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Harold Vance Department of Petroleum Engineering

PETROBRAS Workshop: Scientific Machine Learning (SciML) and Data-Driven Model Reduction for Reservoir Simulation

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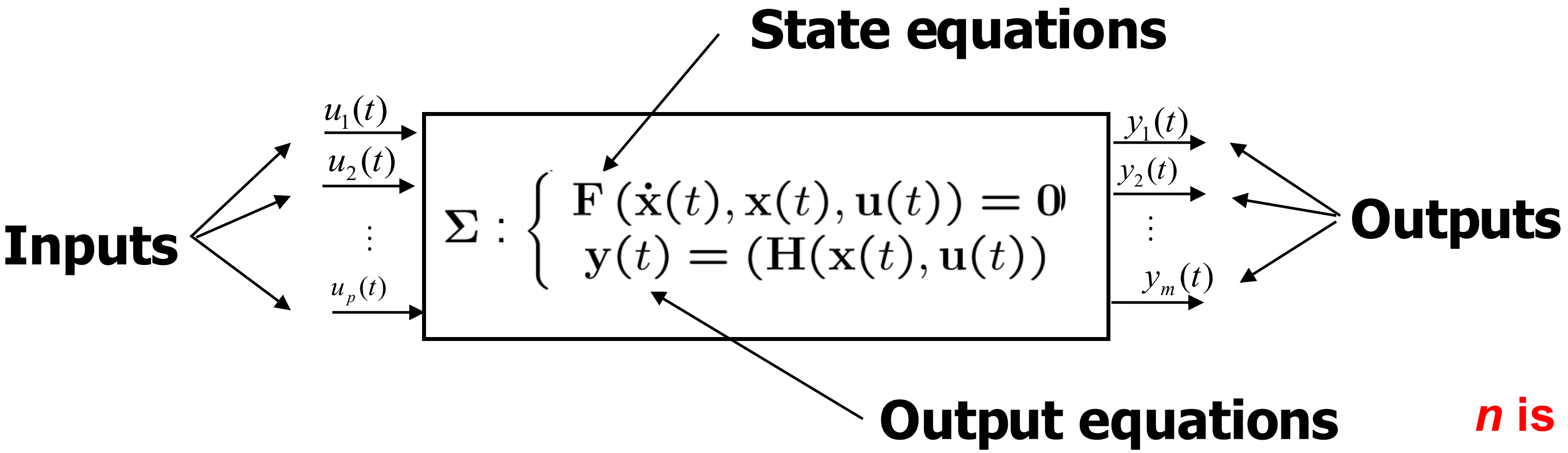
Intro Dynamical Systems

MODEL REDUCTION PROBLEM

- Given



***n* is very large!**

- linear time-invariant (LTI):

$$\Sigma : \begin{cases} \dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{u}(t) \end{cases} \Leftrightarrow \Sigma = \left[\begin{array}{c|c} \mathbf{A} & \mathbf{B} \\ \hline \mathbf{C} & \mathbf{D} \end{array} \right] \in \mathbb{R}^{(n+p)\times(n+m)}$$

LTI/ LTIP

Linear, Time-Invariant (LTI) Systems

$$\begin{aligned} E\dot{x} &= f(t,x,u) &= Ax + Bu, \quad & E, A \in \mathbb{R}^{n\times n}, & B \in \mathbb{R}^{n\times m}, \\ y &= g(t,x,u) &= Cx + Du, \quad & C \in \mathbb{R}^{q\times n}, & D \in \mathbb{R}^{q\times m}. \end{aligned}$$

Linear, Time-Invariant Parametric Systems

$$\begin{aligned} E(p)\dot{x}(t;p) &= A(p)x(t;p) + B(p)u(t), \\ y(t;p) &= C(p)x(t;p) + D(p)u(t), \end{aligned}$$

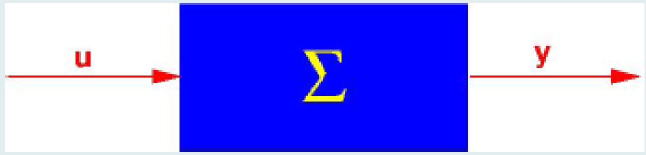
where $A(p), E(p) \in \mathbb{R}^{n\times n}, B(p) \in \mathbb{R}^{n\times m}, C(p) \in \mathbb{R}^{q\times n}, D(p) \in \mathbb{R}^{q\times m}$.

Model Reduction

Original System

$$\Sigma : \begin{cases} \dot{x}(t) = f(t, x(t), u(t)), \\ y(t) = g(t, x(t), u(t)). \end{cases}$$

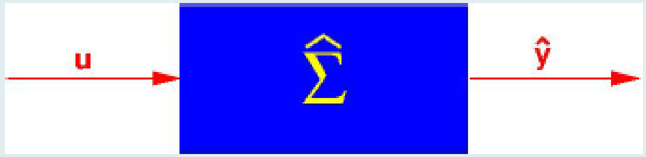
- states $x(t) \in \mathbb{R}^n$,
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $y(t) \in \mathbb{R}^q$.



Reduced-Order Model (ROM)

$$\widehat{\Sigma} : \begin{cases} \dot{\hat{x}}(t) = \widehat{f}(t, \hat{x}(t), u(t)), \\ \hat{y}(t) = \widehat{g}(t, \hat{x}(t), u(t)). \end{cases}$$

- states $\hat{x}(t) \in \mathbb{R}^r$, $r \ll n$
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $\hat{y}(t) \in \mathbb{R}^q$.



Goal:

$\|y - \hat{y}\| <$ tolerance $\cdot \|u\|$ for all admissible input signals.

Secondary goal: reconstruct approximation of x from $\hat{x}$.

The CORE Consortium.

Projection-Based MOR

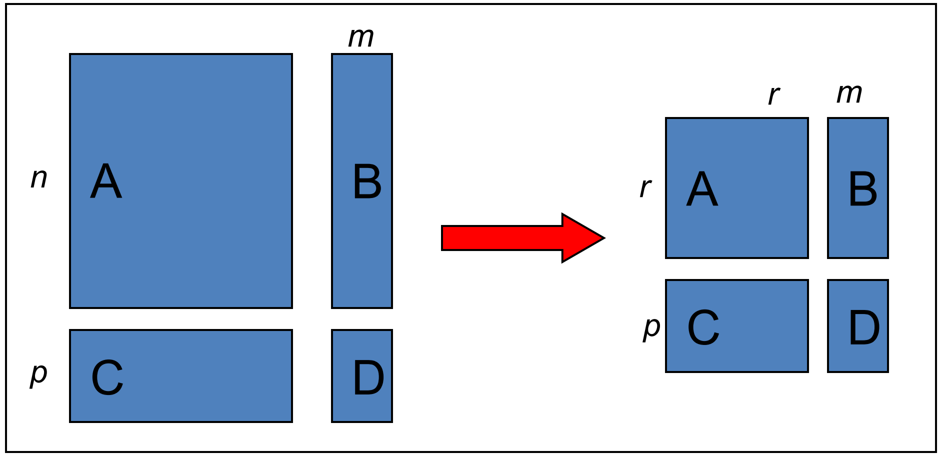
Approximate the states by a linear combination of basis vectors

$$\mathbf{x} \approx \sum_{i=1}^{r} \mathbf{V}_i x_{r_i}$$

$$\Sigma_r : \begin{cases} \dot{\mathbf{x}}_r(t) = \underbrace{\mathbf{W}^T\mathbf{A}\mathbf{V}}_{:=\mathbf{A}_r}\mathbf{x}_r(t) + \underbrace{\mathbf{W}^T\mathbf{B}}_{:=\mathbf{B}_r}\mathbf{u}(t) \\ \mathbf{y}_r(t) = \underbrace{\mathbf{C}\mathbf{V}}_{:=\mathbf{C}_r}\mathbf{x}_r(t) + \underbrace{\mathbf{D}}_{:=\mathbf{D}_r}\mathbf{u}(t) \end{cases}$$

Project

$$n \times 1 \left\{ \begin{bmatrix} \\ \mathbf{x} \\ \\ \end{bmatrix} \right. \approx \begin{bmatrix} \\ \mathbf{V} \\ \\ \end{bmatrix} \left. \begin{bmatrix} \mathbf{x}_r \end{bmatrix} \right\} r \times 1$$



Some definitions

Definition

The Laplace transform of a time domain function $f \in L_{1,\mathrm{loc}}$ with $\mathrm{dom}\,(f) = \mathbb{R}_0^+$ is

$$\mathcal{L} : f(t) \mapsto f(s) := \mathcal{L}\{f(t)\}(s) := \int_0^\infty e^{-st} f(t)\,dt, \quad s \in \mathbb{C}.$$

F is a function in the (Laplace or) frequency domain.

Note: for frequency domain evaluations ("frequency response analysis"), one takes $\operatorname{re} s = 0$ and $\operatorname{im} s \geq 0$. Then $\omega := \operatorname{im} s$ takes the role of a frequency (in [rad/s], i.e., $\omega = 2\pi v$ with v measured in [Hz]).

Lemma

$$\mathcal{L}\{\dot{f}(t)\}(s) = sF(s).$$

Linear Systems in Frequency Domain

Application of Laplace transform $(x(t) \mapsto x(s),\ \dot{x}(t) \mapsto sx(s))$ to linear system

$$E\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t) + Du(t)$$

with $x(0) = 0$ yields:

$$sEx(s) = Ax(s) + Bu(s), \quad y(s) = Cx(s) + Du(s),$$

$\Longrightarrow$ I/O-relation in frequency domain:

$$y(s) = \Big(\underbrace{C(sE - A)^{-1}B + D}_{=:G(s)}\Big)u(s).$$

$G(s)$ is the transfer function of Σ.

Formulating model reduction in frequency domain

Approximate the dynamical system

$$\begin{array}{rcll} E\dot{x} & = & Ax + Bu, & E, A \in \mathbb{R}^{n\times n},\; B \in \mathbb{R}^{n\times m}, \\ y & = & Cx + Du, & C \in \mathbb{R}^{q\times n},\; D \in \mathbb{R}^{q\times m}, \end{array}$$

by reduced-order system

$$\begin{array}{rcll} \hat{E}\dot{\hat{x}} & = & \hat{A}\hat{x} + \hat{B}u, & \hat{E}, \hat{A} \in \mathbb{R}^{r\times r},\; \hat{B} \in \mathbb{R}^{r\times m}, \\ \hat{y} & = & \hat{C}\hat{x} + \hat{D}u, & \hat{C} \in \mathbb{R}^{q\times r},\; \hat{D} \in \mathbb{R}^{q\times m} \end{array}$$

of order $r \ll n$, such that

$$\|y - \hat{y}\| = \|Gu - \hat{G}u\| \leq \|G - \hat{G}\| \cdot \|u\| < \text{tolerance} \cdot \|u\|.$$

$\Longrightarrow$ Approximation problem: $\displaystyle \min_{\text{order}\,(\hat{G}) \leq r} \|G - \hat{G}\|.$

System Norms

Output errors in time-domain

$$
\begin{aligned}
\|y-\hat{y}\|_2 &\leq \|G-\hat{G}\|_\infty \|u\|_2 &&\Longrightarrow \|G-\hat{G}\|_\infty < \mathrm{tol}\\
\|y-\hat{y}\|_\infty &\leq \|G-\hat{G}\|_2 \|u\|_2 &&\Longrightarrow \|G-\hat{G}\|_2 < \mathrm{tol}
\end{aligned}
$$

$\mathcal{H}_\infty$-norm	best approximation problem for given reduced order r in general open; balanced truncation yields suboptimal solution with computable $\mathcal{H}_\infty$-norm bound.
$\mathcal{H}_2$-norm	necessary conditions for best approximation known; (local) optimizer computable with iterative rational Krylov algorithm (IRKA)
Hankel-norm $\|G\|_H := \sigma_{\max}$	optimal Hankel norm approximation (AAK theory).

Similarity Transformations

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Definition

For a linear (time-invariant) system

$$\Sigma : \begin{cases} \dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{cases} \qquad \begin{array}{l} \text{with transfer function} \\ G(s) = C(sI - A)^{-1}B + D, \end{array}$$

the quadruple $(A, B, C, D) \in \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times m} \times \mathbb{R}^{q\times n} \times \mathbb{R}^{q\times m}$ is called a realization of Σ.

Realizations are not unique!

Transfer function is invariant under state-space transformations,

$$\mathcal{T} : \begin{cases} x &\to Tx, \\ (A, B, C, D) &\to (TAT^{-1}, TB, CT^{-1}, D), \end{cases}$$

Realizations are not unique!

Hence,

$$(A, B, C, D), \qquad \left(\begin{bmatrix} A & 0 \\ 0 & A_1 \end{bmatrix}, \begin{bmatrix} B \\ B_1 \end{bmatrix}, \begin{bmatrix} C & 0 \end{bmatrix}, D \right),$$

$$(TAT^{-1}, TB, CT^{-1}, D), \qquad \left(\begin{bmatrix} A & 0 \\ 0 & A_2 \end{bmatrix}, \begin{bmatrix} B \\ 0 \end{bmatrix}, \begin{bmatrix} C & C_2 \end{bmatrix}, D \right),$$

are all realizations of Σ!

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Projection

Definition 3.1 (Projector)

A projector is a matrix $P \in \mathbb{R}^{n \times n}$ with $P^2 = P$. Let $\mathcal{V} = \mathrm{range}(P)$, then P is projector onto $\mathcal{V}$. On the other hand, if $\{v_1, \ldots, v_r\}$ is a basis of $\mathcal{V}$ and $V = [v_1, \ldots, v_r]$, then $P = V(V^T V)^{-1} V^T$ is a projector onto $\mathcal{V}$.

Projection Properties

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Lemma 3.2 (Projector Properties)

- If $P = P^T$, then P is an orthogonal projector (aka: Galerkin projection), otherwise an oblique projector (aka: Petrov-Galerkin projection).
- P is the identity operator on $\mathcal{V}$, i.e., $Pv = v \ \forall v \in \mathcal{V}$.
- $I - P$ is the complementary projector onto $\ker P$.
- If $\mathcal{V}$ is an A-invariant subspace corresponding to a subset of A's spectrum, then we call P a spectral projector.
- Let $\mathcal{W} \subset \mathbb{R}^n$ be another r-dimensional subspace and $W = [\, w_1, \ldots, w_r \,]$ be a basis matrix for $\mathcal{W}$, then $P = V(W^T V)^{-1} W^T$ is an oblique projector onto $\mathcal{V}$ along $\mathcal{W}$.

Example

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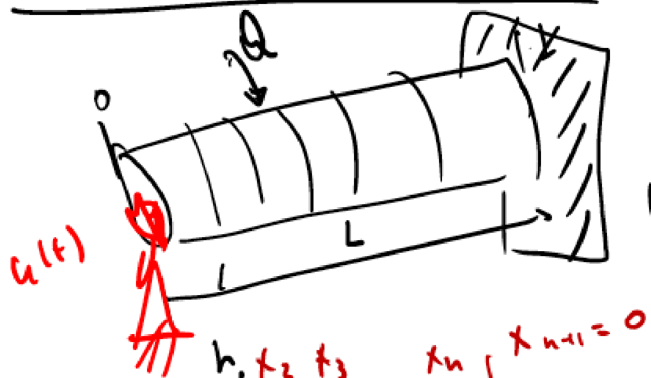
Example Dynamical System

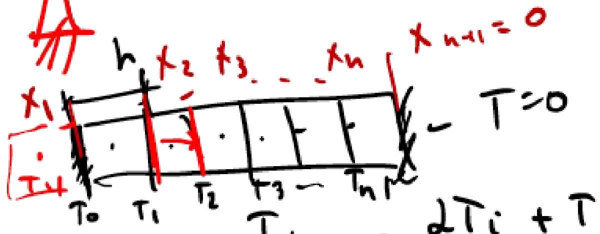


$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \rightarrow O(h^2) \qquad 0 < x < 1$$

BC – $-\left.\frac{\partial T}{\partial t}\right|_{x=0} = u(t)$

$T(1,t) = 0$

I.C. – $T(0,x) = 0$



Using FD on spacing only

$$\frac{\partial T}{\partial t} = \frac{T_{i-1} - 2T_i + T_{i+1}}{h^2} + O$$

x_1 x_2

$$\frac{\partial T_0}{\partial t} = \frac{T_{-1} - 2T_0 + T_1}{h^2}$$

x_3

$$\frac{\partial T_1}{\partial t} = \frac{T_0 - 2T_1 + T_2}{h^2} \; - -$$

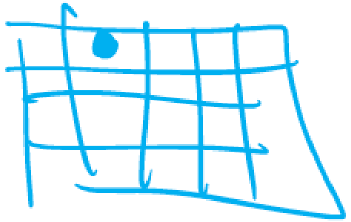
$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = \frac{T_1 - T_0}{h} \quad O(h)$$

$$\boxed{= \frac{T_{-1} - T_1}{2h} \quad O(h^2)}$$

$$\frac{dx}{dt} = \begin{bmatrix} \frac{dx_0}{dt} \\ \frac{dx_1}{dt} \\ \vdots \\ \frac{dx_n}{dt} \end{bmatrix} = n^2 \underbrace{\begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}}_{A \in \mathbb{R}^{n \times n}} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} + n \underbrace{\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}}_{B \in \mathbb{R}^{n \times p}} u(t)$$

$h = \frac{1}{n}$

n = number of grid points



If we can measure Temp everywhere

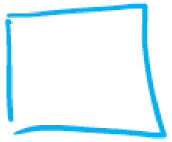
$$y = Cx(t) + Du(t)$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ \vdots \\ T_n \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \end{bmatrix}}_{C = \text{Identity}} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + 0$$

$D = 0$

$C \in \mathbb{R}^{q \times n}$

$D \in \mathbb{R}^{q \times p}$



Now. Suppose measure average temp. @ rod.

$$y(t) = \frac{1}{n}\int_0^T T(t,\xi)\,d\xi \approx \frac{1}{n}\sum_{i=0}^{n} T(t, i/n)$$

$$\approx \frac{1}{n}\sum_{i=1}^{n} x_i(t)$$

$$y(t) = \underbrace{\frac{1}{n}\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & \cdots & 1 \end{bmatrix}}_{C} X + \underbrace{0}_{D}\,u(t)$$

$$\dot{x}_r = A_r \cancel{x}_r + B_r u$$

$$y_r = C_r x_r + D_r u$$

$A_r \in \mathbb{R}^{r \times r}$

$B_r \in \mathbb{R}^{r \times p}$

$C_r \in \mathbb{R}^{q \times r}$

$D_r \in \mathbb{R}^{q \times p}$