Stochastic model reduction of nonlinear dynamics by inference

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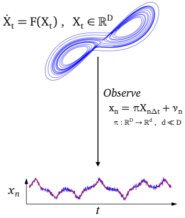
1. Motivation and objective
   - Problem and motivation
   - Example
   - Review
2. Inference-based Model reduction
   - Flow map approximation
   - NARMA: a numerical time series model
   - Example: a chaotic system
3. From nonlinear Galerkin to inference
   - Kuramoto-Sivashinsky Equation
   - Stochastic Burgers equation
   - Optimal space-time reduction

Problem: ensemble prediction of $x(t)$

$$\begin{aligned} x' &= F(x) + U(x,y), && \text{resolved scales} \\ y' &= G(x,y), && \text{subgrid-scales} \end{aligned}$$

Data: $\{x(nh)\}$



Motivation:

- arise from numerical ODE/PDE/SDEs
- Data assimilation: partial noisy observation
  - ensemble prediction
  - can only afford to resolve $x' = F(x)$

Objective: a closed numerical model of x that

- captures key statistical + dynamical properties
- ensemble simulations (with a large time-step)

Example

Numerical stochastic Burgers equation

$$v_t = \nu v_{xx} - v v_x + f(x,t), x \in [0, 2\pi], \text{ periodic BC}$$

- Fourier-Galerkin: N Fourier modes
- Need small space-grid & time-step:
  $N \gtrsim 10/\nu$, $dt \sim 1/N$ by (CFL)
  $\rightarrow$ Costly: e.g. $\nu = 10^{-3} \rightarrow N \sim 10^4$, time steps= $10^4 T$

Interested in: efficient predictions of low modes $(\widehat{v}_{1:K})$, $K << N$.

Question: a reduced model of low modes?

Space-time reduction:
Reduce spatial dimension + Increase time-step size

Closure modeling, model error UQ, subgrid parametrization

Direct constructions:

- non-linear Galerkin [Fioas, Jolly, Kevrekidis, Titi...]
- moment closure [Levermore, Morokoff...]
- Mori-Zwanzig formalism
  memory $\rightarrow$ non-Markov process
  [Chorin, Hald, Kupferman, Stinis, Li, Darve, E, Karniadarkis, Venturi, Duraisamy ...]

Data-driven RM

- PCA/POD, DMD, Kooperman [Holmes, Lumley, Marsden, Wilcox, Kutz, Rowley ...]
- ROM closure [Farhat, Carlberg, Iliescu, Wang...]
- stochastic models: SDEs/GLEs, time series models [Chorin/Majda/Gil groups]
- machine learning (...)

Question:

- when and why data-driven approach work?
- Best space-time time reduction?

This talk: a stochastic modeling perspective — statistical inference

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Flow map approximation

$x' = F(x) + U(x,y)$, $y' = G(x,y)$.
Data $\{x(nh)\}_{n=1}^{N}$

Classical numerical schemes

$$\begin{pmatrix} x_n \\ y_n \end{pmatrix} = \mathbf{F}_n \begin{pmatrix} x_{n-1} \\ y_{n-1} \end{pmatrix}$$

- trajectory-wise Approx.
- fine resolution (stability and accuracy)
- Closure flow map: $x_n = F_n(x_{1:n-1})$:
  - Taylor expansion no longer work
  - depend on subsgrid scale trajectory

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Data-driven methods: approximate the flow map

$$F_n(x_{1:n-1}) \approx \widehat{F}_n(x_{n-p:n-1})$$

- average the subgrid-scales
  KEY: approximate in distribution
- Learning: curse of dimensionality
  - machine learning: blackbox, many parameters
  - parametric inference
    use the structure of the map

NARMA: a numerical time series model

$$(X_n - X_{n-1})/h = R_h(X_{n-1}) + \sum_i c_i \phi_i(x_{n-p:n-1}, \xi_{n-p:n-1}) + \xi_i$$

NARMA(p, q) [Chorin-Lu (15)]

$$\begin{aligned}
&(X_n - X_{n-1})/h = R_h(X_{n-1}) + Z_n, \\
&Z_n = \Phi_n + \xi_n, \\
&\Phi_n = \underbrace{\sum_{j=1}^{p} a_j X_{n-j} + \sum_{j=1}^{r}\sum_{i=1}^{s} b_{i,j} P_i(X_{n-j})}_{\text{Auto-Regression}} + \underbrace{\sum_{j=1}^{q} c_j \xi_{n-j}}_{\text{Moving Average}}
\end{aligned}$$

- $R_h(X_{n-1})$ from a numerical scheme for $x' \approx F(x)$
- Φ_n depends on the past
- NARMAX in system identification $Z_n = \Phi(Z, X) + \xi_n$,

Tasks:

Structure derivation: terms and orders (p, r, s, q) in Φ_n;

Parameter estimation: $a_j, b_{i,j}, c_j$, and σ. Conditional MLE

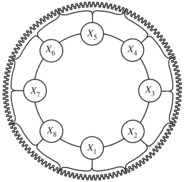
Example: the two-layer Lorenz 96 model

A NARMA model for the X variables

$$\frac{d}{dt}x_k = x_{k-1}(x_{k+1} - x_{k-2}) - x_k + 10 - \frac{1}{J}\sum_j y_{k,j},$$

$$\frac{d}{dt}y_{k,j} = \frac{1}{\varepsilon}[y_{k,j+1}(y_{k,j-1} - y_{k,j+2}) - y_{k,j} + x_k],$$

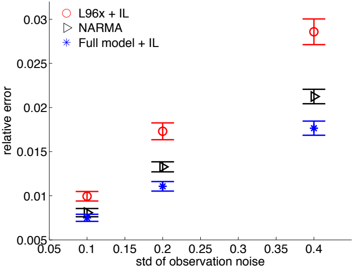
where $x \in \mathbb{R}^{18}$, $y \in \mathbb{R}^{360}$.



- no scale-separation
- Ansatz: polynomial with 2-time lag
- tolerate to large time-step

The NARMA model can

- reproduces statistics: ACF, PDF
  [Chorin-Lu15PNAS]
- improves Data Assimilation
  [Lu-Tu-Chorin17MWR]



- Kuramoto-Sivashinsky: $v_t = -v_{xx} - \nu v_{xxxx} - vv_x$
- Burgers: $v_t = \nu v_{xx} - vv_x + f(x,t)$,

Goal: a closed model for $(\widehat{v}_{1:K})$, $K << N$.

$$\frac{d}{dt}\widehat{v}_k = -q_k^\nu \widehat{v}_k + \frac{ik}{2}\sum_{|l|\le K, |k-l|\le K} \widehat{v}_l \widehat{v}_{k-l} + \widehat{f}_k(t),$$
$$+ \frac{ik}{2}\sum_{|l|>K \text{ or } |k-l|>K} \widehat{v}_l \widehat{v}_{k-l}$$

View $(\widehat{v}_{1:K}) \sim x$, $(\widehat{v}_{k>K}) \sim y$:

$$x' = F(x) + U(x,y), \quad y' = G(x,y).$$

TODO: represent the effects of high modes to the low modes

Derivation of a parametric form (KSE): $v_t = -v_{xx} - \nu v_{xxxx} - v v_x$

Let $v = u + w$. In operator form: $v_t = Av + B(v)$,

$$\frac{du}{dt} = PAu + PB(u) + [PB(u+w) - PB(u)]$$
$$\frac{dw}{dt} = QAw + QB(u+w)$$

Nonlinear Galerkin: approximate inertial manifold (IM)[1]

- $\frac{dw}{dt} \approx 0 \Rightarrow w \approx A^{-1}QB(u+w) \Rightarrow w \approx \psi(u)$
- Need: spectral gap condition ✓;
- $dim(u) > K$:

[1] Foias, Constantin, Temam, Sell, Jolly, Kevrekidis, Titi et al (88-94)

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- Need: spectral gap condition ✓;
- $dim(u) > K$: parametrization with time delay (Lu-Lin17)

A time series (NARMA) model of the form

$$u_k^n = R^\delta(u_k^{n-1}) + g_k^n + \Phi_k^n,$$

with $\Phi_k^n := \Phi_k^n(u^{n-p:n-1}, g^{n-p:n-1})$ in form of

$$\Phi_k^n = \sum_{j=1}^{p} c_{k,j}^v u_k^{n-j} + c_{k,j}^R R^\delta(u_k^{n-j}) + c_{k,j}^w \sum_{\substack{|k-l|\le K, K<|l|\le 2K \\ \text{or } |l|\le K, K<|k-l|\le 2K}} \widetilde{u}_l^{n-1} \widetilde{u}_{k-l}^{n-j}$$

KEY: high-modes = functions of low modes

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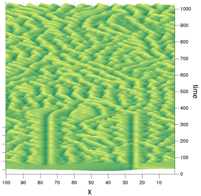
Kuramoto-Sivashinsky Equation

Test setting: $\nu = 3.43$
$N = 128$, $dt = 0.001$
Reduced model: $K = 5, \delta = 100dt$

- 3 unstable modes
- 2 stable modes



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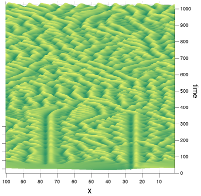
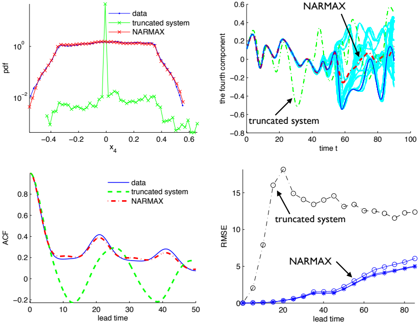


Long-term statistics:

- reproduce PDF /ACF

Prediction: Forecast time:

- truncated sys.: $T \approx 5$
- NARMA: $T \approx$ **50**
  ($\approx$ 2 Lyapunov time)



Derivation of parametric form: stochastic Burgers

$$v_t = \nu v_{xx} - v v_x + f(x,t)$$

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- spectral gap: Burgers ? (likely not)
  $w(t)$ is not function of $u(t)$, but a functional of its path

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Integration instead:

$$w(t) = e^{-QAt} w(0) + \int_0^t e^{-QA(t-s)} [QB(u(s) + w(s))] ds$$
$$w^n \approx c_0 QB(u^n) + c_1 QB(u^{n-1}) + \cdots + c_p QB(u^{n-p})$$

Linear in parameter approximation:

$$PB(u+w) - PB(u) = P[(uw)_x + (u^2)_x]/2 \approx P[(uw)_x]/2 + noise$$
$$\approx \sum_{j=0}^{p} c_j P[(u^n QB(u^{n-j}))_x] + noise$$

KEY: high-modes = functionals of paths of low modes

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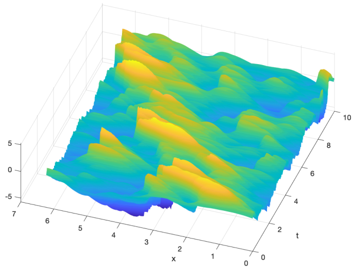
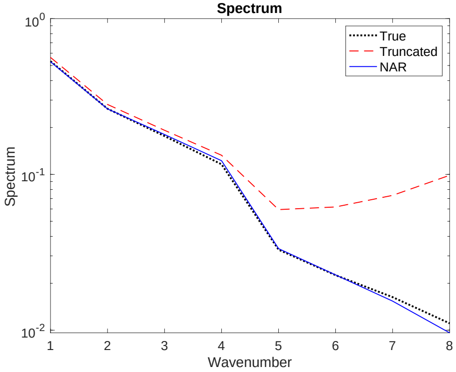
Numerical tests:

$\nu = 0.05$, $K_0 = 4 \to$ random shocks

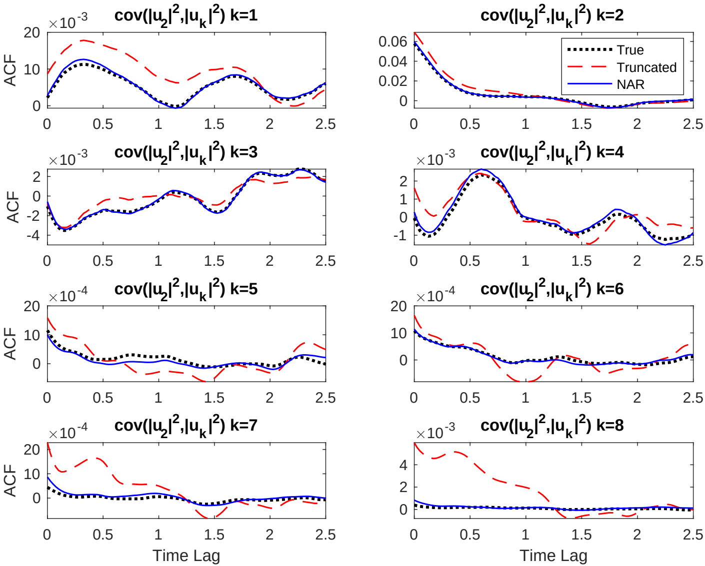




Energy spectrum

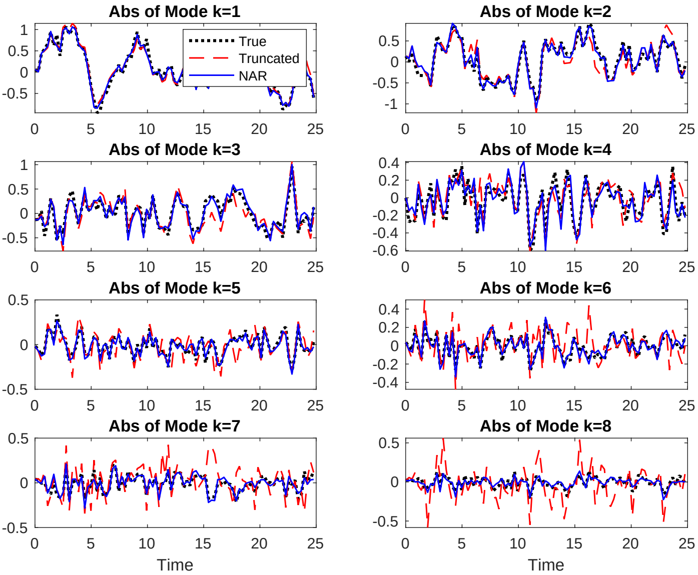
- Full model: $N = 128$, $dt = 0.005$
- Reduced model: $K = 8$, $\delta = 20dt$

Stochastic Burgers equation



Cross-ACF of energy (4th moments!)

Stochastic Burgers equation



Trajectory prediction in response to force

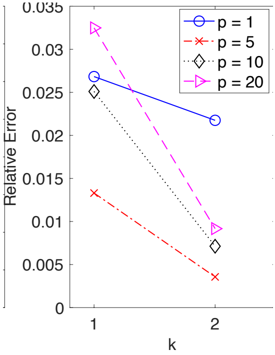
Optimal memory length

$$(X_n - X_{n-1})/h = +R_h(X_{n-1}) + \sum_i c_i \phi_i(x_{n-p:n-1}, \xi_{n-p:n-1}) + \xi_i$$

Best performance at medium memory length?

Relative error of energy spectrum

- first decrease, then increase

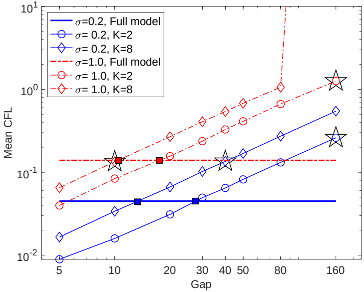


Optimal space-time reduction

- How small can K be? (Space reduction) arbitrary
- How large can δ be? (Time reduction) numerical stability
- What is the optimal space-time reduction ratio?

Best performance when: CFL (truncated Galerkin) $=$ CFL(full model).

- CFL numbers
- NARMA
  - stable up-to large gap
  - best at intersections (squares)



a priori estimate on optimal space-time reduction?

Non-global Lipschitz SDE

Ergodic with non-global Lipschitz drift:

$$dX_t = f(X_t)dt + \sigma dB_t$$

- Explicit scheme: unstable/inaccurate [Mattingly-Stuart-Highm02]
- Implicit scheme: costly (implicit, small Δt)

Infer from data an explicit scheme [Li-Lu-Ye21]

$$(X_n - X_{n-1})/h = \sum_i c_i \phi_i(X_{n-1}, \Delta B_n) + \xi_i$$

- Data from an implicit scheme
- ϕ_i from parametrizing numerical schemes

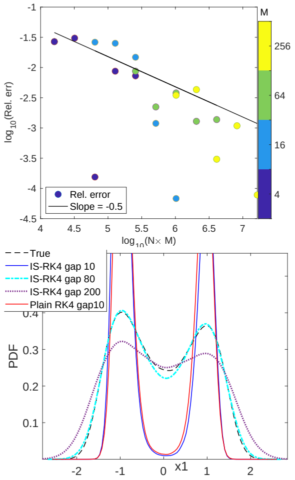
Non-global Lipschitz SDE

Non-global Lipschitz drift:

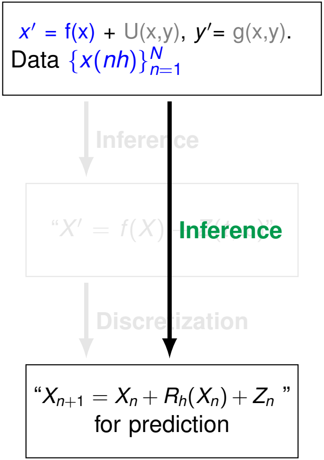
$$dX_t = f(X_t)dt + \sigma dB_t$$

The inferred explicit scheme [Li-Lu-Ye21]

- tolerate large time-step & keep order
- convergent estimators (MLE)
- Insights on optimal time-step
  - medium time-step is the best
  - trade-off: approx. error v.s. sampling /numerical error



Summary



Inference-based stochastic model reduction

- non-intrusive time series (**NARMA**)
- parametrize projections on path space

$$x_n = F_n(x_{1:n-1}) \approx \sum_k c_k \Phi^k_{n-p:n-1}$$

$\rightarrow$ space-time model reduction

Outlook

a bright future for **Numerical + inferential**

- general dissipative systems + model selection
- post-processing to predict shocks
- optimal space-time/time reduction
  - bias-variance tradeoff: “the best in the medium (Zhongyong) ”