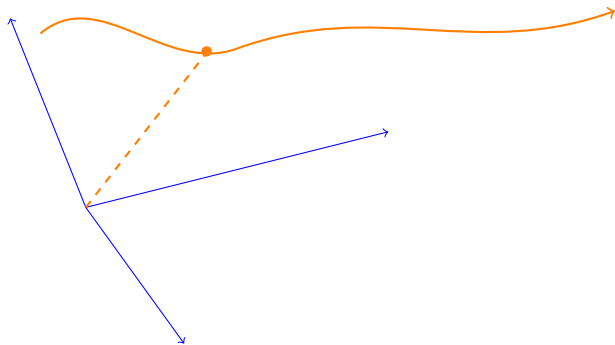


Quantifying Uncertainty

Sai Ravela

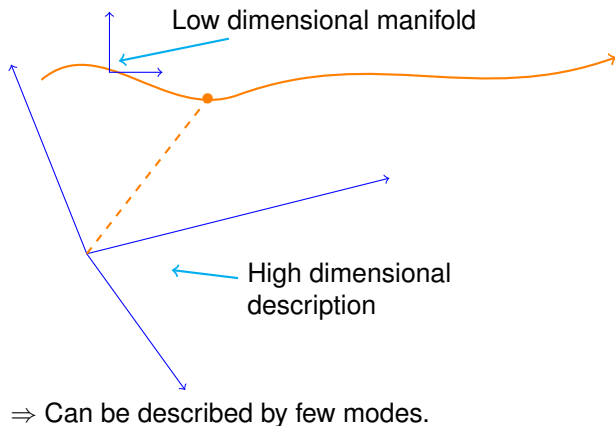
M. I. T

2012



$$\dot{Y}(t) = f(Y(t), t) + \beta u$$

System with **high** dimensions



How to find subspace?

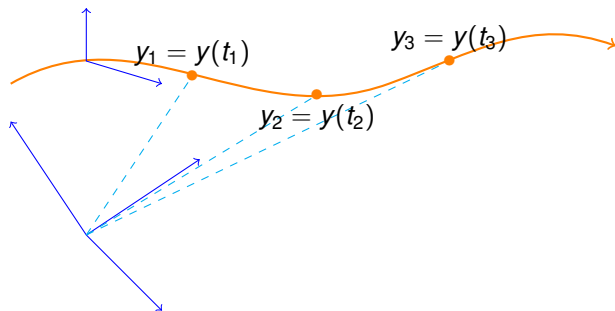
Projection Methods

POD-Proper Orthogonal Decomposition

- ▶ Galerkin Projection
- ▶ Snapshots

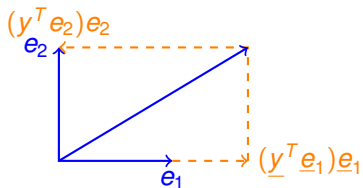
Krylov Subspace

Also Galerkin



$$\sum_{i=1}^n [y_n - \pi_d(y_n)]^2$$

Just minimize a projection error



$$\pi_d(\underline{y}_n) = (\underline{y}_n^T \underline{e}_1) \underline{e}_1 + (\underline{y}_n^T \underline{e}_2) \underline{e}_2$$

$$\therefore \sum_{i=1}^n \left[\underline{y}_n - \sum_{j=1}^d (\underline{y}_n^T \underline{e}_j) \underline{e}_j \right]^2$$

Constraints ?

$$\mathbf{e}_i^T \mathbf{e}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

So, Lagrangian

$$J(\mathbf{e}_1 \dots \mathbf{e}_d) = \sum_{i=1}^n \left[\mathbf{y}_{-n} - \sum_{j=1}^d (\mathbf{y}_{-n}^T \mathbf{e}_j) \mathbf{e}_j \right]^2 + \sum_{k=1}^d \sum_{l=1}^d \lambda_{ij} (\mathbf{e}_i^T \mathbf{e}_j - \delta_{ij})$$

$$\frac{\partial J}{\partial \mathbf{e}_j} = \phi \Rightarrow \sum_{i=1}^n y_i (y_i^T \mathbf{e}_j) = \lambda_{jj} \mathbf{e}_j$$

$\lambda_{ij} = \phi$ for $i \neq j$.

Let y ,

$$Y = [y_1, \dots, y_n] \text{ and } E = [e_1, \dots, e_n]$$

we have

$$\underline{\underline{\lambda}} = \begin{bmatrix} \lambda_{11} & \dots & \lambda_{1d} \\ \vdots & \ddots & \vdots \\ \lambda_{d1} & \dots & \lambda_{dd} \end{bmatrix}$$

$$\underline{\underline{Y}} \underline{\underline{Y}}^T \underline{\underline{E}} = \underline{\underline{\lambda}} \underline{\underline{E}}$$

$$Y Y^T e_j = \lambda_{jj} e_j$$

An eigenvalue problem.

Notice

$$K(s, t) = Y(s)Y(t)$$

$$K = YY^T$$

⇒ Correlation matrix (or Covariance for centered process)

Still, how to do this?

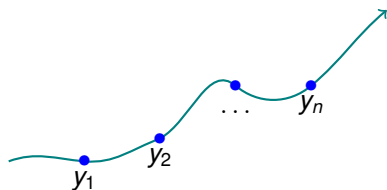
Via SVD

Letting

$$\begin{aligned} Y &= usv^T \\ YY^T &= us^2u^T \\ uu^T &= I, \quad u^T u = I \end{aligned}$$

Where does Y come from?

Snapshots



$$Y = [y_1, \dots, y_n]$$

Typically $n \ll |y_i|$ and modes $d < n$.

But YY^T is huge!

Take 2

$$Y = \underbrace{USV^T}_{\text{svd via iterative methods}} \\ \text{only 'd' leading vectors} \\ \text{or modes}$$

$$\text{Then: } e_j = U_j, \lambda_{jj} = S_{jj}^2$$

Take 3

$$\underbrace{Y^T Y}_{\text{small}} = v s^2 v^T$$

$$Y V S^{-1} = u$$

$$e_i = u_i$$

$$\lambda_{ii} = S_{ii}^2$$

Pod & Model reduction

Let's consider

$$\dot{y}(t) = f(y(t))$$

Let

$$\begin{aligned} y(t) &= u_d s(t) \\ &= \underbrace{u_d}_{\text{Basis}} \underbrace{\chi(t)}_{\substack{\text{time} \\ \text{dependent} \\ \text{decorrelated}}} \end{aligned}$$

$$u_d \dot{\chi}(t) = f(u_d \chi(t))$$
$$\dot{\chi}(t) = u_d^T \underbrace{f(u_d \chi(t))}_{y_d(t)}$$

With initial condition $\chi(0)$ calculated from y_0

$$y_d^{(i)}(0) = [y_0^T(0) u_i] u_i$$

Can this work?

a

Snapshots make it easy, but how badly does it work when dynamics not in steady state (statistical)?

b

How much to truncate by?

$$Residual = \sum_{i=d+1}^n \lambda_{ii}$$

$$Information\ fraction = \frac{\sum_{i=1}^d \lambda_{ii}}{\sum_{j=1}^n \lambda_{jj}}$$

c

Do PoD modes correspond to dynamical modes?

d

Is it sensitive to choice of the inner product?

e

Is a PoD decomposition stable? e.g. $\dot{\chi} = Ax + Bu$ Rom may not have negative eigen values!

How to fix these issues?

- ▶ PoD+ Empirical Grammians (Balanced Truncation) e.g Wilcox
- ▶ Optimization for a stabilizing projection

A Trajectory Piecewise Approach

Via Krylov Subspace



$$\dot{y} = f(y) + B(y)u$$
$$Z = C^T Y$$

$$x' = f(x) + B(x)u$$

$$y = C^T u$$

$Z \Rightarrow$ Reduced state

$$x \cong VZ$$

Residual

$$f(VZ) + B(VZ) - \frac{d(VZ)}{dt}$$

Orthogonal to some reduced space, $V^T v = 0$

$$\frac{d}{dt}[V^T VZ(t)] = V^T f(VZ(t)) + V^T B(VZ(t))u(t)$$

$$y(t) = C^T VZ(t)$$

Is this supposed to be easy?

Linear Case

Say

$$f(x) = Fx$$

$$B(x) = B$$

$$\frac{d}{dt} V^T V Z(t) = V^T F V Z(t) + V^T B u(t)$$

$$y(t) = (V^T C)^T Z(t)$$

Linear Case contd.

$$w \frac{d}{dt} Z(t) = \tilde{A} Z(t) + \tilde{B} u(t)$$

$$y(t) = (V^T C)^T Z(t)$$

Suppose original system was linear and of general form:

$$E \dot{x} = Fx + Bu$$

$$y = C^T x$$

Introduction to Krylov Subspace methods

$$Ax = f$$

Letting $A = M - N$ (say)

$$(M - N)u = f$$

$$Mu^{n+1} = Nu^n + f$$

$$\begin{aligned} u^{n+1} &= M^{-1}Nu^n + M^{-1}f \\ &= u^n + M^{-1}(F - Au^n) \end{aligned}$$

Letting

$$\gamma^n = f - Au^n$$

Iterative method:

$$u^{n+1} = u^n + M^{-1}\gamma^n$$

$$u^0 \rightarrow u^n \rightarrow u^?$$

$$e^n = u^n - u$$

$$e^{n+1} = (I - M^{-1}A)e^n$$

Examples

$$A = D + L + u$$

Jacobi: $M = D, -N = L + u$

Gauss-Sidel: $M = L + D, -N = u$

SOR:

$$M = \left(\frac{1}{w} D + L \right), \quad -N = u - \frac{1-w}{w} D$$

etc.

Letting,

$$\tilde{A} = M^{-1}A \quad \tilde{f} = Mf$$

$$\begin{aligned} u^{n+1} &= u^n + (\tilde{f} - \tilde{A}u^n) \\ &= u^n + \tilde{\gamma}^n \end{aligned}$$

$$\begin{aligned} \tilde{\gamma}^{n+1} &= \tilde{\gamma}^n - \tilde{A}\tilde{\gamma}^n \\ &= (I - \tilde{A})\tilde{\gamma}^n \\ &= (I - \tilde{A})^{n+1}\tilde{\gamma}^0 \end{aligned}$$

$$\boxed{\tilde{\gamma}^n = (I - \tilde{A})^n\tilde{\gamma}^0}$$

$$u^{n+1} = u^0 + \sum_{i=0}^n (I - \tilde{A})^i \tilde{\gamma}^0$$
$$\in u^0 + \underbrace{\text{Span} \left\{ \tilde{\gamma}^0, \tilde{A}\tilde{\gamma}^0, \tilde{A}^2\tilde{\gamma}^0, \dots, \tilde{A}^n\tilde{\gamma}^0 \right\}}_{\text{Krylov Subspace}}$$

So:(after several steps)

$$E\hat{x} = Fx + Bu \quad y = C^T x$$

we look for an orthonormal basis V in Krylov subspace

$$\text{Span} \{ F^{-1}B, F^{-1}EF^{-1}B, \dots, (F^{-1}E)^{v-1}F^{-1}B \}$$

Algo:(F, B, E, v)

Output: V

$$v_1 = B / \|B\|_2$$

for $i = 1$ to q

$$x = Evi$$

Solve $Av = x$

Orthogonalize v

for $j = 1$ to i

$$\alpha = v_j^T V$$

$$v = v - \alpha v_j$$

$$v_i = v / \|v\|_2$$

Reduced System: $E = I$

$$w\tilde{Z} = \tilde{A}Z + \tilde{B}u$$

$$y = \tilde{C}^T Z$$

$$H_\gamma(s) = \tilde{C}^T [sW - \tilde{A}]^{-1} \tilde{B}$$

Original

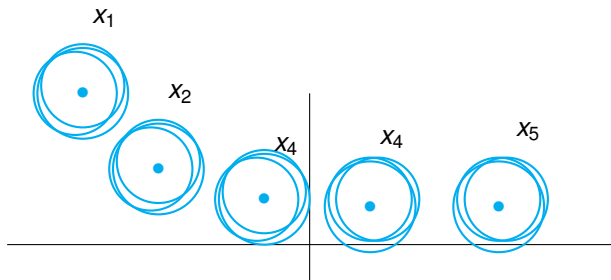
$$H(s) = C^T [sI - A]^{-1} B$$

$H_\gamma(s)$ will match first q moments of H .

However,

- ▶ Still an issue for nonlinear
- ▶ No provable error bounds
- ▶ No guarantee of stability

How does this compare to PoD?



Linearization & model reduction

$$\dot{x}_i = f(x_i) + B(x_i)u$$

$$\dot{x} = f(x_i) + \underbrace{A_i(x - x_i)}_{\text{Jacobian of } f} + B_i u$$

A weighted combination of linearized models.

$$\sum_{i=1}^S w_i(x) \dot{x} = \sum_{j=1}^S w_j(x) [f(x_j) + A_j(x - x_j) + B_j u]$$

$$\sum_i w_i(x) = 1$$

So,

$$\sum_{s=1}^S w_i[VZ] V^T VZ = \sum_{i=1}^S w_i[VZ] \left[\overbrace{V^T f(x_i)}^{\text{Precompute}} + V^T A_i[VZ - x_i] + V^T B_i u \right]$$

Can be fast!

How to get weights?
Kernell estimated!

$$\begin{aligned}\|x - x_i\| &= \|VZ - VZ_i\| \\ &= (Z - Z_i)V^T V(Z - Z_i) \\ &= \|Z - Z_i\|_V\end{aligned}$$

$$d_i \in \|Z - Z_i\|$$

$$\tilde{w}_i = e^{-Kd_i/\sigma^2}$$

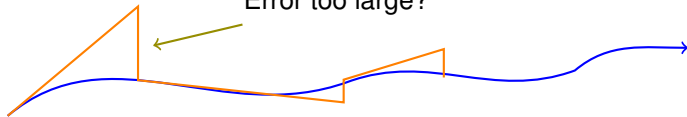
$$\sigma^2 \sim \min d_i$$

$$w_i = \frac{\tilde{w}_i}{\sum \tilde{w}_i}$$

Next time: On the Grassmann Manifold
⇒ Model Interpolation

When to linearize?

Error too large?



Break when error too large

Interpolation also with response surface modeling.

Ideas

- ▶ Is there a way to combine PoD with krylov over MCMC?
- ▶ Can we assemble better collocation points?

$$\frac{\partial \theta}{\partial t}(x, t) = D\theta(x, t)$$

$$R(\theta) = \frac{\partial \theta}{\partial t} - D\theta$$

$$\theta = u\eta(t)$$

$$u^T R = 0$$

$$\frac{\partial \eta}{\partial t} = u^T D u \eta$$

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12.S990 Quantifying Uncertainty

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