

UNIVERSIDAD POLITÉCNICA DE MADRID



# Acceleration of data-driven modal decomposition using

# unsupervised machine learning techniques

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- 1) Describe classical Dynamic Mode Decomposition (DMD)
- 2) DMD as one of many data-driven modal decomposition techniques
- 3) DMD as a matrix factorization technique
- 4) Accelerating DMD methods

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Introduction

**Dynamic Mode Decomposition** 

Alleviating the computational cost

Conclusions

Introduction:

## data-driven modal decomposition techniques



Credit: Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems (Brunton, Kutz, et al.)



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## Matrix factorization techniques



## Matrix factorization techniques



Temporal data sequence acquired at a fixed sampling frequency  $1/\Delta t$ 

Arrange data in a (typically) tall and skinny matrix



**Dynamic Mode Decomposition** Temporal data sequence acquired at a fixed sampling frequency  $1/\Delta t$ Arrange data in a (typically) tall and skinny matrix



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From the complete data set

$$\mathbf{V}_1^{n_t} = [\mathbf{v}_1, \, \mathbf{v}_2, \, \dots, \, \mathbf{v}_{n_t-1}, \, \mathbf{v}_{n_t}] \in \mathbb{R}^{n_p \times n_t}$$

Identify data subsequences as:

$$\mathbf{V}_1^{n_t-1} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{n_t-1}] \equiv \mathbf{X} \quad \text{and} \quad \mathbf{V}_2^{n_t} = [\mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_{n_t-1}, \mathbf{v}_{n_t}] \equiv \mathbf{Y}$$

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$$\mathbf{v}(t_{k+1}) = \mathcal{A} \, \mathbf{v}(t_k)$$

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Koopman assumption

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Assume a linear relationship:

$$\mathbf{V}_{2}^{n_{t}} = \mathcal{A} \mathbf{V}_{1}^{n_{t}-1}$$
$$\mathcal{A} \in \mathbb{R}^{n_{p} \times n_{p}}$$

How does one identify A? Well, you don't need to.

$$\mathbf{V}_1^{n_t-1} \equiv \mathbf{X} \stackrel{SVD}{=} \mathbf{L}_0 \ \mathbf{S}_0 \ \mathbf{R}_0^T = \sum_{j=1}^r s_{0,j} \ \mathbf{l}_{0,j} \cdot \mathbf{r}_{0,j}^T$$
  
The columns of  $\mathbf{L}_0 \Longrightarrow$  Left Singular Vectors

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Project into the reduced Left Singular Vector (sub)space and manipulate  $\mathbf{L}_0 \mathbf{Y} \mathbf{R}_0 \mathbf{S}_0^{-1} = \mathbf{L}_0^T \mathcal{A} \mathbf{L}_0 \equiv \widetilde{\mathcal{A}} \in \mathbb{R}^{r \times r}$ 

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Dynamic modes and Ritz values are obtained via eigendecomposition

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... once the  $\alpha_i$ 's are known.

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# An example



Credit: Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems (Brunton, Kutz, et al.)



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#### Dynamic Mode Decomposition



Synthesis (Reconstruction)

Credit: Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems (Brunton & Kutz)



"Gentle" problem.











Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems (Brunton, Kutz, et al.)

M.R. Jovanovic, P.J. Schmid, J.W. Nichols, Sparsity-promoting dynamic mode decomposition, Phys. Fluids, vol. 26 (2), 2014.

atabase: Re <sub>D</sub> =100 flow around a cylinder			
Method	Reconstruction error	Computing time $[s]$	
Companion $\mathbf{DME}$	N.A.	$4.72\times 10^{-2}$	
$oldsymbol{lpha} = oldsymbol{\Phi}^+  {f v}_1$ .	$1.64  imes 10^{-6}$	1.85	
$\stackrel{\mathrm{min}}{oldsymbol{lpha}} \left\  \mathbf{C}_{1}^{n_{t}-1} - \mathbf{W} \ \mathbf{D}_{lpha} \ \mathbf{V}_{\mu}  ight\ $	$5.85\times10^{-13}$	$6.53 imes10^{-4}$	

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#### Dynamic Mode Decomposition can be understood both

- as a data-driven modal decomposition technique, and
- as matrix factorization technique

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This leads to connections with other decomposition techniques:

FFT, Spectral POD, multi-scale POD, multi-resolution DMD ...

B. Begiashvili *et al.*, Data-driven modal decomposition methods as feature detection techniques for flow problems: a critical assessment, Phys. Fluids 35, 041301 (2023).

### Matrix factorization techniques



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#### **SVD**/DMD are both matrix factorization techniques



#### SVD/DMD are both matrix factorization techniques



Matrix M<sub>µ</sub>: Vandermonde matrix (time, complex, distinct frequencies)

#### **SVD**/DMD are both matrix factorization techniques



## Alleviating the computational cost



There are many  $(n_p)$  spatial points in the system;

most of them will have coherent temporal variations.



Time

There are many  $(n_p)$  spatial points in the system;

most of them will have coherent temporal variations.

Can few data points be representative of the whole database temporal behaviour?



Space

There are  $(n_p)$  many spatial points in the system;

most of them will have coherent temporal variations.

Can few data points be representative of the whole database temporal behaviour?

Yes!

Those representative data points can be identified using *clustering* algorithms (Unsupervised Machine Learning).



Space



Guéniat, Mathelin & Pastur, Phys. Fluids, vol. 27 (2), 2015. Li, Garicano-Mena, Zheng & Valero, Energies, vol. 13 (9), 2020.



Time

Guéniat, Mathelin & Pastur, Phys. Fluids, vol. 27 (2), 2015. Li, Garicano-Mena, Zheng & Valero, Energies, vol. 13 (9), 2020.



Guéniat, Mathelin & Pastur, Phys. Fluids, vol. 27 (2), 2015. Li, Garicano-Mena, Zheng & Valero, Energies, vol. 13 (9), 2020. How can one identify those modes that have a most representative temporal variation?

Group those points that have comparable pdf's.

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It is not easy to identify a pdf from discrete data, though.

Take N<sub>m</sub> statistical moments as representative of the pdf.

#### **Spatially Agglomerated DMD analysis**

1. Compute the first  $\widetilde{N}_M$  (estimated) statistical moments, with  $1 \leq \widetilde{N}_M \ll n_t$ 

2. Arrange those moments into matrix

 $\mathbf{\bar{M}} \in \mathbb{R}^{n_p imes \widetilde{N}_M}$ 

- 3. Spatial Agglomeration feed  $\bar{\mathbf{M}}$ to clustering algorithm retrieve reduced database
- 4. Perform DMD analysis on spatially reduced database retrieve Ritz values & DMD modes
- 5. Reconstruct original DMD modes

Algorithms	Complexity	Parameters
K-Means (scikit-learn)	Spatial: $\mathcal{O}(n_p(\widetilde{N_M} + \widetilde{n_p}))$ . Temporal: $\mathcal{O}(n_p\widetilde{n_p}I)$ .	-
Mini-batch K-Means (scikit-learn)	See above.	-
K-Means (SciPy)	See above.	-
K-Means++ (SciPy)	See above.	2
DBSCAN (scikit-learn)	Spatial: $\mathcal{O}(n_p)$ . Temporal: $\mathcal{O}(n_p^2 t_d)$ .	$d_{max} = 2.2, n_{min} = 2.$
HDBSCAN (HDBSCAN)	Spatial: $\mathcal{O}(n_p \widetilde{N}_M)$ . Temporal: $\mathcal{O}(n_p^2 \widetilde{N}_M)$ .	$n_{min}=2.$
C-Means (SciPy/skfuzzy)	Similar to K-means, affected by fuzzifier [45].	$N_{cluster} = 250, I_{max} = 1000.$
Gaussian Mixture (scikit-learn)	Spatial: $\mathcal{O}(n_p k_G \tilde{N}_M^3)$ . Temporal: $\mathcal{O}(n_p k_G \tilde{N}_M^3)$ [46,47].	$k_G = 50.$
Mean Shift (scikit-learn)	Spatial: $\mathcal{O}(n_p \tilde{N}_M)$ . Temporal: $\mathcal{O}(n_p^2 I)$ [48].	$BW = 15000 / \widetilde{n_p}.$
Affinity Propagation (scikit-learn)	Spatial: $\mathcal{O}(n_p^2)$ . Temporal: $\mathcal{O}(n_p^2 I)$ .	
Agglomerative Clustering (scikit-learn)	Spatial: $\mathcal{O}(n_p^2)$ . Temporal: $\mathcal{O}(n_p^3)$ .	flag = average.
BIRCH (scikit-learn)	Spatial: $\mathcal{O}(n_p \widetilde{N_M})$ . Temporal: $\mathcal{O}(n_p \widetilde{N_M})$ .	-

Li, Garicano-Mena, Zheng & Valero, Dynamic Mode Decomposition Analysis of Spatially Agglomerated Flow Databases, Energies, vol. 13 (9), 2020.





the limit cycle.



 $Re_D = 60$  cylinder flow:  $C_l vs$  time and associated **FFT** spectrum.



DMD spectrum (Ritz values)



 $Re_D = 60$  cylinder flow: most relevant **DMD** modes, and corresponding frequencies and growth rates.

$$\mathbf{F} = \left[ f_0, f_1, f_2, f_3 \right]$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_0, \sigma_1, \sigma_2, \sigma_3 \end{bmatrix}$$

$$\varepsilon_f = \frac{\|\mathbf{F} - \mathbf{F}_C\|_2}{\|\mathbf{F}_C\|_2}$$

$$\varepsilon_{\sigma} = \frac{\|\mathbf{\Sigma}\|_2}{4}$$



 $Re_D = 60$  cylinder flow: Normalized errors  $\varepsilon_f$  (Eq. (12)) and  $\varepsilon_\sigma$  (Eq. (13)) committed on capturing the top 4 frequencies  $f_i$  and corresponding growth rate  $\sigma_i$  with different clustering algorithms over spatial reduction  $\widetilde{n_p}/n_p < 1$ .



 $Re_D = 60$  cylinder flow: time invested (in seconds), for different clustering algorithms (averaged over 10 realizations).
### Database: Re<sub>D</sub>=60 flow around a cylinder



(a) K-means, 
$$\tilde{n_p}/n_p = 0.1\%$$
 ( $\varepsilon_f = 4.26 \times$   
 $10^{-3}, \varepsilon_{\sigma} = 4.23 \times 10^{-3}$ ).  
(b) DBSCAN,  $\tilde{n_p}/n_p = 0.1\%$  ( $\varepsilon_f = 0.1\%$  ( $\varepsilon_f = 0.31, \varepsilon_{\sigma} = 5.37$ ).

 $Re_D = 60$  cylinder flow: The distribution of centroids/cores from different clustering algorithms, with spatial reduction  $\tilde{n_p}/n_p < 0.4\%$ .

### Database: Re<sub>D</sub>=60 flow around a cylinder



(c) Gaussian Mixture,  $\tilde{n_p}/n_p = 0.4\%$  ( $\varepsilon_f = 4.20 \times 10^{-3}, \varepsilon_{\sigma} = 5.02 \times 10^{-3}$ )

(d) Gaussian Mixture,  $\tilde{n_p}/n_p = 0.1\%$  ( $\varepsilon_f = 0.55$ ,  $\varepsilon_{\sigma} = 14.5$ ).

 $Re_D = 60$  cylinder flow: The distribution of centroids/cores from different clustering algorithms, with spatial reduction  $\tilde{n_p}/n_p < 0.4\%$ .



Domain and system of reference for the channel flow problem. The domain is periodic along *x* and *z* directions; bulk flow is along *x* direction.



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	$L_x/\delta$	$L_y/\delta$	$L_z/\delta$	$n_x$	$n_y$	$n_z$	<i>Re</i> <sub>c</sub>	<i>u</i> <sub>c</sub>	$W_0/u_c$	$\lambda_x/L_x$	$u_{ au}$
Standard				0.6	101	0.6	3678.7	0.7699			0.042 33
Actuated	π	2	π/2	96	101	96	3732.7	0.7812	0.5	1	0.031 36
	Forcing				Snaps	hots s	stored n <sub>s</sub>	$\Delta t^s$	Memory (GB)		
14	Constant flow rate					120	0	0.15625	3	52	(c)

### "Small" database

	$L_x/\delta$	$L_y/\delta$	$L_z/\delta$	$n_x$	$n_y$	$n_z$	Rec	<i>u</i> <sub>c</sub>	$W_0/u_c$	$\lambda_x/L_x$	$u_{\tau}$
Standard		2		96	101	96	3678.7	0.7699	1000-1		0.042 33
Actuated	π	2	<i>n</i> / <sub>2</sub>				3732.7	0.7812	0.5	1	0.031 36
	Forcing			Snapshots stored n <sub>s</sub>				$\Delta t^s$	Memory (GB)		\$3 
15	Constant flow rate					120	0	0.15625	3	52	



 $Re_{\tau} = 200$  turbulent channel flow: distribution of centroids along  $y^+$  for different agglomeration strategies.

Re<sub>c</sub>≈3600 TCF Composite DMD





Re<sub>c</sub>≈3600 TCF Composite DMD





Choose those modes that have largest  $\alpha_i$ 

and use

$$\mathbf{v}(\vec{r},t) = \sum_{j=1}^{n_t-1} \alpha_j \, \Phi_j(\vec{r}) \, \boldsymbol{e}^{\lambda_j t} \text{ with } \lambda_j = \frac{\log \mu_j}{\Delta t}$$



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 $V = \Phi D_{\alpha} M_{\mu}$ 

Re<sub>c</sub>≈3600 TCF Composite DMD



## Composite DMD

Temporal data sequence acquired at a fixed sampling frequency  $1/\Delta t$ Arrange data in a (typically) tall and skinny matrix



P.J. Schmid, J. Fluid Mech., vol. 656, 2010

## Composite DMD

Temporal data sequence acquired at a fixed sampling frequency  $1/\Delta t$ Instantaneous data groups two (or more) different variables into single column vector  $\mathbf{v}(t_k)$ Arrange data in a (typically) tall and skinny matrix



T. Sayadi et al., J. Fluid Mech., vol. 748, 2014

#### Composite DMD



Applies to fully developed turbulent channel

K. Fukagata, K. Iwamoto and N. Kasagai, Phys. Fluids vol. 14, 2002

# Analysis on composed $C_f(t_k)$ u'v'(r, $t_k$ ) fields

$$\beta_i \equiv (\phi_i \cdot \mathbf{e}_{C_f})\alpha_i$$

$$\langle u'v'\rangle^{DMD}(y) = \frac{1}{n_s\Delta t^s}\sum_{i=1}^{n_r} \alpha_i \langle \phi_i - (\phi_i \cdot \mathbf{e}_{C_f})\mathbf{e}_{C_f} \rangle \int_0^{n_s\Delta t^s} e^{\lambda_i t} dt.$$

Garicano-Mena, Li, Ferrer & Valero, A composite dynamic mode decomposition analysis of turbulent channel flows, Phys. Fluids, vol. 31, 2019.

Re<sub>c</sub>≈3600 TCF Composite DMD



#### **Composite Parallel DMD**



Standard channel DMD spectra obtained from analysis based on u'v' and composite  $C_{f}$ -u'v' snapshots: amplitudes  $|\alpha_i|/|\alpha_{max}|$  and  $|\beta_i|/|\beta_{max}|$  vs angular pulsation  $\Im(\lambda_i)$ .

#### **Composite Parallel DMD**



Standard channel DMD spectra obtained from analysis based on u'v' and composite  $C_{f}$ -u'v' snapshots: amplitudes  $|\alpha_i|/|\alpha_{max}|$  and  $|\beta_i|/|\beta_{max}|$  vs angular pulsation  $\Im(\lambda_i)$ .

### Composite Parallel DMD





$$Re_{\tau} = 200$$
 turbulent channel flow: **DMD** reconstruction of the field  $-\frac{\langle u'v' \rangle}{u_{\tau}^2}(y^+, z^+)$ 



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## Spatial Agglomeration & DMD

DMD analysis applied on Spatially Agglomerated Databases

allows effective reduction of computational costs

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Succesful example of combination of (Unsupervised) Machine Learning Algorithms & data-driven modal decomposition techniques.

Li, Garicano-Mena, Zheng & Valero, Dynamic Mode Decomposition Analysis of Spatially Agglomerated Flow Databases, Energies, vol. 13 (9), 2020.

Data-driven modal decomposition techniques  $\rightleftharpoons$  matrix factorization:

SVD is univoquely defined, but mixes frequencies.

DMD identifies distinct frequencies, but needs solving an optimization problem.

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SVD (POD) is univoquely defined, but mixes frequencies.

DMD identifies distinct frequencies, but needs solving an optimization problem. Fortunately, a closed solution is available.

Computational cost of data-driven modal decomposition analysis:

Potentially expensive & large memory footprint.

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Strategies to alleviate the computational cost available:

- Spatial Agglomeration,
- Memory-distributed parallelism (not discussed today).

More sophisticated variants available:

Higher-Order SVD (tensor formulation): very robust against noise.

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Higher-Order DMD: uses a generalized, d-lagged Koopman assumption capable of unravel very complex dynamics.

$$\mathbf{v}(t_{k+1}) = \mathcal{A} \, \mathbf{v}(t_k)$$
$$\mathbf{v}(t_{k+d}) = \mathcal{A}_1 \, \mathbf{v}(t_k) + \mathcal{A}_2 \, \mathbf{v}(t_{k+1}) \dots + \mathcal{A}_d \, \mathbf{v}(t_{k+d-1})$$

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Applications also beyond fluid dynamics, e.g. Medical Imaging (echocardiography videos, MRI data)

Groun, Le Clainche et al., Higher order dynamic mode decomposition: From fluid dynamics to heart disease analysis, Computers in Biology and Medicine, Vol 144, 2022. Groun, Le Clainche et al., A novel data-driven method for the analysis and reconstruction of cardiac cine MRI, Computers in Biology and Medicine, Vol. 151, 2022.

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Combinations with Neural Network technology.
## Conclusions

More sophisticated variants available:

Higher-Order SVD (tensor formulation): very robust against noise.

Higher-Order DMD: uses a generalized, d-lagged Koopman assumption capable of unravel very complex dynamics.

Combination with Neural Network technology.

No restriction on data origin.

1) Describe classical Dynamic Mode Decomposition (DMD)

2) DMD as one of many data-driven modal decomposition techniques

3) DMD as a matrix factorization technique

4) Accelerating DMD methods

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## Thank you for your attention



## Questions?