

On the importance of low-dimensional structures for data-driven modeling

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- Maître de Conférences in Fluid Dynamics and Applied Math.
- Machine-learning enthusiast with application to engineering systems.
- Data-efficient models with guarantees of optimality or interpretability.



Given training data $y_i = f(x_i)$ where f is unknown, we want to **learn** a function \hat{f} such that

$$\underset{\hat{f} \in \mathcal{F}}{\text{minimize}} \quad \|\mathbf{f}(x) - \hat{\mathbf{f}}(x)\|$$

where \mathcal{F} is a particular *class* of models. Here, we'll restrict our attention to the class of *linear* models.

A (very) brief overview of SVD

$$\mathbf{A} = \mathbf{U} \ \boldsymbol{\Sigma} \ \mathbf{V}^T$$

Basis for $\text{colspan}(A)$

Basis for $\text{rowspan}(A)$

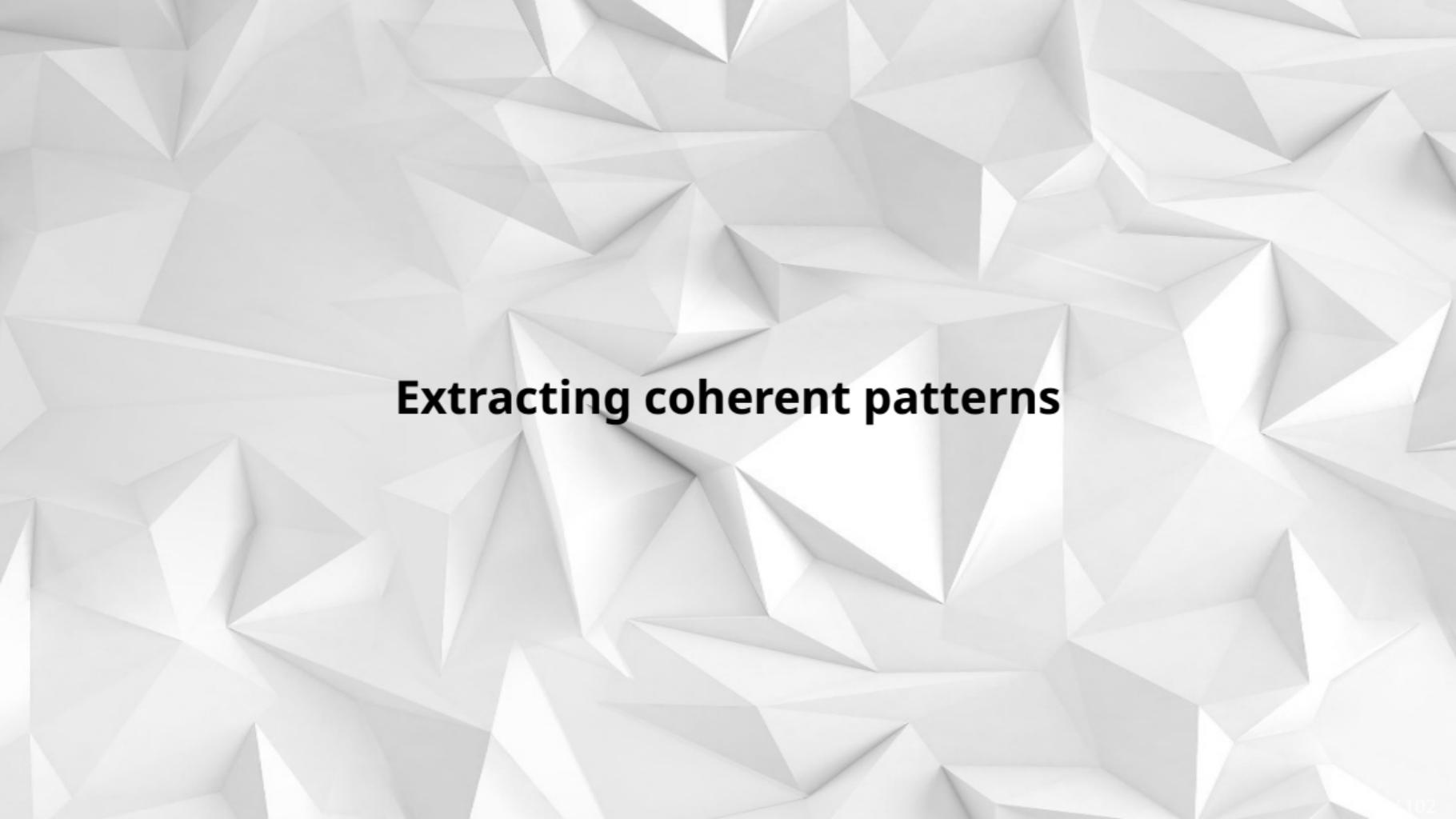
$$A = \color{red}U\color{black} \Sigma \color{blue}V^T$$

Diagonal matrix

Relation to spectral decomposition

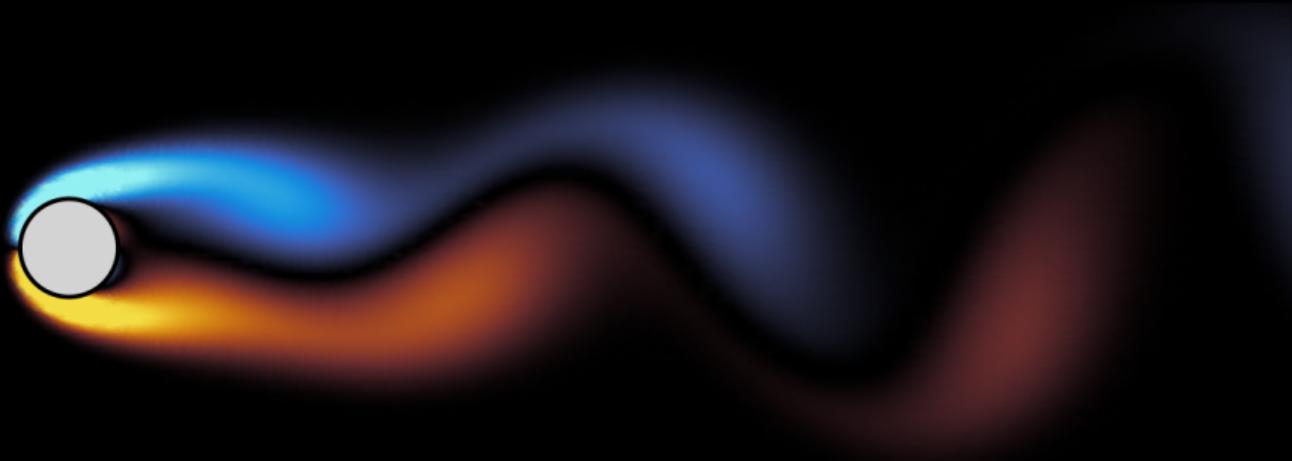
$$\begin{bmatrix} \mathbf{0} & \mathbf{A} \\ \mathbf{A}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u}_i \\ \mathbf{v}_i \end{bmatrix} = \sigma_i \begin{bmatrix} \mathbf{u}_i \\ \mathbf{v}_i \end{bmatrix}$$

Generalization of the *eigenvalue decomposition* to **non-square matrices** by E. Beltrami (1873) and C. Jordan (1874). The first efficient numerical algorithm was developed by G. Golub *et al.* in the late 1960s.

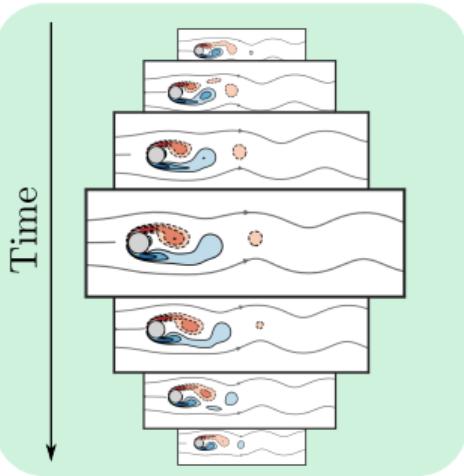
The background of the slide features a complex, abstract pattern of white polygons, likely triangles, arranged in a way that creates a sense of depth and texture. The polygons vary in size and orientation, with some pointing towards the center and others away, giving the appearance of a three-dimensional surface.

Extracting coherent patterns

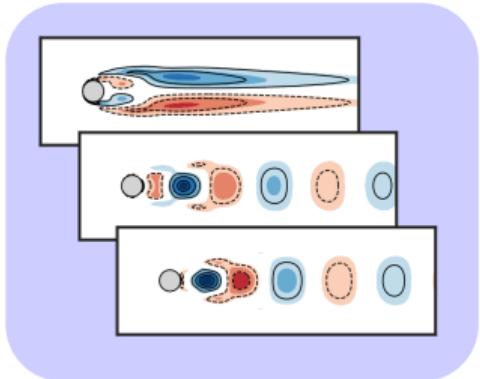




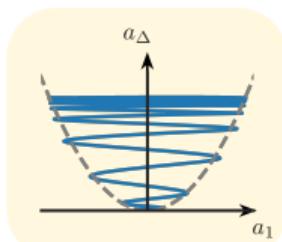
Navier-Stokes simulation

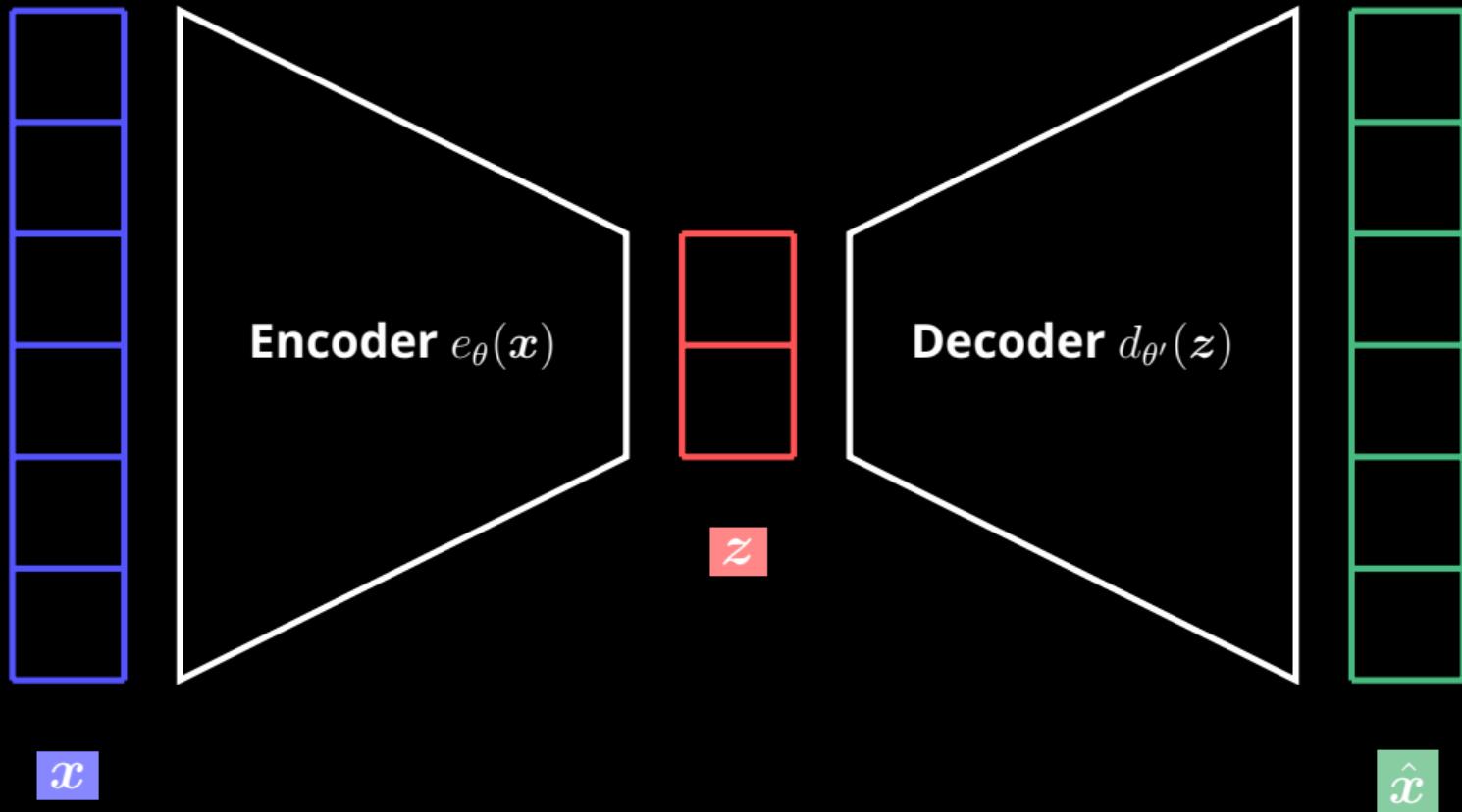


Dimensionality reduction



Simple representation





$$\min_{\theta, \theta'} \sum_{i=1}^N \| \mathbf{x}_i - (d_{\theta'} \circ e_{\theta})(\mathbf{x}_i) \|_2^2$$

Estimate



Ground truth



$$\begin{aligned} & \underset{\boldsymbol{P}, \boldsymbol{Q}}{\text{minimize}} && \sum_{i=1}^N \|\boldsymbol{x}_i - \boldsymbol{P}\boldsymbol{Q}^T\boldsymbol{x}_i\|_2^2 \\ & \text{subject to} && \text{rank } \boldsymbol{P} = \text{rank } \boldsymbol{Q} = r \end{aligned}$$

$$\begin{aligned} & \underset{\boldsymbol{P}}{\text{minimize}} && \sum_{i=1}^N \|\boldsymbol{x}_i - \boldsymbol{P}\boldsymbol{P}^T\boldsymbol{x}_i\|_2^2 \\ & \text{subject to} && \text{rank } \boldsymbol{P} = r \end{aligned}$$

$$\begin{aligned} & \underset{\boldsymbol{P}}{\text{minimize}} && \|\boldsymbol{X} - \boldsymbol{P}\boldsymbol{P}^T\boldsymbol{X}\|_F^2 \\ & \text{subject to} && \boldsymbol{P}^T\boldsymbol{P} = \boldsymbol{I}_r \end{aligned}$$

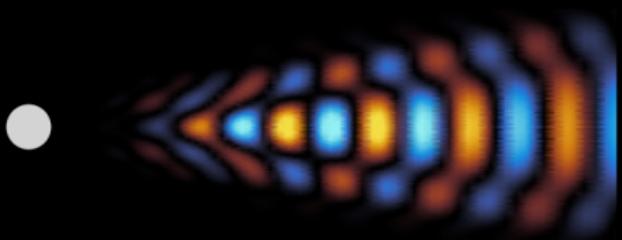
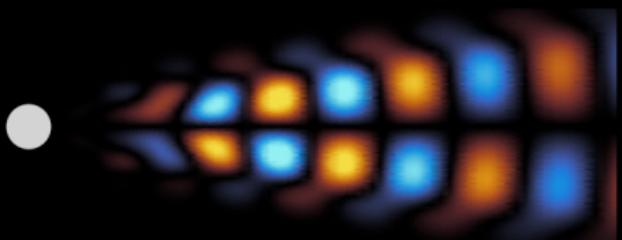
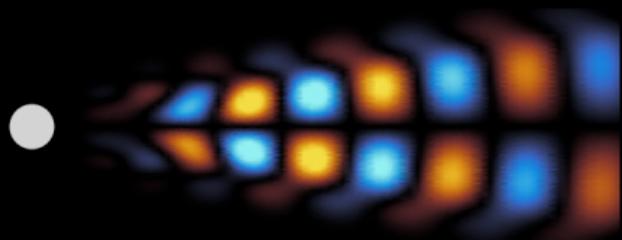
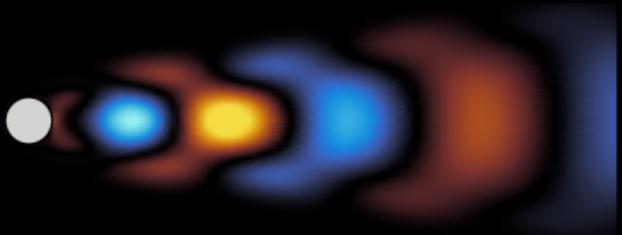
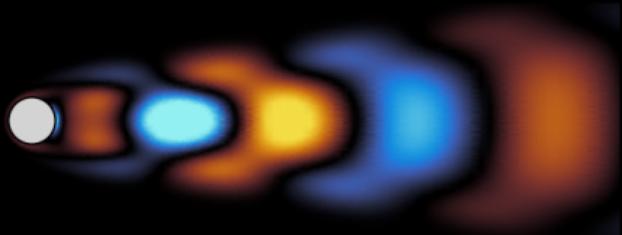
Proper Orthogonal Decomposition

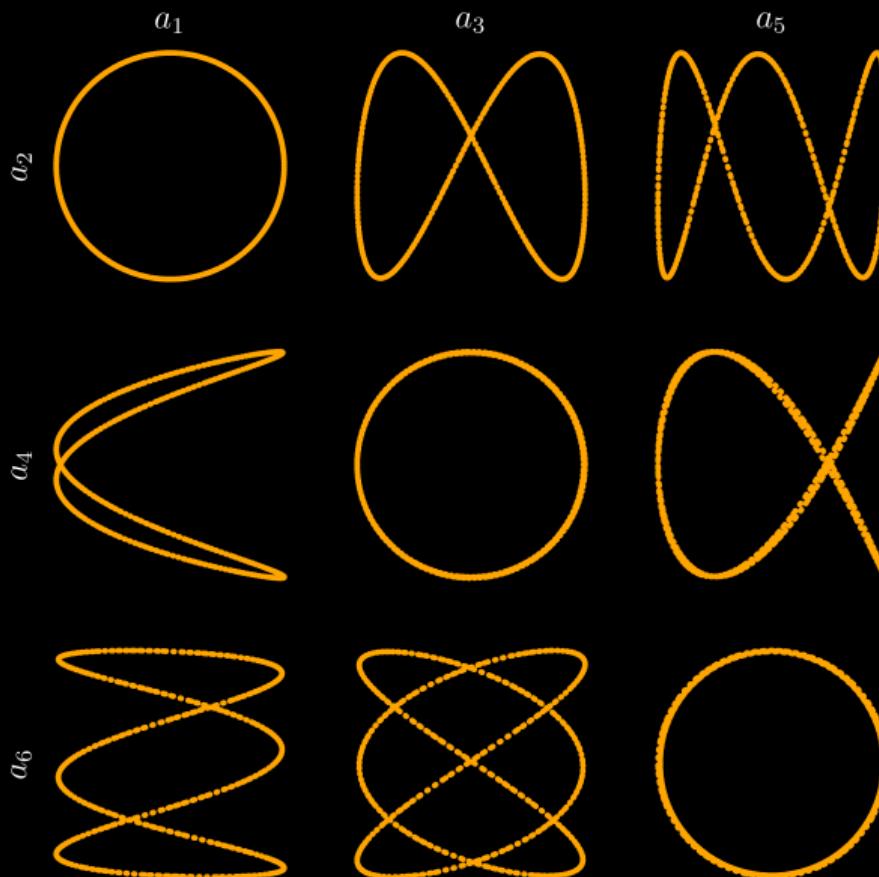
$$P\Lambda = C_{xx}P$$

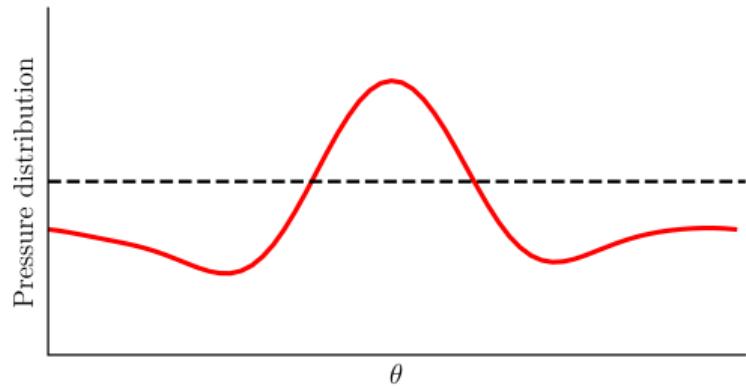
P corresponds to the left singular vectors of X . The latent representation is given by $z_i = P^T x_i$. The optimal rank of the model can be inferred from the distribution of the PCA eigenvalues $\Lambda = \Sigma^2$.

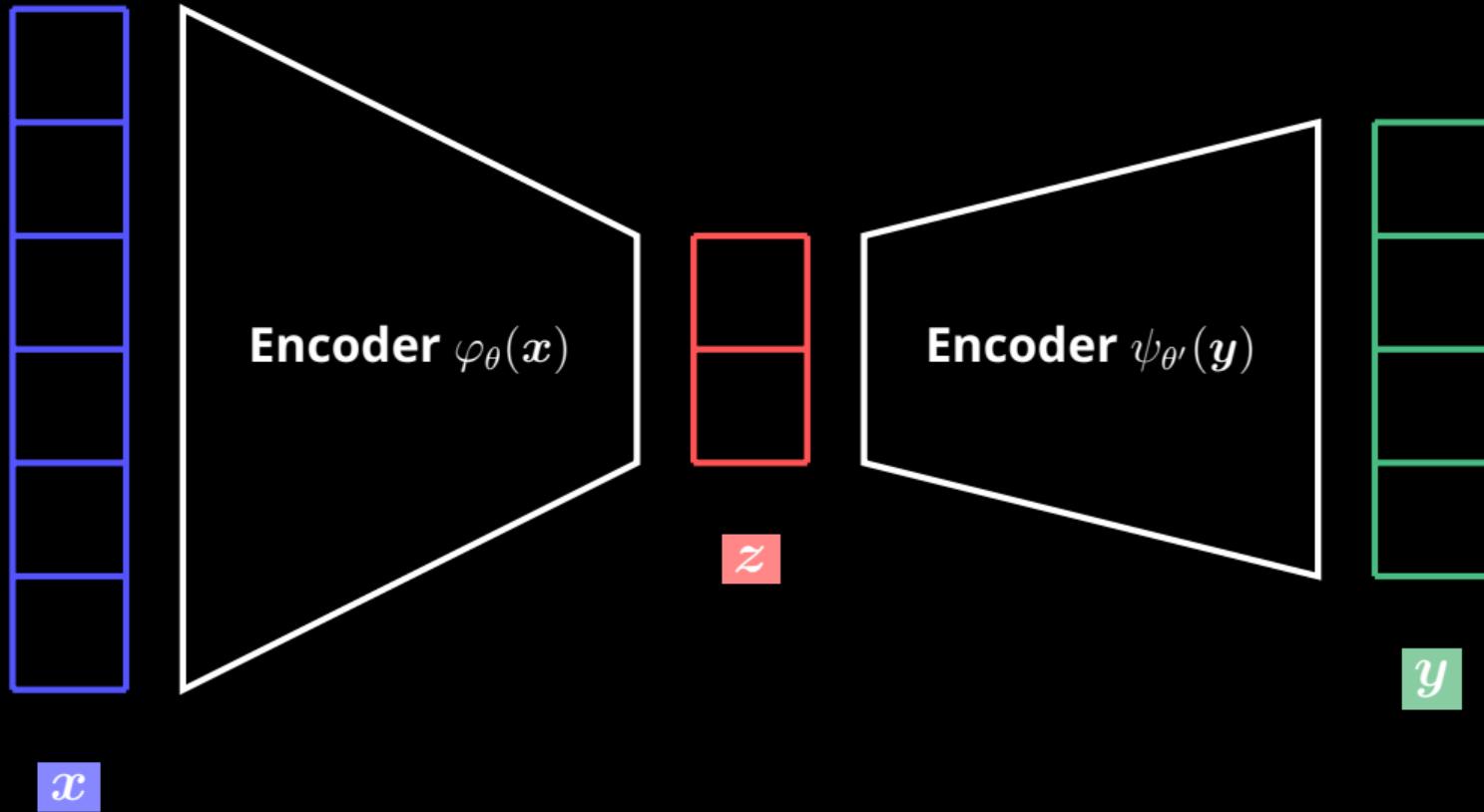


The whole dataset can be correctly approximated using only 500 so-called eigen-faces.









$$\min_{\theta, \theta'} \quad \sum_{i=1}^N \|\varphi_\theta(\mathbf{x}_i) - \psi_{\theta'}(\mathbf{y}_i)\|_2^2$$

$$\begin{aligned} & \underset{\boldsymbol{P}, \boldsymbol{Q}}{\text{minimize}} && \sum_{i=1}^N \|\boldsymbol{P}^T \boldsymbol{y}_i - \boldsymbol{Q}^T \boldsymbol{x}_i\|_2^2 \\ & \text{subject to} && \text{rank } \boldsymbol{P} = \text{rank } \boldsymbol{Q} = r \end{aligned}$$

$$\begin{aligned} & \underset{\boldsymbol{P}, \boldsymbol{Q}}{\text{minimize}} && \|\boldsymbol{P}^T \boldsymbol{Y} - \boldsymbol{Q}^T \boldsymbol{X}\|_F^2 \\ & \text{subject to} && \boldsymbol{P}^T \boldsymbol{C}_{yy} \boldsymbol{P} = \boldsymbol{Q}^T \boldsymbol{C}_{xx} \boldsymbol{Q} = \boldsymbol{I}_r \end{aligned}$$

Canonical Correlation Analysis

$$\begin{bmatrix} C_{yy} & \mathbf{0} \\ \mathbf{0} & C_{xx} \end{bmatrix} \begin{bmatrix} \mathbf{P} \\ \mathbf{Q} \end{bmatrix} \Sigma = \begin{bmatrix} \mathbf{0} & C_{yx} \\ C_{xy} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{P} \\ \mathbf{Q} \end{bmatrix}$$

CCA relies on a *generalized eigenproblem*. \mathbf{P} and \mathbf{Q} describe the encoders such that the latent representations $\mathbf{z} = \mathbf{Q}^T \mathbf{x}$ and $\mathbf{z}' = \mathbf{P}^T \mathbf{Y}$ are as similar as possible. It is closely related to the concept of *mutual information*.

CCA-Encoding

$$z = P^T x$$

$$z' = Q^T y$$

CCA-Encoding

$$z = P^T x$$
$$z' = Q^T y$$

CCA-Latent space

$$z \simeq z'$$

CCA-Encoding

$$z = P^T x$$

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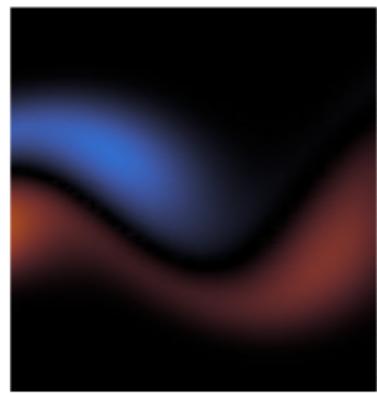
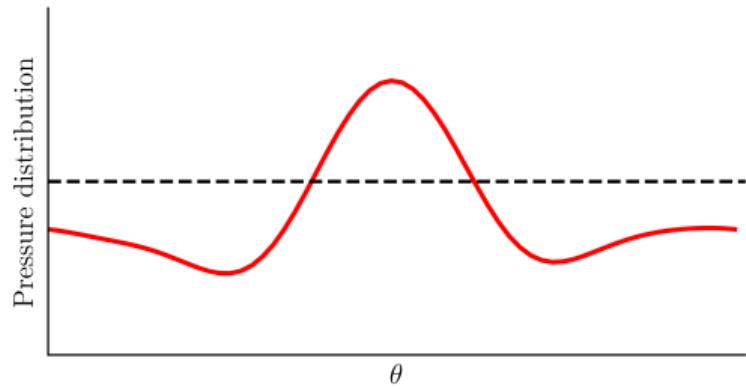
CCA-Latent space

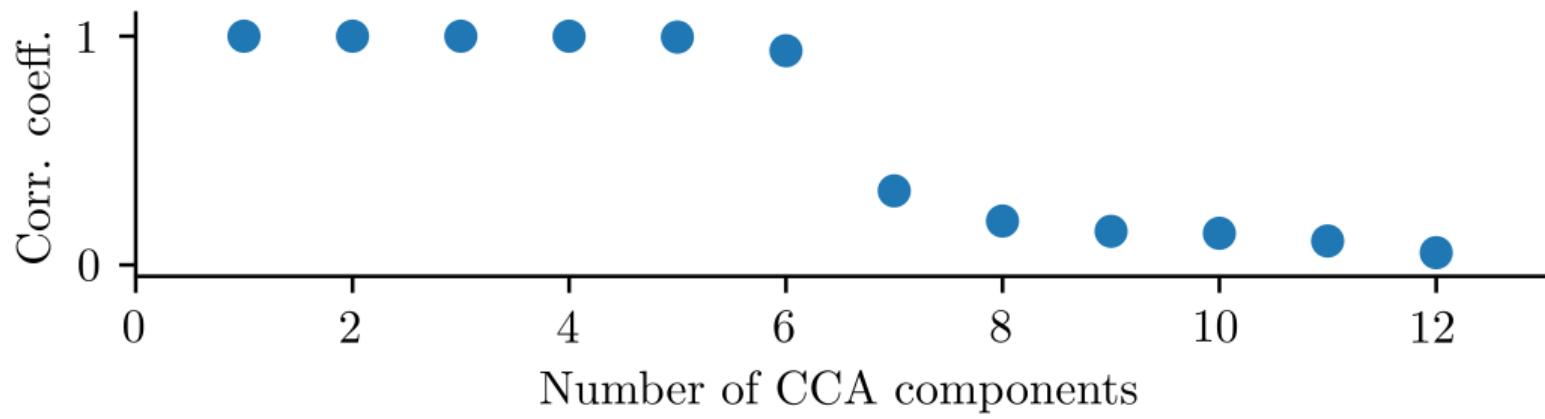
$$z \simeq z'$$

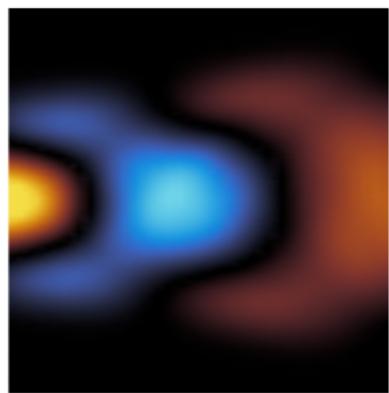
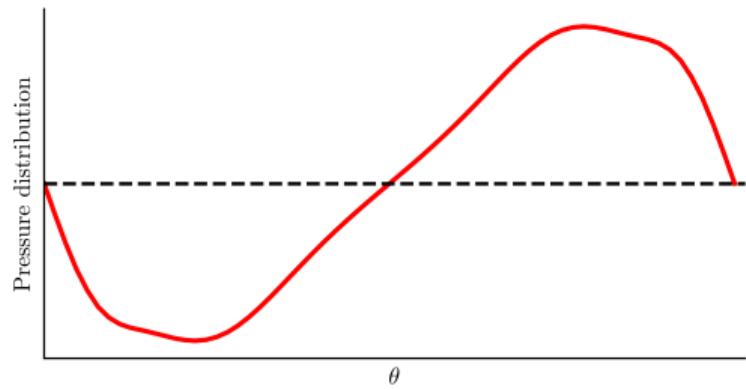
CCA-Decoding

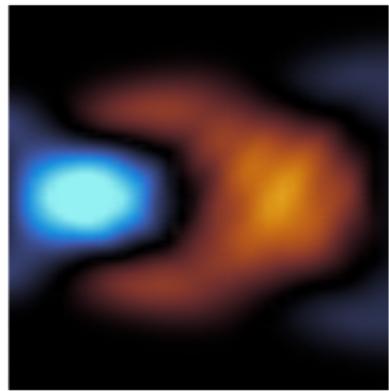
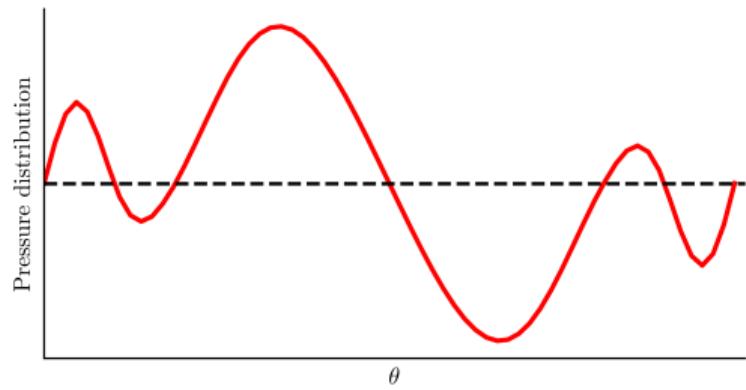
$$\hat{x} = P (P^T P)^{-1} z$$

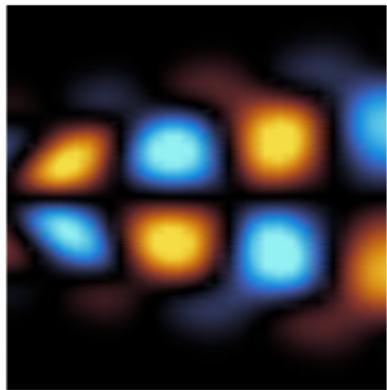
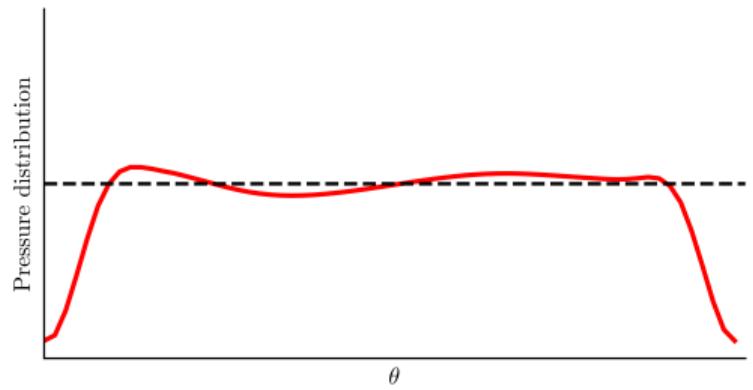
$$\hat{y} = Q (Q^T Q)^{-1} z'$$

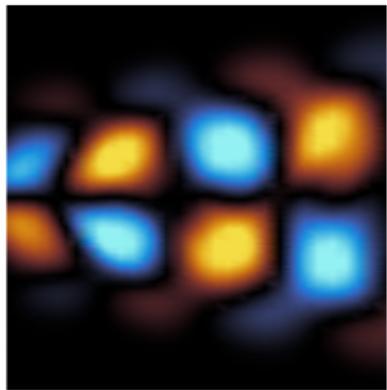
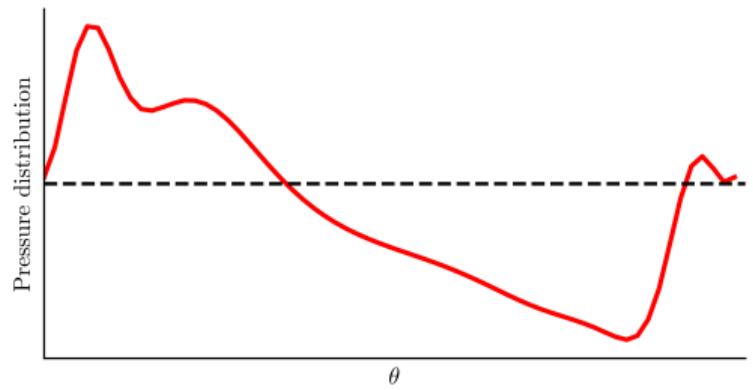


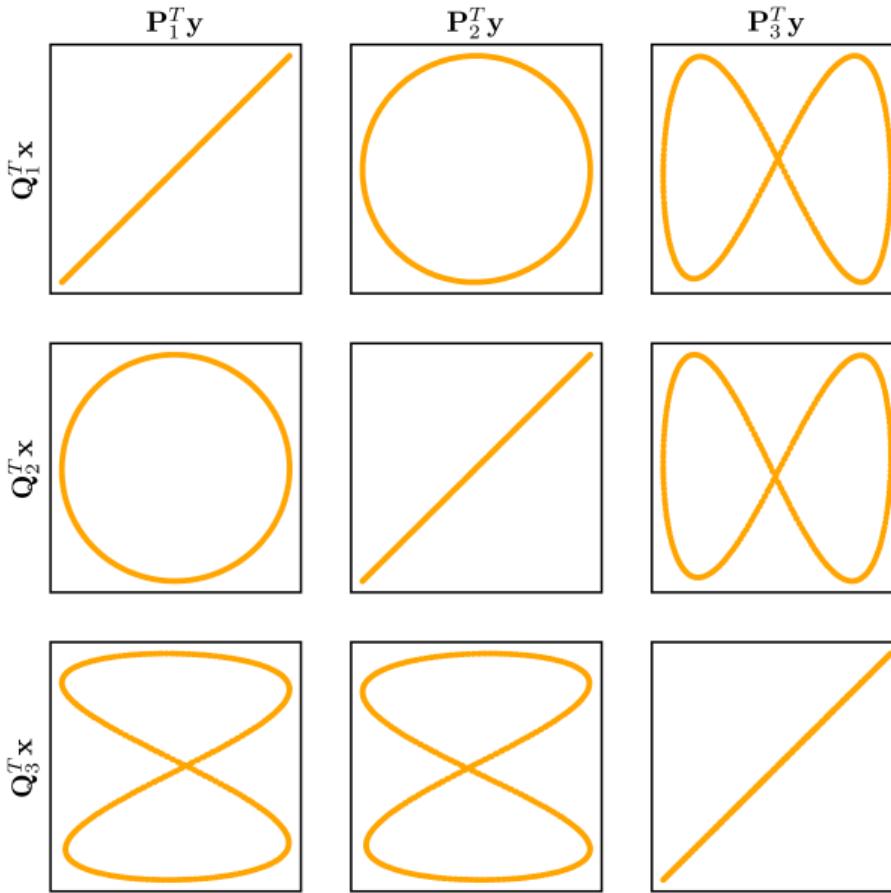


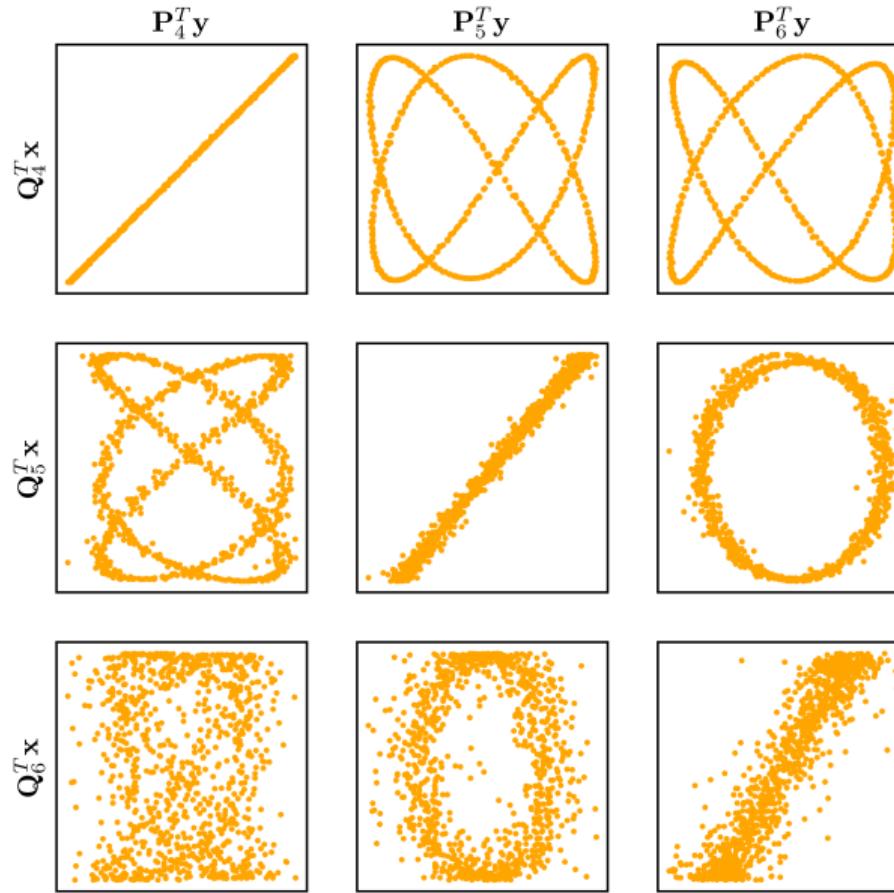








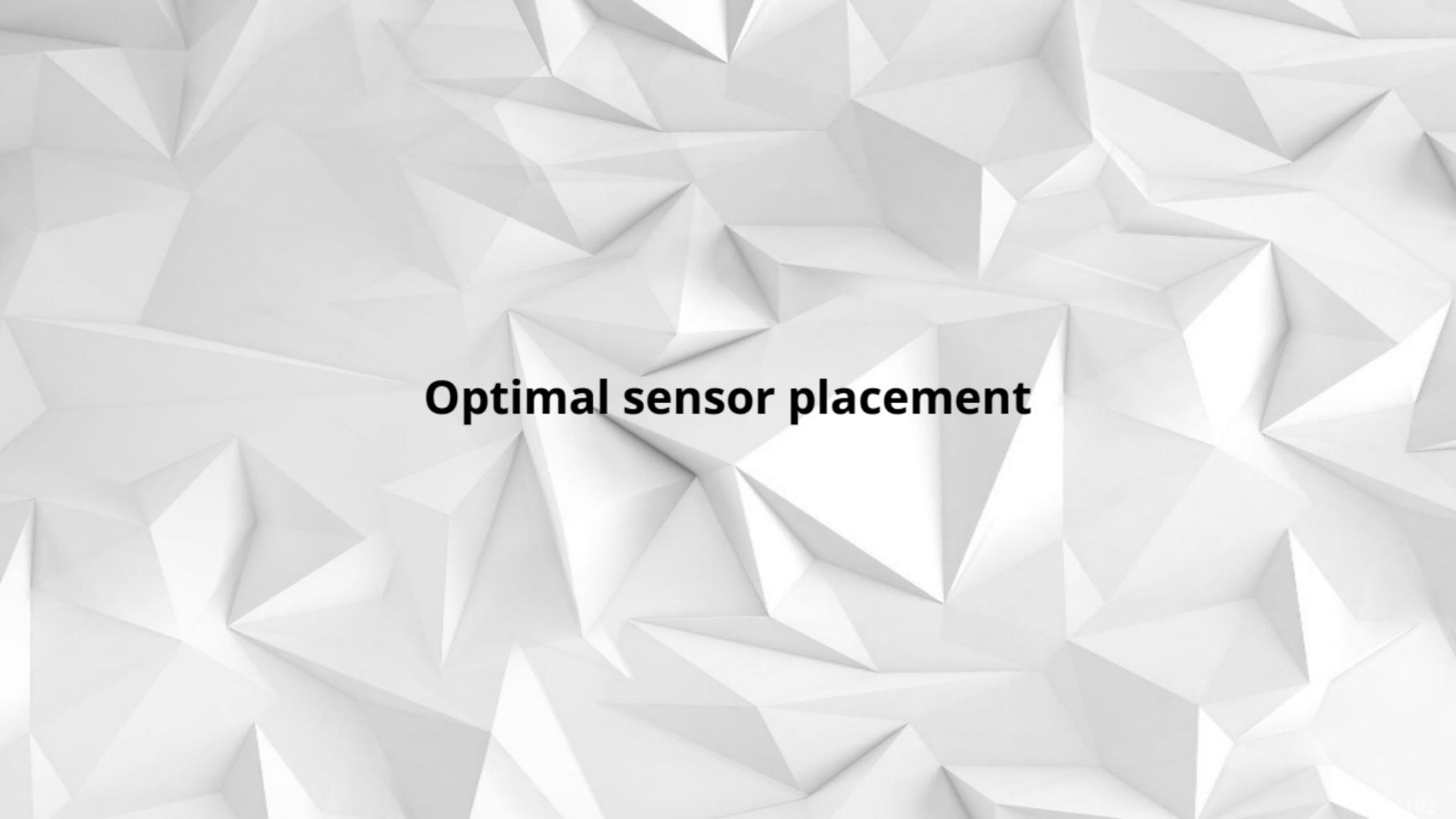




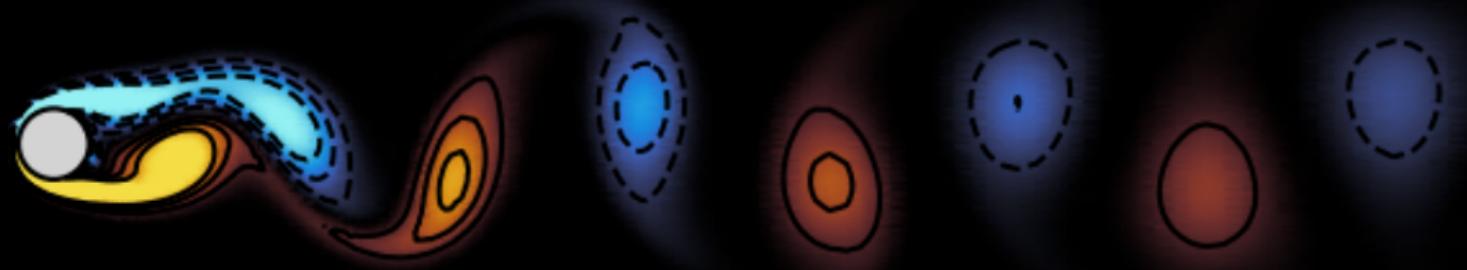
- Relies on extremely efficient numerical linear algebra techniques.
- The singular value distribution provides a simple diagnostic to estimate the dimensional of the embedding Euclidean space.
- Component analysis is well understood from a statistical point of view and benefits from good properties.



- The dimension inferred from the singular value distribution tends to over-estimate the intrinsic dimension of the underlying low-dimensional manifold.
 - This is directly related to the fact the linear dimensionality reduction techniques do not account for *nonlinear correlations*, only linear ones..
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The background of the slide features a complex, abstract pattern of white polygons, resembling a low-poly 3D model or a crystal lattice. The polygons vary in size and orientation, creating a sense of depth and texture. The lighting is soft, with subtle shadows and highlights that emphasize the three-dimensional nature of the surface.

Optimal sensor placement



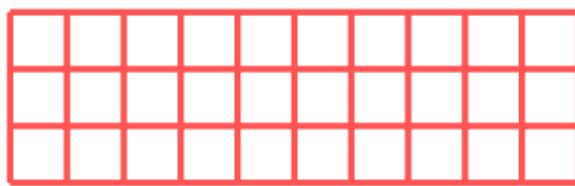
$$\mathbf{y} = \mathbf{C} \mathbf{x}$$

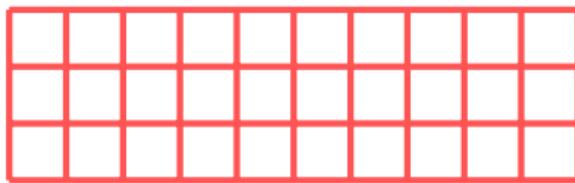
Measurement operator

Full state

Observations

The diagram illustrates a linear relationship between observations \mathbf{y} , a measurement operator \mathbf{C} , and a full state \mathbf{x} . The equation $\mathbf{y} = \mathbf{C} \mathbf{x}$ is shown in the center. A red bracket above the equation is labeled "Measurement operator" and points to the matrix \mathbf{C} . A green bracket below the equation is labeled "Full state" and points to the matrix \mathbf{x} . A blue bracket to the left of the equation is labeled "Observations" and points to the vector \mathbf{y} .

y C x  \sim 

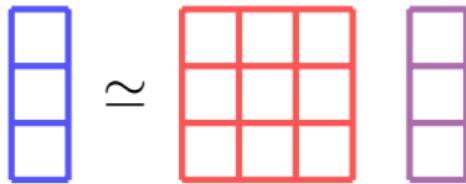
y C U z  \approx 

A large curly brace under the red and green rectangles, labeled Θ .

y

Θ

z



$$\underset{\boldsymbol{z}}{\text{minimize}} \quad \|\boldsymbol{y} - \boldsymbol{\Theta}\boldsymbol{z}\|_2$$

$$z = \Theta^{-1}y$$

$$\underset{\boldsymbol{C}}{\text{maximize}} \quad |\det(\boldsymbol{C}\boldsymbol{U})|$$

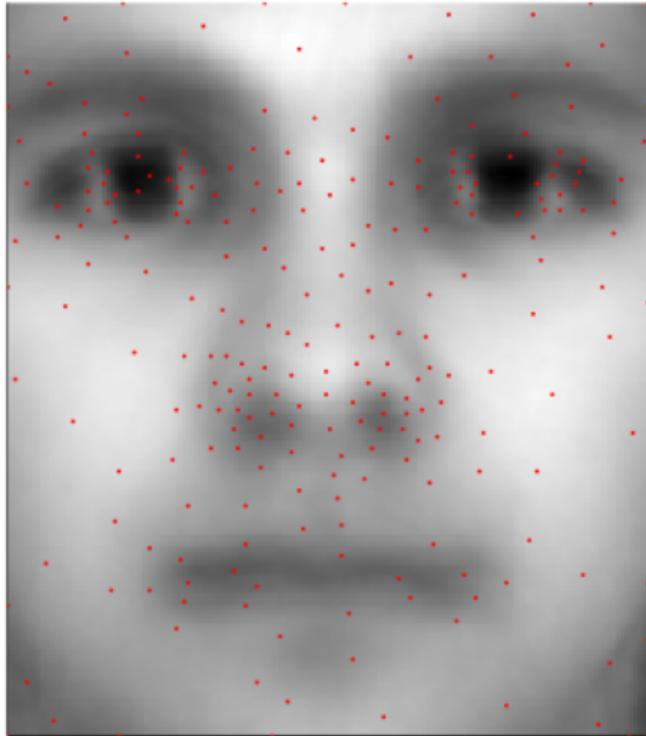
$$\begin{aligned} & \underset{\boldsymbol{C}}{\text{maximize}} && |\det(\boldsymbol{C}\boldsymbol{U})| \\ & \text{subject to} && \boldsymbol{C}_i \in \{\boldsymbol{e}_j\}_{j=1,n} \end{aligned}$$

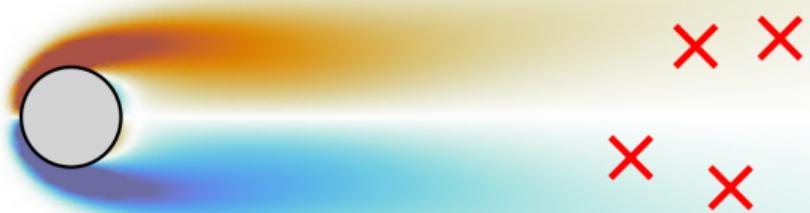
$$\mathbf{U}^T \mathbf{P} = \mathbf{Q} \mathbf{R}$$

Permutation matrix

Low-rank basis

Upper triangular matrix
with $|r_{i-1}| \geq |r_i|$



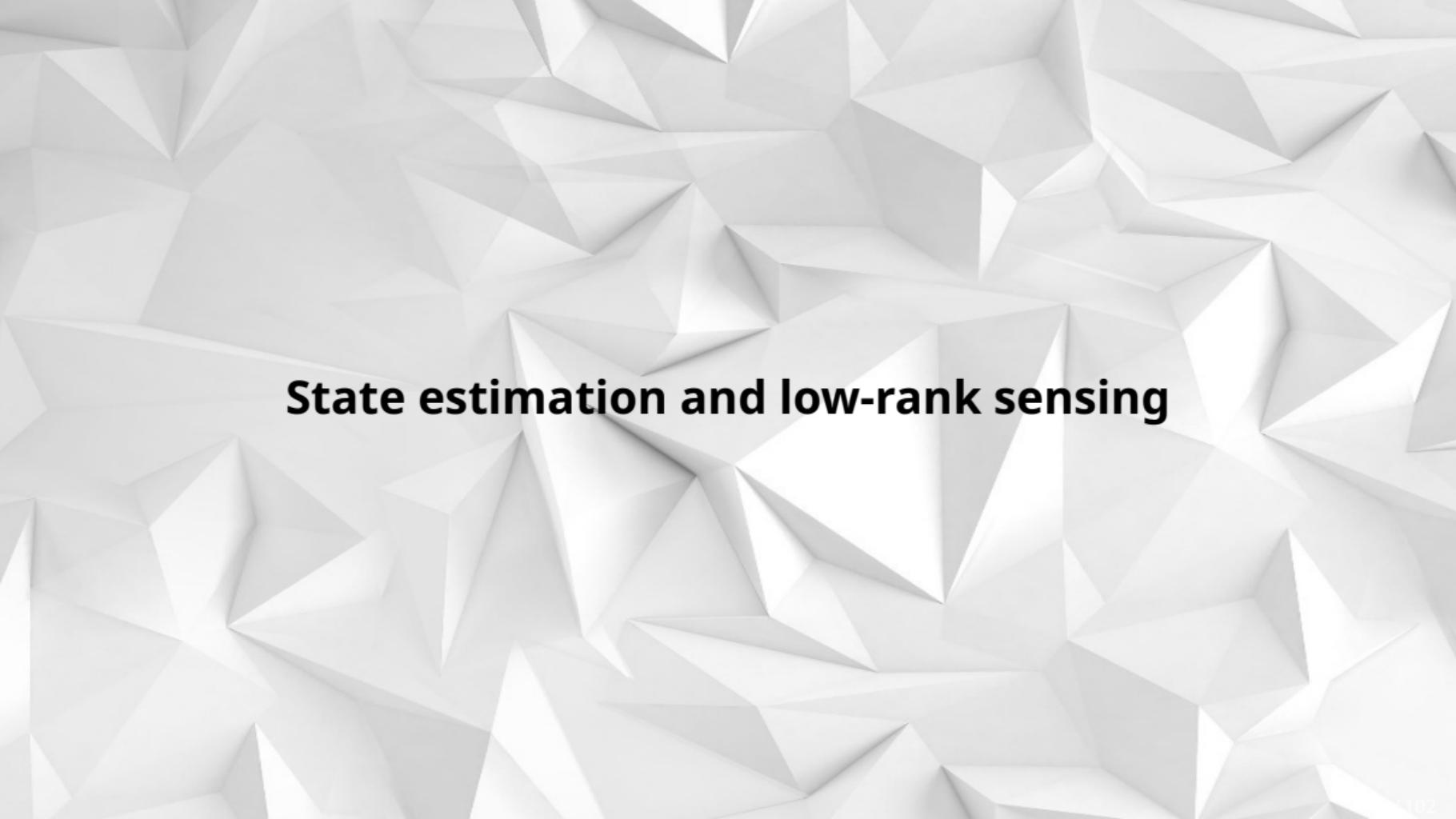


- Relies on extremely efficient numerical linear algebra techniques.
- Greedy solution to an otherwise intractable combinatorial problem.
- Relevant in many situations and benefits from good empirical performances.



- No easy way to estimate how far from the optimum the greedy solution is.

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The background of the slide features a complex, abstract pattern of white polygons, resembling a low-poly 3D model or a crystal lattice. The polygons vary in size and orientation, creating a sense of depth and texture. The lighting is soft, with subtle shadows and highlights that emphasize the three-dimensional nature of the surface.

State estimation and low-rank sensing

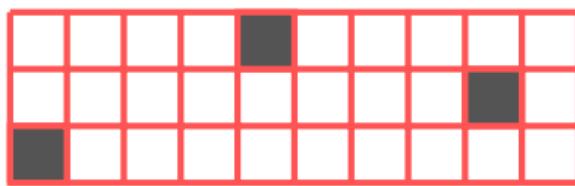
$$\mathbf{y} = \mathbf{C} \mathbf{x}$$

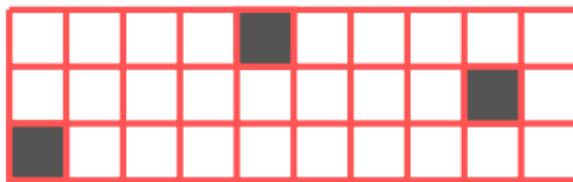
Measurement operator

Full state

Observations

The diagram illustrates a linear measurement model. At the top, a red bracket labeled "Measurement operator" contains a downward-pointing arrow. This arrow points to the matrix \mathbf{C} in the equation $\mathbf{y} = \mathbf{C} \mathbf{x}$. To the right of the equation, a green bracket labeled "Full state" contains an upward-pointing arrow. This arrow points from the matrix \mathbf{x} to the equation. Below the equation, a blue double-headed vertical arrow labeled "Observations" connects the matrices \mathbf{C} and \mathbf{x} to the output vector \mathbf{y} .

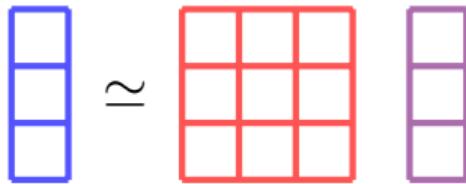
y C x  \sim 

y C U z  \approx  Θ

y

Θ

z



Underdetermined problem

$$\begin{aligned} & \underset{\mathbf{z}}{\text{minimize}} && \|\mathbf{z}\|_2 \\ & \text{subject to} && \mathbf{y} = \Theta\mathbf{z} \end{aligned}$$

Overdetermined problem

$$\underset{\mathbf{z}}{\text{minimize}} \quad \|\mathbf{y} - \Theta\mathbf{z}\|_2^2$$

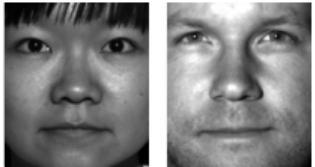
Regularized problem

$$\underset{\mathbf{z}}{\text{minimize}} \quad \|\mathbf{y} - \Theta\mathbf{z}\|_2^2 + \lambda\|\mathbf{z}\|_2^2$$

Regularized and constrained problem

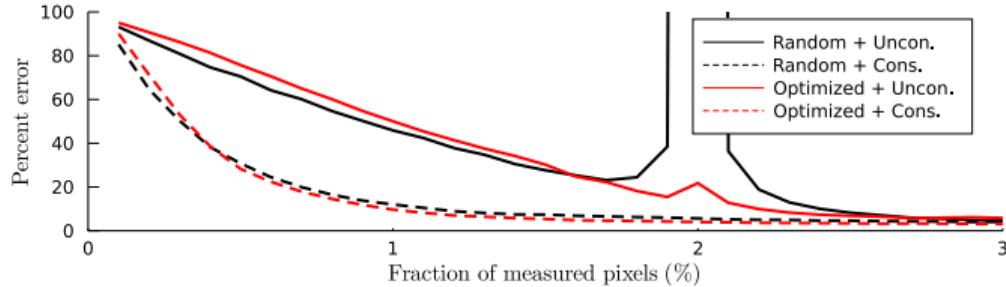
$$\begin{aligned} & \underset{\mathbf{z}}{\text{minimize}} && \|\mathbf{y} - \Theta\mathbf{z}\|_2^2 + \lambda\|\mathbf{z}\|_2^2 \\ & \text{subject to} && |z_i| \leq 2\sigma_i \quad \forall i \end{aligned}$$

Ground truth



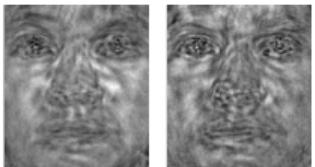
Underdetermined

Overdetermined



Unconstrained

0.5%



1.4%

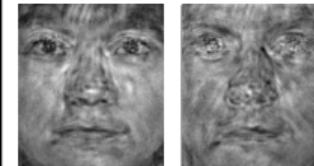
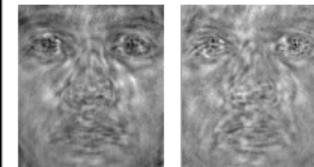


Random sensors

Box-constrained

Unconstrained

Box-constrained



QR-optimized sensors

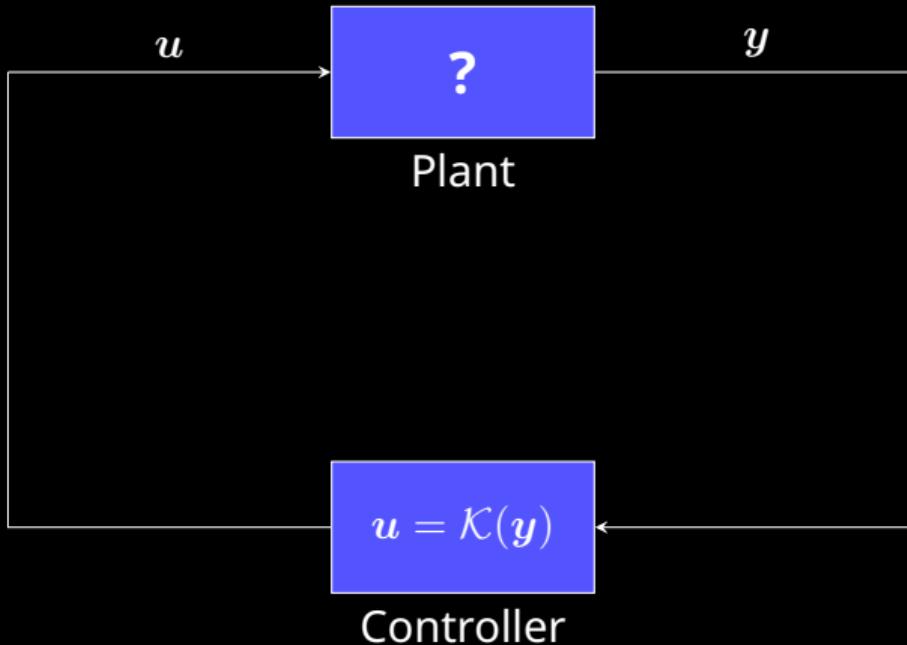
- Low-rank sensing benefits from strong theoretical guarantees.
- Relies on simple yet efficient numerical procedures, both during the training and deployment stages.
- Requires much less data than naïve deep learning alternatives.



- Data needs to be standardized and characterized by an underlying low-rank structure.
 - The state estimator is a **static map**. It does not account for the dynamics (if they exist) of the generating process.
 - The measurement equation needs to be (approximately) linear.
- 

System identification

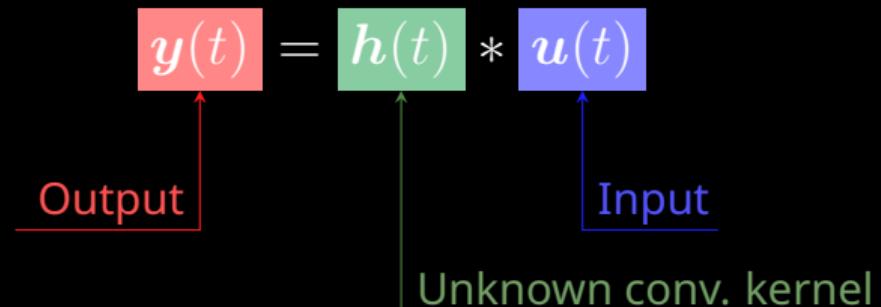




Convolution model

$$y_i = f(u_i, u_{i-1}, u_{i-2}, \dots)$$

Convolution model

$$\mathbf{y}(t) = \mathbf{h}(t) * \mathbf{u}(t)$$


Output

Input

Unknown conv. kernel

$$\begin{array}{l} \text{Natural dynamics} \\ \hline \\ \xrightarrow{\hspace{1cm}} \quad \quad \quad \downarrow \\ \boldsymbol{x}_{i+1} = \boxed{\boldsymbol{A}} \boldsymbol{x}_i + \boxed{\boldsymbol{B}} \boldsymbol{u}_i \\ \quad \quad \quad \uparrow \\ \text{Measurements} \end{array} \quad \quad \quad \begin{array}{l} \text{Actuators} \\ \hline \\ \downarrow \quad \quad \quad \uparrow \\ \boldsymbol{y}_i = \boxed{\boldsymbol{C}} \boldsymbol{x}_i + \boxed{\boldsymbol{D}} \boldsymbol{u}_i \\ \quad \quad \quad \uparrow \\ \text{Feedthrough} \end{array}$$

Input u_i	State x_i	Output y_i
u_0	0	Du_0
u_1	Bu_0	$CBu_0 + Du_1$
u_2	$ABu_0 + Bu_1$	$CABu_0 + CBu_1 + Du_2$
u_3	$A^2Bu_0 + ABu_1 + Bu_2$	$CA^2Bu_0 + CABu_1 + CBu_2 + Du_3$
\vdots	\vdots	\vdots
u_k	$\sum_{i=1}^k A^{i-1}Bu_{k-i}$	$\sum_{i=1}^k CA^{i-1}Bu_{k-i} + Du_k$

$$\mathbf{y}_k = \mathbf{D}\mathbf{u}_k + \sum_{i=1}^k \mathbf{C}\mathbf{A}^{i-1}\mathbf{B}\mathbf{u}_{k-i}$$

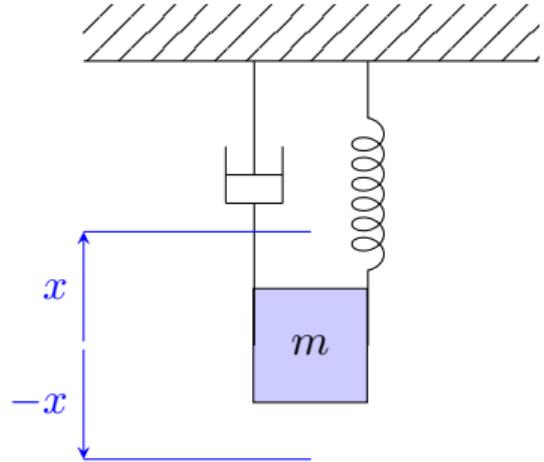
$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} u_0 & \cdots & & & \\ u_1 & u_0 & \cdots & & \\ u_2 & u_1 & u_0 & \cdots & \\ u_3 & u_2 & u_1 & u_0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} D \\ CB \\ CAB \\ CA^2B \\ CA^3B \\ \vdots \end{bmatrix}$$

$$\underset{h}{\text{minimize}} \quad \| \mathbf{y} - \mathcal{T}(u) \mathbf{h} \|_p + \mathcal{R}(h)$$

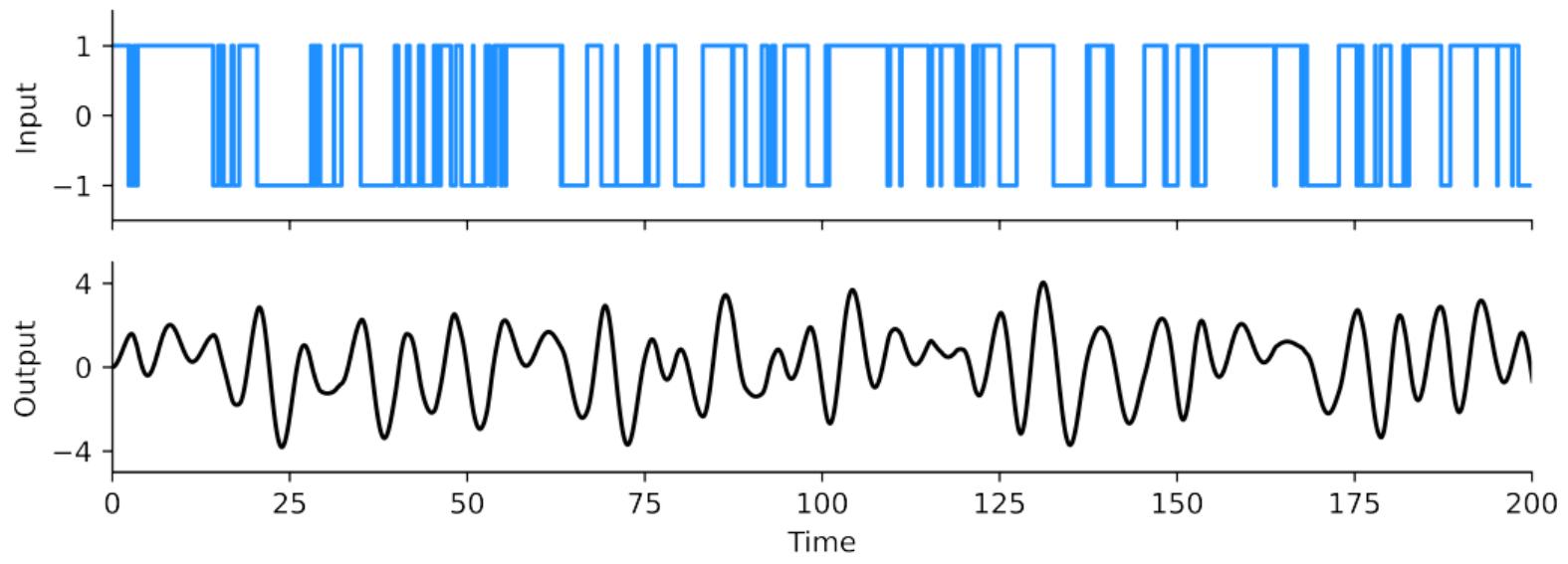
Output sequence

Unknown conv. kernel

Toeplitz matrix built
using the input sequence

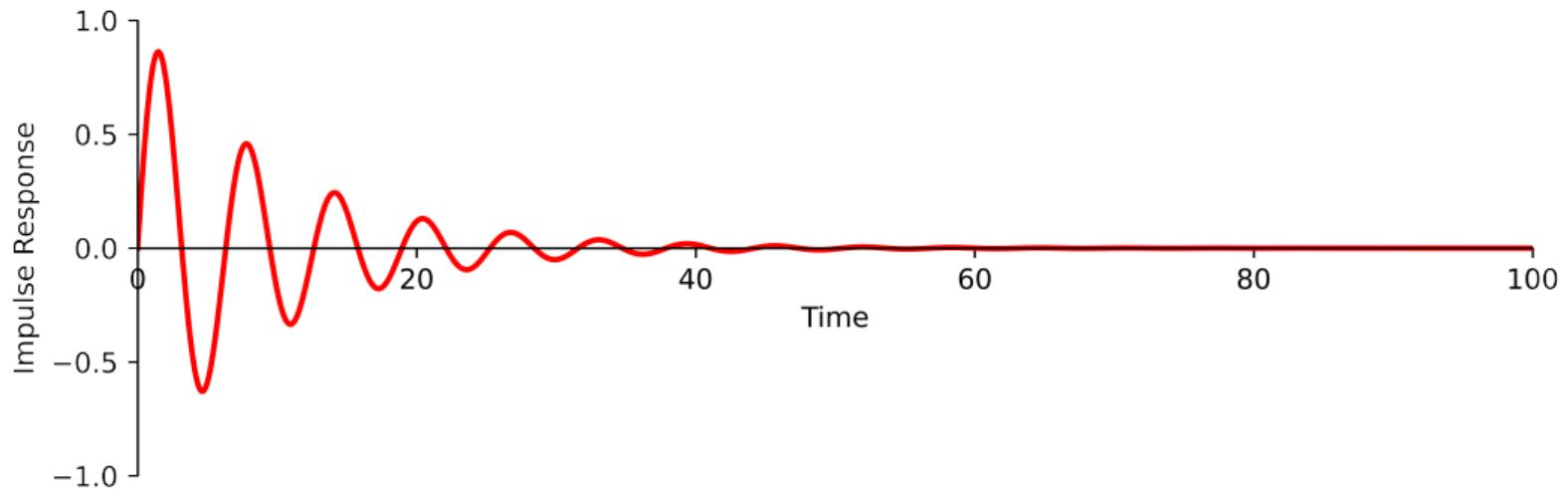


$$\frac{d}{dt} \begin{bmatrix} x \\ v \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -2\zeta \end{bmatrix} \begin{bmatrix} x \\ v \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u$$
$$y = [1 \ 0] \begin{bmatrix} x \\ v \end{bmatrix}$$



Input/Output data for system identification

$$\underset{\mathbf{h}}{\text{minimize}} \quad \|\mathbf{y} - \mathbf{h} * \mathbf{u}\|_2^2$$



- Relies on simple linear regression.
- Easy to extend to nonlinear systems (e.g. LSTM)
- Prior knowledge can be included through regularization or constraints.



- The length of the convolution kernel is *a priori* unknown.
 - The longer the kernel, the more data is needed to obtain converged estimates.
 - It is *a priori* unrelated to the number of degrees of freedom in the system.
-

$$\begin{array}{l} \text{Natural dynamics} \\ \hline \\ \xrightarrow{\hspace{1cm}} \quad \quad \quad \downarrow \\ \boldsymbol{x}_{i+1} = \boxed{\boldsymbol{A}} \boldsymbol{x}_i + \boxed{\boldsymbol{B}} \boldsymbol{u}_i \\ \quad \quad \quad \uparrow \\ \text{Measurements} \end{array} \quad \quad \quad \begin{array}{l} \text{Actuators} \\ \hline \\ \downarrow \quad \quad \quad \uparrow \\ \boldsymbol{y}_i = \boxed{\boldsymbol{C}} \boldsymbol{x}_i + \boxed{\boldsymbol{D}} \boldsymbol{u}_i \\ \quad \quad \quad \uparrow \\ \text{Feedthrough} \end{array}$$

$$\mathcal{O}_k = \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \\ \vdots \\ CA^{k-1} \end{bmatrix} \quad \mathcal{C}_k = [B \ AB \ A^2B \ A^3B \ \dots \ A^{k-1}B]$$

Observability

Controlability

$$h_k = [D \ CB \ CAB \ CA^2B \ CA^3B \ \dots \ CA^{k-1}B]$$

Markov parameters of the system

EigenRealization Algorithm

$$\mathbf{H}_1 = \begin{bmatrix} h_1 & h_2 & h_3 & h_4 & h_5 \\ h_2 & h_3 & h_4 & h_5 & h_6 \\ h_3 & h_4 & h_5 & h_6 & h_7 \\ h_4 & h_5 & h_6 & h_7 & h_8 \\ h_5 & h_6 & h_7 & h_8 & h_9 \end{bmatrix}$$

EigenRealization Algorithm

$$H_1 = \begin{bmatrix} CB & CAB & CA^2B & CA^3B & CA^4B \\ CAB & CA^2B & CA^3B & CA^4B & CA^5B \\ CA^2B & CA^3B & CA^4B & CA^5B & CA^6B \\ CA^3B & CA^4B & CA^5B & CA^6B & CA^7B \\ CA^4B & CA^5B & CA^6B & CA^7B & CA^8B \end{bmatrix}$$

EigenRealization Algorithm

$$H_1 = \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \\ CA^4 \end{bmatrix} [B \ AB \ A^2B \ A^3B \ A^4B]$$

EigenRealization Algorithm

Observability: $\mathcal{O} = U\Sigma^{\frac{1}{2}}$

Controlability: $\mathcal{C} = \Sigma^{\frac{1}{2}}V^T$

EigenRealization Algorithm

$$\mathbf{H}_2 = \begin{bmatrix} h_2 & h_3 & h_4 & h_5 & h_6 \\ h_3 & h_4 & h_5 & h_6 & h_7 \\ h_4 & h_5 & h_6 & h_7 & h_8 \\ h_5 & h_6 & h_7 & h_8 & h_9 \\ h_6 & h_7 & h_8 & h_9 & h_{10} \end{bmatrix}$$

EigenRealization Algorithm

$$H_2 = \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \\ CA^4 \end{bmatrix} A [B \ AB \ A^2B \ A^3B \ A^4B]$$

EigenRealization Algorithm

Natural dynamics

$$A = \mathcal{O}^\dagger H_2 \mathcal{C}^\dagger$$

Actuators

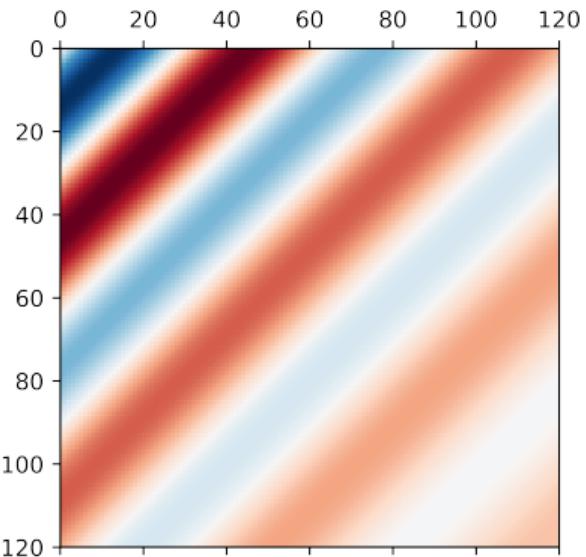
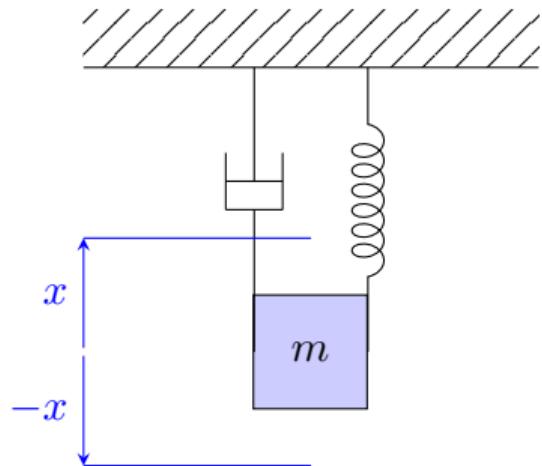
$$B = \left[\Sigma^{\frac{1}{2}} V^T \right]_{:,1:p}$$

Measurements

$$C = \left[U \Sigma^{\frac{1}{2}} \right]_{1:q,:}$$

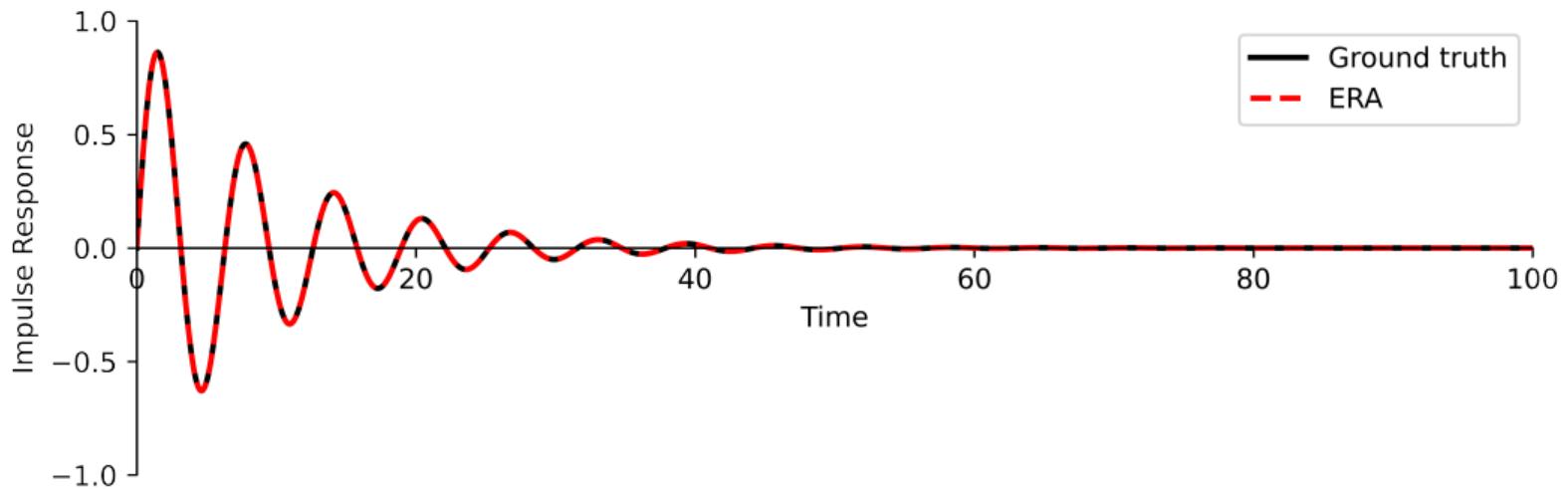
Feedthrough

$$D = h_0$$



$$\Sigma = [27.68 \quad 22.62 \quad 0 \quad 0 \quad \dots]$$

$$\mathbf{A} = \begin{bmatrix} 0.986 & -0.098 \\ 0.098 & 0.984 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} -0.232 \\ 0.210 \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} -0.232 & -0.210 \end{bmatrix}$$



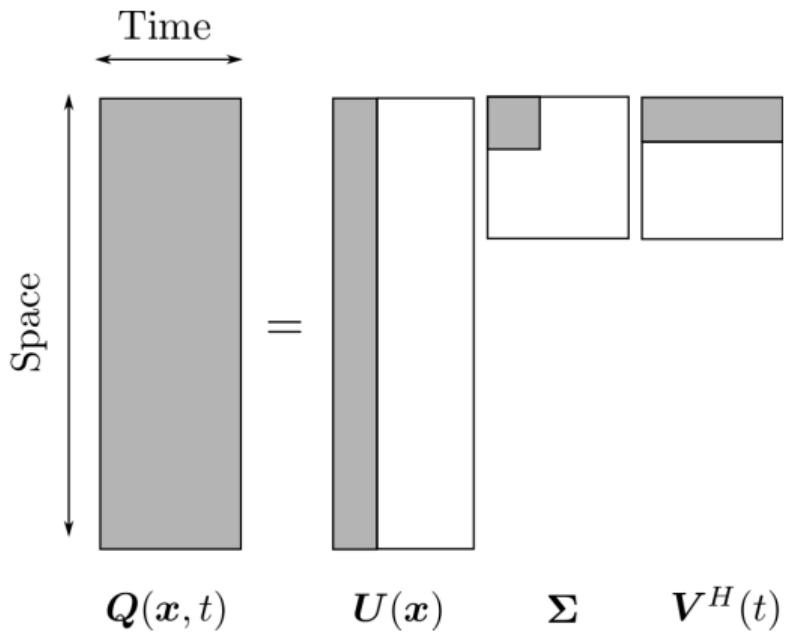
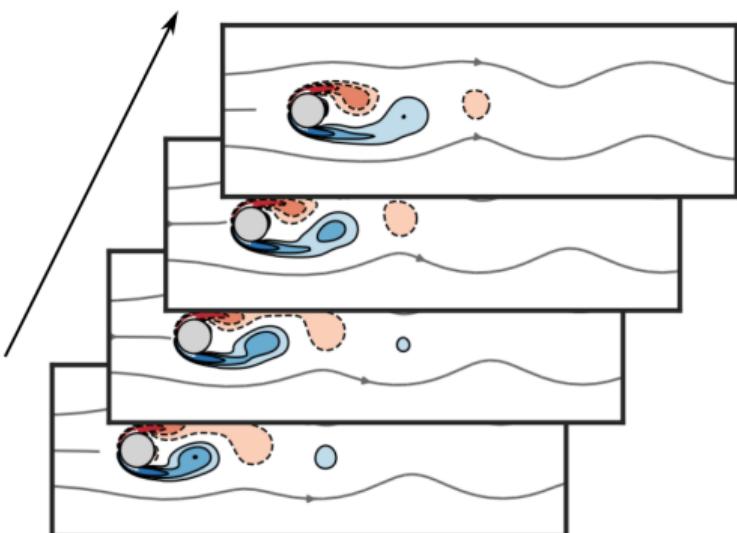
Cylinder flow example

- Relies solely on the impulse response of the system and efficient numerical linear algebra.
- Identifies the minimal number of degrees of freedom needed to represent the dynamics.
- Benefits from strong theoretical guarantees and is well-grounded in control theory.



- Need a really good estimate of the impulse response.
 - Extension to **interpretable** nonlinear systems is not straightforward.
 - Parametric variations cannot be easily included into this framework.
-

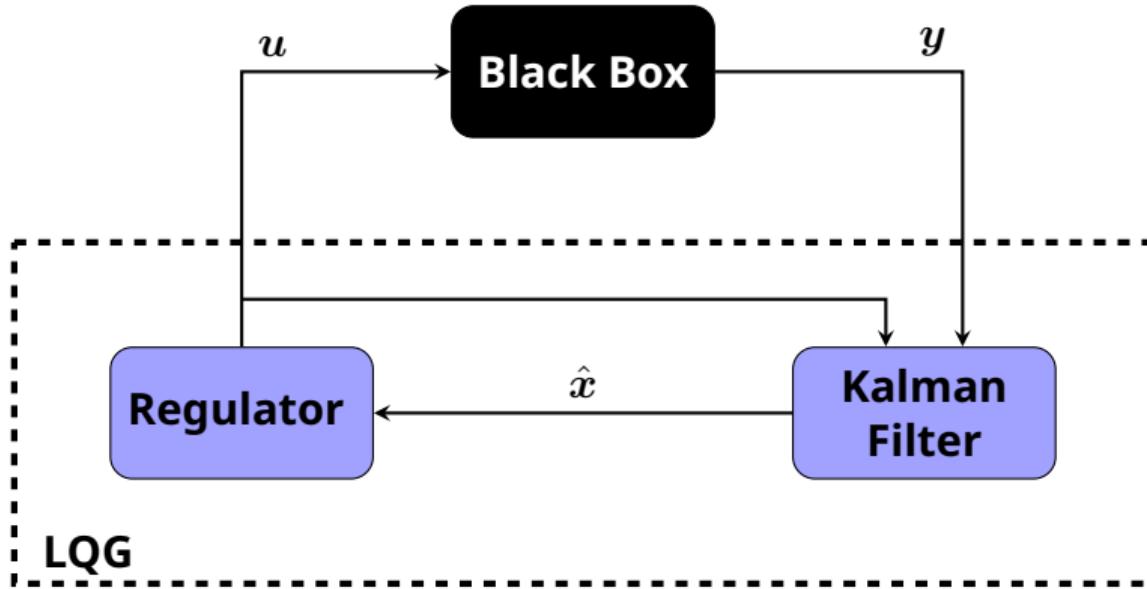
Conclusion





$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}\mathbf{u}_k$$

$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{D}\mathbf{u}_k$$



Thank you for your attention!

Any question?