DYNAMIC ACTIVE SUBSPACES

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A little book

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izabelpaguiar.com/DyAS

What are active subspaces? [1]

Consider a function of m input parameters,

$$f(\mathrm{x}) \in \mathbb{R}$$

Active subspaces identify directions in the parameter space along which $f(\mathrm{x})$ changes the most on average.
Active subspaces are eigenspaces of the matrix,

$$C \;=\; \int \nabla f(\mathrm{x})\, \nabla f(\mathrm{x})^T \rho(\mathrm{x})\, d\mathrm{x}.$$

The eigenvalues of C are equal to the mean-squared directional derivative of $f(\mathrm{x})$ with respect to the corresponding eigenvector.

$$\lambda_i \;=\; \int \left(\mathrm{w}_i^T \nabla f(\mathrm{x})\right)^2 \rho(\mathrm{x})\, d\mathrm{x}, \quad i = 1, \dots, m$$

This enables us to identify important (and unimportant) directions in the parameter space and construct a low-dimensional approximation,

$$f(\mathrm{x}) \approx h(W_1^T \mathrm{x}), \quad W_1^T \mathrm{x} \in \mathbb{R}^n, \; n < m$$

Dynamic Active Subspaces (DyAS)

What about when the output is not only a function of its parameters, but of time as well?

$$f(\mathrm{x}, t)$$

Can we extend active subspaces to dynamical systems? Are we able to construct a time-dependent matrix, $C(t)$ with eigenvectors $\mathrm{w}_i(t)$?

Such an extension would allow for new parameter studies and sensitivity analysis of dynamical systems found in biological and engineering applications.

The state-of-the-art method for computing dynamic active subspaces is to find active subspaces independently and at multiple time steps [2]. This is computationally expensive.

Is there an analytical form for dynamic active subspaces?

DyAS for a linear dynamical system

Consider a linear dynamical system,

$$\mathrm{u} = \mathrm{A}\mathrm{u}, \;\; \mathrm{u}(0) = \eta, \quad \mathrm{u}(t), \eta \in \mathbb{R}^n, \;\; \mathrm{A} \in \mathbb{R}^{n \times n}.$$

The solution to this dynamical system is,

$$\mathrm{u}(t) = e^{\mathrm{A}t}\eta.$$

Consider a time-dependent scalar output of the dynamical system, $f(\eta, t) = \phi^T \mathrm{u}(t)$, for $\phi \in \mathrm{R}^n$. For example, where $f(\eta, t)$ is the ith state of the dynamical system, ϕ is the ith column of the identity matrix. Assume that the initial conditions of the original dynamical system are distributed according to $\eta \sim \rho(\eta)$.

Then the dynamical system of the unnormalized first eigenvector of $\mathrm{C}(t)$ is described by the linear dynamical system,

$$\mathrm{v}'(t) = A^T \mathrm{v}(t), \;\; \mathrm{v}(0) = \phi. \qquad (1)$$

DyAS for an inhomogeneous linear dynamical system

Consider the inhomogeneous linear dynamical system,

$$\mathrm{u} = \mathrm{A}\mathrm{u} + \mu, \;\; \mathrm{u}(0) = \eta, \quad \mathrm{u}(t), \eta, \mu \in \mathbb{R}^n, \;\; \mathrm{A} \in \mathbb{R}^{n \times n}.$$

For invertible A, the solution to this dynamical system is given by *Duhamel's Principle*,

$$\mathrm{u}(t) = e^{\mathrm{A}t}\eta + \mathrm{A}^{-1}(e^{\mathrm{A}t} - I)\mu.$$

Consider a time-dependent scalar output of the dynamical system, $f(\mu, t) = \phi^T \mathrm{u}(t)$, for $\phi \in \mathrm{R}^n$. Assume that μ is distributed according to $\mu \sim \rho(\mu)$.

Then the dynamical system of the unnormalized first eigenvector of $\mathrm{C}(t)$ is described by the linear dynamical system,

$$\mathrm{v}'(t) = A^T \mathrm{v}(t) + \phi, \;\; \mathrm{v}(0) = 0. \qquad (2)$$

Dynamic Mode Decomposition [3]

Consider a dynamical system of n states, as well as *snapshots* of their dynamics at m time steps.
We can form the matrices $\boldsymbol{X}$ and $\boldsymbol{X}'$ such that,

$$\boldsymbol{X} = [x_1 \;\; x_2 \;\; \dots \;\; x_{m-1}]$$
$$\boldsymbol{X}' = [x_2 \;\; x_3 \;\; \dots \;\; x_m]$$

Where each x_i is an $(n \times 1)$ dimensional snapshot vector at time i.
Then we can estimate a matrix $\boldsymbol{A}$ such that,

$$\boldsymbol{X}' \approx \boldsymbol{A}\boldsymbol{X}$$

This is an optimal locally linear approximation.

The dynamic mode decomposition allows us to predict future states of the dynamical system based on information from our snapshots.

Can we use dynamic mode decomposition to inform future states of the eigenvectors of $\boldsymbol{C}$?

Sparse Identification for Nonlinear Dynamical Systems (SINDy) [4]

This method provides an approach for discovering governing equations for dynamical systems from data. We form the matrices $\boldsymbol{X}$ with and $\dot{\boldsymbol{X}}$ with data snapshots and computed time derivatives,

$$\boldsymbol{X} = \begin{bmatrix} \mathrm{x}^T(t_1) \\ \mathrm{x}^T(t_2) \\ \vdots \\ \mathrm{x}^T(t_m) \end{bmatrix} \quad \dot{\boldsymbol{X}} = \begin{bmatrix} \dot{\mathrm{x}}^T(t_1) \\ \dot{\mathrm{x}}^T(t_2) \\ \vdots \\ \dot{\mathrm{x}}^T(t_m) \end{bmatrix}$$

The *library matrix* Θ is formed by taking p functional transformations of the columns of $\boldsymbol{X}$.

$$\Theta(\boldsymbol{X}) = \left[1 \;\; \boldsymbol{X} \;\; \boldsymbol{X}^{P_2} \;\; \boldsymbol{X}^{P_3} \cdots \sin(\boldsymbol{X}) \;\; \cos(\boldsymbol{X}) \cdots \right].$$

We now seek a *coefficient matrix* Ξ such that

$$\dot{\boldsymbol{X}} = \Theta(\boldsymbol{X})\Xi \qquad (3)$$

The coefficients of Ξ will thus indicate which functions of Θ are in the *true* governing system.
Can this approach recover the governing system for a dynamic active subspace?

References

[1] Constantine, P. G. *Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies*. SIAM, Philadelphia (2015).

[2] Louden, T. and Pankavich, S. Mathematical *Analysis and Dynamic Active Subspaces for a Long term model of HIV* (2016).

[3] Kutz, J. N., Brunton, S., Brunton, B., and Proctor, J. *Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems.* SIAM, Philadelphia (2016).

[4] Brunton, S., Proctor, J., and Kutz, J. N. *Discovering governing equations from data by sparse identification of nonlinear dynamical systems.* PNAS (2016).