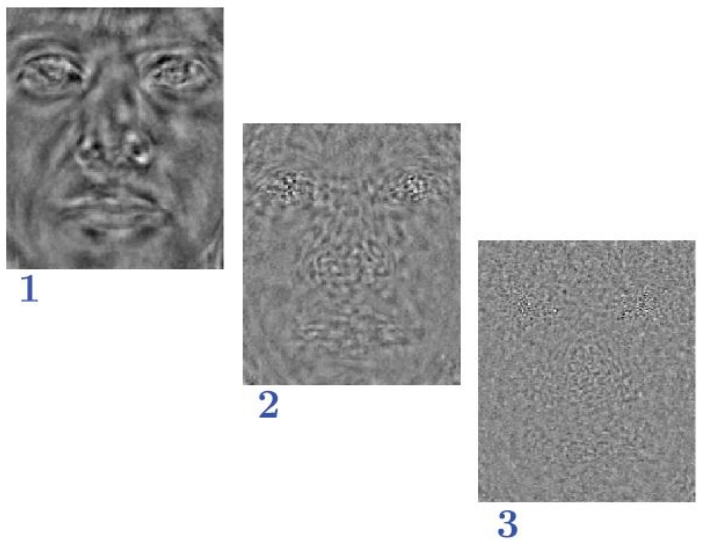



Red: hard threshold ; Blue: 90% energy

# Optimal hard threshold

Eigenfaces

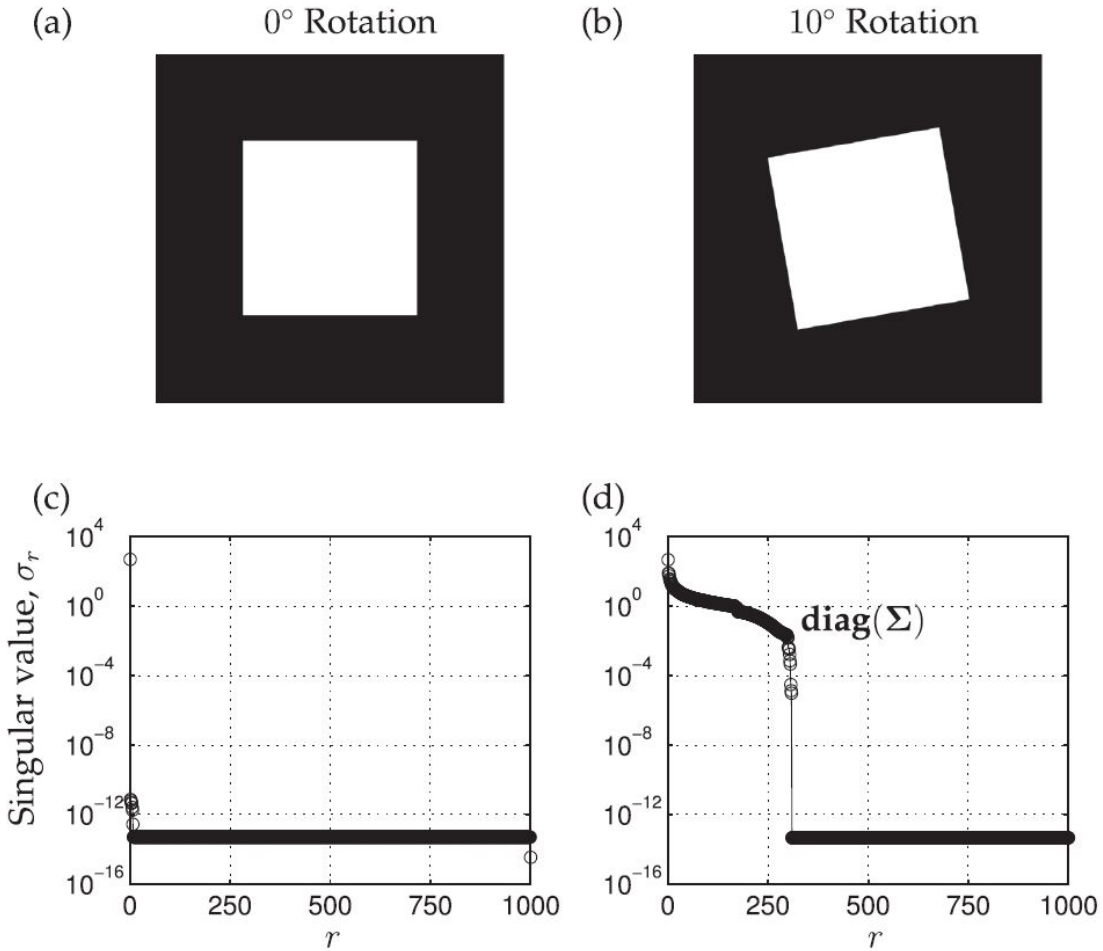



Matrix $X$ rectangular with $\beta = 3/4$. Noise magnitude unknown.

# Data alignment

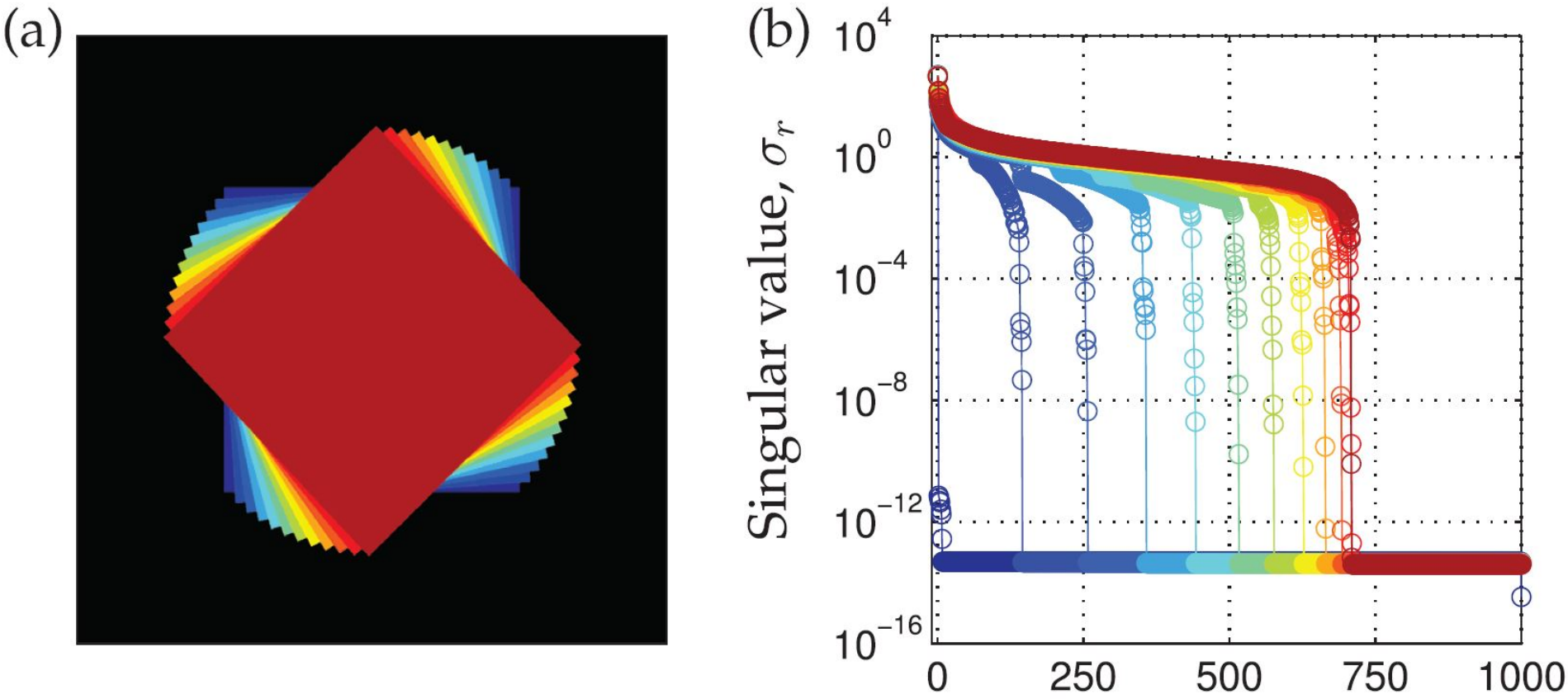
- `jupyter notebook CH01_SEC07_2.ipynb`




The SVD is fundamentally *geometric*. It depends on the coordinate system in which the data is represented.

# Data alignment

- `jupyter notebook CH01_SEC07_3.ipynb`



# Interlude

## Fourier mode expansion

- Fourier mode basis elements given by

$$\psi_k(x) = \exp\left(\jmath \frac{2\pi k x}{L}\right) \quad x \in [0, L] \text{ and } k = -n/2, \cdots, 0, \cdots, n/2 - 1$$

- Search to represent a localized Gaussian function with Fourier modes

$$u(x,t) = \exp\left(-\sigma x^2\right) = \sum_{k=-N}^{N} c_k \psi_k(x)$$

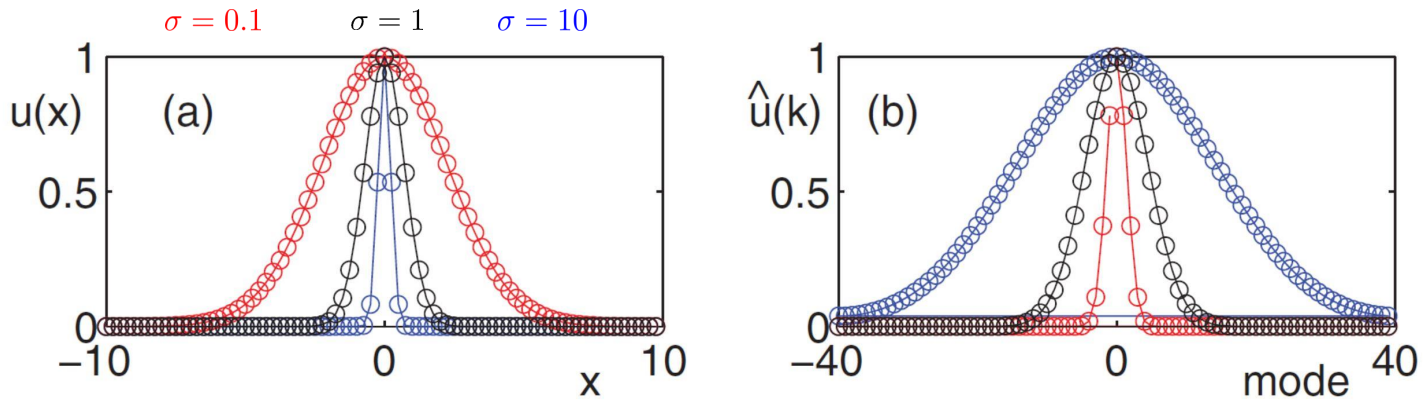
for different values of $\sigma = 0.1,\ 1,\ 10$ and several values of $N = 1, \cdots, 19$.

- `jupyter notebook CH11_SEC01_1_Fig11p1.ipynb`

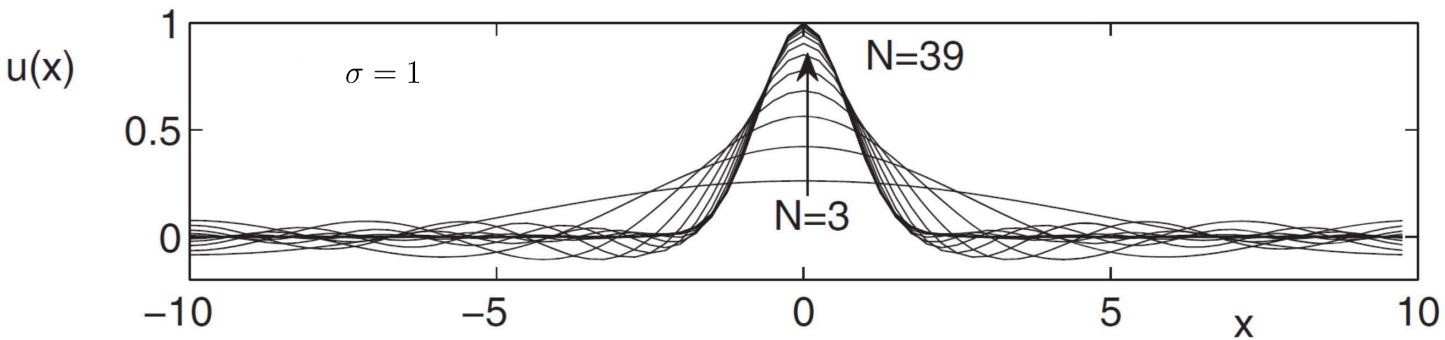
# Interlude

## Fourier mode expansion

- A Gaussian transforms to another Gaussian.

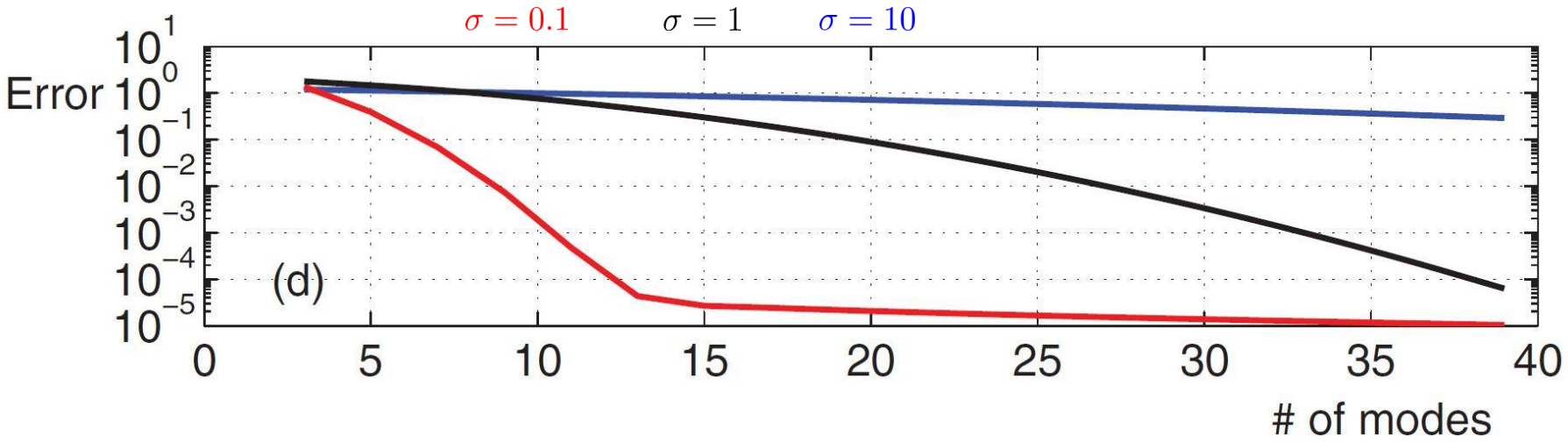



- Fourier approximation with increasing $N$



# Interlude

## Fourier mode expansion




Large number of Fourier modes required to represent simple functions, especially as the Gaussian width is decreased.

# Outline

1. Introduction
2. Preliminaries
   - Eigenvalue Decomposition
   - Singular Value Decomposition
   - Principal Component Analysis
   - Truncation
   - Data alignment
3. Data-based
   - Proper Orthogonal Decomposition
   - Dynamic Mode Decomposition
   - Cluster-based Reduced Order Model
4. Operator-based
   - Global stability analysis
   - Koopman analysis
   - Galerkin projection
5. Perspectives
6. Conclusion

# Proper Orthogonal Decomposition



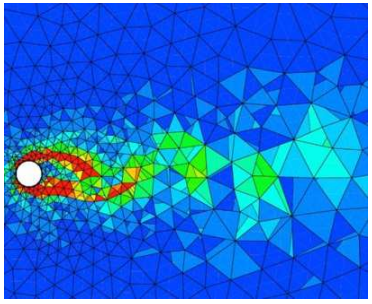
- Also known as:
  - Karhunen-Loève decomposition: Karhunen (1946), Loève (1945) ;
  - Principal Component Analysis: Hotelling (1953) ;
  - Singular Value Decomposition: Golub and Van Loan (1983).
- Applications include:
  - Random variables (Papoulis, 1965) ;
  - Image processing (Rosenfeld and Kak, 1982) ;
  - Signal analysis (Algazi and Sakrison, 1969) ;
  - Data compression (Andrews, Davies and Schwartz, 1967) ;
  - Process identification and control (Gay and Ray, 1986) ;
  - Optimal control (Ravindran, 2000 ; Hinze et Volkwein 2004 ; Bergmann, 2004)

  and of course in fluid mechanics
- Introduced in turbulence by Lumley (1967)

Lumley J.L. (1967) : The structure of inhomogeneous turbulence. *Atmospheric Turbulence and Wave Propagation*, ed. A.M. Yaglom & V.I. Tatarski, pp. 166-178.

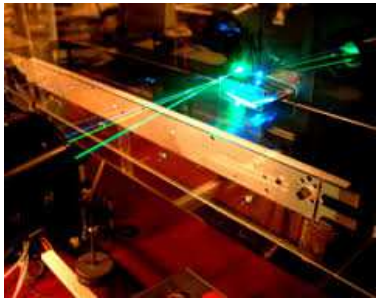
# From data to Snapshot Data Matrix

Simulations



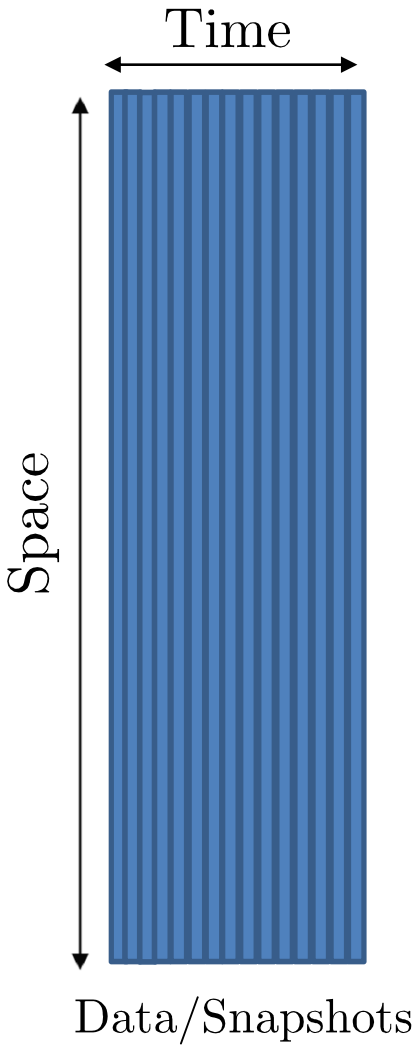
- Velocity fields
- Pressure fields
- Vorticity fields
- Tracers

Experiments



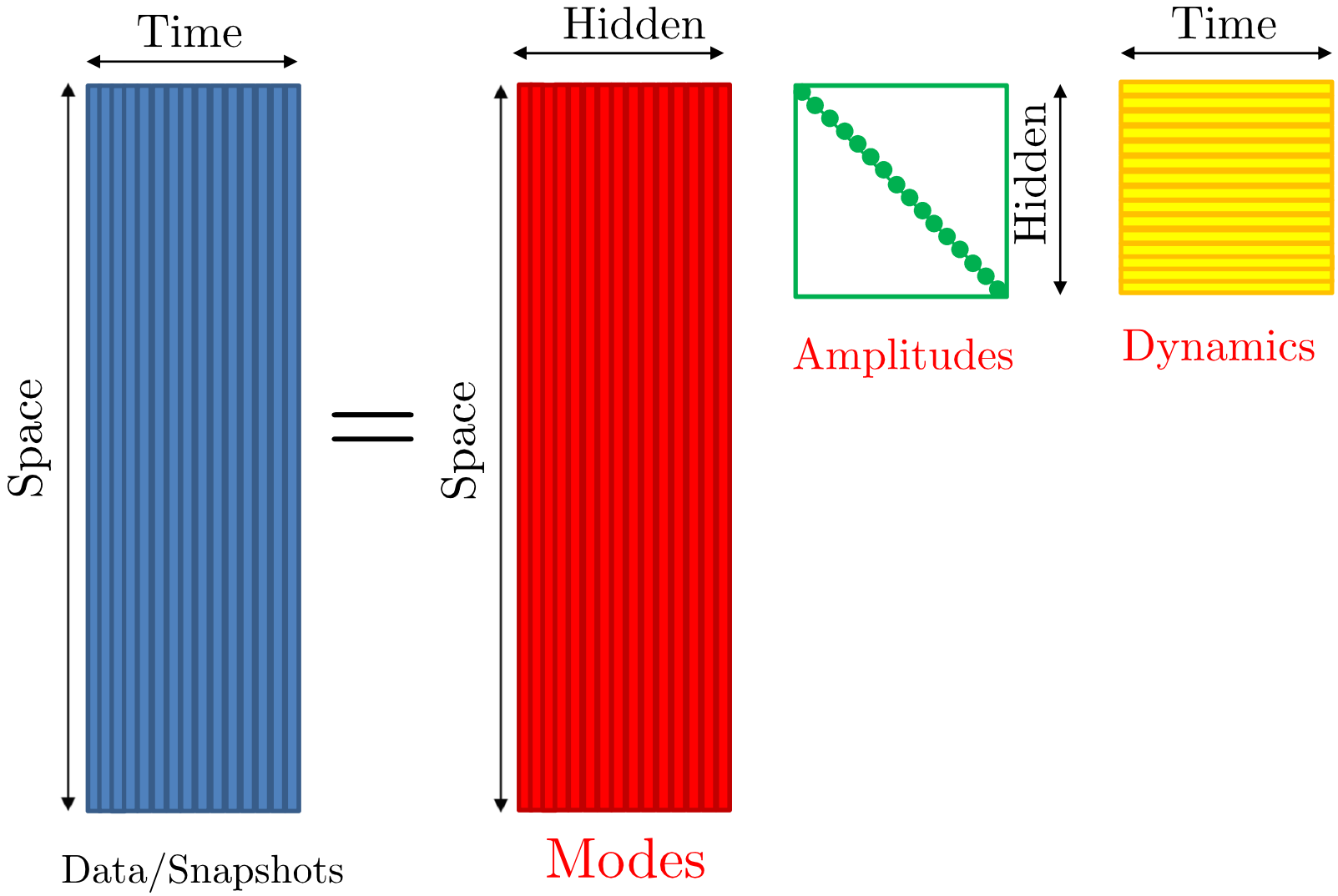
- PIV
- Hot-wires
- LDV
- Visualizations

$\Rightarrow S =$

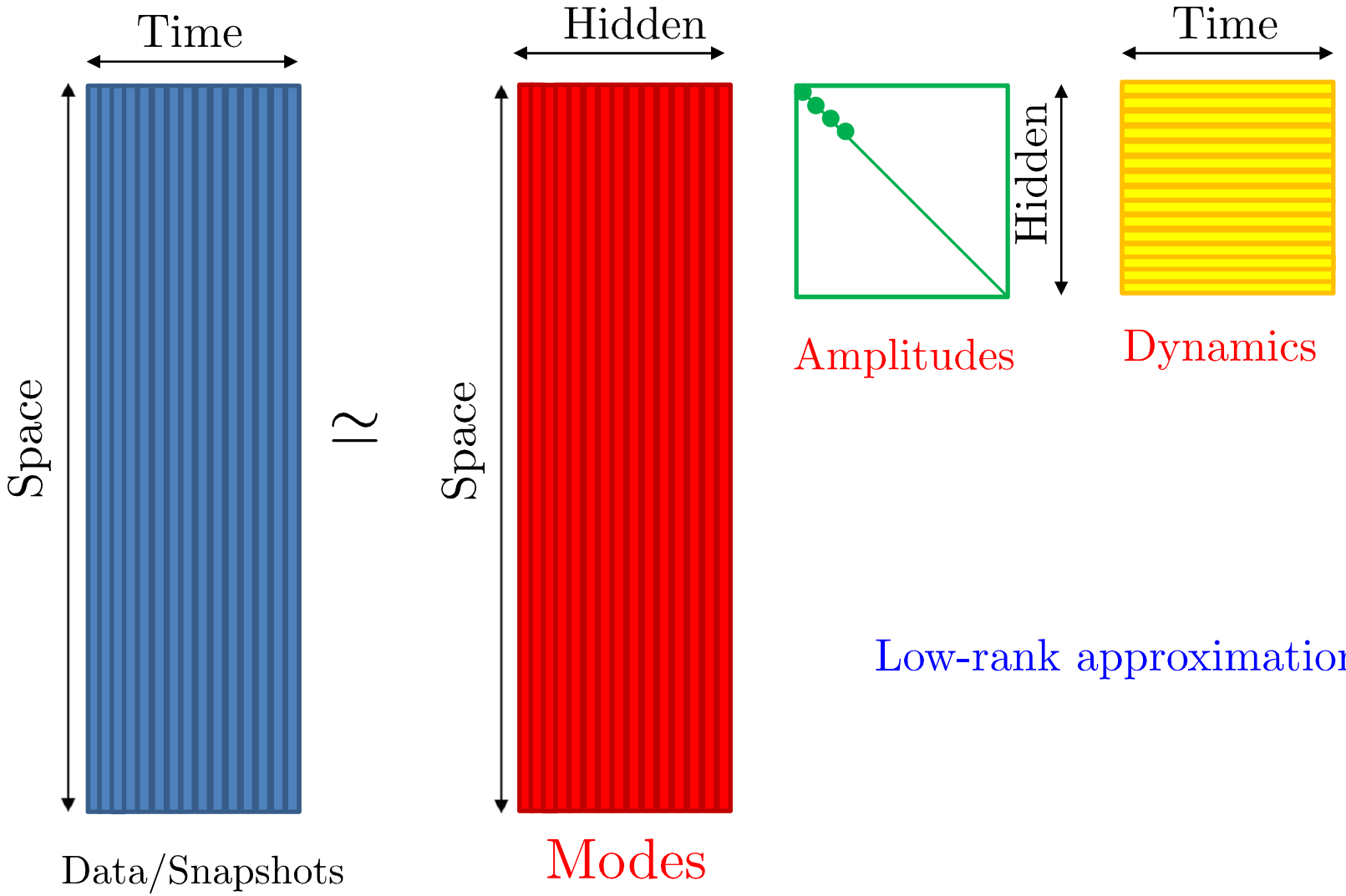



Thanks P. Schmid for the inspiration !

# Data analysis as a matrix decomposition



# Model reduction: exploit the redundancy




Low-rank approximation

# Snapshot Data Matrix

Vectorial case ($n_c$ components)

$$\boldsymbol{u} = (u_1, \cdots, u_{n_c}) \ ; \ \boldsymbol{x} = (x_1, \cdots, x_{n_x}) \ ; \ \boldsymbol{t} = (t_1, \cdots, t_{N_t}) \ ; \ N_x = n_x \times n_c$$

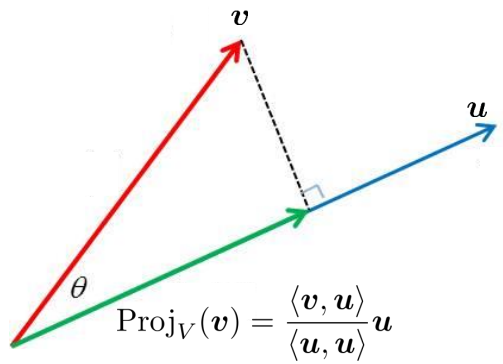
$$S = \left(\begin{array}{c|c|c|c|c}
u_1(x_1,t_1) & u_1(x_1,t_2) & \cdots & u_1(x_1,t_{N_t-1}) & u_1(x_1,t_{N_t}) \\
u_2(x_1,t_1) & u_2(x_1,t_2) & \cdots & u_2(x_1,t_{N_t-1}) & u_2(x_1,t_{N_t}) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
u_{n_c}(x_1,t_1) & u_{n_c}(x_1,t_2) & \cdots & u_{n_c}(x_1,t_{N_t-1}) & u_{n_c}(x_1,t_{N_t}) \\
\hline
u_1(x_2,t_1) & u_1(x_2,t_2) & \cdots & u_1(x_2,t_{N_t-1}) & u_1(x_2,t_{N_t}) \\
u_2(x_2,t_1) & u_2(x_2,t_2) & \cdots & u_2(x_2,t_{N_t-1}) & u_2(x_2,t_{N_t}) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
u_{n_c}(x_2,t_1) & u_{n_c}(x_2,t_2) & \cdots & u_{n_c}(x_2,t_{N_t-1}) & u_{n_c}(x_2,t_{N_t}) \\
\hline
\vdots & \vdots & \vdots & \vdots & \vdots \\
\hline
u_1(x_{N_x},t_1) & u_1(x_{N_x},t_2) & \cdots & u_1(x_{N_x},t_{N_t-1}) & u_1(x_{N_x},t_{N_t}) \\
u_2(x_{N_x},t_1) & u_2(x_{N_x},t_2) & \cdots & u_2(x_{N_x},t_{N_t-1}) & u_2(x_{N_x},t_{N_t}) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
u_{n_c}(x_{N_x},t_1) & u_{n_c}(x_{N_x},t_2) & \cdots & u_{n_c}(x_{N_x},t_{N_t-1}) & u_{n_c}(x_{N_x},t_{N_t})
\end{array}\right)$$

with $S \in \mathbb{R}^{N_x \times N_t}$.

# Orthogonal projection on a subspace $V$

- Let $V$ be a one dimensional subspace spanned by $\boldsymbol{u}$. Given an arbitrary vector $\boldsymbol{v}$ not in $V$, we can project it onto $V$ by:

$$\mathrm{Proj}_V(\boldsymbol{v}) = \frac{\langle \boldsymbol{v}, \boldsymbol{u} \rangle}{\langle \boldsymbol{u}, \boldsymbol{u} \rangle} \boldsymbol{u}$$



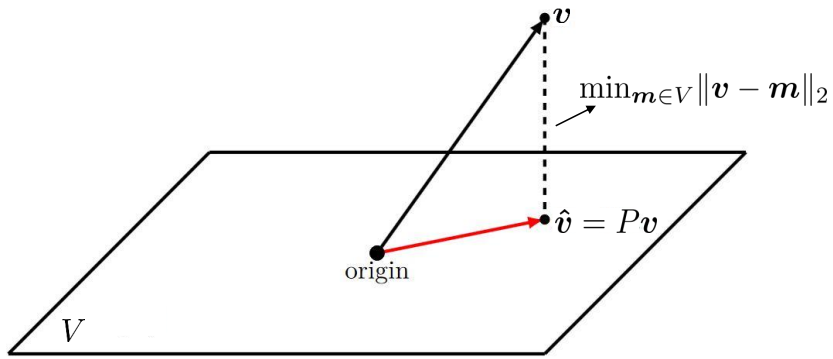

- Let $V$ be a subspace of dimension $k$. If the orthogonal vectors $\boldsymbol{u}_i$, $i = 1, \cdots, k$ is a basis of $V$, then we write:

$$V = \mathrm{span}(\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k)$$

$$\mathrm{Proj}_V(\boldsymbol{v}) = \sum_{i=1}^{k} \frac{\langle \boldsymbol{v}, \boldsymbol{u}_i \rangle}{\langle \boldsymbol{u}_i, \boldsymbol{u}_i \rangle} \boldsymbol{u}_i = \frac{\langle \boldsymbol{v}, \boldsymbol{u}_1 \rangle}{\langle \boldsymbol{u}_1, \boldsymbol{u}_1 \rangle} \boldsymbol{u}_1 + \cdots + \frac{\langle \boldsymbol{v}, \boldsymbol{u}_k \rangle}{\langle \boldsymbol{u}_k, \boldsymbol{u}_k \rangle} \boldsymbol{u}_k.$$

# Closest point theorem

$$\boxed{\min_{\boldsymbol{m}\in V}\|\boldsymbol{v}-\boldsymbol{m}\|_2 = \|\boldsymbol{v}-P\boldsymbol{v}\|_2}$$




Dem: If $\hat{\boldsymbol{v}} = P\boldsymbol{v}$, then $\hat{\boldsymbol{v}} - \boldsymbol{m} \in V$ for all $\boldsymbol{m} \in V$ and

$$\boldsymbol{v} - \hat{\boldsymbol{v}} = (\boldsymbol{I} - P)\,\boldsymbol{v} \in V^{\perp}$$

so $(\hat{\boldsymbol{v}} - \boldsymbol{m}) \perp (\boldsymbol{v} - \hat{\boldsymbol{v}})$. The Pythagorean theorem says $\|\boldsymbol{x}+\boldsymbol{y}\|^2 = \|\boldsymbol{x}\|^2 + \|\boldsymbol{y}\|^2$ whenever $\boldsymbol{x} \perp \boldsymbol{y}$, and hence

$$\|\boldsymbol{v}-\boldsymbol{m}\|_2^2 = \|\boldsymbol{v}-\hat{\boldsymbol{v}}+\hat{\boldsymbol{v}}-\boldsymbol{m}\|_2^2 = \|\boldsymbol{v}-\hat{\boldsymbol{v}}\|_2^2 + \|\hat{\boldsymbol{v}}-\boldsymbol{m}\|_2^2 \geq \|\boldsymbol{v}-\hat{\boldsymbol{v}}\|_2^2.$$

# The POD basis problem in $\mathbb{R}^{N_x}$



- Find a $k$ dimensional subspace $V_k^{\mathrm{POD}} = \mathrm{span}\,(\boldsymbol{\Phi}_1, \cdots, \boldsymbol{\Phi}_k)$ s.t.

$$\min_{\Pi_{\mathrm{POD}}} \sum_{i=1}^{N_t} \|\boldsymbol{u}(\boldsymbol{x}, t_i) - \Pi_{\mathrm{POD}}\boldsymbol{u}(\boldsymbol{x}, t_i)\|^2_{\mathbb{R}^{N_x}} \qquad s.t. \quad \|\boldsymbol{\Phi}_k\|^2_{\mathbb{R}^{N_x}} = 1$$

or equivalently

$$\max_{\Pi_{\mathrm{POD}}} \sum_{i=1}^{N_t} \|\Pi_{\mathrm{POD}}\boldsymbol{u}(\boldsymbol{x}, t_i)\|^2_{\mathbb{R}^{N_x}} \qquad s.t. \quad \|\boldsymbol{\Phi}_k\|^2_{\mathbb{R}^{N_x}} = 1$$

with $\Pi_{\mathrm{POD}}$: orthogonal projector on $V_k^{\mathrm{POD}}$, and

$$\Pi_{\mathrm{POD}}\boldsymbol{u}(\boldsymbol{x}, t_i) = \sum_{j=1}^{k} \left(\boldsymbol{u}(\boldsymbol{x}, t_i), \boldsymbol{\Phi}_j(\boldsymbol{x})\right)_{\mathbb{R}^{N_x}} \boldsymbol{\Phi}_{\boldsymbol{j}}(\boldsymbol{x}) = U_k U_k^{\mathrm{H}} \boldsymbol{u}(\boldsymbol{x}, t_i).$$

- Solutions:

$$\left(SS^{\mathsf{T}}\right)\boldsymbol{\Phi}_i = \lambda_i \boldsymbol{\Phi}_i, \quad i = 1, \cdots, k, \ \ i.e. \ \boxed{V_k^{\mathrm{POD}} \equiv U_k}$$

# The POD basis problem with a weighted inner product

- Weighted inner product: $W$ symmetric, positive semidefinite[1]

$$(\boldsymbol{\psi}_1, \boldsymbol{\psi}_2)_W = \boldsymbol{\psi}_1^{\mathsf{T}} \underbrace{W}_{W^{1/2}W^{1/2}} \boldsymbol{\psi}_2 = \left(W^{1/2}\boldsymbol{\psi}_1, W^{1/2}\boldsymbol{\psi}_2\right)_{\mathbb{R}^{N_x}}$$

- Find a $k$ dimensional subspace $V_k^{\mathrm{POD}} = \mathrm{span}\left(\boldsymbol{\Phi}_1, \cdots, \boldsymbol{\Phi}_k\right)$ s.t.

$$\max_{\Pi_{\mathrm{POD}}} \sum_{i=1}^{N_t} \|\Pi_{\mathrm{POD}}\boldsymbol{u}(\boldsymbol{x}, t_i)\|_W^2 \qquad s.t. \quad \|\boldsymbol{\Phi}_k\|_W^2 = 1$$

- Solutions:

$$\left(\tilde{S}\tilde{S}^{\mathsf{T}}\right)\tilde{\boldsymbol{\Phi}}_i = \lambda_i \tilde{\boldsymbol{\Phi}}_i, \quad i = 1, \cdots, k$$

with

$$\boxed{\tilde{S} = W^{1/2}S} \qquad \text{and} \qquad \boxed{\tilde{\boldsymbol{\Phi}}_i = W^{1/2}\boldsymbol{\Phi}_i}$$

[1] A symmetric real $n \times n$ matrix $A$ is called positive semidefinite if $\boldsymbol{x}^T A\boldsymbol{x} \geq 0$ for all $\boldsymbol{x} \in \mathbb{R}^n$

# POD expansion

## Quantum harmonic oscillator

- Schrodinger equation with a parabolic potential

$$\jmath u_t + \frac{1}{2} u_{xx} - \frac{V(x)}{2} u = 0 \text{ with } V(x) = x^2 \text{ and } u \longrightarrow 0 \text{ as } x \longrightarrow \pm\infty \quad (1)$$

- Solution ansatz of the form

$$u(x,t) = a_k \psi_k(x) \exp\left[-\jmath\left(k + 1/2\right) t\right]$$

- Analytic solution given by

$$u(x,t) = \sum_{k=0}^{+\infty} a_k \left(2^k\, k!\, \sqrt{\pi}\right)^{-1/2} \exp\left(-x^2/2\right) H_k(x) \exp\left[-\jmath\left(k + 1/2\right) t\right]$$

where $H_k(x)$ are the Gaussian-Hermite functions.

- $a_k = \langle u(x,t), \psi_k \rangle$ with

$$u(x,0) = \exp\left(-0.2\left(x - x_0^2\right)\right) \quad \text{Gaussian pulse centered at } x = x_0$$

for $x_0 = 0$ and $x_0 = 1$.

# POD expansion

## Quantum harmonic oscillator

- `jupyter notebook CH11_SEC02_1_HarmonicOscillator.ipynb`
- Equation solved with a Fourier mode expansion. See appendix on Fourier decomposition.
- Rewriting (1) in the Fourier domain, we get:

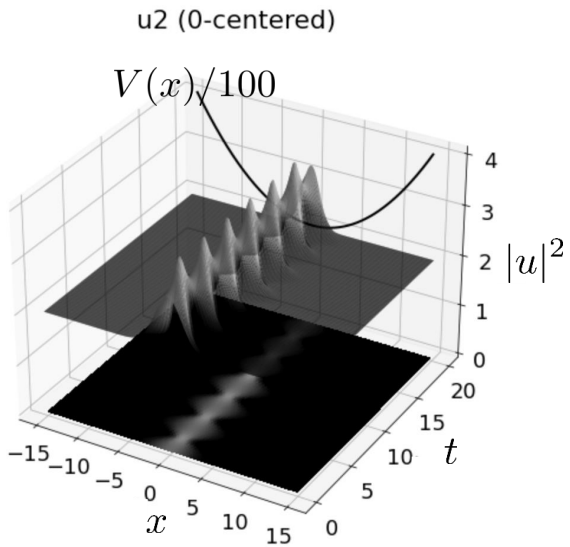
$$\widehat{u}_t = -\frac{\jmath}{2}k^2\widehat{u} - \frac{\jmath}{2}\widehat{Vu}$$

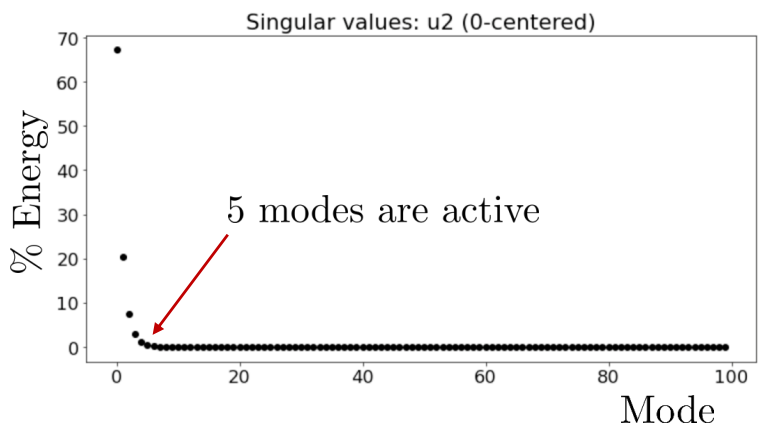
See Fourier Appendix for details.

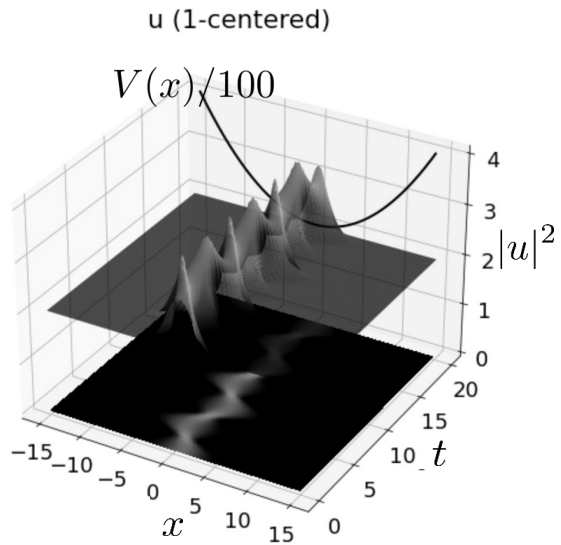
# POD expansion

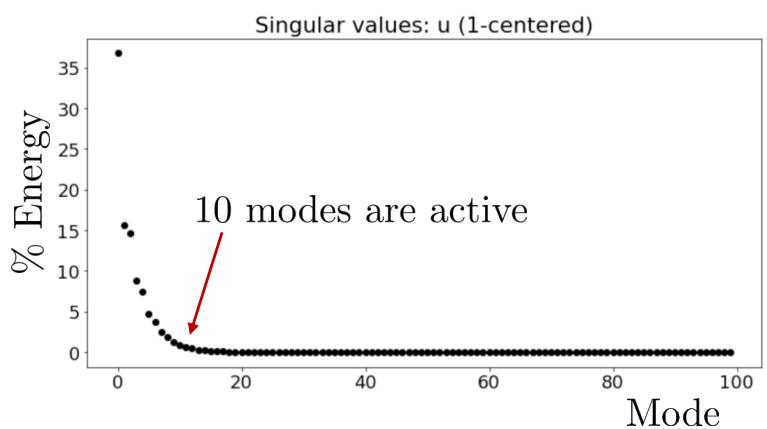
## Quantum harmonic oscillator

Dynamics and singular values.



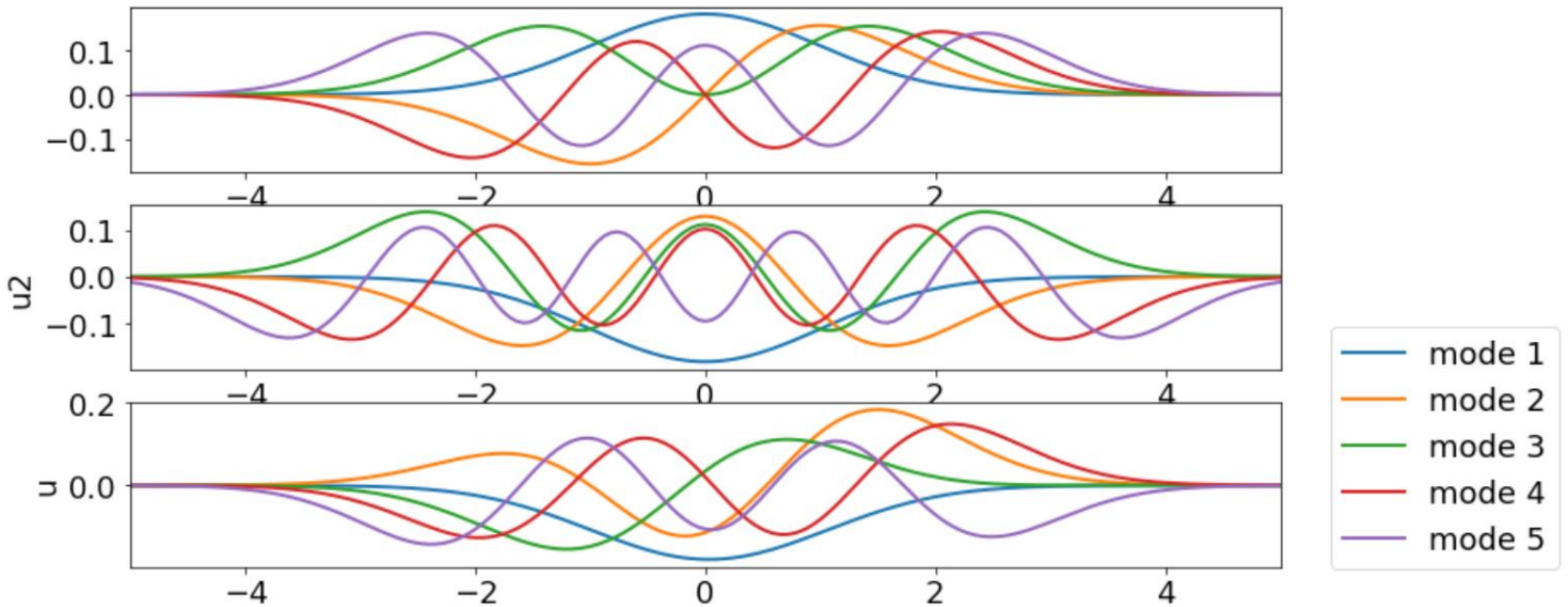



# POD expansion

## Quantum harmonic oscillator

First five modes of the quantum harmonic oscillator.




Top: Gauss Hermite functions
Middle: Symmetric initial condition $x_0 = 0$
Bottom: Asymmetric initial condition $x_0 = 1$

A purely snapshot-based method is capable of reproducing the nearly ideal basis set for the harmonic oscillator.

# Hermite polynomials I

- The "physicist's Hermite polynomials" are given by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

- Orthogonality. Let $w(x) = e^{-x^2}$, then

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) w(x) dx = \sqrt{\pi} 2^n n! \delta_{mn},$$

where $\delta_{mn}$ denotes the Kronecker delta.

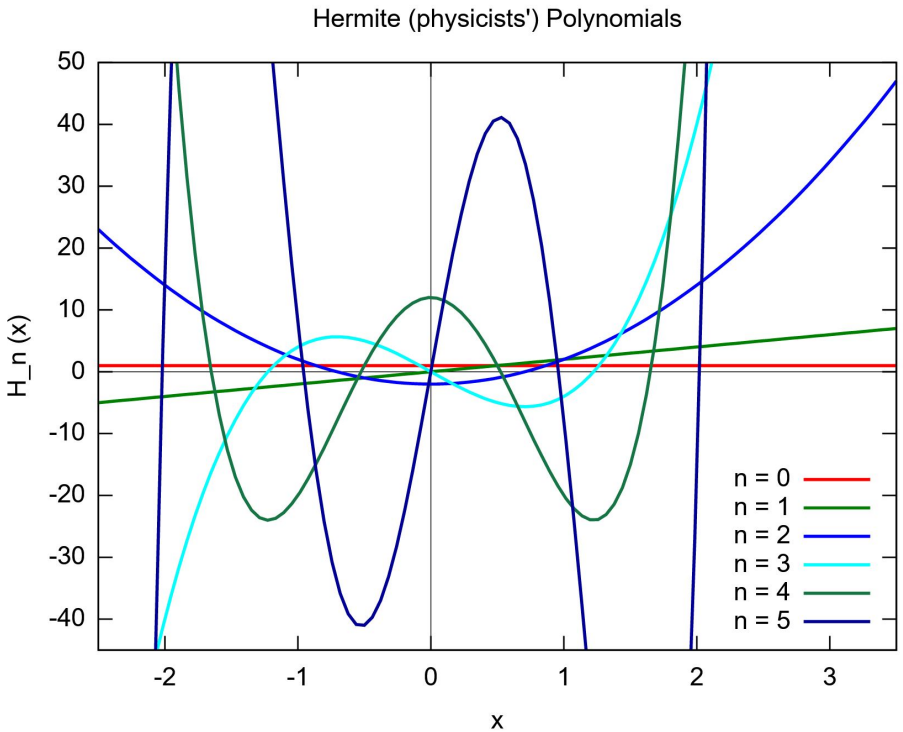
- A set of formulas

$$H_{n+1}(x) = 2xH_n(x) - H_n'(x)$$
$$H_n'(x) = 2nH_{n-1}(x)$$

# Hermite polynomials II

The first eleven physicist's Hermite polynomials are:

$$H_0(x) = 1,$$
$$H_1(x) = 2x,$$
$$H_2(x) = 4x^2 - 2,$$
$$H_3(x) = 8x^3 - 12x,$$
$$H_4(x) = 16x^4 - 48x^2 + 12,$$
$$H_5(x) = 32x^5 - 160x^3 + 120x$$



# POD for Partial Differential Equations



- Consider a system of nonlinear PDEs given by

$$\boldsymbol{u}_t = \boldsymbol{N}\left(\boldsymbol{u}, \boldsymbol{u}_x, \boldsymbol{u}_{xx}, \cdots, \boldsymbol{x}, t; \boldsymbol{\Theta}\right) \quad \text{with } \boldsymbol{x} \in \Omega \text{ and } t \in [0; T] \tag{2}$$

- Consider a **separation of variables** solution ansatz of the form

$$\begin{aligned} \boldsymbol{u}(\boldsymbol{x}, t) &= \sum_{k=1}^{n} a_k(t) \boldsymbol{\Phi}_k(\boldsymbol{x}) \\ &\simeq \boldsymbol{\Phi} \boldsymbol{a}(t) \quad \text{where} \end{aligned}$$

$$\boldsymbol{\Phi} = \begin{bmatrix} | & | & \cdots & | \\ \boldsymbol{\Phi}_1 & \boldsymbol{\Phi}_2 & \cdots & \boldsymbol{\Phi}_n \\ | & | & \cdots & | \end{bmatrix} \text{ and } \boldsymbol{a}(t) = \begin{bmatrix} a_1(t) \\ a_2(t) \\ | \\ a_n(t) \end{bmatrix}$$

with $n$ large enough to represent correctly the dynamics.

# POD for Partial Differential Equations

## POD Galerkin

1. Insert the POD ansatz into (2)

$$\sum_{k=1}^{n} \boldsymbol{\Phi}_k(\boldsymbol{x}) \frac{da_k(t)}{dt} = \boldsymbol{N}\left(\sum_k a_k \boldsymbol{\Phi}_k, \sum_k a_k \left(\boldsymbol{\Phi}_k\right)_x, \sum_k a_k \left(\boldsymbol{\Phi}_k\right)_{xx}, \cdots, \boldsymbol{x}, t; \boldsymbol{\Theta}\right)$$

2. Take the inner product (function space) with $\boldsymbol{\Phi}_i, i = 1, \cdots, n$, *i.e.*

$$\frac{da_k}{dt} = \left(\boldsymbol{N}\left(\sum_k a_k \boldsymbol{\Phi}_k, \sum_k a_k \left(\boldsymbol{\Phi}_k\right)_x, \sum_k a_k \left(\boldsymbol{\Phi}_k\right)_{xx}, \cdots, \boldsymbol{x}, t; \boldsymbol{\Theta}\right), \boldsymbol{\Phi}_i\right)_\Omega$$

where by construction

$$\left(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_k\right)_\Omega = \int_\Omega \boldsymbol{\Phi}_i \cdot \boldsymbol{\Phi}_k^* \, \mathrm{d}\boldsymbol{x} = \delta_{ik} = \begin{cases} 0, & \text{if } i \neq k \\ 1, & \text{otherwise} \end{cases}$$

# Non linear Schrodinger equation



$$\jmath u_t + \frac{1}{2}u_{xx} + |u|^2 u = 0 \quad \text{with } u \longrightarrow 0 \text{ as } x \longrightarrow \pm\infty \tag{3}$$

- Equation solved with a Fourier mode expansion. Rewriting (3) in the Fourier domain, we get:

$$\widehat{u}_t = -\frac{\jmath}{2}k^2\widehat{u} + \jmath\widehat{|u|^2 u}$$

- Solve (3) with $u(x,0) = N\,\mathrm{sech}(x)$ (soliton initial conditions) where

$$\mathrm{sech}(x) = \frac{1}{\cosh(x)} = \frac{2}{e^x + e^{-x}} = \frac{2e^x}{e^{2x}+1} \quad \text{(hyperbolic secant)}$$

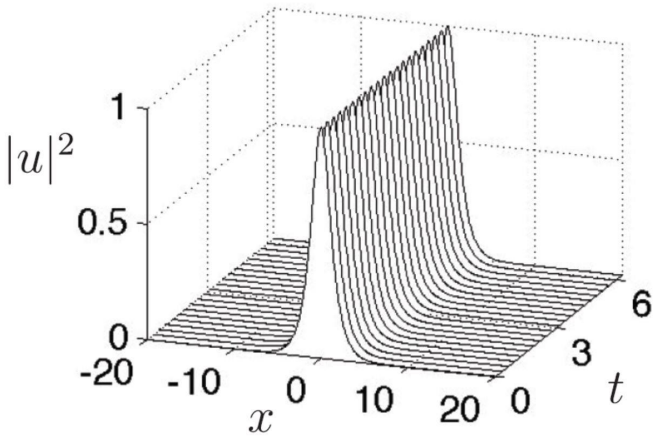
- `jupyter notebook CH11_SEC03_1_NonlinearSchrodinger.ipynb`

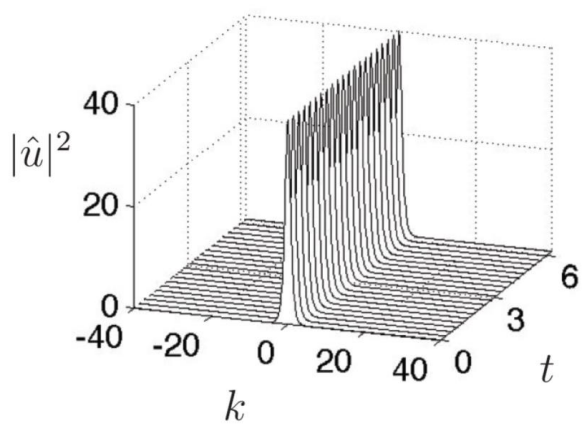
1. Solve (3)
2. Apply the SVD decomposition
3. Apply the Galerkin projection for $N = 1$ and $N = 2$ (black board).

# Non linear Schrodinger equation

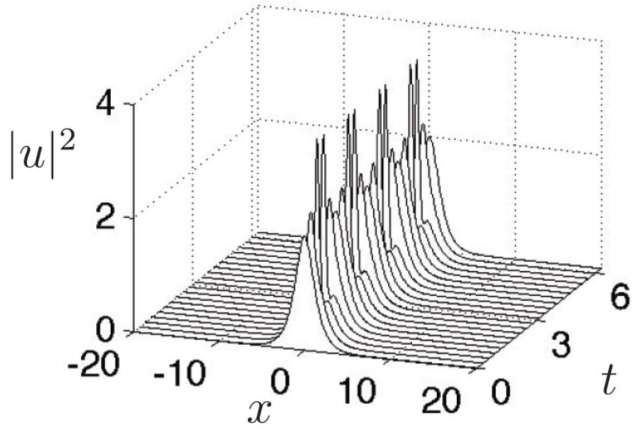
## POD approximation

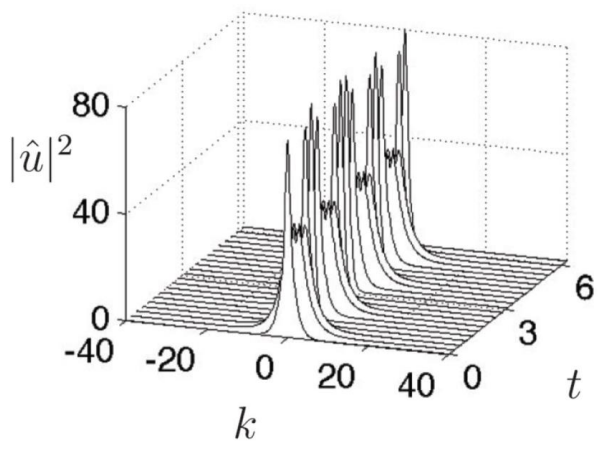
$N = 1$
50 Fourier modes necessary




$N = 2$
200 Fourier modes necessary

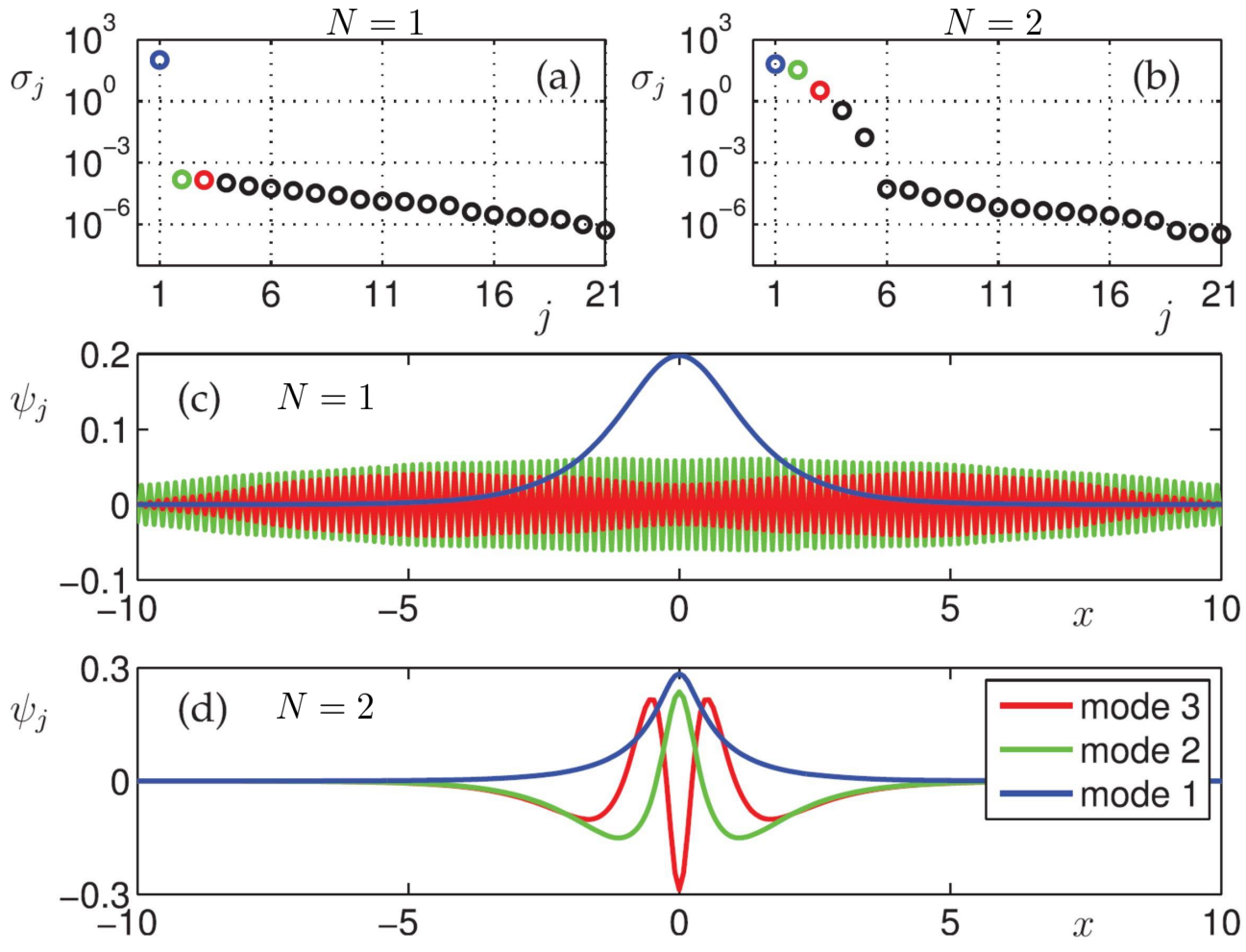



Is is really necessary to keep 50 or 200 degrees of freedom to describe the soliton dynamics.

# Non linear Schrodinger equation

## POD approximation




- $N = 1$: one mode is necessary
- $N = 2$: two modes are necessary for representing 95% of the variance.

# Non linear Schrodinger equation

## Galerkin projection

- Galerkin projection for $N = 1$. A single mode is kept.

$$u(x,t) = a(t)\phi(x)$$

Plugging this into (3) yields:

$$\jmath a_t \phi + \frac{1}{2} a \phi_{xx} + |a|^2 a |\phi|^2 \phi = 0$$

Taking the inner product with $\phi$ gives

$$\jmath a_t + \frac{\alpha}{2} a + \beta |a|^2 a = 0 \tag{4}$$

where

$$\alpha = \frac{(\phi, \phi_{xx})_\Omega}{(\phi,\phi)_\Omega} \quad \beta = \frac{\left(\phi, |\phi|^2 \phi\right)_\Omega}{(\phi,\phi)_\Omega}$$

# Non linear Schrodinger equation



(4) can be solved explicitly to yield

$$a(t) = a(0) \exp\left[\jmath\left(\frac{\alpha}{2}t + \beta|a(0)|^2 t\right)\right]$$

To find $a(0)$, recall that

$$u(x,0) = N\,\mathrm{sech}(x) = a(0)\phi(x)$$

Taking the inner product with $\phi$ gives $(N = 1)$

$$a(0) = \frac{(\phi, \mathrm{sech}(x))_\Omega}{(\phi,\phi)_\Omega}$$

Approximated solution given by:

$$u(x,t) = a(0)\left[\jmath\left(\frac{\alpha}{2}t + \beta|a(0)|^2 t\right)\right]\phi(x)$$

# Non linear Schrodinger equation



- Galerkin projection for $N = 2$. Two modes are kept.

$$u(x,t) = a_1(t)\phi_1(x) + a_2(t)\phi_2(x)$$

Plugging this into (3) yields:

$$\jmath\left(a_{1t}\phi_1 + a_{2t}\phi_2\right) + \frac{1}{2}\left(a_1\phi_{1xx} + a_2\phi_{2xx}\right) + \left(a_1\phi_1 + a_2\phi_2\right)^2\left(a_1^*\phi_1^* + a_2^*\phi_2^*\right) = 0$$

The cubic term gives:

$$|a_1|^2 a_1|\phi_1|^2\phi_1 + |a_2|^2 a_2|\phi_2|^2\phi_2 + 2|a_1|^2 a_2|\phi_1|^2\phi_2 + 2|a_2|^2 a_1|\phi_2|^2\phi_1 + a_1^2 a_2^*\phi_1^2\phi_2^* + a_2^2 a_1^*\phi_2^2\phi_1^*$$

We take the inner product with $\phi_1$ and $\phi_2$, and recall that these two modes are orthonormal.

# Non linear Schrodinger equation



We get the $2 \times 2$ nonlinear system of equations:

$$\jmath a_{1t} + \alpha_{11} a_1 + \alpha_{12} a_2 + \left(\beta_{111} |a_1|^2 + 2\beta_{211} |a_2|^2\right) a_1 + \left(\beta_{121} |a_1|^2 + 2\beta_{221} |a_2|^2\right) a_2 + \sigma_{121} a_1^2 a_2^* + \sigma_{211} a_2^2 a_1^* = 0$$

$$\jmath a_{2t} + \alpha_{21} a_1 + \alpha_{22} a_2 + \left(\beta_{112} |a_1|^2 + 2\beta_{212} |a_2|^2\right) a_1 + \left(\beta_{122} |a_1|^2 + 2\beta_{222} |a_2|^2\right) a_2 + \sigma_{122} a_1^2 a_2^* + \sigma_{212} a_2^2 a_1^* = 0$$

where

$$\alpha_{jk} = \frac{\left(\phi_{j\,xx}, \phi_k\right)_\Omega}{2\left(\phi_k, \phi_k\right)_\Omega} \qquad \beta_{jkl} = \frac{\left(|\phi_j|^2 \phi_k, \phi_l\right)_\Omega}{\left(\phi_l, \phi_l\right)_\Omega} \qquad \sigma_{jkl} = \frac{\left(\phi_j^2 \phi_k^{\mathrm{H}}, \phi_l\right)_\Omega}{\left(\phi_l, \phi_l\right)_\Omega}$$

Initial conditions

$$a_1(0) = \frac{\left(2\,\mathrm{sech}(x), \phi_1\right)_\Omega}{\left(\phi_1, \phi_1\right)_\Omega} \qquad a_2(0) = \frac{\left(2\,\mathrm{sech}(x), \phi_2\right)_\Omega}{\left(\phi_2, \phi_2\right)_\Omega}$$

# POD with symmetries

## Rotation: Spiral waves ($u$)

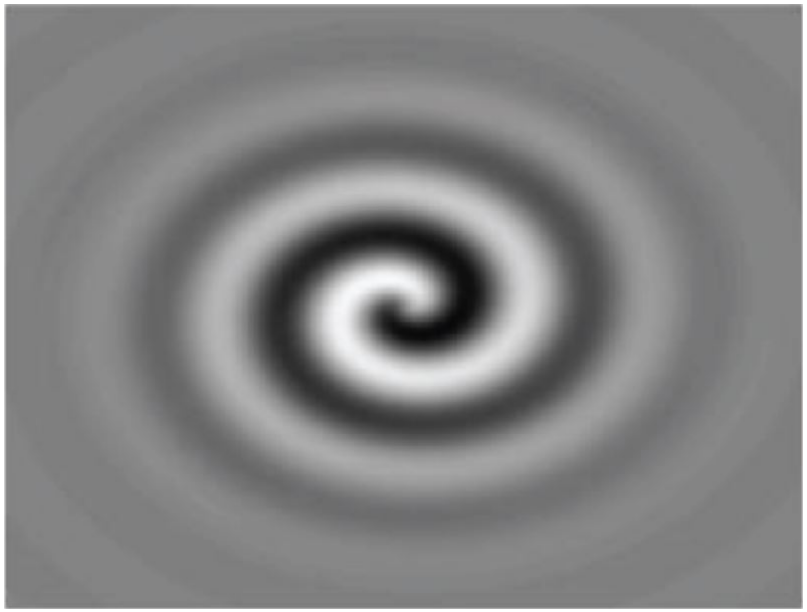
- A spiral wave centered at the origin can be defined as:

$$u(x,y) = \tanh\left[\sqrt{x^2+y^2}\cos\left(\angle(x+\jmath y) - \sqrt{x^2+y^2}\right)\right]$$

where $\angle z$ denotes the phase angle of $z$.

- To localize the spiral on a spatial domain, it is multiplied by a Gaussian centered at the origin. The function of interest is:

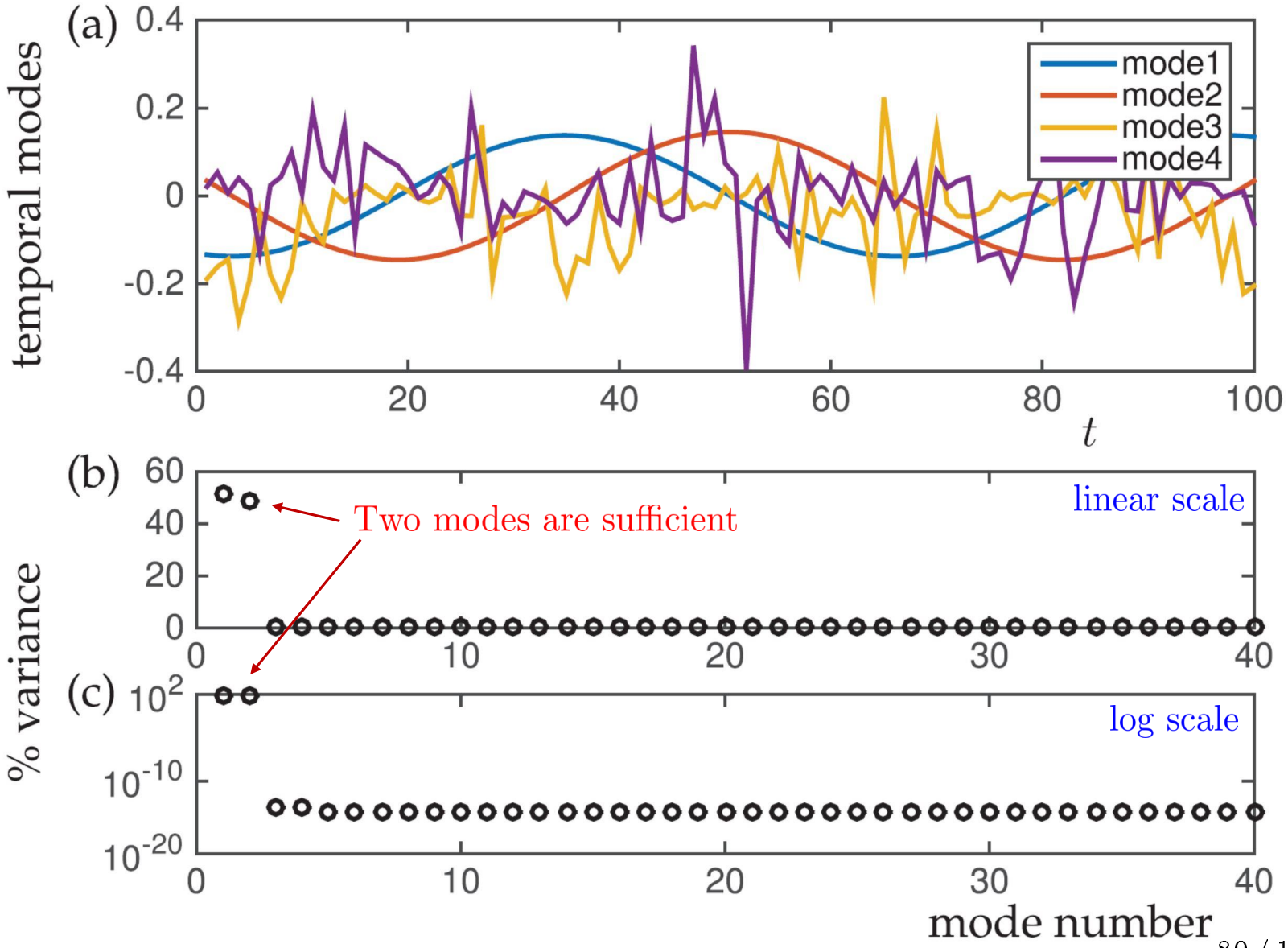
$$f(x,y) = u(x,y)\exp\left[-0.01(x^2+y^2)\right]$$



with $x \in [-20,20]$ and $y \in [-20,20]$.

# POD with symmetries

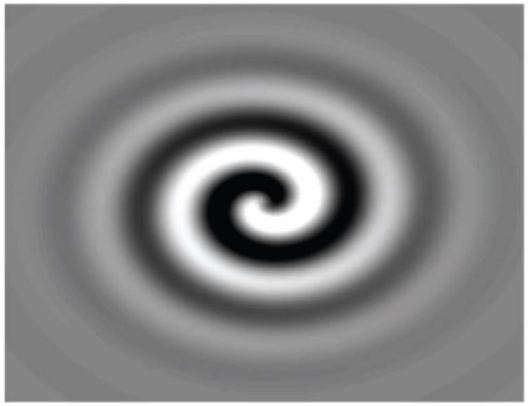
## Rotation: Spiral waves ($u$)

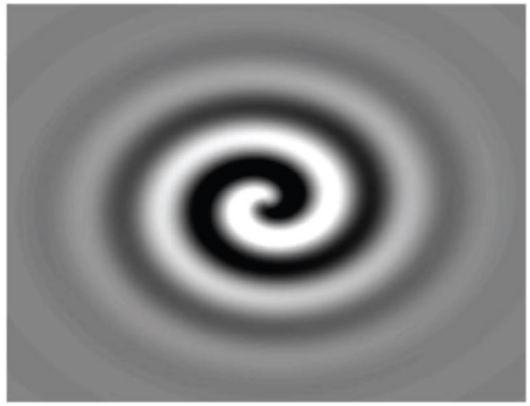


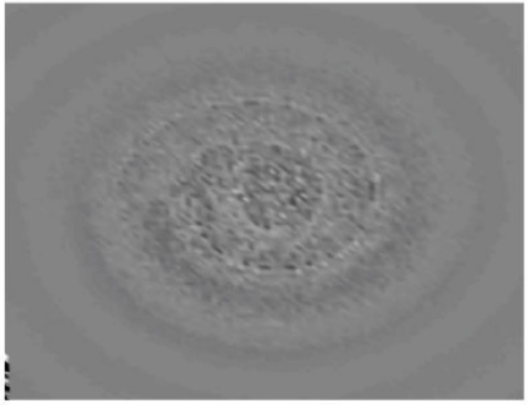
# POD with symmetries

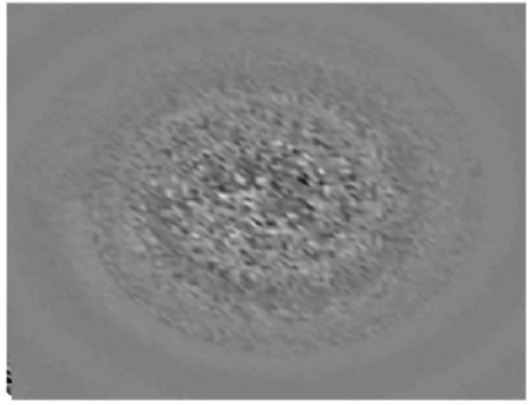
## Rotation: Spiral waves ($u$)

First four POD modes. The first two modes capture all the variance while the third and fourth are noisy.

$\psi_1$ 

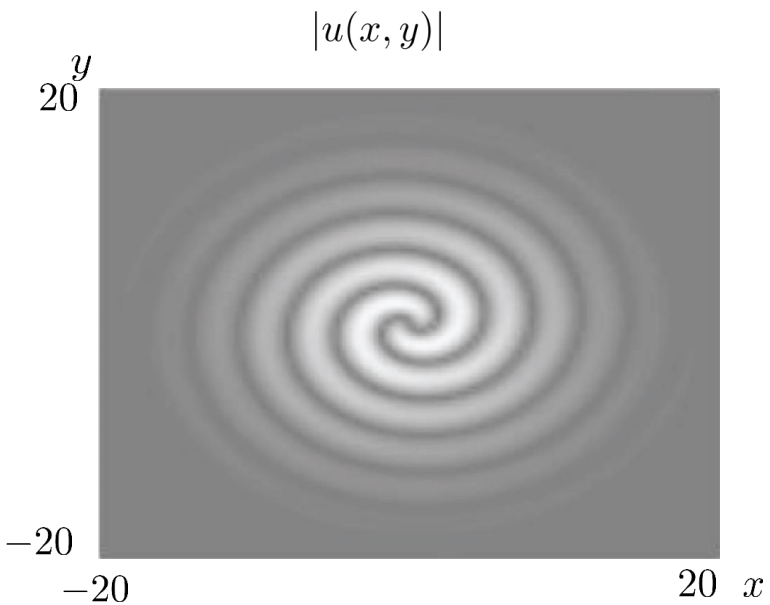
$\psi_2$ 

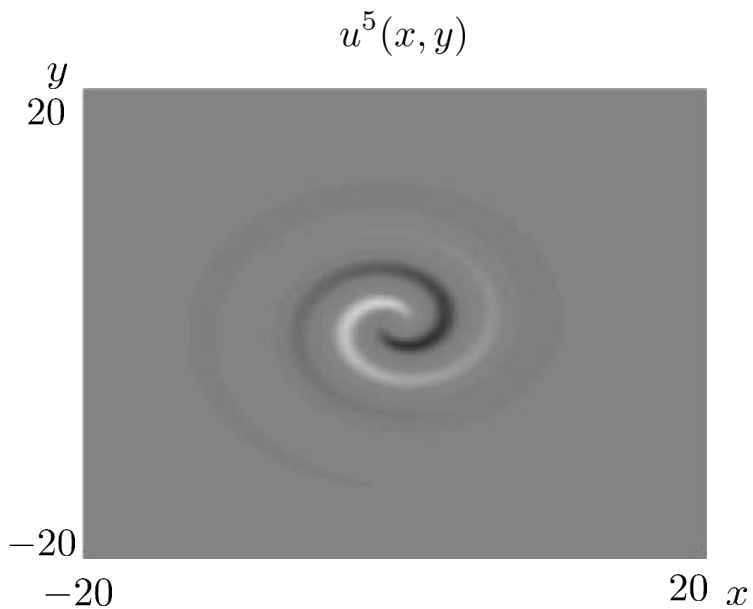
$\psi_3$ 

$\psi_4$ 

# POD with symmetries

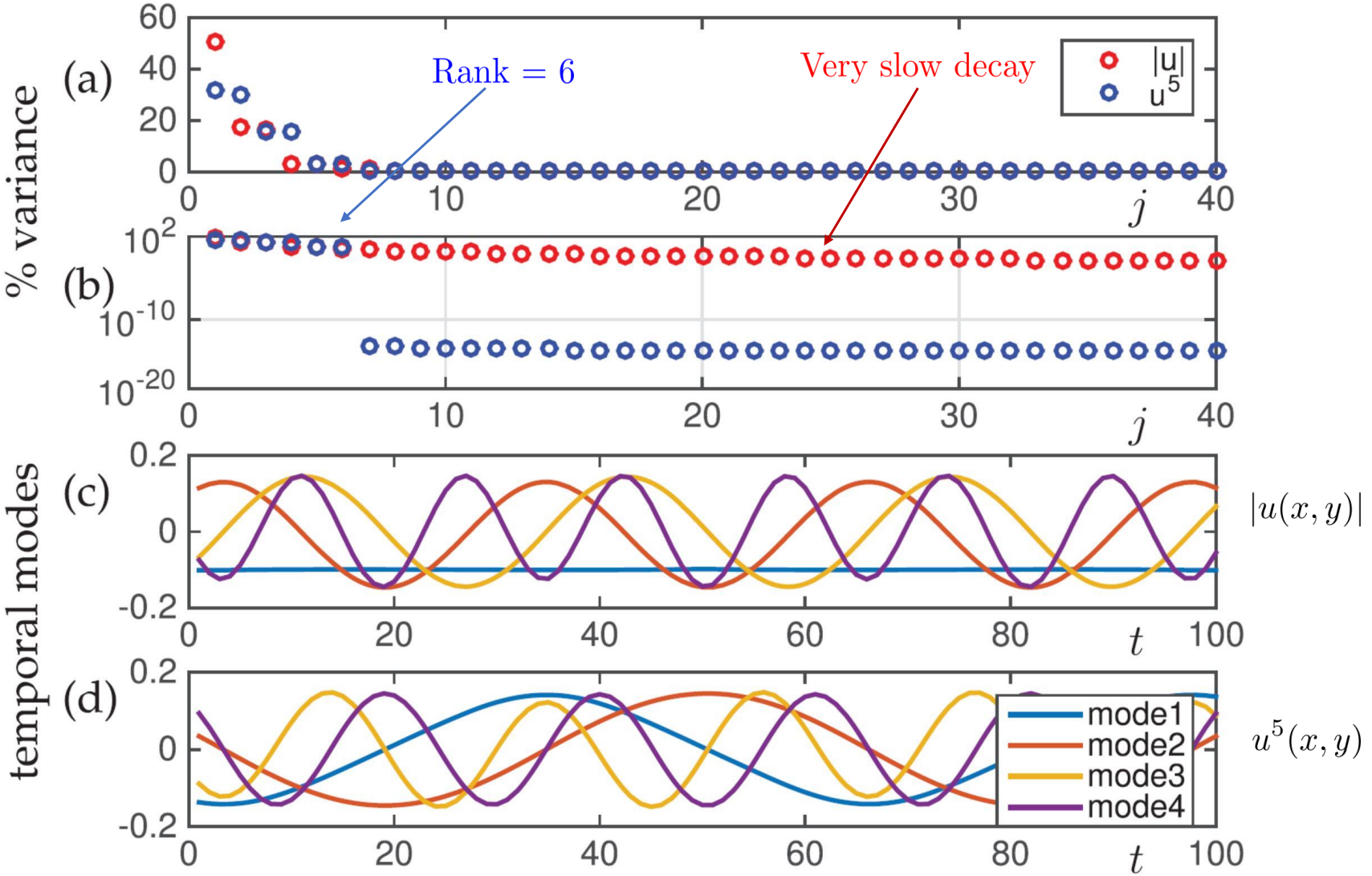
## Rotation: Spiral waves ($|u|$ and $u^5$)



# POD with symmetries

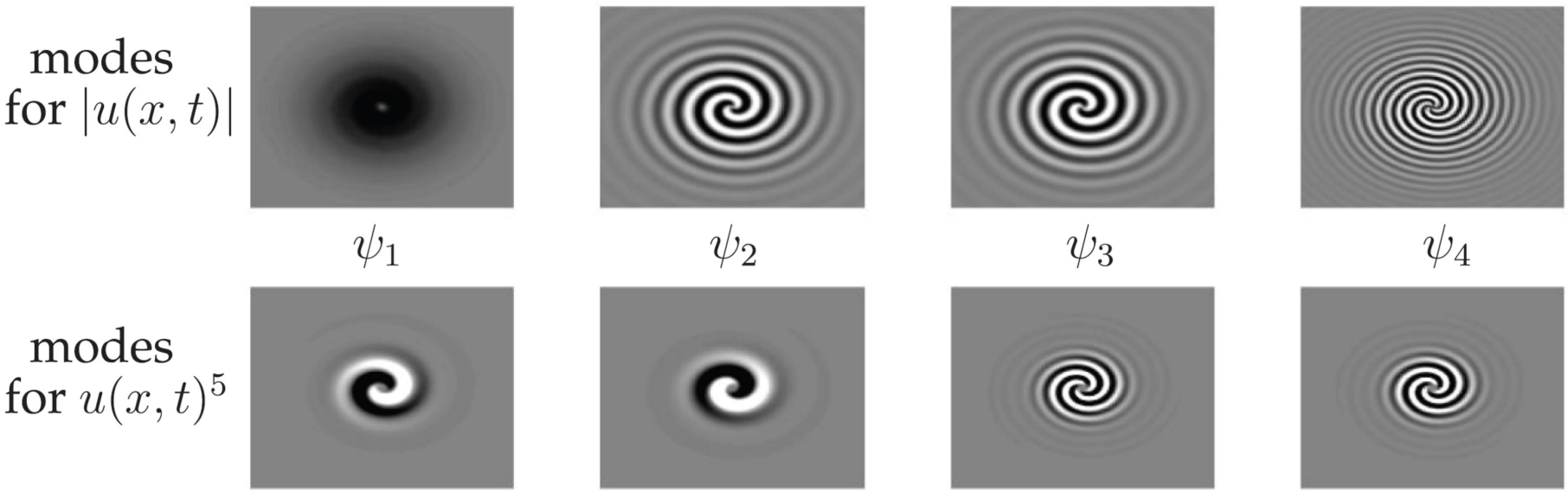
## Rotation: Spiral waves ($|u|$ and $u^5$)



# POD with symmetries

## Rotation: Spiral waves ($|u|$ and $u^5$)

First four POD modes.




Rotational invariance complicates the POD reduction procedure.

# POD with symmetries

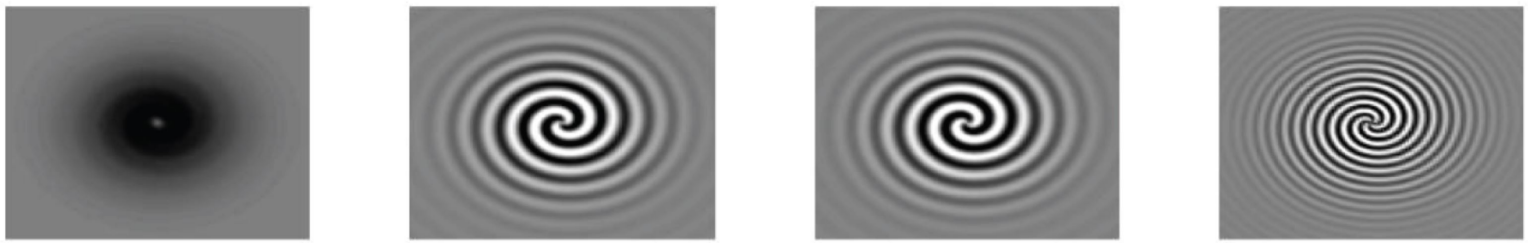
## Translation: Wave propagation

- Consider a Gaussian propagating with velocity $c$:

$$u(x,y) = \exp\left[-\left(x - ct + 15\right)\right] \quad \text{with} \quad x \in [-20, 20] \quad \text{and} \quad t \in [0, 10]$$

where $c = 3$.

modes for $|u(x,t)|$



$\psi_1$ $\psi_2$ $\psi_3$ $\psi_4$

modes for $u(x,t)^5$

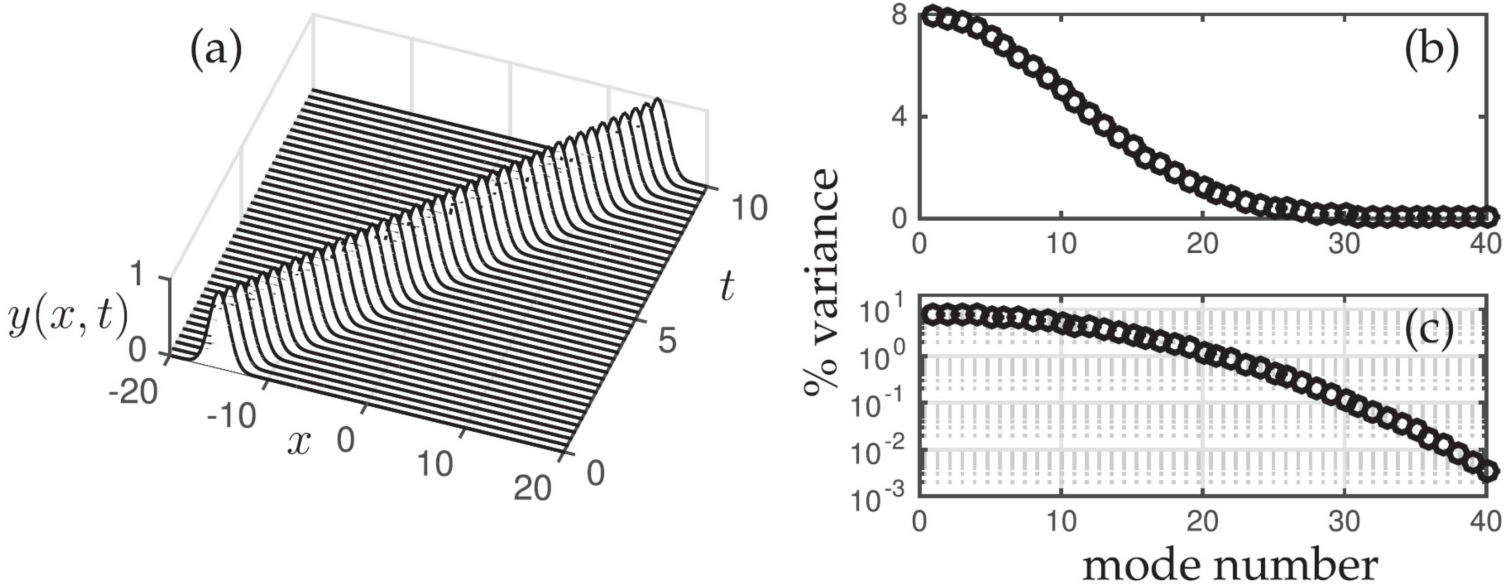
# POD with symmetries

## Translation: Wave propagation

- Consider a Gaussian propagating with velocity $c$:

$$u(x,y) = \exp\left[-\left(x - ct + 15\right)\right] \quad \text{with} \quad x \in [-20, 20] \quad \text{and} \quad t \in [0, 10]$$

where $c = 3$.

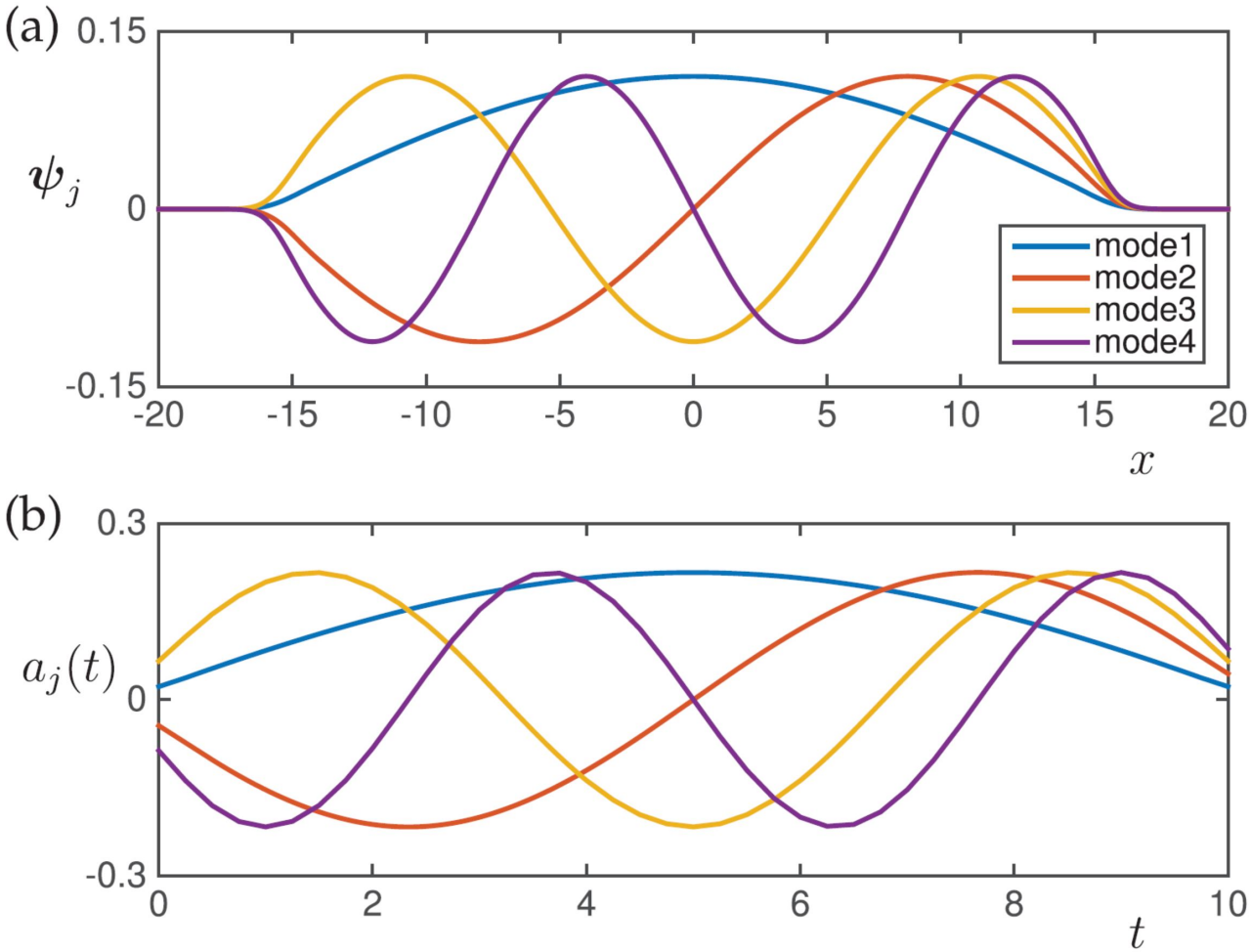



Very slow decay of the singular values.

# POD with symmetries

## Translation: Wave propagation

Spatial and temporal SVD modes. Modes are global, they appear to be Fourier modes.




This is due to the spatial invariance.

# Proper Orthogonal Decomposition

SVD/POD results in a hierarchy of modes based entirely on correlations and variances (energy) content.

# Dynamic Mode Decomposition (DMD) The Arnoldi approach

Objective: (Schmid)2010

Determine the leading eigenvectors/values of $A$, **the best-fit linear mapping** that relates two successive snapshots sampled uniformly.

## Hypothesis 1

$\exists A \in \mathbb{R}^{N_x \times N_x}$, linear operator, such that

$$\boldsymbol{u}_{k+1} = A\boldsymbol{u}_k, \quad \forall k \in [1, N-1] \quad \Longrightarrow$$

$$U_2^N = \{\boldsymbol{u}_2, \ldots, \boldsymbol{u}_N\} = AU_1^{N-1} = A\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_{N-1}\}$$

## Hypothesis 2

- $\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_{N-1}\}$ linearly independent.
- $\boldsymbol{u}_N = c_1\boldsymbol{u}_1 + \cdots + c_{N-1}\boldsymbol{u}_{N-1} + \boldsymbol{r}$.

Remark: Since $A$ is NOT known, the DMD algorithm resembles an Arnoldi algorithm.

# Dynamic Mode Decomposition (DMD) The Arnoldi approach

(Schmid)2010

## Combining Hyp. 1 and Hyp. 2

$$AU_1^{N-1} = U_1^{N-1}C + \boldsymbol{r}\boldsymbol{e}_{N-1}^{\mathsf{T}}$$

*Similarity transformation*

with $C$ the Companion matrix:

$$C = \begin{pmatrix} 0 & \dots & 0 & c_1 \\ 1 & \dots & 0 & c_2 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & 1 & c_{N-1} \end{pmatrix}$$

$c_i$ can be found by pseudo-inverse of $U_1^{N-1}$.

$$\boldsymbol{u}_N = U_1^{N-1}\boldsymbol{c} \Rightarrow \boxed{\boldsymbol{c} = \left(U_1^{N-1}\right)^{+}\boldsymbol{u}_N}$$

## Eigen-elements of A

If $C\boldsymbol{y}_i = \lambda_i \boldsymbol{y}_i$ then $A\boldsymbol{\Phi}_i \approx \lambda_i \boldsymbol{\Phi}_i$,

with $\boldsymbol{\Phi}_i = U_1^{N-1}\boldsymbol{y}_i$ defined up to a constant.

Reconstruction using Comp. matrix properties:

$$\boldsymbol{u}_k = \sum_{i=1}^{N-1} \boldsymbol{\Phi}_i \lambda_i^{k-1}$$

# DMD

## The SVD-based approach

- Use of pseudo-inverse

$$U_2^N = AU_1^{N-1} \quad \Longrightarrow \quad A = U_2^N \left(U_1^{N-1}\right)^+$$

- SVD of $U_1^{N-1}$

$$U_1^{N-1} = U_r \Sigma_r V_r^{\mathrm{H}} \quad \Longrightarrow \quad \left(U_1^{N-1}\right)^+ = V_r \Sigma_r^+ U_r^{\mathrm{H}}$$

- Similarity matrix of $A$

$$A = U_2^N V_r \Sigma_r^+ U_r^{\mathrm{H}} \quad \Longrightarrow \quad \boxed{U_r^{\mathrm{H}} A U_r = U_r^{\mathrm{H}} U_2^N V_r \Sigma_r^+ = S_r}$$

- Eigen-elements of $A$ (*Tu et al., 2014*)

$$\text{If} \quad S_r \boldsymbol{y}_i = \lambda_i \boldsymbol{y}_i \quad \text{then} \quad A\boldsymbol{\Phi}_i \approx \lambda_i \boldsymbol{\Phi}_i$$

with

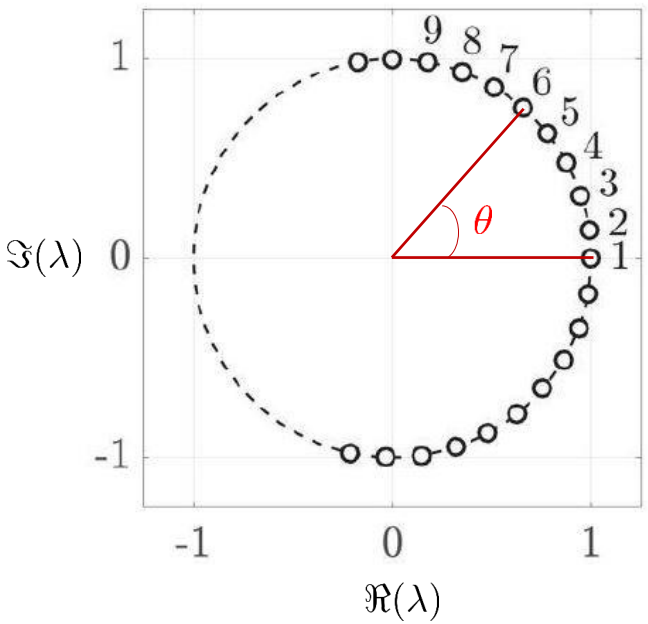
$$\boldsymbol{\Phi}_i = \lambda_i^{-1} U_2^N V_r \Sigma_r^+ \boldsymbol{y}_i$$

# DMD

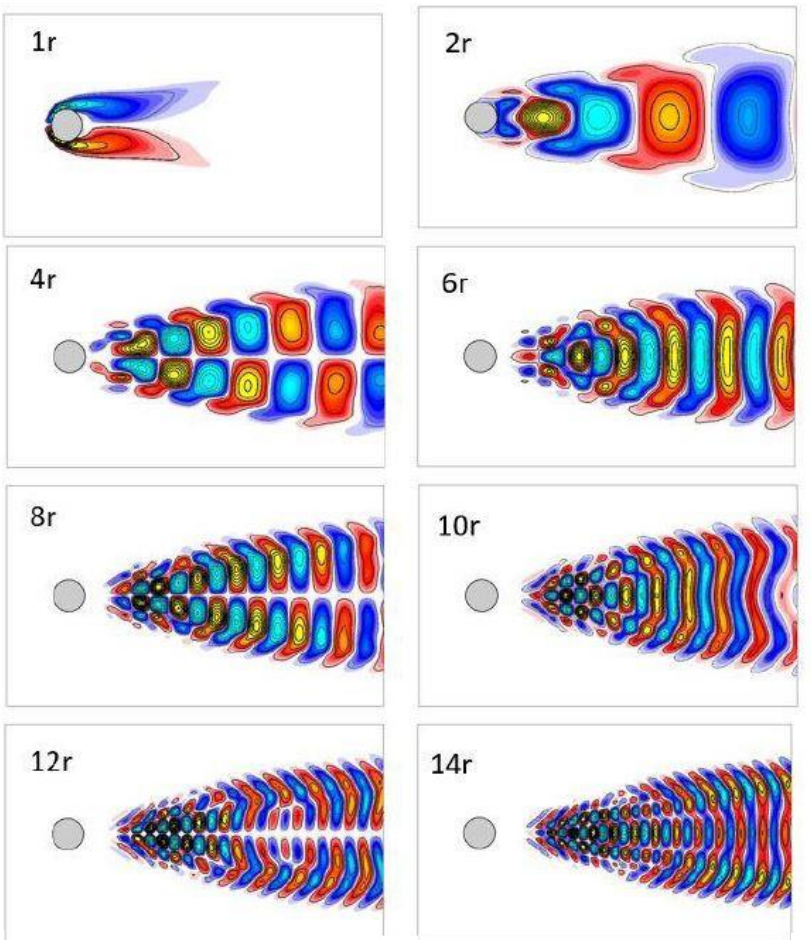
## Cylinder wake flow (DMD)

- See `jupyter notebook CH07_SEC02_DMD_Cylinder.ipynb` (Python)
- See also Kutz et al. (2016) for Matlab codes.

$\lambda = \Re(\lambda) + \jmath\Im(\lambda) = e^{\jmath\theta}$
$|\lambda| = 1$



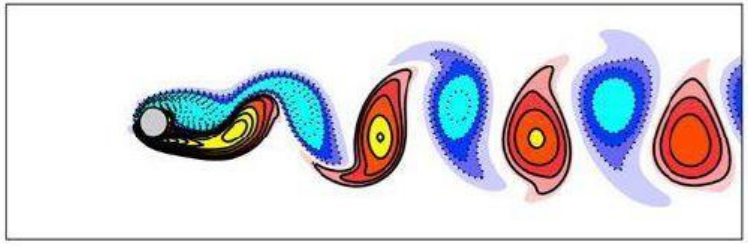

Each mode is associated with a particular eigenvalue with a particular frequency of oscillation $\Im(\lambda)$ and growth rate or decay rate $\Re(\lambda)$.

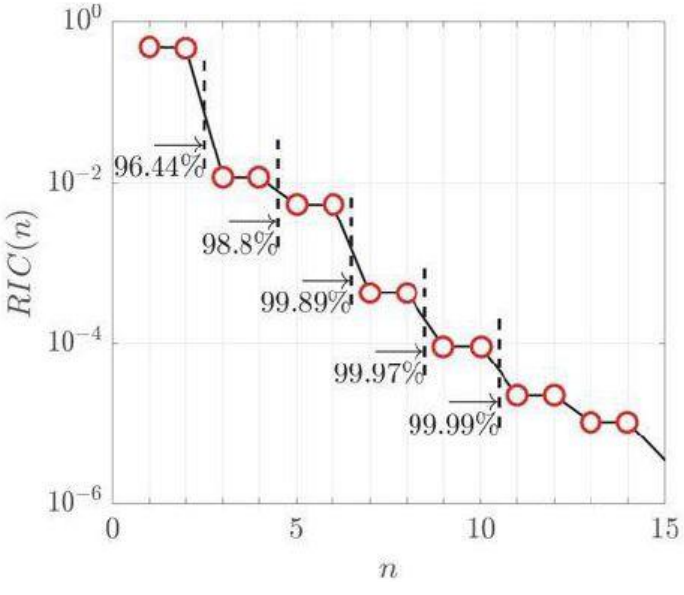


# DMD

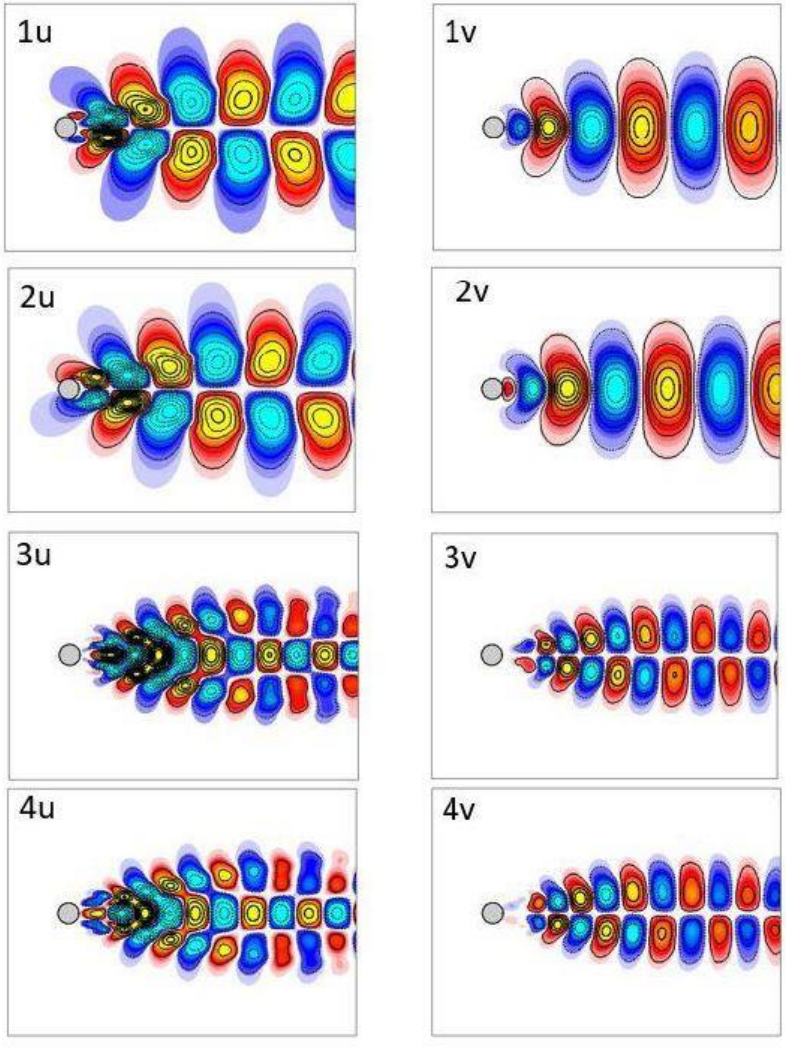
## Cylinder wake flow (POD)

- See Kutz et al. (2016) for Matlab codes.






Modes are ranked by energy.



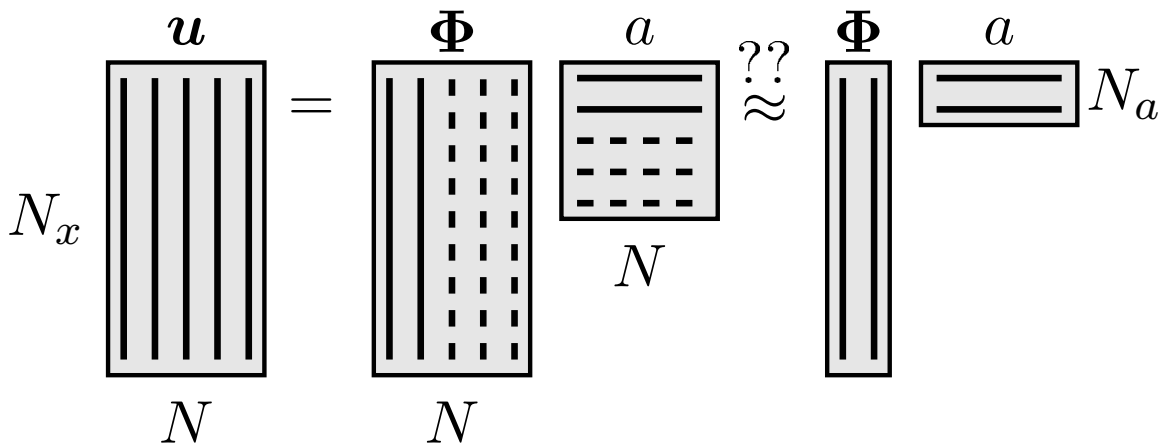
# DMD

## Modes' selection

### How to perform a truncation?

$$\boldsymbol{u}_k = \sum_{i=1}^{N-1} \boldsymbol{\Phi}_i(\boldsymbol{x}) a_i(t_k) \qquad \text{Complete basis.}$$

### Modes' selection




- POD / Balanced truncation: Modes sorted by eigenvalues.
- DMD: Choice not obvious!

# DMD

## Modes' selection

**How to perform a truncation in DMD?**

$$\boldsymbol{u}_k = \sum_{i=1}^{N-1} \boldsymbol{\Phi}_i \lambda_i^{k-1} \qquad N-1 \text{ modes with linear dynamics behavior.}$$

Modes' selection: Choice depends on the objective.

# DMD

## Modes' selection

**How to perform a truncation in DMD?**

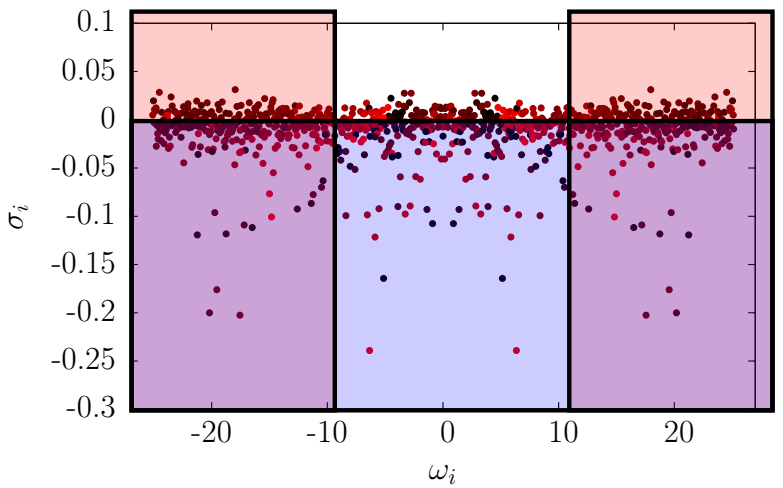
$$\boldsymbol{u}_k = \sum_{i=1}^{N-1} \boldsymbol{\Phi}_i \lambda_i^{k-1} \qquad N-1 \text{ modes with linear dynamics behavior.}$$

Modes' selection: Choice depends on the objective.

Frequency / Growth-decay rate:

$\lambda_i^{k-1} = e^{(\sigma_i + i\omega_i)t_k}$ with

$$\omega_i = \frac{\arg(\lambda_i)}{\Delta t} \; ; \; \sigma_i = \frac{\log(|\lambda_i|)}{\Delta t}$$



# DMD

## Modes' selection

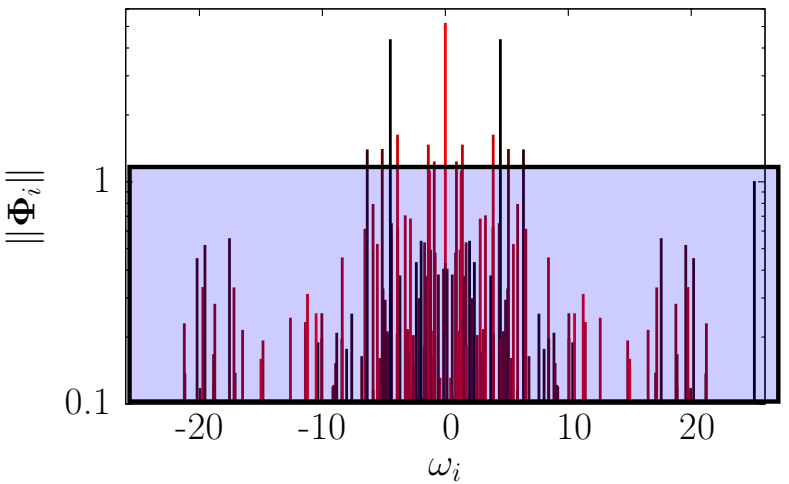
**How to perform a truncation in DMD?**

$$\boldsymbol{u}_k = \sum_{i=1}^{N-1} \boldsymbol{\Phi}_i \lambda_i^{k-1} \qquad N-1 \text{ modes with linear dynamics behavior.}$$

Modes' selection: Choice depends on the objective.

Mode amplitude:

$$A_i = \|\boldsymbol{\Phi}_i\|^2$$



# DMD

## Modes' selection

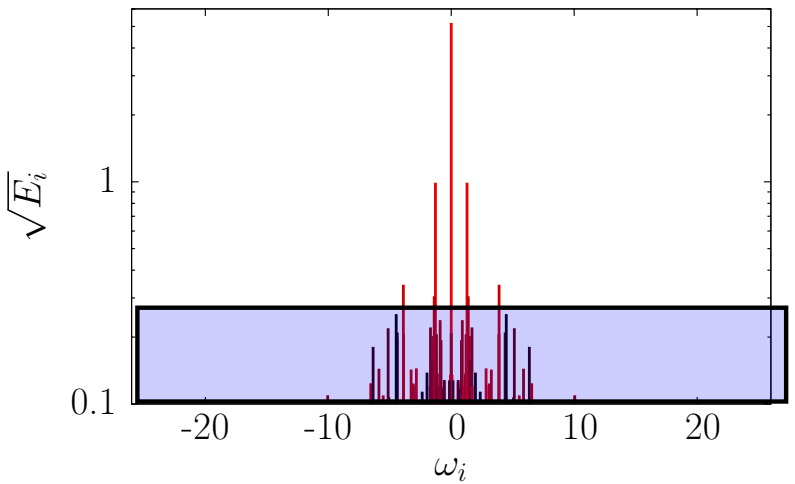
**How to perform a truncation in DMD?**

$$\boldsymbol{u}_k = \sum_{i=1}^{N-1} \boldsymbol{\Phi}_i \lambda_i^{k-1} \qquad N-1 \text{ modes with linear dynamics behavior.}$$

Modes' selection: Choice depends on the objective.

Energy contribution:

$$E_i = \frac{1}{T} \int_0^T \left\| \boldsymbol{\Phi}_i \lambda_i^{t/\Delta t} \right\|^2 \mathrm{d}t$$
$$= \|\boldsymbol{\Phi}_i\|^2 \frac{e^{2\sigma_i T} - 1}{2\sigma_i T}$$



# DMD

## Modes' selection

**How to perform a truncation in DMD?**

$$\boldsymbol{u}_k = \sum_{i=1}^{N-1} \boldsymbol{\Phi}_i \lambda_i^{k-1} \qquad N-1 \text{ modes with linear dynamics behavior.}$$

Modes' selection: Choice depends on the objective.

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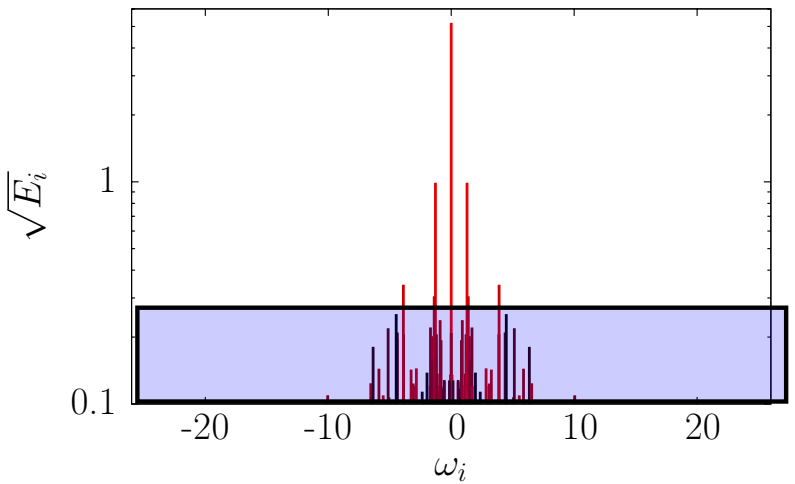
$$E_i = \frac{1}{T} \int_0^T \left\| \boldsymbol{\Phi}_i \lambda_i^{t/\Delta t} \right\|^2 \mathrm{d}t$$
$$= \|\boldsymbol{\Phi}_i\|^2 \frac{e^{2\sigma_i T} - 1}{2\sigma_i T}$$




Non-orthogonality of modes $\Longrightarrow$ Difficulty of modes' selection.

# Variants of DMD

## Optimized DMD

### Optimized DMD: (Chen *et al.*)2012

- $\boldsymbol{u}_k = \sum_{i=1}^{N_a} \hat{\boldsymbol{\Phi}}_i \hat{\lambda}_i^{k-1} + \boldsymbol{r}_k \quad \text{with} \quad N_a \ll N-1$
- Find the best $(\hat{\boldsymbol{\Phi}}_i, \hat{\lambda}_i)$ such that $\Gamma = \sum_{k=1}^{N} \|\boldsymbol{r}_k\|^2$ minimal.

Minimize the residual under the linear dynamics constraint
Computationally expensive. $\Rightarrow$ Analytical gradient computation.

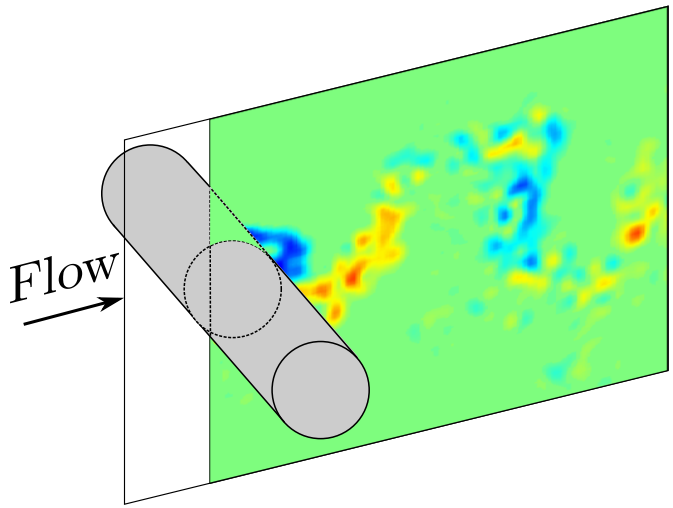
- Other variants:
  - Low-rank and sparse DMD (*Jovanović et al., 2012*).
  - Optimal mode decomposition (*Goulart et al., 2012*).
  - Chronos-Koopman analysis (*Cammilleri et al., 2013*).
  - Compressive sampling DMD (*Brunton et al., 2013*).
  - Extended DMD (*Williams et al., 2015*).

# DMD

## DMD vs. Optimized DMD

*N. Bénard*

Data: PIV data of a cylinder wake $Re = 13000$.




Classical DMD:

- $N = 1000$.
- 25 periods of vortex shedding.
- $N_a = 7$ modes selected with $E_i$ criterion.

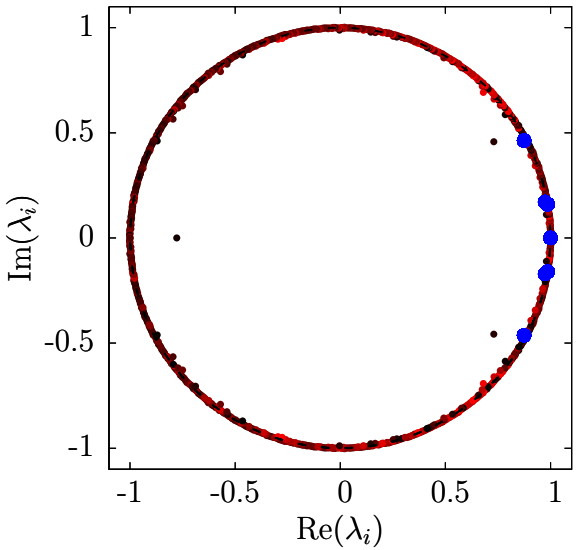
Optimized DMD:

- $N = 256$.
- 6 periods of vortex shedding.
- $N_a = 7$ Optimized DMD modes.

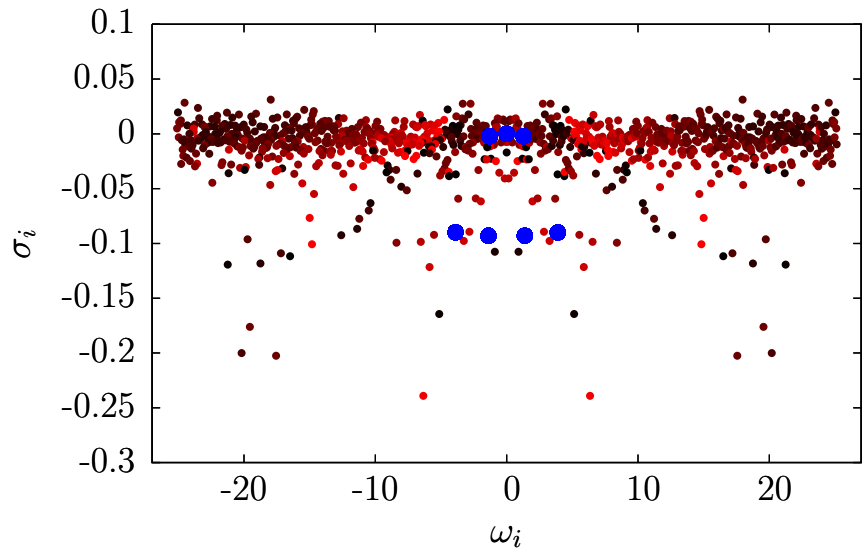
# DMD

## DMD vs. Optimized DMD

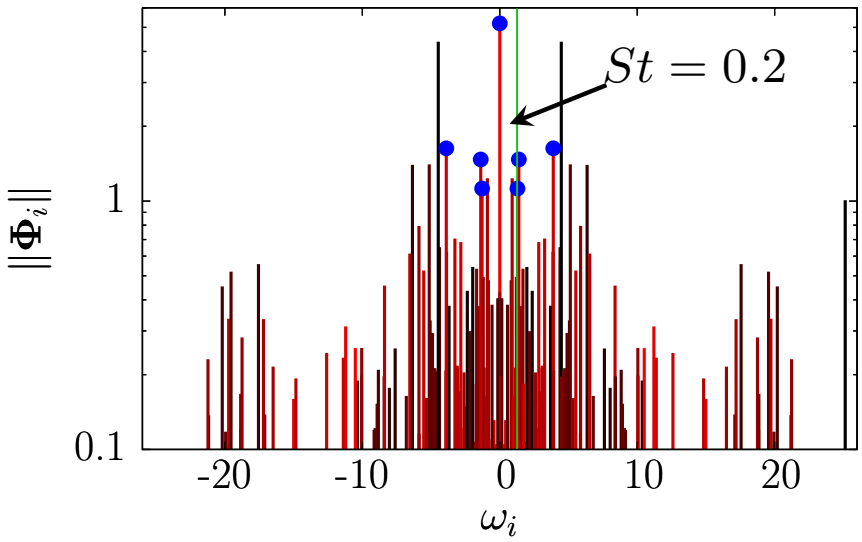
### DMD eigenvalues:



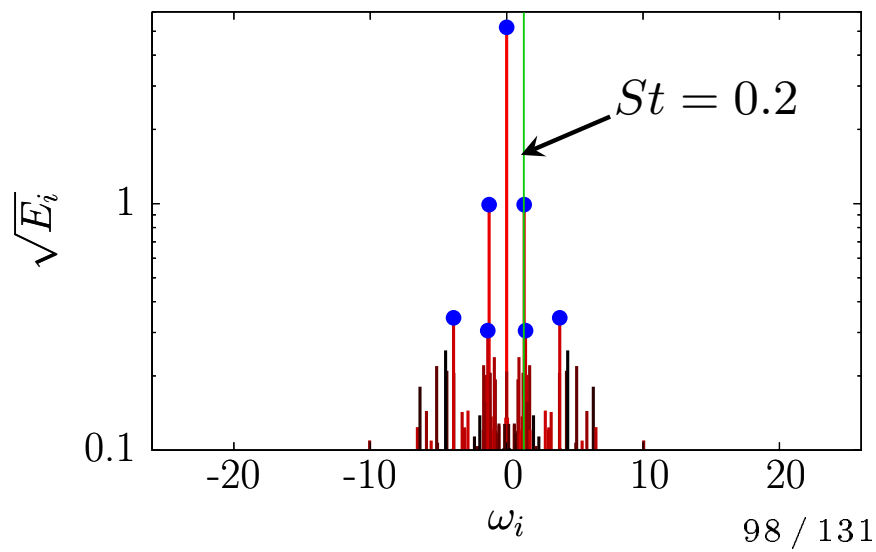

### Frequencies/growth rates:




### Modes amplitude:



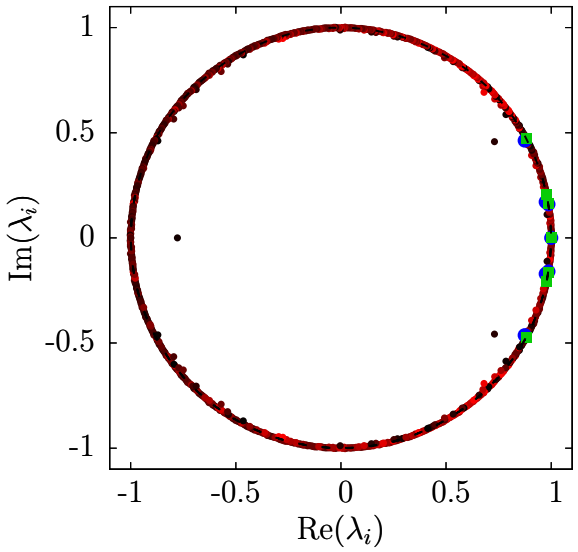

### Energy contribution:



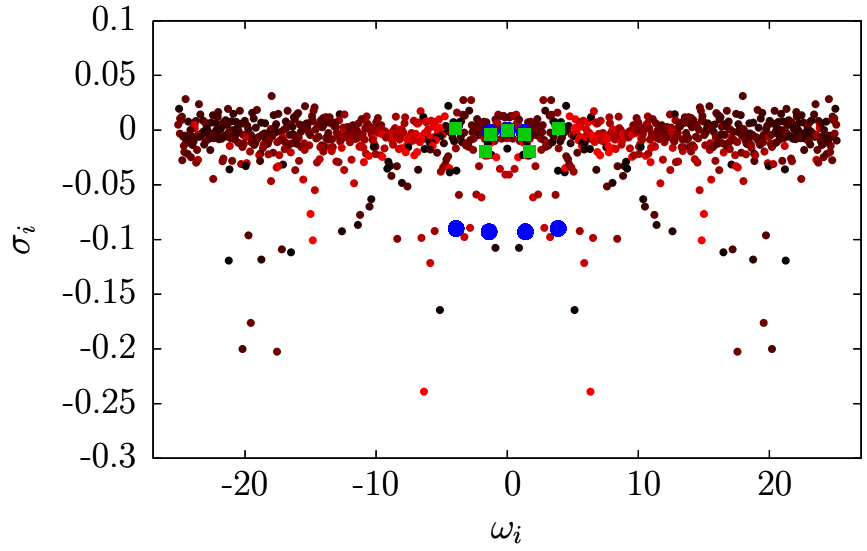
# DMD

## DMD vs. Optimized DMD

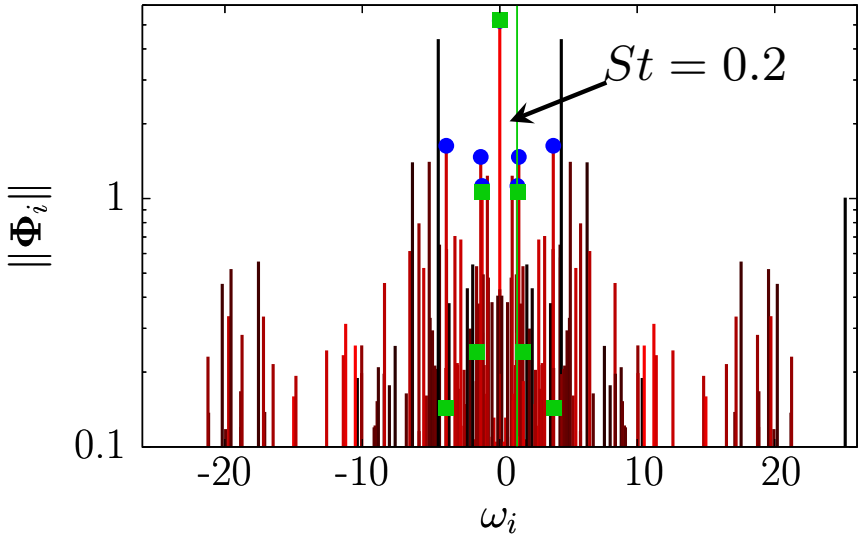
### DMD eigenvalues:



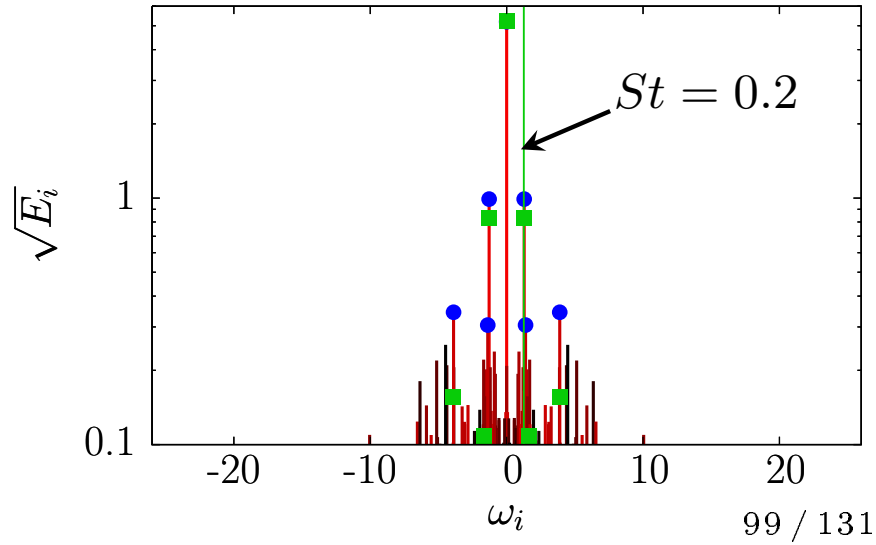

### Frequencies/growth rates:




### Modes amplitude:




### Energy contribution:

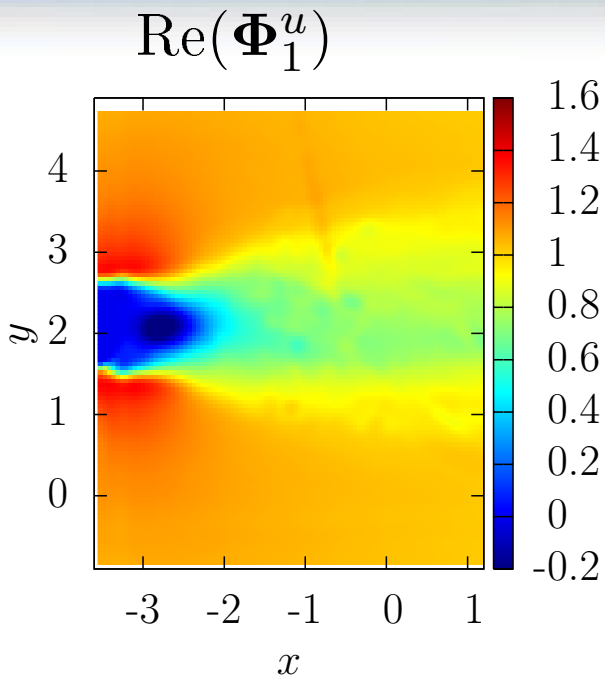


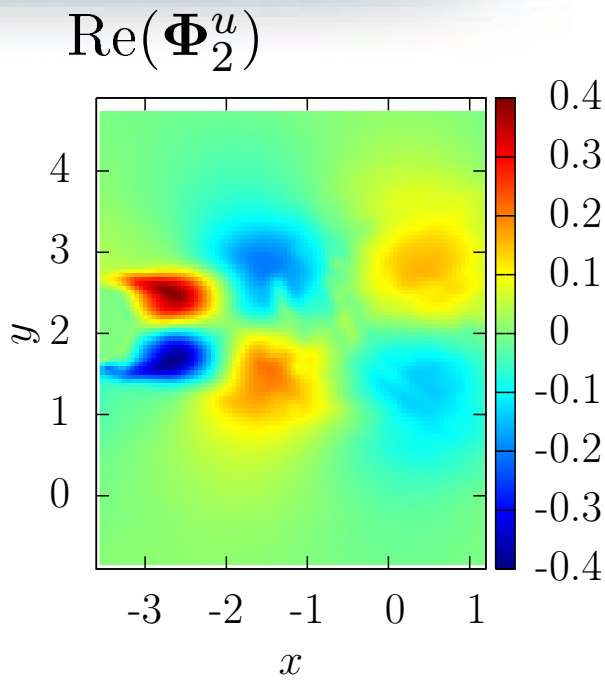
# DMD

## DMD vs. Optimized DMD

### Classical DMD

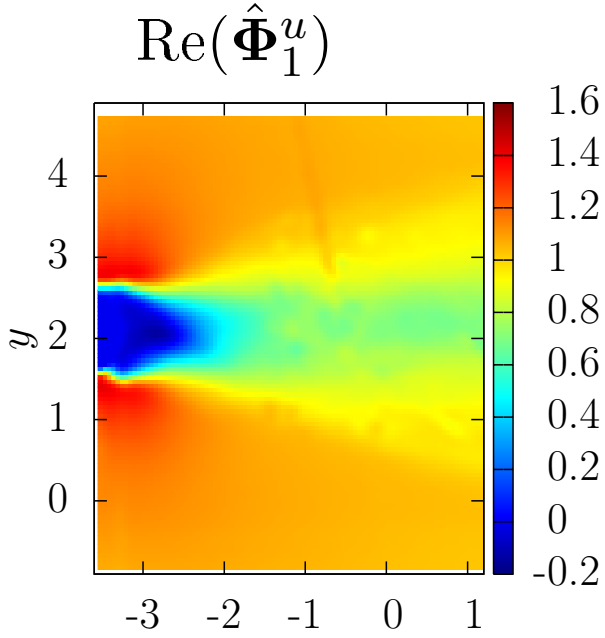
*Modes with higher energy contribution.*

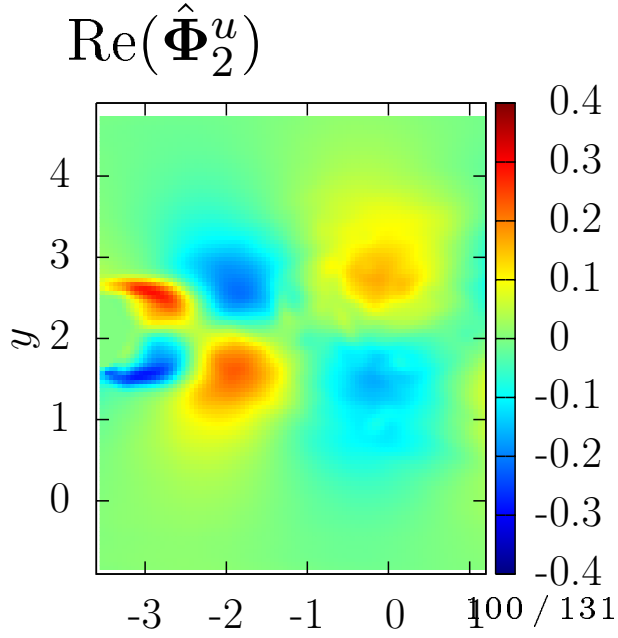



### Optimized DMD

*Selected DMD modes as initial condition.*



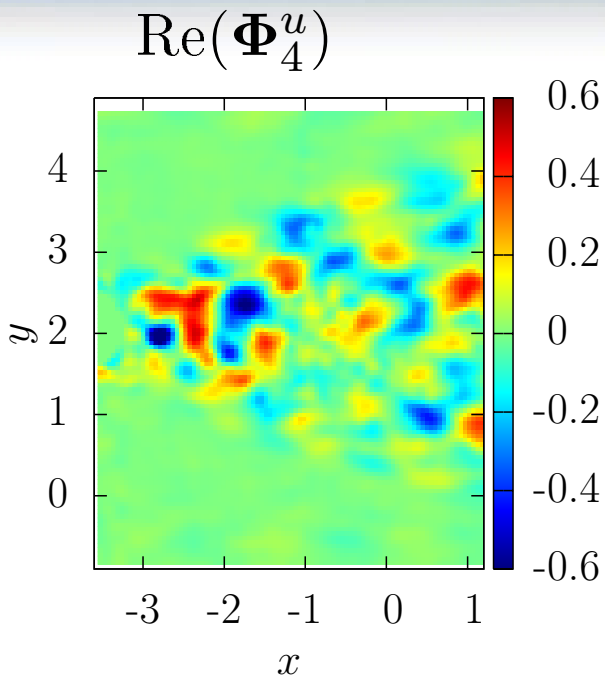



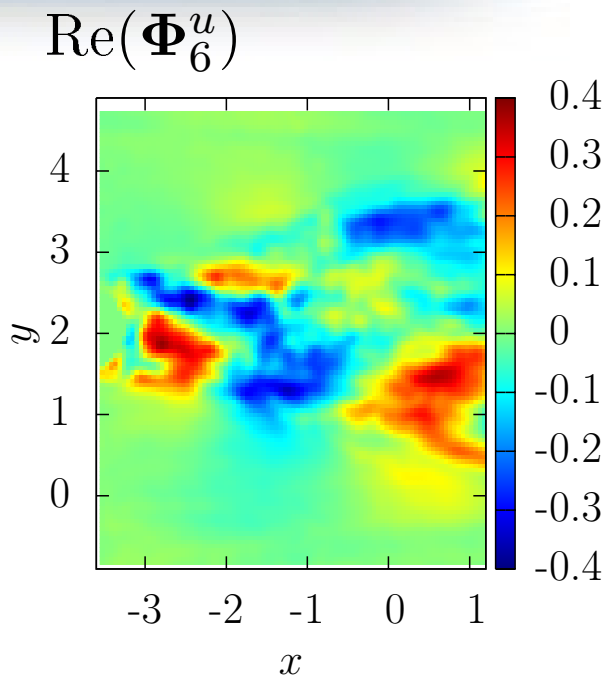
# DMD

## DMD vs. Optimized DMD

### Classical DMD

*Modes with higher energy contribution.*

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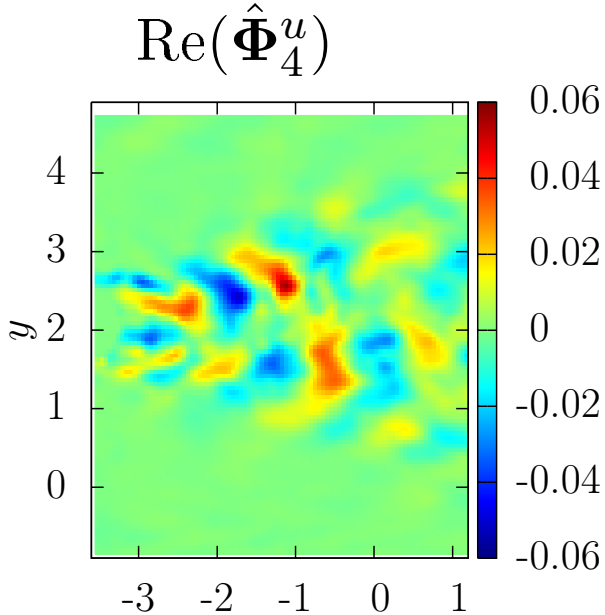
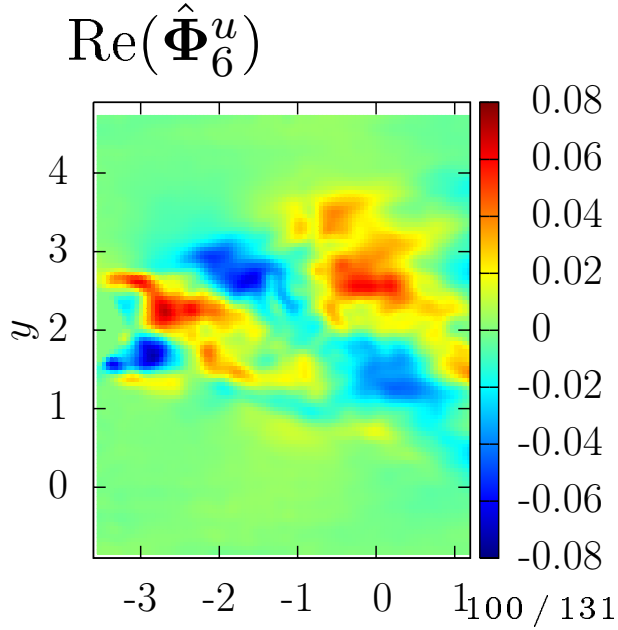
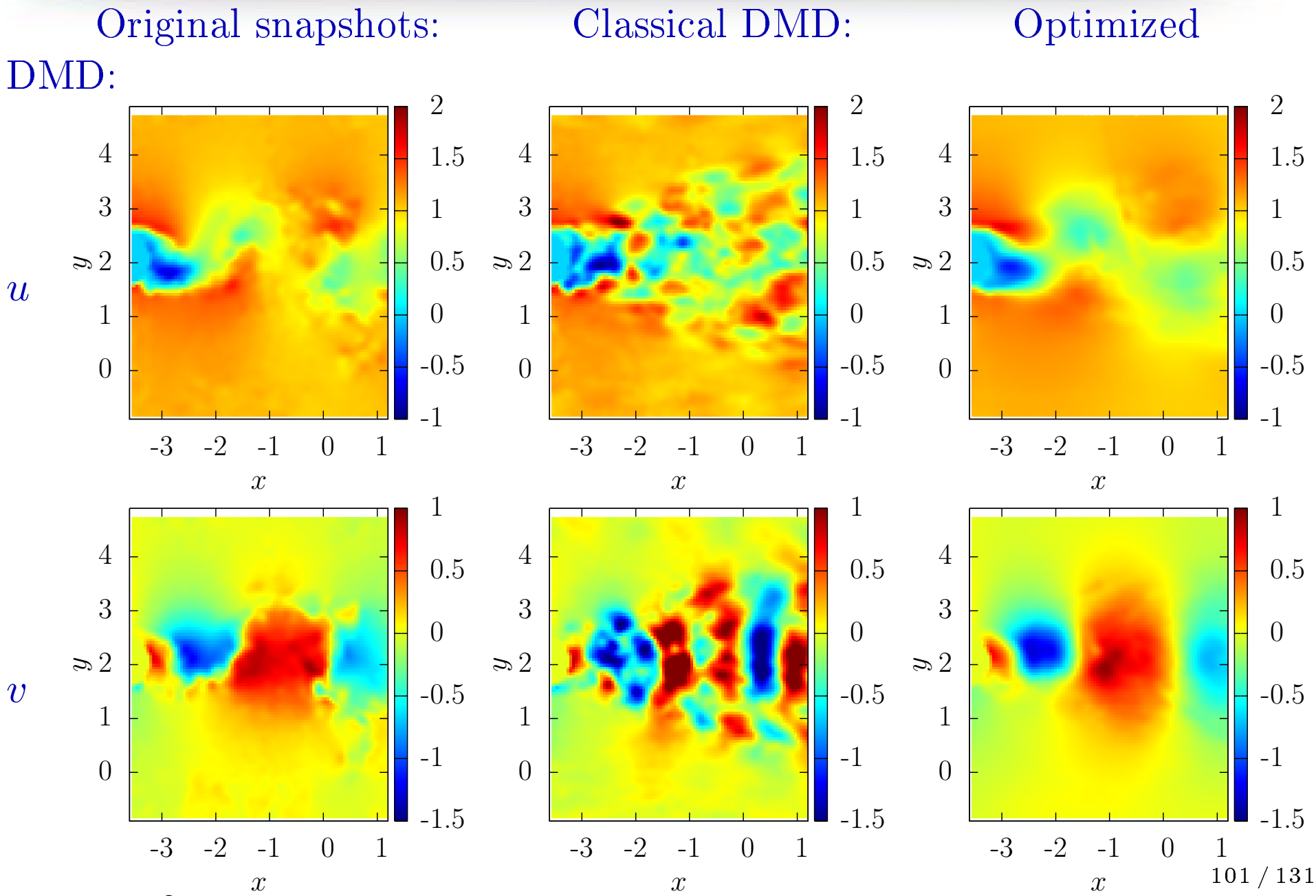


# DMD vs. Optimized DMD

$5^{\text{th}}$ snapshot reconstruction



# K-means algorithm

**Input** : $\{\boldsymbol{v}^m\}$, set of snapshots
**Input** : $K$, number of clusters
**Output:** $\boldsymbol{c}_1, \cdots, \boldsymbol{c}_K$, centroids

0. Initialize $K$ means $\boldsymbol{c}_1^{(0)}, \cdots, \boldsymbol{c}_K^{(0)}$ (random, kmeans++);

**for** $l \leftarrow 0$ **to** $L$ **do**

1. **Assignment step**;
   Assign each snapshot to the nearest cluster;

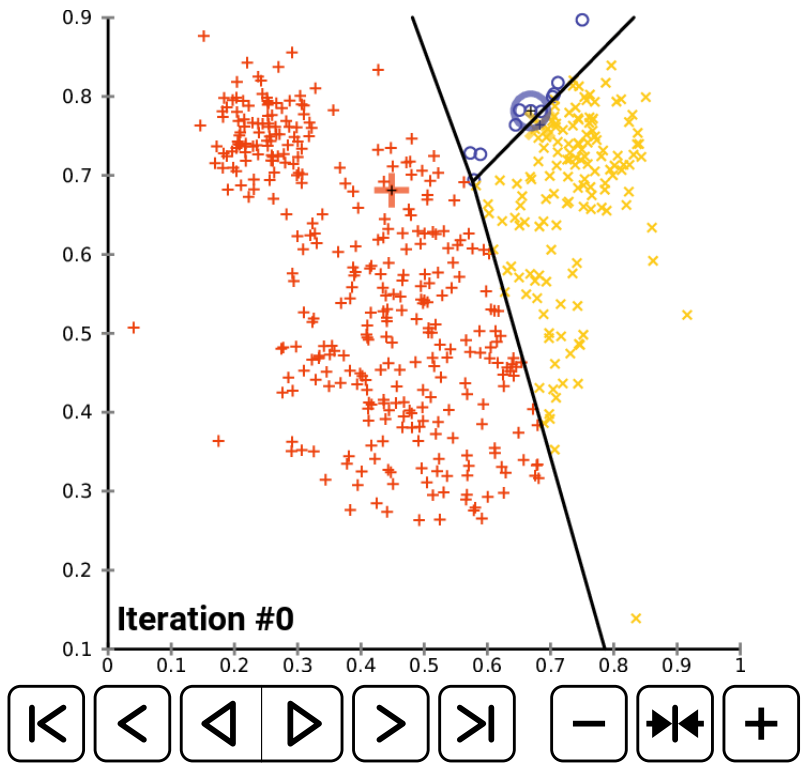
$$\mathcal{C}_k^{(l)} = \{\boldsymbol{v}^m : \|\boldsymbol{v}^m - \boldsymbol{c}_k^{(l)}\|^2 \leq \|\boldsymbol{v}^m - \boldsymbol{c}_j^{(l)}\|^2 \quad \forall j \in [1:K]\}$$

2. **Update step**;
   Compute new means (centroids);

$$\boldsymbol{c}_k^{(l+1)} = \frac{1}{|\mathcal{C}_k^{(l)}|} \sum_{\boldsymbol{v}^m \in \mathcal{C}_k^{(l)}} \boldsymbol{v}^m$$

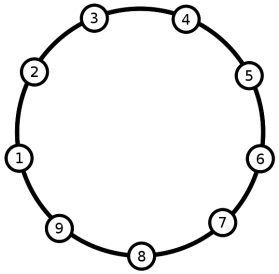
3. **Test convergence**;

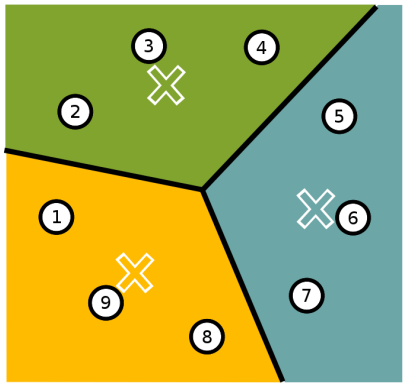
**end**

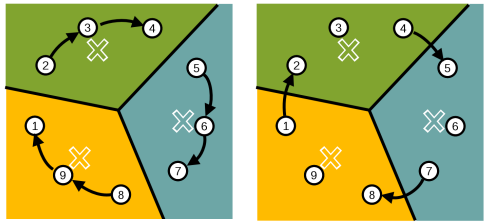


# Cluster-based Reduced-Order Modelling

| | Kinematics | Dynamics |
|---|---|---|
| **1** **Data** | **2** **Discretised state space** (cluster analysis) | **3** Construct **cluster transition matrix** → Markov model |
| Discrete snapshots of a limit cycle | | |

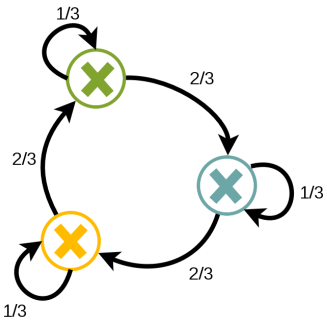


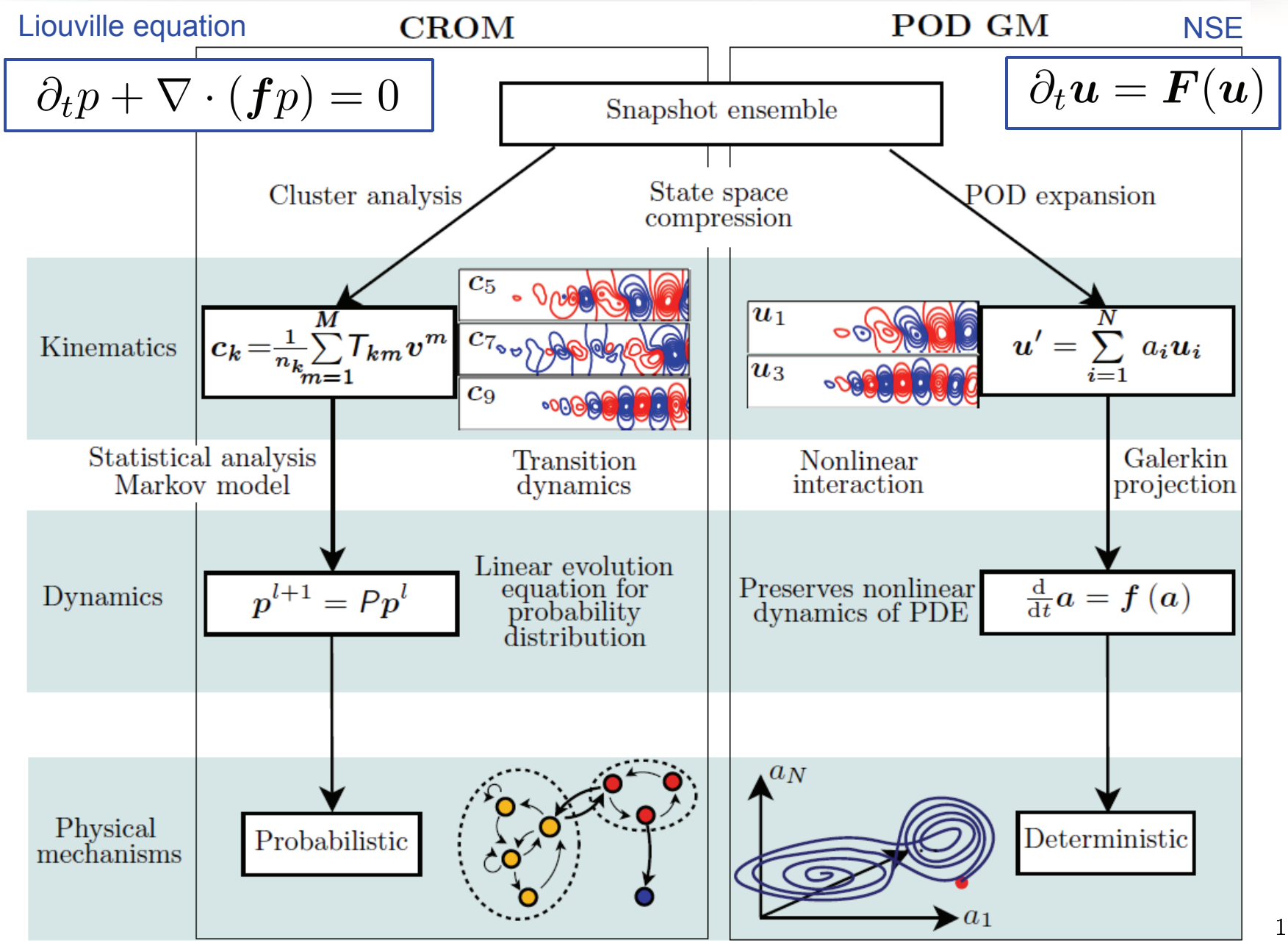

$$\boldsymbol{p}^l = P^l\,\boldsymbol{p}^0$$

| $P_{jk}$ | k=1 1→j | k=2 2→j | k=3 3→j |
|---|---|---|---|
| j=1 | 2/3 | 0 | 1/3 |
| j=2 | 1/3 | 2/3 | 0 |
| j=3 | 0 | 1/3 | 2/3 |




| | | |
|---|---|---|
| Time resolved velocity snapshots | Cluster analysis (k-means) (Steinhaus 1956, MacQueen 1967) | Discrete-time Markov model |
| $\boldsymbol{v}^m(\boldsymbol{x}) := \boldsymbol{v}(\boldsymbol{x}, t_m)$ | $J = \sum_{k=1}^{K} \sum_{\boldsymbol{v}^m \in \mathcal{C}_k} \|\boldsymbol{v}^m - \boldsymbol{c}_k\|_\Omega^2$ | $\boldsymbol{p}^l = P^l\,\boldsymbol{p}^0$ with $P_{jk} = \frac{n_{jk}}{n_k}$ |

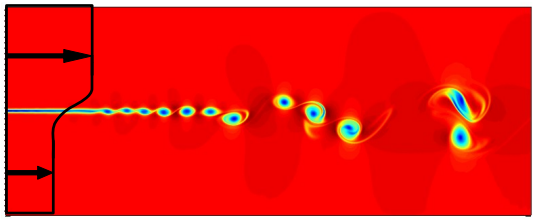
# Comparison CROM vs. POD GM



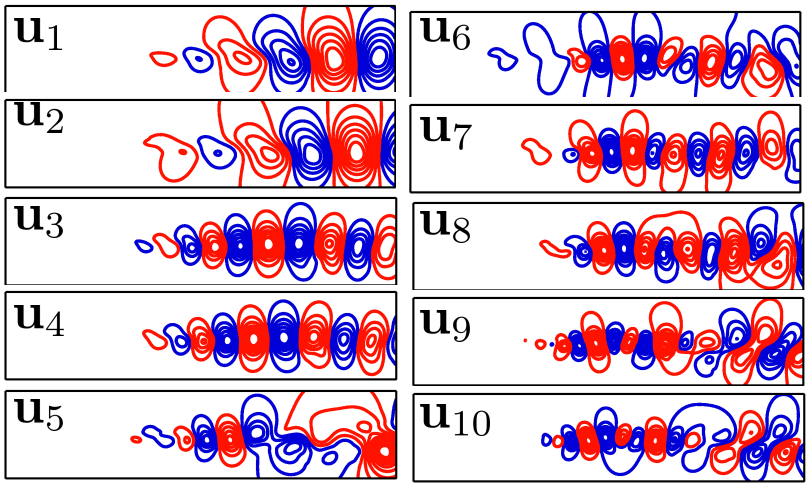
# CROM

## Mixing layer

1. **Data**
   - 2D incompressible
   - $Re = 500$
   - $M = 2000$ snapshots



Snapshot POD modes

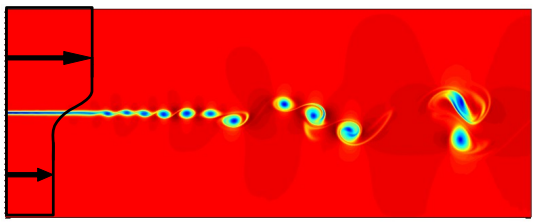


# CROM

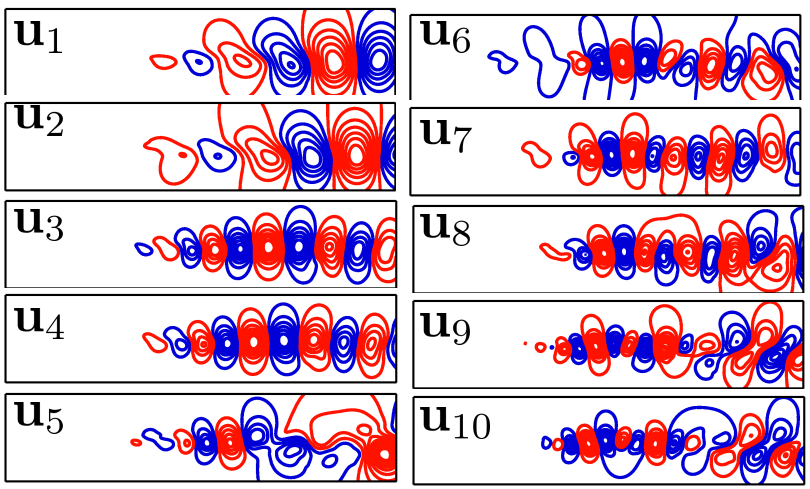
## Mixing layer

### 1 Data

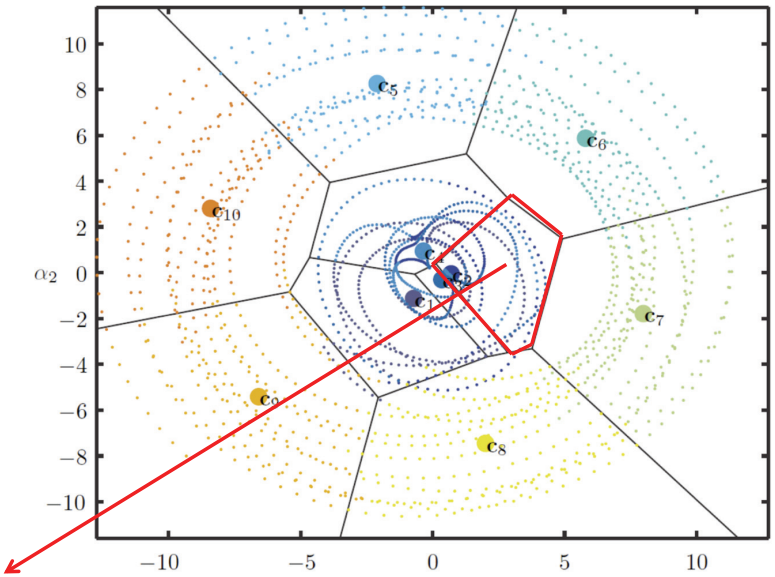
- 2D incompressible
- $Re = 500$
- $M = 2000$ snapshots



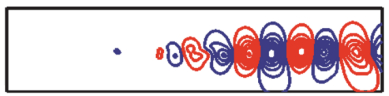
Snapshot POD modes



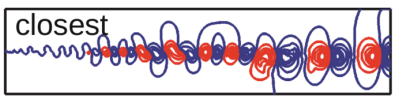

### 2 Cluster analysis ($K = 10$)



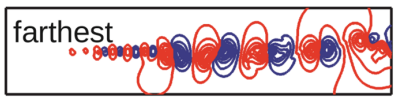

Cluster centroid c2:



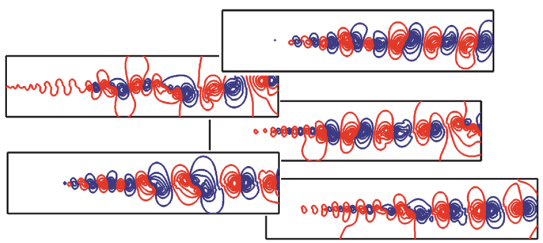
closest



farthest



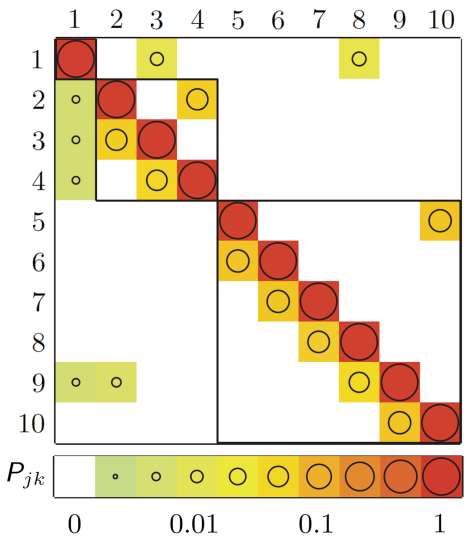
Some snapshots in this cluster:

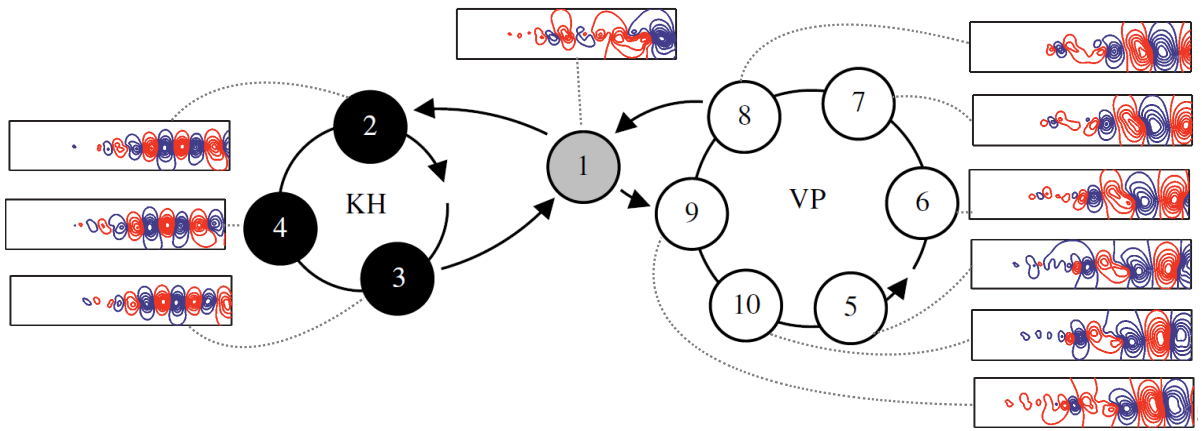


# CROM

## Mixing layer

### 3 Cluster transition matrix and simplified cluster transitions




- Identification of two shedding regimes:
  KH: Kelvin Helmoltz and VP: Vortex pairing
- Flipper cluster $c_1$ acts as a switch between both regimes

# Outline

1. Introduction
2. Preliminaries
   - Eigenvalue Decomposition
   - Singular Value Decomposition
   - Principal Component Analysis
   - Truncation
   - Data alignment
3. Data-based
   - Proper Orthogonal Decomposition
   - Dynamic Mode Decomposition
   - Cluster-based Reduced Order Model
4. Operator-based
   - Global stability analysis
   - Koopman analysis
   - Galerkin projection
5. Perspectives
6. Conclusion

# Global modes



- Flow dynamics:

$$\dot{\boldsymbol{q}} = \boldsymbol{f}(\boldsymbol{q}). \tag{5}$$

- Hypothesis: Steady base flow $\boldsymbol{Q}$

$$\boldsymbol{q}(x,y,z,t) = \boldsymbol{Q}(x,y,z) + \epsilon \boldsymbol{q'}(x,y,z,t) \quad \text{with} \quad \epsilon \ll 1 \tag{6}$$

- Substitute (6) into (5), expand in Taylor series, at order 1

$$\dot{\boldsymbol{q}}' = A\boldsymbol{q}' \quad \text{with } A \text{ Jacobian matrix of } \boldsymbol{f} \text{ at } \boldsymbol{Q}$$

- Different levels of expansion for $\boldsymbol{q}(x,y,z,t)$

$$\boldsymbol{Q}(x,y,z) + \epsilon \left\{ \hat{\boldsymbol{q}}(x,y,z) \exp\left[-\jmath\Omega t\right] + \text{c.c.} \right\} \qquad \text{3D global modes}$$

$$\boldsymbol{Q}(x,y) + \epsilon \left\{ \hat{\boldsymbol{q}}(x,y) \exp\left[\jmath\left(\beta z - \Omega t\right)\right] + \text{c.c.} \right\} \qquad \text{2D global modes}$$

$$\boldsymbol{Q}(y) + \epsilon \left\{ \hat{\boldsymbol{q}}(y) \exp\left[\jmath\left(\alpha x + \beta z - \Omega t\right)\right] + \text{c.c.} \right\} \qquad \text{Local stability}$$

- 3D global modes leads to generalized eigenvalue problem

$$\boxed{-\jmath\Omega\hat{\boldsymbol{q}} = A\hat{\boldsymbol{q}}}$$

# 2D global modes

## Incompressible Navier-Stokes (1)

- Incompressible Navier-Stokes $\boldsymbol{u} = (u, v, w)$

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\, \boldsymbol{u} = -\boldsymbol{\nabla} p + \frac{1}{Re} \boldsymbol{\Delta u}$$
$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0,$$

- Base flow equations $\boldsymbol{Q}(x, y) = (\boldsymbol{U}, P) = (U, V, 0, P)$

$$(\boldsymbol{U} \cdot \boldsymbol{\nabla})\, \boldsymbol{U} = -\boldsymbol{\nabla} P + \frac{1}{Re} \boldsymbol{\Delta U}$$
$$\boldsymbol{\nabla} \cdot \boldsymbol{U} = 0.$$

- Perturbation equations $\boldsymbol{q'}(x, y, z, t) = (u', v', w', p')$

$$\partial_t \boldsymbol{u'} + (\boldsymbol{u'} \cdot \boldsymbol{\nabla})\, \boldsymbol{U} + (\boldsymbol{U} \cdot \boldsymbol{\nabla})\, \boldsymbol{u'} = -\boldsymbol{\nabla} p' + \frac{1}{Re} \boldsymbol{\Delta u'}$$
$$\boldsymbol{\nabla} \cdot \boldsymbol{u'} = 0.$$

- Hypothesis: Base flow homogeneous in the transverse direction

$$\boldsymbol{q'}(x, y, z, t) = \frac{1}{2} \left\{ (\hat{u}, \hat{v}, \hat{w}, \hat{p})\, (x, y) \exp\left[\jmath \beta z + \sigma t\right] + \text{c.c.} \right\} \text{ with } \sigma \in \mathbb{C}$$

# 2D global modes

## Incompressible Navier-Stokes (2)

$\boxed{A\,\hat{\boldsymbol{q}} = \sigma\, B\,\hat{\boldsymbol{q}}}$ with $\hat{\boldsymbol{q}} = (\hat{\boldsymbol{u}}, p) = (\hat{u}, \hat{v}, \jmath\hat{w}, \hat{p})$ global mode.

$$A = \begin{pmatrix} \mathcal{D} - \mathcal{C} - \partial_x U & -\partial_y U & 0 & -\partial_x \\ -\partial_x V & \mathcal{D} - \mathcal{C} - \partial_y V & 0 & -\partial_y \\ 0 & 0 & \mathcal{D} - \mathcal{C} & \beta \\ \partial_x & \partial_y & \beta & 0 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

where

$\mathcal{D} = \frac{1}{Re}\left(\partial_{x^2} + \partial_{y^2} - \beta^2\right)$ viscous diffusion of perturbation

$\mathcal{C} = U\partial_x + V\partial_y$ advection by base flow

# Koopman operator

*(Koopman, 1931)*

- Nonlinear dynamical system $\boldsymbol{f} : \mathcal{M} \longrightarrow \mathcal{M}$ ($\mathcal{M}$ finite dimensional)

$$\boldsymbol{\mathcal{X}}_{k+1} = \boldsymbol{f}(\boldsymbol{\mathcal{X}}_k)$$

- Let $g : \mathcal{M} \to \mathbb{R}$ be a scalar observable. $\mathcal{K}_{\boldsymbol{f}}$ Koopman operator

$$\mathcal{K}_{\boldsymbol{f}} g(\boldsymbol{\mathcal{X}}_k) := g(\boldsymbol{f}(\boldsymbol{\mathcal{X}}_k)) = g \circ \boldsymbol{f}(\boldsymbol{\mathcal{X}}_k) = g(\boldsymbol{\mathcal{X}}_{k+1}).$$

- $\mathcal{K}_{\boldsymbol{f}}$: linear operator of infinite dimension

$$\mathcal{K}_{\boldsymbol{f}}(\alpha_1 g_1(\boldsymbol{\mathcal{X}}_k) + \alpha_2 g_2(\boldsymbol{\mathcal{X}}_k)) = \alpha_1 \mathcal{K}_{\boldsymbol{f}} g_1(\boldsymbol{\mathcal{X}}_k) + \alpha_2 \mathcal{K}_{\boldsymbol{f}} g_2(\boldsymbol{\mathcal{X}}_k)$$

- Eigenfunctions and eigenvalues

$$\mathcal{K}_{\boldsymbol{f}}\, \phi^{(j)}(\boldsymbol{\mathcal{X}}_k) = \lambda^{(j)} \phi^{(j)}(\boldsymbol{\mathcal{X}}_k)$$

- Let define $\boxed{z^{(j)} = \phi^{(j)}(\boldsymbol{\mathcal{X}})}$ nonlinear change of coordinates. We have:

$$z^{(j)}_{k+1} = \phi^{(j)}(\boldsymbol{\mathcal{X}}_{k+1}) = \phi^{(j)}(\boldsymbol{f}(\boldsymbol{\mathcal{X}}_k)) = \mathcal{K}_{\boldsymbol{f}} \phi^{(j)}(\boldsymbol{\mathcal{X}}_k) = \lambda^{(j)} \phi^{(j)}(\boldsymbol{\mathcal{X}}_k) = \lambda^{(j)} z^{(j)}_k$$

Dynamics linear in $z^{(j)}$ ; $\mathcal{K}_{\boldsymbol{f}}$ may have enough eigenfunctions !!!

# Koopman operator

## Connection with DMD

- Let $\boldsymbol{g} : \mathcal{M} \to \mathbb{R}^p$ be a vectorial observable. We have:

$$\boldsymbol{g}(\boldsymbol{\mathcal{X}}_k) = \sum_{j=1}^{+\infty} \phi_j(\boldsymbol{\mathcal{X}}_k)\boldsymbol{k}_j \quad \text{with} \quad \boldsymbol{k}_j : \text{Koopman modes}$$

- We can show that:

$$\boldsymbol{g}(\boldsymbol{\mathcal{X}}_k) = \sum_{j=1}^{+\infty} \phi_j(\boldsymbol{\mathcal{X}}_k)\boldsymbol{k}_j = \sum_{j=1}^{+\infty} \mathcal{K}_{\boldsymbol{f}}^{k-1}\phi_j(\boldsymbol{\mathcal{X}}_1)\boldsymbol{k}_j = \sum_{j=1}^{+\infty} \lambda_j^{k-1}\phi_j(\boldsymbol{\mathcal{X}}_1)\boldsymbol{k}_j$$

$\Longrightarrow$ Koopman modes can be obtained by DMD algorithm.

# Reduced-Order Modelling



- Full-order model (FOM)

$$\mathcal{S}: \begin{cases} \dot{\boldsymbol{\mathcal{X}}}(t) = \boldsymbol{f}\left(\boldsymbol{\mathcal{X}}(t), \boldsymbol{c}(t)\right), & \text{where} \quad \boldsymbol{\mathcal{X}} \in \mathbb{R}^{n_{\mathcal{X}}} \\ \boldsymbol{\mathcal{Y}}(t) = \boldsymbol{g}\left(\boldsymbol{\mathcal{X}}(t), \boldsymbol{c}(t)\right), & \text{where} \quad \boldsymbol{\mathcal{Y}} \in \mathbb{R}^{n_{\mathcal{Y}}}. \end{cases}$$

- Reduced-order model (ROM)

$$\widehat{\mathcal{S}}: \begin{cases} \dot{\widehat{\boldsymbol{\mathcal{X}}}}(t) = \widehat{\boldsymbol{f}}\left(\widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)\right), & \text{where} \quad \widehat{\boldsymbol{\mathcal{X}}} \in \mathbb{R}^{n_k} \quad \text{with} \quad \boxed{n_k \ll n_{\mathcal{X}}} \\ \widehat{\boldsymbol{\mathcal{Y}}}(t) = \widehat{\boldsymbol{g}}\left(\widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)\right), & \text{where} \quad \widehat{\boldsymbol{\mathcal{Y}}} \in \mathbb{R}^{n_{\mathcal{Y}}}. \end{cases}$$

---

- Requirements for deriving $\widehat{\mathcal{S}}$
  1. low approximation error $\forall \boldsymbol{c}$ *i.e.*

$$\|\boldsymbol{\mathcal{Y}} - \widehat{\boldsymbol{\mathcal{Y}}}\| < \epsilon \times \|\boldsymbol{c}\| \qquad \text{with } \epsilon \text{ a tolerance}$$

$$\Longrightarrow \text{Need computable error bound estimates!!}$$

  2. stability and passivity (no generation of energy) preserved ;
  3. procedure of model reduction numerically stable and efficient ;
  4. if possible, automatic generation of models.

# Reduced-Order Modelling — Projection method (Petrov-Galerkin)

- We introduce $W_1$ and $W_2$, two biorthogonal matrices of size $\mathbb{R}^{n_{\mathcal{X}} \times n_k}$, such that $\boxed{W_2^{\mathrm{H}} Q W_1 = I_{n_k}}$ where $Q \in \mathbb{R}^{n_{\mathcal{X}} \times n_{\mathcal{X}}}$ is the weight matrix.
- We consider: i) the projection $\boldsymbol{\mathcal{X}} = W_1 \widehat{\boldsymbol{\mathcal{X}}}$ and ii) $\widehat{\boldsymbol{\mathcal{Y}}} \simeq \boldsymbol{\mathcal{Y}}$.
- Algorithm:
  1. $\boldsymbol{\mathcal{X}} \simeq W_1 \widehat{\boldsymbol{\mathcal{X}}}$

$$\boldsymbol{\mathcal{R}} = W_1 \dot{\widehat{\boldsymbol{\mathcal{X}}}}(t) - \boldsymbol{f}\left(W_1 \widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)\right),$$
$$\widehat{\boldsymbol{\mathcal{Y}}}(t) = \boldsymbol{g}\left(W_1 \widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)\right).$$

  2. Petrov-Galerkin projection: $W_2^{\mathrm{H}} Q\, \boldsymbol{\mathcal{R}} = \mathbf{0}_{n_k}$ *i.e.*

$$\widehat{\mathcal{S}} : \begin{cases} \dot{\widehat{\boldsymbol{\mathcal{X}}}}(t) = \widehat{\boldsymbol{f}}(\widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)) = W_2^{\mathrm{H}} Q\, \boldsymbol{f}(W_1 \widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)), \\ \widehat{\boldsymbol{\mathcal{Y}}}(t) = \widehat{\boldsymbol{g}}(\widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)) = \boldsymbol{g}(W_1 \widehat{\boldsymbol{\mathcal{X}}}(t), \boldsymbol{c}(t)), \end{cases}$$

For $W_1 \neq W_2$: oblique projection.
For $W_1 \equiv W_2$: Galerkin projection (orthogonal projection).

# Reduced-Order Modelling Projection method: choice of $W_1$ and $W_2$

▷ For linear systems, various projection methods exist:

1. Krylov methods (Gugercin et Antoulas, 2006)
   proj. on the Krylov subspace of the controllability gramian: identification of the moments of the transfer function.
2. Balanced realizations
   proj. on dominant modes of the controllability and observability gramians
   - Balanced Truncation (Moore, 1981) ; Balanced POD (Rowley, 2005)
3. Instability methods
   proj. on global modes and adjoint global modes (Sipp, 2008)

▷ For non-linear systems: *a posteriori* methods

1. Proper Orthogonal Decomposition or POD (Lumley 1967 ; Sirovich 1987)
   proj. on the subspace determined with snapshots of the system.
2. Dynamic Mode Decomposition (Schmid, 2010)

# POD Reduced-order model

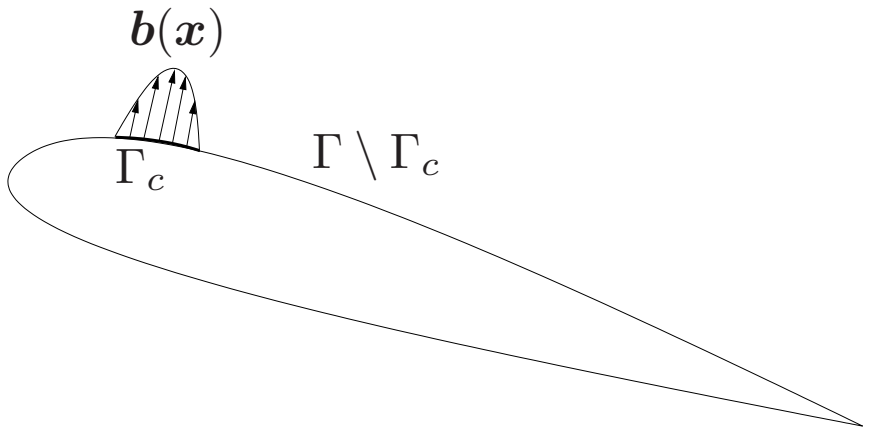


▷ Boundary control of the Navier-Stokes equations $(\boldsymbol{x} \in \Omega \text{ and } t \geq 0)$

$$\begin{cases} \dfrac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{f}(\boldsymbol{u}, P) \\ \boldsymbol{u}(\boldsymbol{x}, t = 0) = \boldsymbol{u}_0(\boldsymbol{x}) \quad (I.C.) \\ \boldsymbol{u}(\boldsymbol{x}, t) = \gamma(t)\boldsymbol{b}(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \Gamma_c, \quad (B.C.) \\ \boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{h}(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \Gamma \setminus \Gamma_c \quad (B.C.). \end{cases}$$

where

$$\boldsymbol{f}(\boldsymbol{u}, P) = -(\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} - \boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}} \Delta \boldsymbol{u}.$$



# POD Reduced-order model

## Choice of the decomposition variable

▷ B.C. independent of time, *i.e.* $\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{u}_{\mathrm{BC}}(\boldsymbol{x})$ on $\Gamma$

- $\mathcal{U} = \{\boldsymbol{u}(\boldsymbol{x}, t_1), \cdots, \boldsymbol{u}(\boldsymbol{x}, t_{N_t})\}$
- $\boldsymbol{u_m}(\boldsymbol{x})$: ensemble average of $\mathcal{U}$ (time average)

$$\boldsymbol{u_m}(\boldsymbol{x}) = \frac{1}{N_t} \sum_{k=1}^{N_t} \boldsymbol{u}(\boldsymbol{x}, t_k)$$

- $\mathcal{U}' = \{\boldsymbol{u}(\boldsymbol{x}, t_1) - \boldsymbol{u_m}(\boldsymbol{x}), \cdots, \boldsymbol{u}(\boldsymbol{x}, t_{N_t}) - \boldsymbol{u_m}(\boldsymbol{x})\}$
- $\boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{u_m}(\boldsymbol{x})$ is solenoidal
- $\boldsymbol{u}_{\mathrm{POD}}(\boldsymbol{x}, t) = \boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{u_m}(\boldsymbol{x})$ verify homogeneous B.C. i.e.

$$\boxed{\boldsymbol{\Phi}_i(\boldsymbol{x})|_{\boldsymbol{x}\in\Gamma} = \boldsymbol{0}}.$$

- $\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{u_m}(\boldsymbol{x}) + \sum_{i=1}^{N_{\mathrm{POD}}} a_i(t)\boldsymbol{\Phi}_i(\boldsymbol{x})$.

# POD Reduced-order model — Choice of the decomposition variable

▷ B.C. dependent of time, *i.e.* $\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{u}_{\mathrm{BC}}(\boldsymbol{x}, t)$ on $\Gamma$

- $\mathcal{U} = \{\boldsymbol{u}(\boldsymbol{x}, t_1), \cdots, \boldsymbol{u}(\boldsymbol{x}, t_{N_t})\}$
- $\boldsymbol{u_m}(\boldsymbol{x})$: ensemble average of $\mathcal{U}$ (time average)
- $\mathcal{U}' = \{\boldsymbol{u}(\boldsymbol{x}, t_1) - \gamma(t_1)\boldsymbol{u_c}(\boldsymbol{x}) - \boldsymbol{u_m}(\boldsymbol{x}), \cdots, \boldsymbol{u}(\boldsymbol{x}, t_{N_t}) - \gamma(t_{N_t})\boldsymbol{u_c}(\boldsymbol{x}) - \boldsymbol{u_m}(\boldsymbol{x})\}$
- $\boxed{\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{u_m}(\boldsymbol{x}) + \gamma(t)\boldsymbol{u_c}(\boldsymbol{x}) + \sum_{i=1}^{N_{\mathrm{POD}}} a_i(t)\boldsymbol{\Phi}_i(\boldsymbol{x})}$ where

$$\begin{aligned} \boldsymbol{u_c}(\boldsymbol{x}) &= \boldsymbol{b}(\boldsymbol{x}) \quad \text{on } \Gamma_c \text{ and} \\ \boldsymbol{u_c}(\boldsymbol{x}) &= \boldsymbol{0} \qquad \text{on } \Gamma \setminus \Gamma_c. \end{aligned}$$

- $\boldsymbol{u}_{\mathrm{POD}}(\boldsymbol{x}, t) = \boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{u_m}(\boldsymbol{x}) - \gamma(t)\boldsymbol{u_c}(\boldsymbol{x})$ verify homogeneous B.C. i.e.

$$\boxed{\boldsymbol{\Phi}_i(\boldsymbol{x})|_{\boldsymbol{x}\in\Gamma} = \boldsymbol{0}}.$$

# POD Reduced-order model

## Galerkin projection (1)

- Galerkin Projection of the Navier-Stokes equations onto the POD basis:

$$\left(\boldsymbol{\Phi}_i,\ \frac{\partial \boldsymbol{u}}{\partial t} - \boldsymbol{f}(\boldsymbol{u}, P)\right)_\Omega = \left(\boldsymbol{\Phi}_i,\ \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\,\boldsymbol{u} + \boldsymbol{\nabla} p - \frac{1}{\mathrm{Re}}\Delta \boldsymbol{u}\right)_\Omega = 0 \quad \forall i$$

$$\Longrightarrow \left(\boldsymbol{\Phi}_i,\ \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}\right)_\Omega = \left(\boldsymbol{\Phi}_i,\ -\boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}}\Delta \boldsymbol{u}\right)_\Omega .$$

- Integration by parts (Green formula):

$$\left(\boldsymbol{\Phi}_i,\ \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}\right)_\Omega = (p,\ \boldsymbol{\nabla}\cdot\boldsymbol{\Phi}_i)_\Omega - \frac{1}{\mathrm{Re}}\left((\boldsymbol{\nabla}\otimes\boldsymbol{\Phi}_i)^\mathsf{T},\ \boldsymbol{\nabla}\otimes\boldsymbol{u}\right)_\Omega$$
$$- [p\,\boldsymbol{\Phi}_i]_\Gamma + \frac{1}{\mathrm{Re}}[(\boldsymbol{\nabla}\otimes\boldsymbol{u})\boldsymbol{\Phi}_i]_\Gamma .$$

with $[\boldsymbol{a}]_\Gamma = \int_\Gamma \boldsymbol{a}\cdot\boldsymbol{n}\,\mathrm{d}\boldsymbol{x}$ and $(\overline{\overline{A}},\ \overline{\overline{B}})_\Omega = \int_\Omega \overline{\overline{A}} : \overline{\overline{B}}\,d\Omega = \sum_{i,j}\int_\Omega A_{ij}B_{ji}\,\mathrm{d}\boldsymbol{x}$

# POD Reduced-order model

## Galerkin projection (2)

- We decompose the velocity fields on $N_{\text{POD}}$ modes:

$$\boldsymbol{u}(\boldsymbol{x},t) = \boldsymbol{u_m}(\boldsymbol{x}) + \gamma(t)\,\boldsymbol{u_c}(\boldsymbol{x}) + \sum_{k=1}^{N_{\text{POD}}} a_k(t)\boldsymbol{\Phi}_k(\boldsymbol{x}).$$

- Dynamical system with $N_{\text{gal}}$ ($\ll N_{\text{POD}}$) modes kept:

$$\begin{aligned}\frac{d\,a_i(t)}{d\,t} =& \mathcal{A}_i + \sum_{j=1}^{N_{\text{gal}}} \mathcal{B}_{ij}\,a_j(t) + \sum_{j=1}^{N_{\text{gal}}}\sum_{k=1}^{N_{\text{gal}}} \mathcal{C}_{ijk}\,a_j(t)a_k(t) \\ &+ \mathcal{D}_i\,\frac{d\,\gamma}{d\,t} + \left(\mathcal{E}_i + \sum_{j=1}^{N_{\text{gal}}} \mathcal{F}_{ij}\,a_j(t)\right)\gamma + \mathcal{G}_i\gamma^2\end{aligned}$$

$$a_i(0) = (\boldsymbol{u}(\boldsymbol{x},0) - \boldsymbol{u_m}(\boldsymbol{x}) - \gamma(0)\,\boldsymbol{u_c}(\boldsymbol{x}),\ \boldsymbol{\Phi}_i(\boldsymbol{x}))_\Omega.$$

$\mathcal{A}_i$, $\mathcal{B}_{ij}$, $\mathcal{C}_{ijk}$, $\mathcal{D}_i$, $\mathcal{E}_i$, $\mathcal{F}_{ij}$ et $\mathcal{G}_i$ depend only on $\boldsymbol{\Phi}$, $\boldsymbol{u_m}$, $\boldsymbol{u_c}$ and Re.

- Dynamics predicted by the POD ROM may be not sufficiently accurate

$\Longrightarrow$ need of identification techniques (Data Assimilation)

# POD Reduced-order model

## Coefficients for $\gamma = 0$

$$\mathcal{A}_i = -\left(\boldsymbol{\Phi}_i, \left(\boldsymbol{u_m} \cdot \boldsymbol{\nabla}\right) \boldsymbol{u_m}\right)_\Omega - \frac{1}{\mathrm{Re}} \left(\boldsymbol{\nabla}\boldsymbol{\Phi}_i, \boldsymbol{\nabla}\boldsymbol{u_m}\right)_\Omega + \frac{1}{\mathrm{Re}} \left[\boldsymbol{\Phi}_i \, \boldsymbol{\nabla}\boldsymbol{u_m}\right]_\Gamma$$

$$\mathcal{B}_{ij} = -\left(\boldsymbol{\Phi}_i, \left(\boldsymbol{u_m} \cdot \boldsymbol{\nabla}\right) \boldsymbol{\Phi}_j\right)_\Omega - \left(\boldsymbol{\Phi}_i, \left(\boldsymbol{\Phi}_j \cdot \boldsymbol{\nabla}\right) \boldsymbol{u_m}\right)_\Omega$$
$$-\frac{1}{\mathrm{Re}} \left(\boldsymbol{\nabla}\boldsymbol{\Phi}_i, \boldsymbol{\nabla}\boldsymbol{\Phi}_j\right)_\Omega + \frac{1}{\mathrm{Re}} \left[\boldsymbol{\Phi}_i \, \boldsymbol{\nabla}\boldsymbol{\Phi}_j\right]_\Gamma$$

$$\mathcal{C}_{ijk} = -\left(\boldsymbol{\Phi}_i, \left(\boldsymbol{\Phi}_j \cdot \boldsymbol{\nabla}\right) \boldsymbol{\Phi}_k\right)_\Omega$$

# POD Reduced-order model

## Coefficients for $\gamma \neq 0$

$$\mathcal{D}_i = -\left(\boldsymbol{\Phi}_i, \boldsymbol{u_c}\right)_\Omega$$

$$\mathcal{E}_i = -\left(\boldsymbol{\Phi}_i, \left(\boldsymbol{u_m}\cdot\boldsymbol{\nabla}\right)\boldsymbol{u_c}\right)_\Omega - \left(\boldsymbol{\Phi}_i, \left(\boldsymbol{u_c}\cdot\boldsymbol{\nabla}\right)\boldsymbol{u_m}\right)_\Omega - \frac{1}{\mathrm{Re}}\left(\boldsymbol{\nabla}\boldsymbol{\Phi}_i, \boldsymbol{\nabla}\boldsymbol{u_c}\right)_\Omega + \frac{1}{\mathrm{Re}}\left[\boldsymbol{\Phi}_i\,\boldsymbol{\nabla}\boldsymbol{u_c}\right]_\Gamma$$

$$\mathcal{F}_{ij} = -\left(\boldsymbol{\Phi}_i, \left(\boldsymbol{\Phi}_j\cdot\boldsymbol{\nabla}\right)\boldsymbol{u_c}\right)_\Omega - \left(\boldsymbol{\Phi}_i, \left(\boldsymbol{u_c}\cdot\boldsymbol{\nabla}\right)\boldsymbol{\Phi}_j\right)_\Omega$$

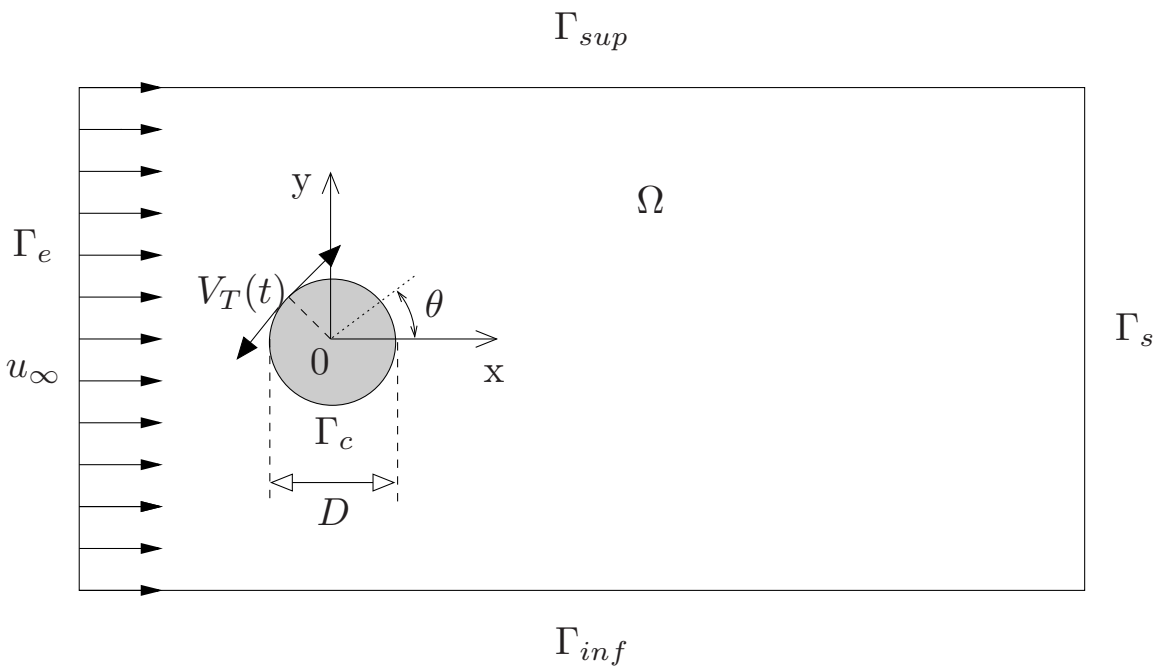
$$\mathcal{G}_i = -\left(\boldsymbol{\Phi}_i, \left(\boldsymbol{u_c}\cdot\boldsymbol{\nabla}\right)\boldsymbol{u_c}\right)_\Omega$$

# Cylinder wake flow



- Two dimensional flow around a circular cylinder at $\mathrm{Re} = 200$
- Viscous, incompressible and Newtonian fluid
- Cylinder oscillation with a tangential velocity $\gamma(t)$

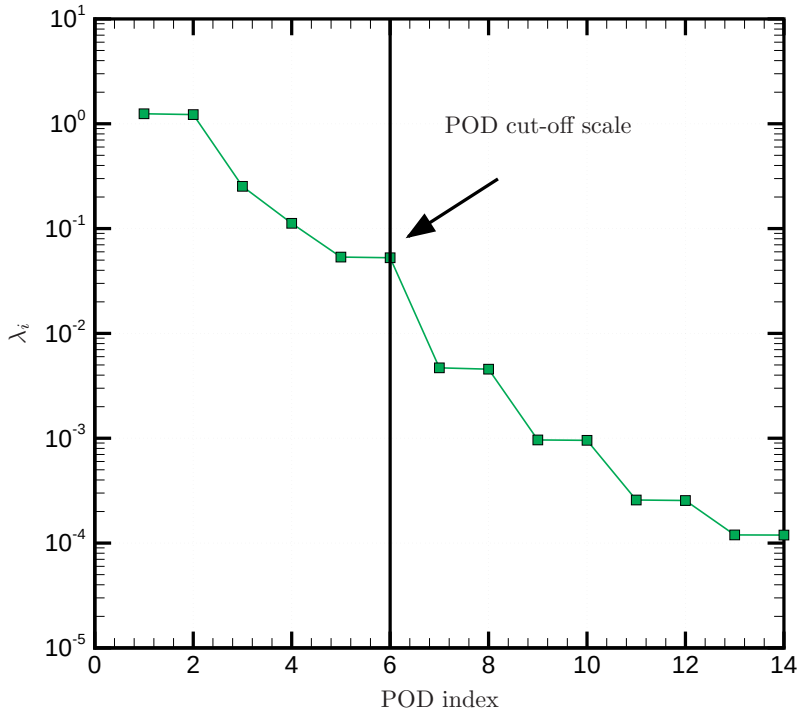
$$\gamma(t) = \frac{V_T}{u_\infty} = A \sin(2\pi St_f t)$$

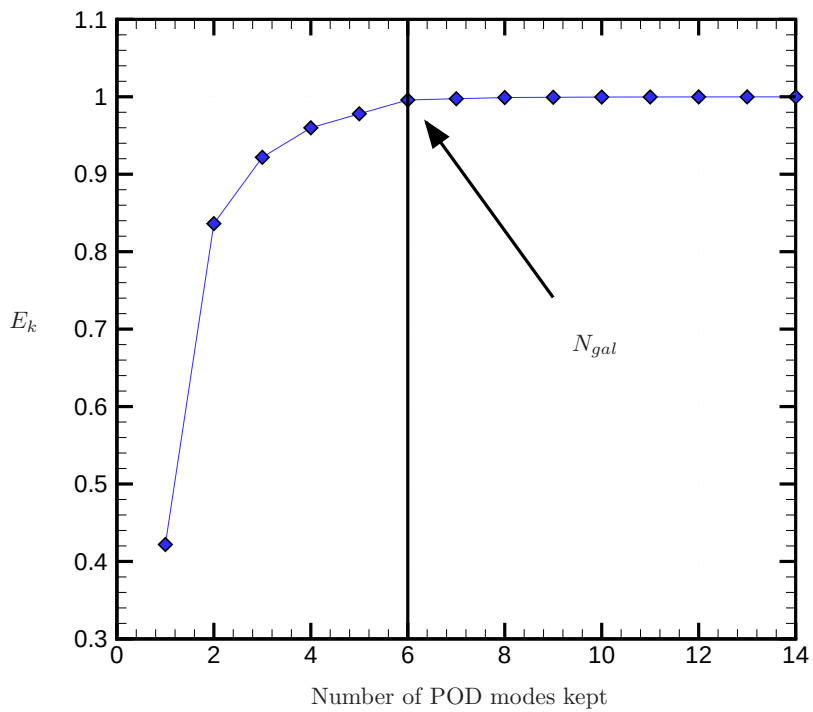


# POD of the controlled wake flow ($\gamma \neq 0$) $A = 2$ and $St_f = 0,5$

- 361 snapshots taken uniformly over $T = 18$
- Energetic Content: $E_k = \sum_{i=1}^{k} \lambda_i \Big/ \sum_{i=1}^{N_{\mathrm{POD}}} \lambda_i$

*Objective: Determine POD truncation with 99% of relative energy*




$$N_{gal} = \arg\min_k E_k \text{ such that } E_{N_{\mathrm{gal}}} > 99\% \quad \Rightarrow \quad \boldsymbol{N_{\mathrm{gal}} = 6} \text{ !}$$

# POD controlled wake flow ($\gamma \neq 0$)

## Velocity modes

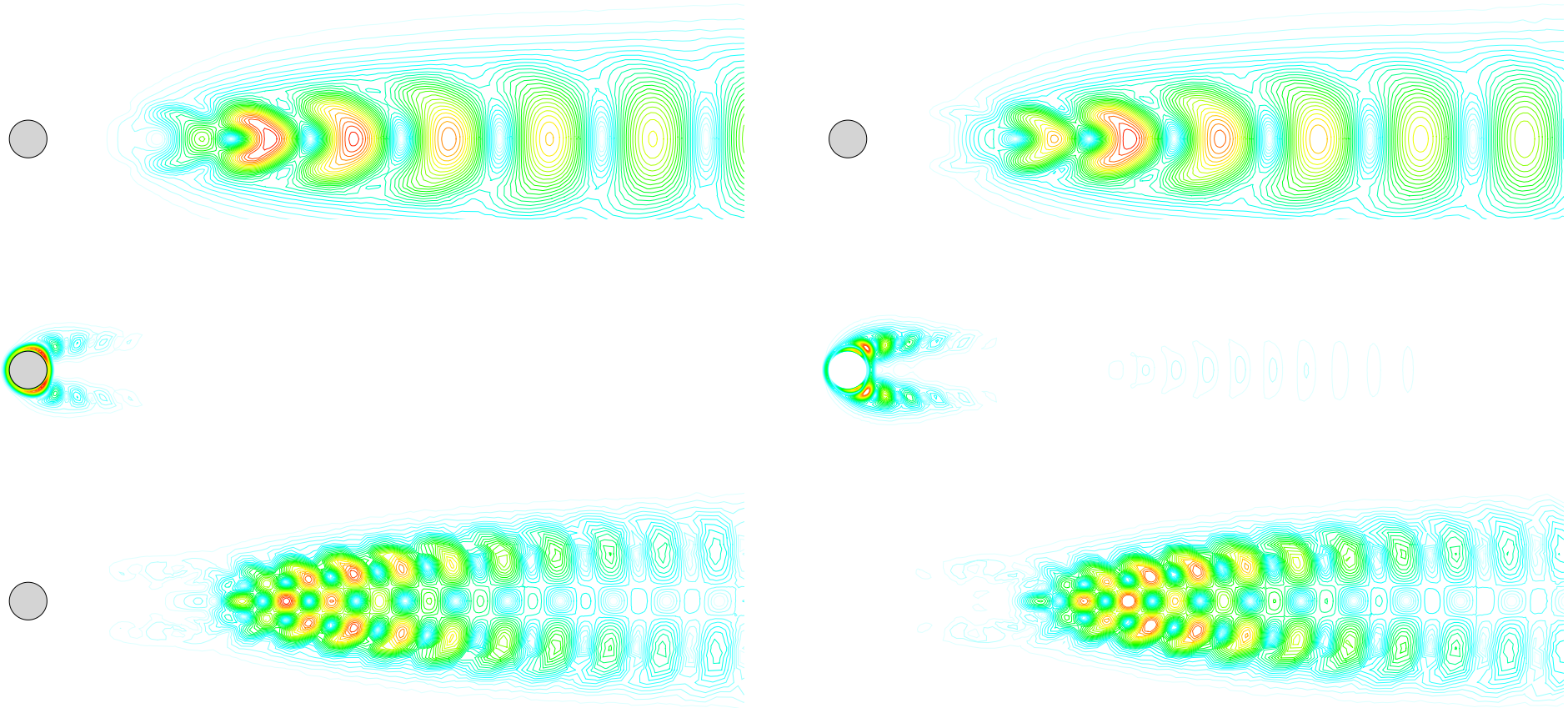


**Fig.** : *Iso-values of the first 6 POD modes*

$\gamma(t) = A\sin(2\pi St_f t)$ *with* $A = 2$ *and* $St_f = 0,5$.

# POD controlled wake flow ($\gamma \neq 0$)

## Integration and calibration

Reconstruction errors of POD ROM $\Rightarrow$ time amplification of the modes

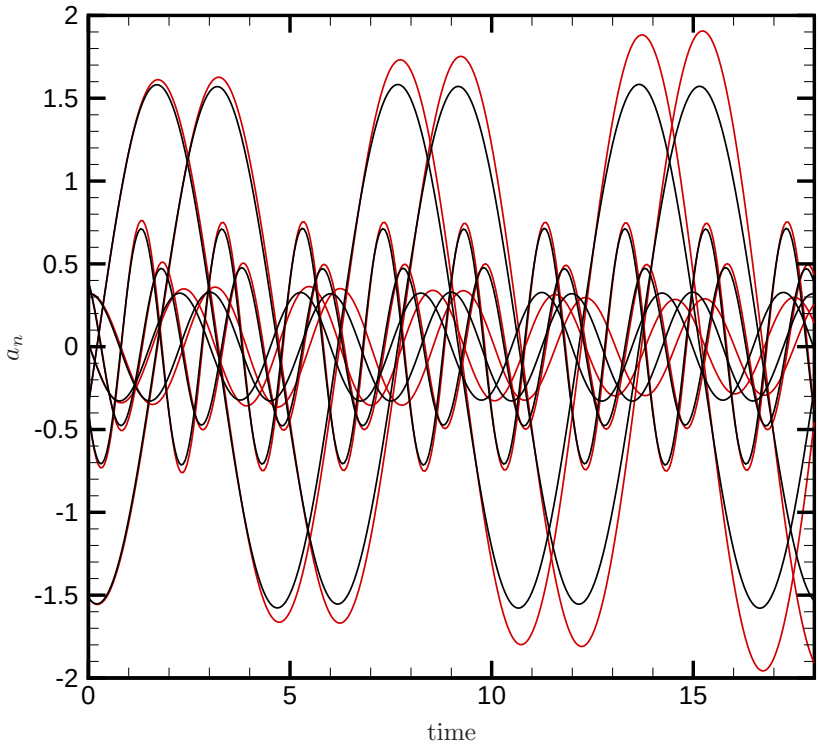



**Fig.** : *Time evolution of the first 6 POD modes ($A = 2$ and $St_f = 0,5$).*

▷ Reasons:

- Extraction of large scale structures carrying energy
- Main of the dissipation contained in the small structures

▷ Solutions:

- Identification method, Data Assimilation for instance

——— projection (Navier-Stokes) : $a^P(t)$

——— prediction before identification (POD ROM)

# Outline

1. Introduction
2. Preliminaries
   - Eigenvalue Decomposition
   - Singular Value Decomposition
   - Principal Component Analysis
   - Truncation
   - Data alignment
3. Data-based
   - Proper Orthogonal Decomposition
   - Dynamic Mode Decomposition
   - Cluster-based Reduced Order Model
4. Operator-based
   - Global stability analysis
   - Koopman analysis
   - Galerkin projection
5. Perspectives
6. Conclusion

# Perspectives



- For linear models
  - Balanced Truncation
  - Balanced Proper Orthogonal Decomposition (BPOD)
  - Eigensystem Realization Algorithm (ERA)
- Non linear dimensionality reduction methods
  - Kernel Principal Component Analysis (K-PCA)
  - MultiDimensional Scaling (MDS)
  - Isomap
  - Locally Linear Embedding (LLE)
- High-Order Principal Component Analysis (HO-PCA)
- Resolvent analysis
- ...
- ...

# Outline

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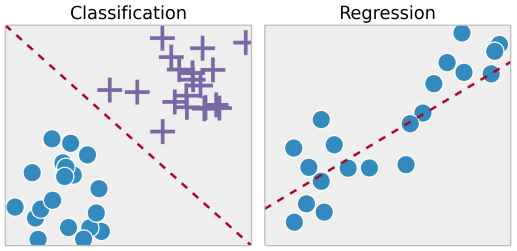
# Machine Learning

## Sub categories

1. **Supervised Learning**

   Learn a mapping from inputs $\boldsymbol{x}$ to outputs $\boldsymbol{y}$ given a labeled set $\mathcal{D}_{\text{SL}} = \{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$.

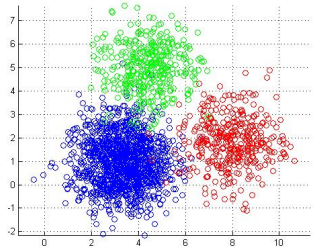
   - Classification or pattern recognition
   - Regression Genetic Programming




2. **Unsupervised Learning**

   Given only inputs $\mathcal{D}_{\text{UL}} = \{\boldsymbol{x}_i\}_{i=1}^N$, discover "interesting patterns"

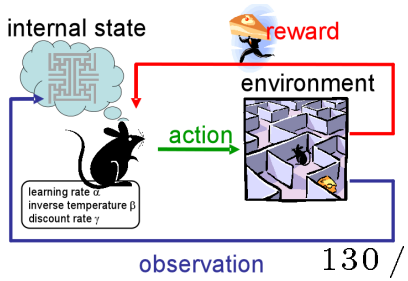
   - Clustering: CROM
   - Dimensionality Reduction: PCA, POD, DMD



3. **Reinforcement Learning**

   How to take actions in an environment so as to maximize a cumulative reward.

   Discretized and continuous RL




QUESTIONS??
Fish '11

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# Outline

7 Fourier series and Fourier transforms

8 Linear algebra recap

# Fourier series

## Orthogonal functions

- Hermitian inner product of (complex) functions defined on $x \in [a, b]$

$$\langle f(x), g(x) \rangle = \int_a^b f^*(x)\, g(x)\, \mathrm{d}x$$

This inner product induces a norm on functions, given by

$$\|f\|_2 = \sqrt{\langle f, f \rangle} = \left( \int_a^b f^*(x)\, f(x)\, \mathrm{d}x \right)^{\frac{1}{2}}$$

- $f$ and $g$ (non zero functions) are orthogonal when

$$\langle f(x), g(x) \rangle = 0$$

A set of non-zero functions, $\{f_i(x)\}$, is said to be mutually orthogonal if

$$\int_a^b f_i(x)\, f_j(x)\ \mathrm{d}x = \begin{cases} 0 & i \neq j \\ c > 0 & i = j \end{cases}$$

# Fourier series

## Periodic functions

- If $f$ is continuous and periodic with period $T$ ($f(x) = f(x+T)$), then

$$\int_0^T f(t)\,\mathrm{d}t = \int_b^{b+T} f(t)\,\mathrm{d}t \quad \forall b \in \mathbb{R}$$

Dem: Let $H(x) = \int_x^{x+T} f(t)\,\mathrm{d}t$, then

$$\frac{dH}{dx} = f(x+T) - f(x) = 0$$

It follows that $H(x)$ is constant. In particular, $H(b) = H(0)$.

- If $f$ and $g$ are both periodic functions with period $T$ then so is $f+g$ and $fg$. Dem:

$$(f+g)(x+T) = f(x+T) + g(x+T) = f(x) + g(x) = (f+g)(x)$$
$$(fg)(x+T) = f(x+T)\,g(x+T) = f(x)\,g(x) = (fg)(x)$$

# Fourier series

## Orthogonality of sine and cosine integrals

$\forall L_x$, we have:

- $$\int_{-L_x}^{L_x} \cos\left(\frac{n\pi x}{L_x}\right) \cos\left(\frac{m\pi x}{L_x}\right) \, \mathrm{d}x = \begin{cases} 2L_x & \text{if } n = m = 0 \\ L_x & \text{if } n = m \neq 0 \\ 0 & \text{if } n \neq m \end{cases}$$
- $$\int_{0}^{L_x} \cos\left(\frac{n\pi x}{L_x}\right) \cos\left(\frac{m\pi x}{L_x}\right) \, \mathrm{d}x = \begin{cases} L_x & \text{if } n = m = 0 \\ \frac{L_x}{2} & \text{if } n = m \neq 0 \\ 0 & \text{if } n \neq m \end{cases}$$
- $$\int_{-L_x}^{L_x} \sin\left(\frac{n\pi x}{L_x}\right) \sin\left(\frac{m\pi x}{L_x}\right) \, \mathrm{d}x = \begin{cases} L_x & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$
- $$\int_{0}^{L_x} \sin\left(\frac{n\pi x}{L_x}\right) \sin\left(\frac{m\pi x}{L_x}\right) \, \mathrm{d}x = \begin{cases} \frac{L_x}{2} & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$
- $$\int_{-L_x}^{L_x} \sin\left(\frac{n\pi x}{L_x}\right) \cos\left(\frac{m\pi x}{L_x}\right) \, \mathrm{d}x = 0$$

# Fourier series

## Orthogonality of sine and cosine integrals (Dem)

$$\sin\alpha\cos\beta = \frac{1}{2}\left[\sin\left(\alpha-\beta\right)+\sin\left(\alpha+\beta\right)\right]$$

$$\sin\alpha\sin\beta = \frac{1}{2}\left[\cos\left(\alpha-\beta\right)-\cos\left(\alpha+\beta\right)\right]$$

$$\cos\alpha\cos\beta = \frac{1}{2}\left[\cos\left(\alpha-\beta\right)+\cos\left(\alpha+\beta\right)\right]$$

$$\sin(2\theta) = 2\sin\theta\cos\theta = (\sin\theta+\cos\theta)^2 - 1 = \frac{2\tan\theta}{1+\tan^2\theta}$$

$$\cos(2\theta) = \cos^2\theta - \sin^2\theta = 2\cos^2\theta - 1 = 1 - 2\sin^2\theta = \frac{1-\tan^2\theta}{1+\tan^2\theta}$$

# Fourier series

## Orthogonality of sine and cosine integrals (Dem)

Dem: Show that $\left\{\cos\left(\frac{n\pi x}{L_x}\right)\right\}_{n=0}^{\infty}$ is mutually orthogonal

$$I = \int_{-L_x}^{L_x} \cos\left(\frac{n\pi x}{L_x}\right)\cos\left(\frac{m\pi x}{L_x}\right)\,\mathrm{d}x = 2\int_{0}^{L_x} \cos\left(\frac{n\pi x}{L_x}\right)\cos\left(\frac{m\pi x}{L_x}\right)\,\mathrm{d}x$$

$\underline{n = m = 0}$

$$\int_{-L_x}^{L_x} dx = 2\int_{0}^{L_x} dx = 2L_x$$

$\underline{n = m \neq 0}$

$$I = 2\int_{0}^{L_x} \cos^2\left(\frac{n\pi x}{L_x}\right)\,dx = \int_{0}^{L_x}\left(1+\cos\left(\frac{2n\pi x}{L_x}\right)\right)\,\mathrm{d}x$$

$$= \left[x + \frac{L_x}{2n\pi}\sin\left(\frac{2n\pi x}{L_x}\right)\right]_0^{L_x} = L_x + \frac{L_x}{2n\pi}\sin\left(2n\pi\right)$$

$$= L_x$$

# Fourier series

## Orthogonality of sine and cosine integrals (Dem)

$\underline{n \neq m}$

$$
\begin{aligned}
I &= 2\int_0^{L_x} \cos\left(\frac{n\pi x}{L_x}\right)\cos\left(\frac{m\pi x}{L_x}\right)\,dx \\
&= \int_0^{L_x}\left(\cos\left(\frac{(n-m)\,\pi x}{L_x}\right)+\cos\left(\frac{(n+m)\,\pi x}{L_x}\right)\right)\,dx \\
&= \left[\frac{L_x}{(n-m)\,\pi}\sin\left(\frac{(n-m)\,\pi x}{L_x}\right)+\frac{L_x}{(n+m)\,\pi}\sin\left(\frac{(n+m)\,\pi x}{L_x}\right)\right]_0^{L_x} \\
&= \frac{L_x}{(n-m)\,\pi}\sin\left((n-m)\,\pi\right)+\frac{L_x}{(n+m)\,\pi}\sin\left((n+m)\,\pi\right) \\
&= 0 \quad \text{since } n-m \text{ and } n+m \text{ are integers}
\end{aligned}
$$

# Fourier series

## Orthogonality of sine and cosine integrals (Dem)

Dem: Show that $\left\{\sin\left(\frac{n\pi x}{L_x}\right)\right\}_{n=1}^{\infty}$ is mutually orthogonal

$$I = \int_{-L_x}^{L_x} \sin\left(\frac{n\pi x}{L_x}\right) \sin\left(\frac{m\pi x}{L_x}\right) \, \mathrm{d}x$$

$n = m$

$$\int_{-L_x}^{L_x} \sin^2\left(\frac{n\pi x}{L_x}\right) \, \mathrm{d}x = 2\int_{0}^{L_x} \sin^2\left(\frac{n\pi x}{L_x}\right) \, \mathrm{d}x = \int_{0}^{L_x} \left(1 - \cos\left(\frac{2n\pi x}{L_x}\right)\right)$$

$$= \left[x - \frac{L_x}{2n\pi}\sin\left(\frac{2n\pi x}{L_x}\right)\right]_0^{L_x} = L_x - \frac{L_x}{2n\pi}\sin\left(2n\pi\right)$$

$$= L_x$$

# Fourier series

## Orthogonality of sine and cosine integrals (Dem)

$\underline{n \neq m}$

$$
\begin{aligned}
I &= 2\int_0^{L_x} \sin\left(\frac{n\pi x}{L_x}\right)\sin\left(\frac{m\pi x}{L_x}\right)\,\mathrm{d}x \\
&= \int_0^{L_x}\left(\cos\left(\frac{(n-m)\,\pi x}{L_x}\right)-\cos\left(\frac{(n+m)\,\pi x}{L_x}\right)\right)\,\mathrm{d}x \\
&= \left[\frac{L_x}{(n-m)\,\pi}\sin\left(\frac{(n-m)\,\pi x}{L_x}\right)-\frac{L_x}{(n+m)\,\pi}\sin\left(\frac{(n+m)\,\pi x}{L_x}\right)\right]_0^{L_x} \\
&= \frac{L_x}{(n-m)\,\pi}\sin\left((n-m)\,\pi\right)-\frac{L_x}{(n+m)\,\pi}\sin\left((n+m)\,\pi\right) \\
&= 0 \quad \text{since } n-m \text{ and } n+m \text{ are integers}
\end{aligned}
$$

# Fourier series

## Orthogonality of sine and cosine integrals (Dem)

Dem: Show that $\left\{\sin\left(\frac{n\pi x}{L_x}\right)\right\}_{n=1}^{\infty}$ and $\left\{\cos\left(\frac{m\pi x}{L_x}\right)\right\}_{m=0}^{\infty}$ are mutually orthogonal

$$\int_{-L_x}^{L_x} \underbrace{\underbrace{\sin\left(\frac{n\pi x}{L_x}\right)}_{\text{odd}}\underbrace{\cos\left(\frac{m\pi x}{L_x}\right)}_{\text{even}}}_{\text{odd}} \mathrm{d}x = 0$$

The integral of an odd function over a symmetric interval is equal to zero.

# Fourier series

$L$ periodic on $[0, L[$

If $f$ is $L$ periodic on $[0, L[$, then it can be written in terms of a Fourier series, *i.e.*

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} \left( a_k \cos\left(\frac{2\pi}{L} kx\right) + b_k \sin\left(\frac{2\pi}{L} kx\right) \right)$$

and

$$a_k = \frac{2}{L} \int_0^L f(x) \cos\left(\frac{2\pi}{L} kx\right) \, \mathrm{d}x = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \cos\left(\frac{2\pi}{L} kx\right) \, \mathrm{d}x$$
$$= \frac{\left\langle f(x), \cos\left(\frac{2\pi}{L} kx\right) \right\rangle}{\left\| \cos\left(\frac{2\pi}{L} kx\right) \right\|_2^2}$$

$$b_k = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{2\pi}{L} kx\right) \, \mathrm{d}x = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \sin\left(\frac{2\pi}{L} kx\right) \, \mathrm{d}x$$
$$= \frac{\left\langle f(x), \sin\left(\frac{2\pi}{L} kx\right) \right\rangle}{\left\| \sin\left(\frac{2\pi}{L} kx\right) \right\|_2^2}$$

# Fourier series

## $L$ periodic on $[0, L[$ (Dem)

Dem:

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\left(\frac{2n\pi x}{L}\right) + \sum_{n=1}^{\infty} B_n \sin\left(\frac{2n\pi x}{L}\right)$$

- Projection on $\left\{\cos\left(\frac{2m\pi x}{L}\right)\right\}_{m=0}^{\infty}$, *i.e.* determine $I = \int_{-L/2}^{L/2} f(x) \cos\left(\frac{2m\pi x}{L}\right) \, dx$.

$$I = \int_{-L/2}^{L/2} \sum_{n=0}^{\infty} A_n \cos\left(\frac{2n\pi x}{L}\right) \cos\left(\frac{2m\pi x}{L}\right) dx + \int_{-L/2}^{L/2} \sum_{n=1}^{\infty} B_n \sin\left(\frac{2n\pi x}{L}\right) \cos\left(\frac{2m\pi x}{L}\right) dx$$

$$= \sum_{n=0}^{\infty} A_n \int_{-L/2}^{L/2} \cos\left(\frac{2n\pi x}{L}\right) \cos\left(\frac{2m\pi x}{L}\right) dx + \sum_{n=1}^{\infty} B_n \int_{-L/2}^{L/2} \sin\left(\frac{2n\pi x}{L}\right) \cos\left(\frac{2m\pi x}{L}\right) dx$$

The second integral is always zero. The first summation term reduces to

$$\int_{-L/2}^{L/2} f(x) \cos\left(\frac{2m\pi x}{L}\right) dx = \begin{cases} A_m(L) & \text{if } n = m = 0 \\ A_m\left(\frac{L}{2}\right) & \text{if } n = m \neq 0 \end{cases}$$

We get

$$A_0 = \frac{1}{L} \int_{-L/2}^{L/2} f(x) \, dx \quad ; \quad A_m = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \cos\left(\frac{2m\pi x}{L}\right) dx \qquad m = 1, 2, 3, \ldots$$

# Fourier series

## $L$ periodic on $[0, L[$ (Dem)

- Projection on $\left\{\sin\left(\frac{2m\pi x}{L}\right)\right\}_{m=1}^{\infty}$, *i.e.* determine $I = \int_{-L/2}^{L/2} f(x) \sin\left(\frac{2m\pi x}{L}\right) \mathrm{d}x$.

$$I = \int_{-L/2}^{L/2} \sum_{n=0}^{\infty} A_n \cos\left(\frac{2n\pi x}{L}\right) \sin\left(\frac{2m\pi x}{L}\right) \mathrm{d}x + \int_{-L/2}^{L/2} \sum_{n=1}^{\infty} B_n \sin\left(\frac{2n\pi x}{L}\right) \sin\left(\frac{2m\pi x}{L}\right) \mathrm{d}x$$

$$= \sum_{n=0}^{\infty} A_n \int_{-L/2}^{L/2} \cos\left(\frac{2n\pi x}{L}\right) \sin\left(\frac{2m\pi x}{L}\right) \mathrm{d}x + \sum_{n=1}^{\infty} B_n \int_{-L/2}^{L/2} \sin\left(\frac{2n\pi x}{L}\right) \sin\left(\frac{2m\pi x}{L}\right) \mathrm{d}x$$

The first integral is always zero. The second summation term reduces to

$$\int_{-L/2}^{L/2} f(x) \sin\left(\frac{2m\pi x}{L}\right) dx = B_m \left(\frac{L}{2}\right)$$

We get

$$B_m = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \sin\left(\frac{2m\pi x}{L}\right) dx \qquad m = 1, 2, 3, \ldots$$

# Fourier sine and cosine series

$L$ periodic on $[0, L[$

- If $f$ is $L$ periodic on $[0, L[$, and odd, then we have:

$$a_k = 0 \quad \text{and} \quad b_k = \frac{4}{L} \int_0^{L/2} f(x) \sin\left(\frac{2\pi}{L} kx\right) \, dx$$

- If $f$ is $L$ periodic on $[0, L[$, and even, then we have:

$$b_k = 0 \quad \text{and} \quad a_k = \frac{4}{L} \int_0^{L/2} f(x) \cos\left(\frac{2\pi}{L} kx\right) \, dx$$

# Fourier series

## $2\pi$ periodic on $[-\pi, \pi[$

If $f$ is $2\pi$ periodic on $[-\pi, \pi[$, we get:

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} \left( a_k \cos(kx) + b_k \sin(kx) \right)$$

and

$$a_k = \frac{1}{\pi} \int_0^{2\pi} f(x) \cos(kx)\, dx = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(kx)\, dx = \frac{\langle f(x), \cos(kx) \rangle}{\|\cos(kx)\|_2^2}$$

$$b_k = \frac{1}{\pi} \int_0^{2\pi} f(x) \sin(kx)\, dx = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(kx)\, dx = \frac{\langle f(x), \sin(kx) \rangle}{\|\sin(kx)\|_2^2}$$

# Fourier series in complex form

$L$ periodic on $[0, L[$

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{\jmath \frac{2\pi}{L} kx} \quad \text{with} \quad c_k = \begin{cases} \dfrac{a_k - \jmath b_k}{2} & \text{if } k > 0 \\ c_{-k}^* & \text{if } k < 0 \\ \frac{a_0}{2} & \text{if } k = 0 \end{cases}$$

By introducing $a_k$ and $b_k$, we obtain:

$$c_k = \frac{1}{L} \int_{-L/2}^{L/2} f(x) e^{-\jmath \frac{2\pi}{L} kx} \, \mathrm{d}x \quad \forall k \in \mathbb{Z}$$

If $f$ is real-valued then $c_{-k} = c_k^*$.

# Fourier series in complex form

*$L$ periodic on $[0, L[$ (Dem)*

Dem: Let $\theta_k = \frac{2\pi}{L} kx$, we have ($c_k \in \mathbb{C}$):

$$
\begin{aligned}
f(x) &= \frac{a_0}{2} + \sum_{k=1}^{\infty} \left( a_k \cos\left(\theta_k\right) + b_k \sin\left(\theta_k\right) \right) \\
&= \frac{a_0}{2} + \sum_{k=1}^{\infty} \left( a_k \frac{e^{\jmath\,\theta_k} + e^{-\jmath\,\theta_k}}{2} + b_k \frac{e^{\jmath\,\theta_k} - e^{-\jmath\,\theta_k}}{2\jmath} \right) \quad \text{Euler} \\
&= \frac{a_0}{2} + \sum_{k=1}^{\infty} \left( \frac{a_k - \jmath b_k}{2} e^{\jmath\,\theta_k} + \frac{a_k + \jmath b_k}{2} e^{-\jmath\,\theta_k} \right) = \sum_{k=-\infty}^{\infty} c_k e^{\jmath\,\theta_k}
\end{aligned}
$$

After identification, we get:

$$
c_k = \begin{cases} \dfrac{a_k - \jmath b_k}{2} & \text{if } k > 0 \\ c_{-k}^* & \text{if } k < 0 \end{cases} \qquad \text{and} \qquad c_0 = \frac{a_0}{2}
$$

# Fourier series as orthogonal basis

$L$ periodic on $[0, L[$

The functions $\psi_k(x) = e^{\jmath \frac{2\pi}{L} kx}$ for $k \in \mathbb{Z}$ provide a basis for $L$-periodic complex-valued functions on an interval $[0, L[$. These functions are orthogonal. Let $\theta_k = \frac{2\pi}{L} kx$, we have

$$\langle \psi_k(x), \psi_\ell(x) \rangle = \int_{-L/2}^{L/2} \psi_k(x), \psi_\ell^*(x) \, \mathrm{d}x = \int_{-L/2}^{L/2} e^{\jmath(\theta_k - \theta_\ell)} \, \mathrm{d}x$$

$$= \left[ \frac{e^{\jmath(\theta_k - \theta_\ell)}}{\jmath(\theta_k - \theta_\ell)} \right]_{-L/2}^{L/2} = \begin{cases} 0 & \text{if } k \neq \ell \\ L & \text{if } k = \ell \end{cases}$$

A Fourier series is a change of coordinates of a function $f$ into an infinite-dimensional orthogonal function space spanned by sines and cosines:

$$f(x) = \sum_{k=-\infty}^{\infty} c_k \psi_k(x) = \frac{1}{L} \sum_{k=-\infty}^{\infty} \langle f(x), \psi_k(x) \rangle \psi_k(x)$$

$$= \sum_{k=-\infty}^{\infty} \frac{\langle f(x), \psi_k(x) \rangle}{\|\psi_k(x)\|_2^2} \psi_k(x)$$

# Fourier decomposition



The Fourier transform integral is the limit of a Fourier series as the length of the domain goes to infinity.
Since different conventions are used, the Fourier transform pair may be defined in general with two arbitrary constants $a$ and $b$ (Wolfram):

$$\boxed{\hat{f}(\omega) = \mathcal{F}\left[f(t)\right] = C_{a,b} \int_{-\infty}^{\infty} f(t) e^{\jmath b \omega t} \, \mathrm{d}t}$$

$$\boxed{f(t) = \mathcal{F}^{-1}\left[\hat{f}(\omega)\right] = D_{a,b} \int_{-\infty}^{\infty} \hat{f}(\omega) e^{-\jmath b \omega t} \, \mathrm{d}\omega}$$

where

$$C_{a,b} = \sqrt{\frac{|b|}{(2\pi)^{1-a}}} \quad \text{and} \quad D_{a,b} = \sqrt{\frac{|b|}{(2\pi)^{1+a}}}$$

# Fourier decomposition



- $(a, b) = (1, -1)$ in pure mathematics and systems engineering,

$$C_{a,b} = 1 \quad \text{and} \quad D_{a,b} = \frac{1}{2\pi}$$

- $(a, b) = (1, 1)$ in probability theory for the computation of the characteristic function,

$$C_{a,b} = 1 \quad \text{and} \quad D_{a,b} = \frac{1}{2\pi}$$

- $(a, b) = (0, 1)$ in modern physics,

$$C_{a,b} = \frac{1}{\sqrt{2\pi}} \quad \text{and} \quad D_{a,b} = \frac{1}{\sqrt{2\pi}}$$

- $(a, b) = (-1, 1)$ in classical physics, and

$$C_{a,b} = \frac{1}{2\pi} \quad \text{and} \quad D_{a,b} = 1$$

- $(a, b) = (0, -2\pi)$ in signal processing.

$$C_{a,b} = 1 \quad \text{and} \quad D_{a,b} = 1$$

# Fourier decomposition



- For $(a, b) = (1, -1)$ (pure mathematics, systems engineering), we get:

$$\boxed{\hat{f}(\omega) = \mathcal{F}\left[f(t)\right] = \int_{-\infty}^{\infty} f(t) e^{-\jmath \omega t}\, \mathrm{d}t}$$

$$\boxed{f(t) = \mathcal{F}^{-1}\left[\hat{f}(\omega)\right] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(\omega) e^{\jmath \omega t}\, \mathrm{d}\omega}$$

where $\omega = 2\pi f$ is the angular frequency.

- For $(a, b) = (1, 1)$ (probability theory), we get:

$$\boxed{\hat{f}(\omega) = \mathcal{F}\left[f(t)\right] = \int_{-\infty}^{\infty} f(t) e^{\jmath \omega t}\, \mathrm{d}t}$$

$$\boxed{f(t) = \mathcal{F}^{-1}\left[\hat{f}(\omega)\right] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(\omega) e^{-\jmath \omega t}\, \mathrm{d}\omega}$$

The variables $(t, \omega)$ (time/angular frequency) are interchangeable with the variables $(x, k)$ (space/wave number).

# Fourier decomposition



- For $(a, b) = (0, 1)$ (modern physics), we get:

$$\boxed{\hat{f}(\omega) = \mathcal{F}\left[f(t)\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{\jmath \omega t} \, \mathrm{d}t}$$

$$\boxed{f(t) = \mathcal{F}^{-1}\left[\hat{f}(\omega)\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(\omega) e^{-\jmath \omega t} \, \mathrm{d}\omega}$$

where $\omega = 2\pi f$ is the angular frequency.

- For $(a, b) = (-1, 1)$ (classical physics), we get:

$$\boxed{\hat{f}(\omega) = \mathcal{F}\left[f(t)\right] = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) e^{\jmath \omega t} \, \mathrm{d}t}$$

$$\boxed{f(t) = \mathcal{F}^{-1}\left[\hat{f}(\omega)\right] = \int_{-\infty}^{\infty} \hat{f}(\omega) e^{-\jmath \omega t} \, \mathrm{d}\omega}$$

The variables $(t, \omega)$ (time/angular frequency) are interchangeable with the variables $(x, k)$ (space/wave number).

# Fourier decomposition



- For $(a, b) = (0, -2\pi)$ (signal processing), we get:

$$\boxed{\hat{f}(\omega) = \mathcal{F}\left[f(t)\right] = \int_{-\infty}^{\infty} f(t) e^{-2\pi \jmath \omega t} \, \mathrm{d}t}$$

$$\boxed{f(t) = \mathcal{F}^{-1}\left[\hat{f}(\omega)\right] = \int_{-\infty}^{\infty} \hat{f}(\omega) e^{2\pi \jmath \omega t} \, \mathrm{d}\omega}$$

where $\omega = 2\pi f$ is the angular frequency.

The variables $(t, \omega)$ (time/angular frequency) are interchangeable with the variables $(x, k)$ (space/wave number).

- Duality time/space where

$$\omega = 2\pi f = \frac{2\pi}{T} \quad \text{and} \quad k = 2\pi\xi = \frac{2\pi}{L}$$

with $T$ and $L$, the period over time and space, respectively.
$\xi$: wavenumber.

# Fourier decomposition



- **Linearity**

$$\boxed{\mathcal{F}[\alpha f(x) + \beta g(x)] = \alpha \mathcal{F}[f(x)] + \beta \mathcal{F}[g(x)] = \alpha \hat{f}(k) + \beta \hat{g}(k)}$$

$$\boxed{\mathcal{F}^{-1}[\alpha \hat{f}(k) + \beta \hat{g}(k)] = \alpha \mathcal{F}^{-1}[\hat{f}(k)] + \beta \mathcal{F}^{-1}[\hat{g}(k)] = \alpha f(x) + \beta g(x)}$$

Dem: with $(a, b) = (0, -2\pi)$

$$\begin{aligned}
\mathcal{F}[\alpha f(x) + \beta g(x)] &= \int [\alpha f(x) + \beta g(x)]\, e^{-2\pi \jmath k x}\, \mathrm{d}x \\
&= \alpha \int_{-\infty}^{\infty} f(x)\, e^{-2\pi \jmath k x}\, \mathrm{d}x + \beta \int_{-\infty}^{\infty} g(x) e^{-2\pi \jmath k x}\, \mathrm{d}x \\
&= \alpha \hat{f}(k) + \beta \hat{g}(k)
\end{aligned}$$

- **Symmetry**: $\boxed{\hat{f}(-k) = \mathcal{F}\left[f(-x)\right]}$
- **Convolutions**:

$$\boxed{(f * g)(x) = \int_{-\infty}^{\infty} f(x')\, g(x - x')\, \mathrm{d}x'} \quad \text{(Def.)}$$

# Fourier decomposition



$$\boxed{\mathcal{F}[f * g] = \mathcal{F}[f]\mathcal{F}[g]}$$

$$\boxed{\mathcal{F}[fg] = \mathcal{F}[f] * \mathcal{F}[g]}$$

$$\boxed{\mathcal{F}^{-1}[\mathcal{F}(f)\mathcal{F}(g)] = f * g}$$

$$\boxed{\mathcal{F}^{-1}[\mathcal{F}(f) * \mathcal{F}(g)] = fg}$$

Dem: with $(a, b) = (0, -2\pi)$

$$\begin{aligned}
\mathcal{F}[f * g] &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-2\pi\jmath k x} f(x')\, g(x - x')\, \mathrm{d}x'\, \mathrm{d}x \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left[e^{-2\pi\jmath k x'} f(x')\, \mathrm{d}x'\right] \left[e^{-2\pi\jmath k (x-x')} g(x - x')\, \mathrm{d}x\right] \\
&= \left[\int_{-\infty}^{\infty} e^{-2\pi\jmath k x'} f(x')\, \mathrm{d}x'\right] \left[\int_{-\infty}^{\infty} e^{-2\pi\jmath k x''} g(x'')\, \mathrm{d}x''\right] \\
&= \mathcal{F}[f]\mathcal{F}[g]
\end{aligned}$$

where $x'' = x - x'$.

# Fourier decomposition



- **Derivatives of functions**:

$$\mathcal{F}[f'(x)] = \int_{-\infty}^{\infty} \overbrace{f'(x)}^{v'} \overbrace{e^{-2\pi\jmath k x}}^{u} \,\mathrm{d}x \quad \text{with} \quad (a,b) = (0,-2\pi)$$

$$= \underbrace{\left[ \underbrace{f(x)e^{-2\pi\jmath k x}}_{uv} \right]_{-\infty}^{\infty}}_{} - \int_{-\infty}^{\infty} \underbrace{f(x)}_{v} \underbrace{\left( \underbrace{-2\pi\jmath k\, e^{-2\pi\jmath k x}}_{u'} \right)}_{} \,\mathrm{d}x$$

$$= (2\pi\jmath k) \int_{-\infty}^{\infty} f(x)\, e^{-2\pi\jmath k x} \,\mathrm{d}x \quad \text{since} \quad \lim_{x\to\pm\infty} f(x) = 0$$

$$\boxed{\mathcal{F}[f'(x)] = (2\pi\jmath k)\,\mathcal{F}[f(x)]}$$

For the $n$-th derivative:

$$\boxed{\mathcal{F}[f^{(n)}(x)] = (2\pi\jmath k)^n\,\mathcal{F}[f(x)] \quad \text{for} \quad (a,b) = (0,-2\pi)}$$

$$\boxed{\mathcal{F}[f^{(n)}(x)] = (\jmath k)^n\,\mathcal{F}[f(x)] \quad \text{for} \quad (a,b) = (1,-1)}$$

# Fourier decomposition



- **Parseval's theorem**:

$$\boxed{\int_{-\infty}^{\infty} |f(t)|^2 \, \mathrm{d}t = \frac{1}{(2\pi)^a} \int_{-\infty}^{\infty} |\hat{f}(\omega)|^2 \, \mathrm{d}\omega \quad \forall (a,b)}$$

Dem:

$$\begin{aligned}
\int_{-\infty}^{\infty} |f(t)|^2 \, \mathrm{d}t &= \int_{-\infty}^{\infty} f(t) f^*(t) \, \mathrm{d}t \\
&= D_{a,b}^2 \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} \hat{f}(\omega) e^{-\jmath\, b\, \omega\, t} \, \mathrm{d}\omega \right\} \left\{ \int_{-\infty}^{\infty} \hat{f}^*(\omega') e^{\jmath\, b\, \omega'\, t} \, \mathrm{d}\omega' \right\} \, \mathrm{d}t \\
&= D_{a,b}^2 \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} e^{\jmath\, b\, (\omega' - \omega)\, t} \, \mathrm{d}t \right] \hat{f}^*(\omega') \, \mathrm{d}\omega' \right] \hat{f}(\omega) \, \mathrm{d}\omega
\end{aligned}$$

By use of the integral identity for the Dirac delta function:

$$\delta(s - s') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{\jmath x (s - s')} \, \mathrm{d}x \quad \text{we conclude that}$$

$$\int_{-\infty}^{\infty} e^{\jmath\, b\, (\omega' - \omega)\, t} \, \mathrm{d}t = \frac{2\pi}{|b|} \delta(\omega' - \omega)$$

# Fourier decomposition



$$\begin{aligned}
\int_{-\infty}^{\infty} |f(t)|^2 \, \mathrm{d}t &= D_{a,b}^2 \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} e^{\jmath \, b \, (\omega' - \omega) \, t} \, \mathrm{d}t \right] \hat{f}^*(\omega') \, \mathrm{d}\omega' \right] \hat{f}(\omega) \, \mathrm{d}\omega \\
&= \frac{1}{(2\pi)^a} \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \delta(\omega' - \omega) \hat{f}^*(\omega') \, \mathrm{d}\omega' \right] \hat{f}(\omega) \, \mathrm{d}\omega \\
&= \frac{1}{(2\pi)^a} \int_{-\infty}^{\infty} \hat{f}(\omega) \hat{f}^*(\omega) \, \mathrm{d}\omega \\
&= \frac{1}{(2\pi)^a} \int_{-\infty}^{\infty} |\hat{f}(\omega)|^2 \, \mathrm{d}\omega
\end{aligned}$$

# Fourier decomposition



- **Fourier transform of a Gaussian function** ($\sigma > 0$):

$$\boxed{\mathcal{F}[e^{-\sigma\, x^2}] = C_{a,b}\sqrt{\frac{\pi}{\sigma}}e^{-\frac{b^2}{4\sigma}\, k^2} \quad \forall (a,b)}$$

A Gaussian transforms to another Gaussian.

Dem:

$$\begin{aligned}\mathcal{F}[e^{-\sigma\, x^2}] &= C_{a,b}\int_{-\infty}^{\infty} e^{-\sigma\, x^2} e^{\jmath\, b\, k\, x}\ \mathrm{d}x \\ &= C_{a,b}\int_{-\infty}^{\infty} \underbrace{e^{-\sigma\, x^2}}_{\text{even}}\underbrace{\cos(b\, k\, x)}_{\text{even}}\ \mathrm{d}x + \jmath\int_{-\infty}^{\infty} \underbrace{e^{-\sigma\, x^2}}_{\text{even}}\underbrace{\sin(b\, k\, x)}_{\text{odd}}\ \mathrm{d}x\end{aligned}$$

The second integrand ($I_2$) is odd, so integration over a symmetrical range gives 0. The first integrand ($I_1$) is even, so integration over a symmetrical range is equal to two times the integral over a mid range.

$$I_1 = 2\int_0^{\infty} e^{-\sigma\, x^2}\cos(b\, k\, x)\ \mathrm{d}x$$

# Fourier decomposition



After Abramowitz and Stegun (1972, p. 302, eq. 7.4.6), we have

$$\int_0^\infty e^{-\alpha t^2} \cos(2X t)\ \mathrm{d}t = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}} e^{-\frac{X^2}{\alpha}} \quad \text{with} \quad \alpha > 0$$

From which we deduce that

$$\mathcal{F}[e^{-\sigma x^2}] = C_{a,b}\sqrt{\frac{\pi}{\sigma}} e^{-\frac{b^2}{4\sigma} k^2}$$

Dem: for $(a, b) = (0, -2\pi)$, we get $C_{a,b} = 1$, *i.e.*

$$\mathcal{F}[e^{-\sigma x^2}] = \sqrt{\frac{\pi}{\sigma}} e^{-\frac{\pi^2 k^2}{\sigma}} \quad \text{(Wolfram)}$$

# Outline

7 Fourier series and Fourier transforms

8 Linear algebra recap

# Vector space

Definition

A vector space consists of a set $V$ (elements of $V$ are called vectors), a field $K$ (elements of $K$ are called scalars), and two operations:

- An operation called **vector addition** that takes two vectors $\boldsymbol{v}, \boldsymbol{w} \in V$, and produces a third vector, written $\boldsymbol{v} + \boldsymbol{w} \in V$.
- An operation called **scalar multiplication** that takes a scalar $c \in F$ and a vector $\boldsymbol{v} \in V$, and produces a new vector, written $c\boldsymbol{v} \in V$.

which satisfy the following conditions (called axioms):

1. *Associativity of vector addition*:
$$(\boldsymbol{u} + \boldsymbol{v}) + \boldsymbol{w} = \boldsymbol{u} + (\boldsymbol{v} + \boldsymbol{w}) \quad \forall \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in V$$
2. *Commutativity of vector addition*:
$$\boldsymbol{u} + \boldsymbol{v} = \boldsymbol{v} + \boldsymbol{u} \quad \forall \boldsymbol{u}, \boldsymbol{v} \in V$$
3. *Identity element of vector addition*: there exists a vector $\mathbf{0} \in V$, called the zero vector, such that:
$$\boldsymbol{u} + \mathbf{0} = \boldsymbol{u} \quad \forall \boldsymbol{u} \in V$$

4. *Inverse element of vector addition*: there exists a vector $-\boldsymbol{u} \in V$, called the negative of $\boldsymbol{u}$, such that:

$$\boldsymbol{u} + (-\boldsymbol{u}) = \boldsymbol{0} \quad \forall \boldsymbol{u} \in V$$

5. *Compatibility of scalar multiplication with field multiplication*:

$$a(b\boldsymbol{u}) = (ab)\boldsymbol{u} \quad \forall \boldsymbol{u} \in V \quad \text{and} \quad a, b \in F$$

6. *Identity element of scalar multiplication*:

$$1\boldsymbol{u} = \boldsymbol{u} \quad \forall \boldsymbol{u} \in V$$

7. *Distributivity of scalar multiplication with respect to vector addition*:

$$a(\boldsymbol{u} + \boldsymbol{v}) = a\boldsymbol{u} + a\boldsymbol{v} \quad \forall \boldsymbol{u}, \boldsymbol{v} \in V \quad \text{and} \quad a \in F$$

8. Distributivity of scalar multiplication with respect to vector addition.

$$(a + b)\boldsymbol{u} = a\boldsymbol{u} + b\boldsymbol{u} \quad \forall \boldsymbol{u} \in V \quad \text{and} \quad a, b \in F$$

# Inner product

Definition

Let $V$ be a vector space over the field $K$ (real numbers $\mathbb{R}$ or complex numbers $\mathbb{C}$). The map

$$\langle \cdot, \cdot \rangle : V \times V \to K$$

is called an **inner product**, if the following conditions (1), (2) and (3) are satisfied for all vectors $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in V$ and all scalars $a \in K$:

1. *Linearity* in the second[2] argument:

$$\langle \boldsymbol{x}, a\boldsymbol{y} \rangle = a\langle \boldsymbol{x}, \boldsymbol{y} \rangle$$
$$\langle \boldsymbol{x}, \boldsymbol{y} + \boldsymbol{z} \rangle = \langle \boldsymbol{x}, \boldsymbol{y} \rangle + \langle \boldsymbol{x}, \boldsymbol{z} \rangle$$

2. *Hermitian* symmetry:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \langle \boldsymbol{y}, \boldsymbol{x} \rangle^{\mathrm{H}}.$$

3. *Positive-definite*:

$$\langle \boldsymbol{x}, \boldsymbol{x} \rangle > 0, \qquad \text{if } \boldsymbol{x} \neq \mathbf{0}_V$$

[2] In mathematics, $\langle \cdot, \cdot \rangle$ is linear in the first argument. Here, we adopt the convention that $\langle \cdot, \cdot \rangle$ is linear in the second argument, which is more common in applied mathematics and physics.

Assuming (1) holds, condition (3) will hold if and only if conditions (4) and (5) below hold:

4. *Positive semi-definite* or nonnegative-definite:

$$\langle \boldsymbol{x}, \boldsymbol{x} \rangle \geq 0$$

5. *Definite condition*

$$\langle \boldsymbol{x}, \boldsymbol{x} \rangle = 0 \Rightarrow \boldsymbol{x} = \mathbf{0}_V$$

Conditions (1) through (5) are satisfied by every inner product.

We call *pre-Hilbert space* or *inner product space* a vector space with an inner product.

Inner product spaces are normed vector spaces for the norm defined by

$$\|x\| = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$$

# Examples of inner products

- The **Euclidean vector space** is defined in $\mathbb{R}^n$ with the dot product:

$$\left\langle \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \right\rangle_{\mathbb{R}^n} := \boldsymbol{x} \cdot \boldsymbol{y} = \boldsymbol{x}^\top \boldsymbol{y} = \sum_{i=1}^{n} x_i y_i = x_1 y_1 + \cdots + x_n y_n.$$

- The **Hermitian vector space** is defined in $\mathbb{C}^n$ with the inner product:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle := \boldsymbol{x}^{\mathrm{H}} \boldsymbol{y} = \left( \boldsymbol{y}^{\mathrm{H}} \boldsymbol{x} \right)^{\mathrm{H}} = \sum_{i=1}^{n} x_i^* y_i = x_1^* y_1 + \cdots + x_n^* y_n.$$

- Let $C([a, b])$ denote the **space of all complex-valued continuous functions defined on** $[a, b]$. We define an Hermitian inner product by

$$\langle f(x), g(x) \rangle = \int_a^b f^*(x)\, g(x)\, \mathrm{d}x.$$

# Inner product with respect to matrix I

- Let $\boldsymbol{A} \in \mathbb{C}^{n \times n}$ be any Hermitian positive-definite[3] matrix. The inner product with respect to $\boldsymbol{A}$ of $\boldsymbol{x} \in \mathbb{C}^n$ and $\boldsymbol{y} \in \mathbb{C}^n$ is given by

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{A}} := \boldsymbol{x}^{\mathrm{H}} \boldsymbol{A} \boldsymbol{y} = \left( \boldsymbol{y}^{\mathrm{H}} \boldsymbol{A} \boldsymbol{x} \right)^{\mathrm{H}}.$$

The inner product can be used to define a norm

$$\|\boldsymbol{x}\|_{\boldsymbol{A}} = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle_{\boldsymbol{A}}},$$

which is called the $\boldsymbol{A}$-norm. When $\boldsymbol{A} = \boldsymbol{I}$, this is just the 2-norm.

[3] $\boldsymbol{A}$ is said to be positive-definite if the scalar $\boldsymbol{z}^{\mathrm{H}} \boldsymbol{A} \boldsymbol{z}$ is strictly positive for every non-zero column vector $\boldsymbol{z}$ of $n$ complex numbers.

# Inner product with respect to matrix II

- $\boldsymbol{A}$ is an Hermitian positive semidefinite matrix if and only if it can be decomposed as a product

$$\boldsymbol{A} = \boldsymbol{M}^{\mathrm{H}} \boldsymbol{M}.$$

With that in mind, the $\boldsymbol{A}$ inner product can be written:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{A}} = \boldsymbol{x}^{\mathrm{H}} \boldsymbol{A} \boldsymbol{y} = \boldsymbol{x}^{\mathrm{H}} \boldsymbol{M}^{\mathrm{H}} \boldsymbol{M} \boldsymbol{y} = (\boldsymbol{M}\boldsymbol{x})^{\mathrm{H}} (\boldsymbol{M}\boldsymbol{y}) = \langle \boldsymbol{M}\boldsymbol{x}, \boldsymbol{M}\boldsymbol{y} \rangle_{\mathbb{C}^n}.$$

In terms of norm, we obtain:

$$\|\boldsymbol{x}\|_{\boldsymbol{A}} = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle_{\boldsymbol{A}}} = \sqrt{\langle \boldsymbol{M}\boldsymbol{x}, \boldsymbol{M}\boldsymbol{x} \rangle_{\mathbb{C}^n}} = \|\boldsymbol{M}\boldsymbol{x}\|_{\mathbb{C}^n}.$$

# Orthogonality and orthonormality

Definition

- Two vectors, $\boldsymbol{x}$ and $\boldsymbol{y}$, in an inner product space, $V$, are orthogonal if their inner product $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = 0$. We denote this relation $\boldsymbol{x} \perp \boldsymbol{y}$. These vectors are $\boldsymbol{A}$-orthogonal if $\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{A}} = 0$.

Let $\langle \cdot, \cdot \rangle$ be the inner product defined over $V$. A set of vectors $\{\boldsymbol{u_1}, \boldsymbol{u_2}, \ldots, \boldsymbol{u_n}\} \in V$ is called *orthonormal* if and only if

$$\langle \boldsymbol{u_i}, \boldsymbol{u_j} \rangle = \delta_{ij}, \quad \forall i, j$$

where $\delta_{ij}$ is the Kronecker delta. $\boldsymbol{A}$-orthonormality is defined by extension with the $\boldsymbol{A}$-inner product. Every orthonormal set of vectors is linearly independent.

# Unitary/orthogonal matrices



$\boldsymbol{A} \in \mathbb{C}^{n \times n}$ is *unitary*, if

$$\boldsymbol{A}^{\mathrm{H}} \boldsymbol{A} = \boldsymbol{A} \boldsymbol{A}^{\mathrm{H}} = \boldsymbol{I}_n.$$

By extension, if $\boldsymbol{A} \in \mathbb{R}^{n \times n}$, we define an *orthogonal* matrix as:

$$\boldsymbol{A}^{\top} \boldsymbol{A} = \boldsymbol{A} \boldsymbol{A}^{\top} = \boldsymbol{I}_n.$$

The columns and rows of $\boldsymbol{A}$ are orthonormal for the usual inner product.

# Unitary/orthogonal matrices

## Properties

If $\boldsymbol{A}$ is a unitary matrix, then the following hold:

1. Let $\boldsymbol{x}$ and $\boldsymbol{y}$ be two complex vectors, multiplication by $\boldsymbol{A}$ preserves their inner product, *i.e.* $\langle \boldsymbol{Ax}, \boldsymbol{Ay} \rangle = \langle \boldsymbol{x}, \boldsymbol{y} \rangle$. See Pt. 6 next slide for the consequence.
2. $\boldsymbol{A}$ is *normal*: $\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}^{\mathrm{H}}$. See Pt. 3 and Pt. 7 next slide for the consequence.
3. $\boldsymbol{A}$ is diagonalizable and its eigenvectors form an orthonormal basis, *i.e.* $\boldsymbol{A}$ has a decomposition of the form

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^{\mathrm{H}}$$

   where $\boldsymbol{U}$ is unitary, and $\boldsymbol{\Lambda}$ is diagonal and unitary. $\boldsymbol{A}$ is similar to the diagonal matrix $\boldsymbol{\Lambda}$.
4. $|\det(\boldsymbol{A})| = 1$. See Pt. 7 next slide for the consequence in terms of eigenvalues of $\boldsymbol{A}$.

# Unitary/orthogonal matrices

## Equivalent conditions

If $\boldsymbol{A} \in \mathbb{C}^{n\times n}$, then the following conditions are equivalent:

1. $\boldsymbol{A}$ is unitary.
2. $\boldsymbol{A}^{\mathrm{H}}$ is unitary.
3. $\boldsymbol{A}$ is invertible with $\boldsymbol{A}^{-1} = \boldsymbol{A}^{\mathrm{H}}$.
4. The columns of $\boldsymbol{A}$ form an orthonormal basis of $\mathbb{C}^n$ with respect to the usual inner product, *i.e.* $\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A} = \boldsymbol{I}_n$.
5. The rows of $\boldsymbol{A}$ form an orthonormal basis of $\mathbb{C}^n$ with respect to the usual inner product, *i.e.* $\boldsymbol{A}\boldsymbol{A}^{\mathrm{H}} = \boldsymbol{I}_n$.
6. $\boldsymbol{A}$ is an *isometry* with respect to the usual norm, *i.e.*

   $\|\boldsymbol{A}\boldsymbol{x}\|_2 = \|\boldsymbol{x}\|_2$ for all $\boldsymbol{x} \in \mathbb{C}^n$, where $\|\boldsymbol{x}\|_2 = \sqrt{\sum_{i=1}^{n} |x_i|^2}$.

   Orthogonal matrices $\boldsymbol{A}$ are often called rotations or reflections.
7. $\boldsymbol{A}$ is a normal matrix (equivalently, there is an orthonormal basis formed by eigenvectors of $\boldsymbol{A}$). Since $|\det(\boldsymbol{A})| = 1$ (see Pt. 4 previous slide), then the eigenvalues of $\boldsymbol{A}$ lie on the unit circle.

# Matrix similarity

- In linear algebra, two $n$-by-$n$ matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are called *similar* if there exists an invertible $n$-by-$n$ matrix $\boldsymbol{P}$ such that:

$$\boldsymbol{B} = \boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{P}.$$

- Similar matrices represent the same linear map under two (possibly) different bases, with $\boldsymbol{P}$ being the change of basis matrix.

- A transformation $\boldsymbol{A} \mapsto \boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{P}$ is called a *similarity transformation* or *conjugation* of the matrix $\boldsymbol{A}$. The matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ share the same eigenvalues.

# Normal matrix

- Let $\boldsymbol{A}$ be a complex matrix. $\boldsymbol{A}$ is normal, if and only if, we have:

$$\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}^{\mathrm{H}}.$$

- The *spectral theorem* states that a matrix $\boldsymbol{A}$ is normal if and only if there exists a diagonal matrix $\boldsymbol{\Lambda}$ and a unitary matrix $\boldsymbol{U}$ such that $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^{\mathrm{H}}$. Since $\boldsymbol{U}^{-1} = \boldsymbol{U}^{\mathrm{H}}$, the matrix $\boldsymbol{A}$ is similar to a diagonal matrix $\boldsymbol{\Lambda}$. Since $\boldsymbol{U}$ is unitary, the eigenvectors of $\boldsymbol{A}$ form an orthonormal basis for the usual inner product.

- A symmetric matrix $\boldsymbol{C} \in \mathbb{R}^{n\times n}$ is a special case of normal matrix. As a consequence $\boldsymbol{C}$ is necessarily orthogonally diagonalizable. This implies that there always exists an orthogonal matrix $\boldsymbol{S} \in \mathbb{R}^{n\times n}$ (*i.e.* $\boldsymbol{S}^{\top}\boldsymbol{S} = \boldsymbol{I}_n$) such that $\boldsymbol{S}^{-1}\boldsymbol{C}\boldsymbol{S}$ is diagonal. The columns of the matrix $\boldsymbol{S}$ correspond to the eigenvectors of $\boldsymbol{C}$.

# Basis

Let $V$ be a vector space over a field $K$ (real numbers $\mathbb{R}$ or complex numbers $\mathbb{C}$). A subset $B$ of $V$ is a *basis* if it satisfies the two conditions:

1. the *linear independence* property, *i.e.* for every finite subset $\{\boldsymbol{v_1}, \ldots, \boldsymbol{v_n}\}$ of $B$:

$$c_1\boldsymbol{v_1} + \cdots + c_n\boldsymbol{v_n} = 0, \text{for some } c_1, \ldots, c_n \in K \quad \text{then} \quad c_1 = \cdots = c_n = 0;$$

2. the *spanning* property, *i.e.* for every vector $\boldsymbol{v}$ in $V$, one can write:

$$\boldsymbol{v} = c_1\boldsymbol{v_1} + \cdots + c_n\boldsymbol{v_n} \text{ with } c_1, \ldots, c_n \in K \quad \text{and} \quad \boldsymbol{v_1}, \ldots, \boldsymbol{v_n} \in B.$$

The scalars $c_i$ are called the coordinates of the vector $\boldsymbol{v}$ with respect to the basis $B$. By the first property, the coordinates are uniquely determined. The *dimension* of a subspace is the largest number of vectors in the subspace that are linearly independent.

# Vector norm

Definition

- Given a vector space $V$ over a field $K$ (real numbers $\mathbb{R}$ or complex numbers $\mathbb{C}$), a norm on $V$ is a non negative-valued function $p : V \to \mathbb{R}^+$ with the following properties:

For all $a \in K$ and all $\boldsymbol{u}, \boldsymbol{v} \in V$,

1. $p(\boldsymbol{u} + \boldsymbol{v}) \leq p(\boldsymbol{u}) + p(\boldsymbol{v})$ (*triangle inequality*).
2. $p(a\boldsymbol{u}) = |a|\, p(\boldsymbol{u})$ (*absolutely homogeneous* or *absolutely scalable*).
3. if $p(\boldsymbol{u}) = 0$ then $\boldsymbol{u} = \boldsymbol{0}$ (*positive definite*).

The norm of a vector $\boldsymbol{u} \in V$ is usually denoted by $p(\boldsymbol{u}) = \|\boldsymbol{u}\|$.

# Vector norm



- A *seminorm* on $V$ is a function $p : V \to \mathbb{R}^+$ with only the properties 1 and 2 above.

- Suppose that $p$ and $q$ are two norms (or seminorms) on a vector space $V$. Then $p$ and $q$ are called *equivalent*, if there exists two real constants $c$ and $C$ with $c > 0$ such that for every vector $\boldsymbol{v} \in V$, we have

$$cq(\boldsymbol{v}) \leq p(\boldsymbol{v}) \leq Cq(\boldsymbol{v}).$$

In a finite-dimensional space, any two norms are equivalent but this is not true in infinite-dimensional spaces.

# Vector norm

*p*-norm ($p \geq 1$)

- The $p$-norm (also called $\ell_p$-norm) of vector $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ is

$$\|\boldsymbol{x}\|_p := \left( \sum_{i=1}^{n} |x_i|^p \right)^{1/p}.$$

- For $p = 1$, we get the Taxicab norm or Manhattan norm $\|\boldsymbol{x}\|_1 := \sum_{i=1}^{n} |x_i|$. It can be viewed as counting the number of blocks you would have to walk on a $n$-dimensional grid.
- For $p = 2$, we get the Euclidean norm $\|\boldsymbol{x}\|_2 := \sqrt{x_1^2 + \cdots + x_n^2}$.
- As $p$ approaches $\infty$, the $p$-norm approaches the infinity norm or maximum norm: $\|\boldsymbol{x}\|_\infty := \max_i |x_i|$.

The norm is a measure of length. All these norms are equivalent, since

$$\|\boldsymbol{x}\|_\infty \leq \|\boldsymbol{x}\|_p \leq n^{\frac{1}{p}} \|\boldsymbol{x}\|_\infty.$$

# Matrix norm

Definition

- Let $K^{m\times n}$ be the vector space of all matrices of size $m \times n$ with entries in the field $K$ (real numbers $\mathbb{R}$ or complex numbers $\mathbb{C}$). A matrix norm is a function $\|\cdot\| : K^{m\times n} \to \mathbb{R}$ that must satisfy the following properties:
  - $\|\alpha \boldsymbol{A}\| = |\alpha| \|\boldsymbol{A}\|$ (*absolutely homogeneous*)
  - $\|\boldsymbol{A} + \boldsymbol{B}\| \leq \|\boldsymbol{A}\| + \|\boldsymbol{B}\|$ (*sub-additive* or *triangle inequality*)
  - $\|\boldsymbol{A}\| \geq 0$ (*positive-valued*)
  - $\|\boldsymbol{A}\| = 0 \iff \boldsymbol{A} = 0_{m,n}$ (*definite*)

  for all scalars $\alpha \in K$ and for all matrices $\boldsymbol{A}, \boldsymbol{B} \in K^{m\times n}$.
- Additionally, in the case of square matrices ($m = n$), some (but not all) matrix norms satisfy the additional property given by

$$\|\boldsymbol{AB}\| \leq \|\boldsymbol{A}\| \|\boldsymbol{B}\|.$$

A matrix norm that satisfies this additional property is called a *submultiplicative* norm.

# Matrix norm

## Matrix norms induced by vector norms (I)

Let $\|\cdot\|$ be a vector norm for both spaces $K^m$ and $K^n$. The *induced norm* on the space $K^{m\times n}$ of all $m \times n$ matrices is defined as follows:

$$\begin{aligned}\|\boldsymbol{A}\| &= \sup\{\|\boldsymbol{A}\boldsymbol{x}\| : \boldsymbol{x} \in K^n \text{ with } \|\boldsymbol{x}\| = 1\} \\ &= \sup\left\{\frac{\|\boldsymbol{A}\boldsymbol{x}\|}{\|\boldsymbol{x}\|} : \boldsymbol{x} \in K^n \text{ with } \boldsymbol{x} \neq \boldsymbol{0}\right\}.\end{aligned}$$

If the $p$-norm for vectors $(1 \leq p \leq \infty)$ is used, then

$$\|\boldsymbol{A}\|_p = \sup_{\boldsymbol{x}\neq\boldsymbol{0}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|_p}{\|\boldsymbol{x}\|_p}.$$

# Matrix norm

## Matrix norms induced by vector norms (II)

When $p = 1, 2, \infty$, the induced matrix norms can be computed as

$$\|\boldsymbol{A}\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |a_{ij}|,$$

which is simply the maximum absolute column sum of the matrix;

$$\|\boldsymbol{A}\|_\infty = \max_{1 \le i \le m} \sum_{j=1}^{n} |a_{ij}|,$$

which is simply the maximum absolute row sum of the matrix;

$$\|\boldsymbol{A}\|_2 = \sigma_{\max}(\boldsymbol{A}) \le \|\boldsymbol{A}\|_{\mathrm{F}} = \left( \sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2 \right)^{\frac{1}{2}},$$

where $\sigma_{\max}(\boldsymbol{A})$ represents the largest singular value of matrix $\boldsymbol{A}$ and where $\|\boldsymbol{A}\|_{\mathrm{F}}$ is the Frobenius norm.

# Matrix norm

## Matrix norms induced by vector norms (III)

The *Frobenius* norm or the *Hilbert–Schmidt* norm is defined as:

$$\|\boldsymbol{A}\|_{\mathrm{F}} = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2} = \sqrt{\operatorname{trace}\left(\boldsymbol{A}^{\mathrm{H}}\boldsymbol{A}\right)} = \sqrt{\sum_{i=1}^{\min\{m,n\}}\sigma_i^2(\boldsymbol{A})},$$

where $\sigma_i(\boldsymbol{A})$ are the singular values of $\boldsymbol{A}$.

# Injectivity, surjectivity and bijection I

Let $f$ be a function mapping the domain $X$ to the *codomain* $Y$, *i.e.* $f : X \to Y$.

- By definition, the function $f$ is said to be *injective*, if

$$\forall \boldsymbol{x_1}, \boldsymbol{x_2} \in X, \quad f(\boldsymbol{x_1}) = f(\boldsymbol{x_2}) \Rightarrow \boldsymbol{x_1} = \boldsymbol{x_2},$$

or, using the contrapositive, if

$$\forall \boldsymbol{x_1}, \boldsymbol{x_2} \in X, \quad \boldsymbol{x_1} \neq \boldsymbol{x_2} \Rightarrow f(\boldsymbol{x_1}) \neq f(\boldsymbol{x_2}).$$

An injective function (also known as *injection*, or *one-to-one* function) is a function that maps distinct elements of its domain to distinct elements of its codomain. In other words, every element of the function's codomain is the image of at most one element of its domain.

# Injectivity, surjectivity and bijection II

- By definition, the function $f$ is said to be *surjective*, if

$$\forall \boldsymbol{y} \in Y, \exists \boldsymbol{x} \in X, \quad f(\boldsymbol{x}) = \boldsymbol{y}.$$

A surjective function is also known as *surjection*, or *onto* function. It is not required that $\boldsymbol{x}$ be unique; the function $f$ may map one or more elements of $X$ to the same element of $Y$.

- By definition, the function $f$ is a *bijection*, *bijective function*, *one-to-one correspondence*, or *invertible* function, if $f$ is a one-to-one (injective) and onto (surjective) mapping of a set $X$ to a set $Y$. In other words, each element of $X$ is paired with exactly one element of $Y$, and each element of $Y$ is paired with exactly one element of $X$. There are no unpaired elements.

# Range space, Null space and Rank



Let $\boldsymbol{A} \in \mathbb{R}^{n \times m}$ be an arbitrary matrix, we can associate to $\boldsymbol{A}$ the linear map $f : \mathbb{R}^n \to \mathbb{R}^m$ such that $\boldsymbol{x} \mapsto \boldsymbol{A}\boldsymbol{x}$ where $\boldsymbol{x} \in \mathbb{R}^n$. For $f$ to be an injective function, it is necessary that $n \leq m$ and that the columns of $\boldsymbol{A}$ be linearly independent. If the columns are not linearly independent, then there exists $\boldsymbol{z} \in \mathbb{R}^n$ such that $\boldsymbol{A}\boldsymbol{z} = \boldsymbol{0}$. Due to the linearity, there are an infinite number of vectors that map to zero. This set of vectors is called the *null space* of $\boldsymbol{A}$ and is denoted

$$\mathcal{N}(\boldsymbol{A}) = \{\boldsymbol{x} \in \mathbb{R}^n \mid \boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}\}.$$

Due to the linearity of the mapping, $\mathcal{N}(\boldsymbol{A})$ is a subspace.

# Range space, Null space and Rank



Now consider the range of $f$. The range

$$\mathcal{R}(\boldsymbol{A}) = \{\boldsymbol{A}\boldsymbol{x} \mid \boldsymbol{x} \in \mathbb{R}^n\}.$$

is the set of vectors mapped to $\mathbb{R}^m$ by $\boldsymbol{x} \mapsto \boldsymbol{A}\boldsymbol{x}$. For an arbitrary $\boldsymbol{x} \in \mathbb{R}^n$, $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ is a linear combination of the columns of $\boldsymbol{A}$. The range of $\boldsymbol{A}$ is then the span of the columns of $\boldsymbol{A}$:

$$\mathcal{R}(\boldsymbol{A}) = \text{Span}(\boldsymbol{a_1}, \boldsymbol{a_2}, \cdots, \boldsymbol{a_n}).$$

The column-rank is the dimension of $\mathcal{R}(\boldsymbol{A})$ and the row-rank is the dimension of $\mathcal{R}(\boldsymbol{A}^\top)$. The column-rank of a matrix is equal to its row-rank and is called the *rank* of the matrix. A matrix is said to have *full rank* if $\text{Rank}(\boldsymbol{A}) = \min(m, n)$.

# Range space, Null space and Rank



$f$ is an injective function if $m \geq n$ and $\boldsymbol{A}$ has full rank. In that case, we have

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}\boldsymbol{y} \Rightarrow \boldsymbol{x} = \boldsymbol{y}.$$

For $f$ to be a surjective function, the column rank must be $m$. A square matrix is full rank if and only if $f$ is a bijective function. Such a matrix is called *non singular*. For a non singular matrix, there exists a unique *inverse*. A square matrix with rank less than its size is called *singular*.

For a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, we have:

$$\dim\left(\mathcal{R}\left(\boldsymbol{A}\right)\right) + \dim\left(\mathcal{N}\left(\boldsymbol{A}\right)\right) = n.$$