Inference based model reduction for complex dynamical systems

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Department of Mathematics, Duke University

Inference based stochastic model reduction

1. Motivation and objective
2. An inference approach
3. Data assimilation with reduced models
4. Model reduction for PDEs
    - Kuramoto-Sivashinsky
    - **Stochastic Burger equation**

Motivation: data assimilation in weather/climate prediction

$x' = f(x) + U(x,y)$,
$y' = g(x,y)$.

Observe only
$\{x(nh)\}_{n=1}^{N}$.

Forecast
$x(t), t \geq Nh$.

- HighD multiscale full chaotic/ergodic systems:
  - can only afford to resolve $x' = f(x)$ online
  - y: unresolved variables (subgrid-scales)
- Discrete noisy observations: missing i.c.
- Ensemble prediction: need many simulations

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

Goal: Develop a closed reduced model of x that

- captures key statistical + dynamical properties
- use it for online state estimation and prediction

reduce spatial dimension + increase time step-size

Various efforts in closure model reduction:

- Direct constructions:
  - Mori-Zwanzig formalism
  - relaxiation approximations
  - Galerkin methods: non-linear Galerkin, Petrov - Galerkin
  - linear response (Fluctuation-dissipation theory)
    (filtering / feedback control /)

- Inference
  - hypoellitpic SDEs, GLE and SDDEs
  - manifold learning
  - neural network learning
  - discrete-time (time series) models

(system identification / parametrization / error quantification)

Inference-based model reduction

SDEs and time series – dynamical models

Differential system or discrete-time system?

$X' = f(X) + Z(t,\omega)$	$X_{n+1} = X_n + R_h(X_n) + Z_n$
informative, neat	messy but non-intrusive
Inference[1]	likelihood
Discretization[2]	error correction by data

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[1] Brockwell, Sørensen, Pokern, Wiberg, Samson,. . .

[2] Milstein, Tretyakov, Talay, Mattingly, Stuart, Higham, . . .

Discrete-time stochastic parametrization

NARMA(p, q)

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

- $R_h(X_{n-1})$ 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.

Structure derivation: derive the terms in Φ_n

$$X_n = X_{n-1} + R_h(X_{n-1}) + Z_n,$$
$$Z_n = \Phi_n + \xi_n,$$
$$\Phi_n = \sum_{j=1}^{p} a_j X_{n-j} + \sum_{j=1}^{r} \sum_{i=1}^{s} b_{i,j} P_i(X_{n-j}) + \sum_{j=1}^{q} c_j \xi_{n-j}.$$

The nonlinear structure is problem dependent.

Techniques: drive terms from

- the reduced differential systems (IDEs/SDEs)
- numerical schemes
- inertial manifolds

and estimate their coefficients from data.

Parameter estimation: conditional maximum likelihood[1]

$$\begin{aligned} X_n &= X_{n-1} + R_h(X_{n-1}) + Z_n, \\ Z_n &= \Phi_n + \xi_n, \\ \Phi_n &= \sum_{j=1}^{p} a_j X_{n-j} + \sum_{j=1}^{r} \sum_{i=1}^{s} b_{i,j} P_i(X_{n-j}) + \sum_{j=1}^{q} c_j \xi_{n-j}; \end{aligned}$$

Conditioned on $\xi_1, \ldots, \xi_q$, the log-likelihood of $X_{q+1:N}$ is

$$l(\theta|\xi_1, \ldots, \xi_q) = -\sum_{n=q+1}^{N} \frac{|Z_n - \Phi_n|^2}{2\sigma^2} - \frac{N-q}{2} \ln \sigma^2.$$

- compute Φ_n and ξ_n recursively for $n > q$
- maximum likelihood estimator (MLE) by optimization
- $\{\xi_n\}$ can be non-Gaussian to get other lost fucntions
- when $q = 0$: a least squares regression

[1] e.g. Hamilton 94: Time Series Analysis

Overview:

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

Discrete-time stochastic parametrization

NARMA

$$
\begin{aligned}
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&\quad + \sum_{j=1}^{r} \sum_{i=1}^{s} b_{i,j} P_i(X_{n-j}).
\end{aligned}
$$

1. compute $R_h(x)$
2. derive structure
3. estimate parameters

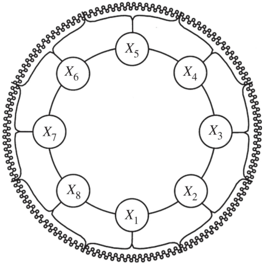
Data assimilation with model reduction

$$x' = f(x) + U(x,y), \; y' = g(x,y).$$
Noisy data: $x(nh) + W(n), \;\; n = 1, 2, \ldots$

Data assimilation:

- estimate the state of a forward model (FM):
  - (x, y) for the full model
  - x for a reduced model of x
- predict x (by ensembles of solutions of FM)
  - Widely used method: Ensemble Kalman filters (EnKF)

The Lorenz 96 system



Wilks 2005

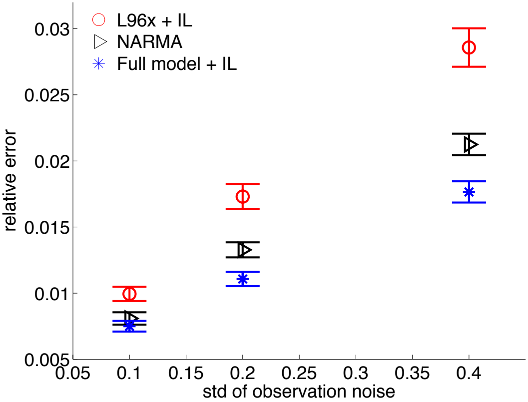
Estimate and predict x based on

➢ Noisy Data $z(n) = x(nh) + \mathbf{W(n)}$

➢ **Forward models**

- **L96x**: the truncated model
  $\frac{d}{dt}x_k \approx x_{k-1}\left(x_{k+1} - x_{k-2}\right) - x_k + 10$
  (account for the model error by IL in EnKF)
- **NARMA** (account for the model error by parametrization in the forward model)

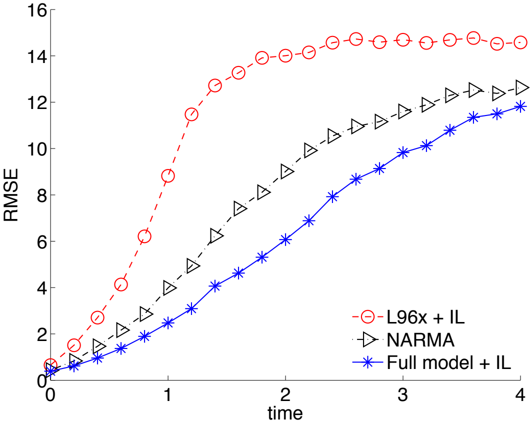
Relative error of state estimation



Relative error for different observation noises.

(ensemble size: =1000 for L96x and NARMA; =10 for the full model)

RMSE of state prediction



RMSE of 10^4 ensemble forecasts.

(ensemble size: =1000 for L96x and NARMA; =10 for the full model)

Summary: NARMA improves performance of DA.

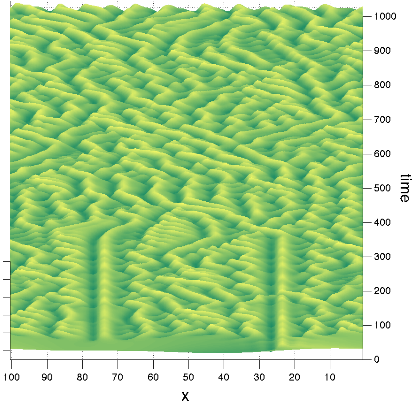
Model reduction for PDEs

(chaotic/stochastic PDEs)

The Kuramoto-Sivashinsky equation

$$v_t + v_{xx} + v_{xxxx} + vv_x = 0\ , t > 0, x \in [0, 2\pi\nu], \textit{periodic}.$$

Spatio-temporally chaotic



solved with 128 Fourier modes

Problem setting: $\nu = 3.43$

- Observing only 5 Fourier modes every 10 time steps
- to predict their evolution
- 100-fold reduction

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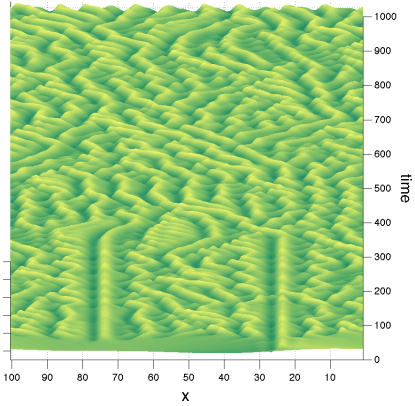

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Reduced models:

- the truncated system not accurate
- Mori-Zwanzig reduction[a]: complicated
- Discrete-time sto. paramtrization[b]: derive structure from inertial manifold
  $\rightarrow$ an effective NARMA model

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[a] Stinis 12
[b] Lu-Lin-Chorin17

Key point 1: long-term statistics $\leftrightarrow$ Large time behavior of PDE[2]

Inertial manifolds $\mathcal{M}$: - finite-dimensional, positively invariant manifolds

- exponentially attracts all trajectories

Let $v = u + w$. Rewrite the KSE:

$$\frac{du}{dt} = Au + PB(u+w)$$
$$\frac{dw}{dt} = Aw + QB(u+w)$$

On $\mathcal{M}$, $w = \psi(u)$

$$\frac{du}{dt} = PAu + PB(u + \psi(u)).$$

Approximate inertial manifolds (AIMs): approximate $w = \psi(u)$

- $\frac{dw}{dt} \approx 0 \Rightarrow w \approx A^{-1}QB(u+w)$,
- Fixed point: $\psi_0 = 0$; $\psi_{n+1} = A^{-1}QB(u + \psi_n)$.

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

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Key point 2: parametrize the AIM

- AIM with 5 modes: unstable
  (An accurate AIM requires $m = dim(u)$ to be large!)
- use the terms; estimate their coefficients from data
  $\rightarrow$ an effective NARMA model

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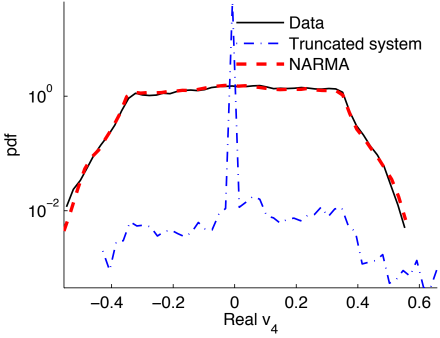
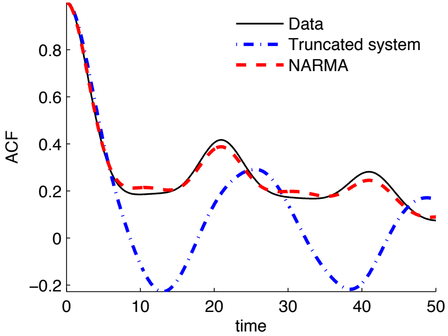
Long-term statistics:



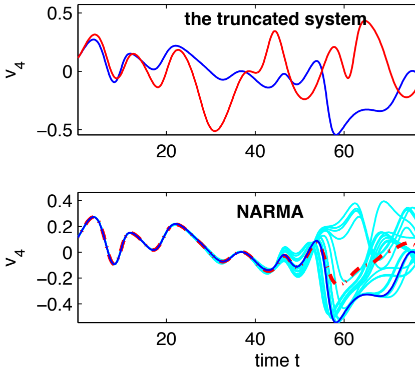
probability density function



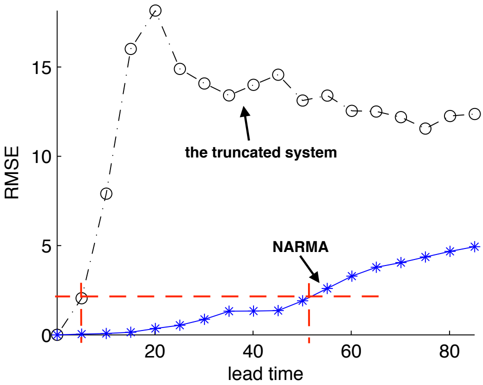
auto-correlation function

Prediction

A typical forecast:



RMSE of many forecasts:



Forecast time:

the truncated system: $T \approx 5$
the NARMA system: $T \approx \mathbf{50}$

Stochastic Burgers equation:

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

where $f(x,t) = \sum_{k=1}^{K_0} \sin(kx) dW(t)$.

- $N \gtrsim 5/\nu$ Fourier modes are needed to resolve the Eq.

Goal: a closed model for $(\widehat{v}_{1:K})$, $K = 2K_0 \leq 1/\nu$.

- to capture energy spectrum and correlations (>PDF, ACF)
- Test setting:
  - Full model: $\nu = 0.05$, $K_0 = 4 \to$ random shocks
    $N = 128, dt \to$ CFL ≈ 0.2;
  - Reduced model: $K = 8$, $\delta = 20dt \to$ CFL ≈ 4;

Let $v = u + w$. In operator form:

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

$$\frac{dw}{dt} = QAw + QB(u+w)$$

- No spectral gap $\rightarrow$ no inertial manifold (IM)
  No Approximate IM: ~~$\frac{dw}{dt} \approx 0 \Rightarrow w \approx A^{-1}QB(u+w)$.~~

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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:

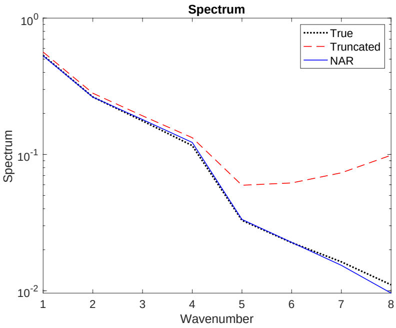
$$PB(u+w) - PB(u) = P[(uw)_x + (w^2)_x]/2 \approx P[(uw)_x]/2 + noise$$
$$\approx \sum_{j=0}^{p} c_j P[(u^n QB(u^{n-j}))_x] + noise$$

The NAR model has the form

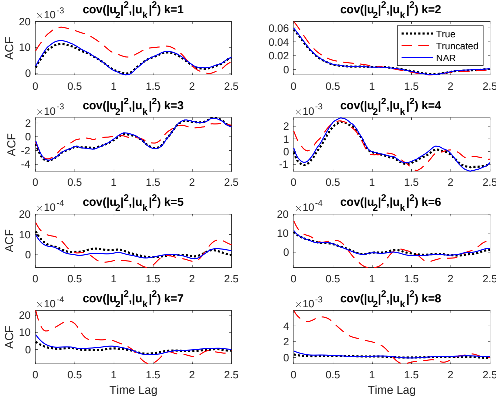
$$u_k^n = R^\delta(u_k^{n-1}) + f_k^n + g_k^n + \Phi_k^n,$$

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

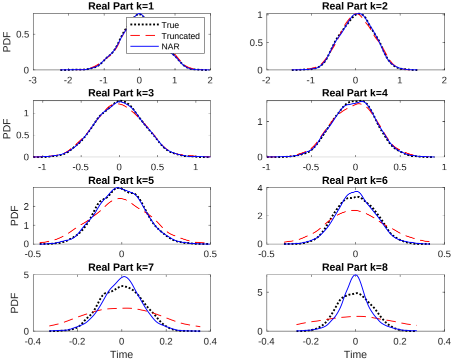
$$\Phi_k^n = \sum_{j=1}^{p} c_{k,j}^v u_k^{n-j} + c_{k,j}^R R^\delta(u_k^{n-j}) + c_{k,j}^w \sum_{\substack{|k-l|\le K, K<|l|\le 2K \\ \text{or } |l|\le K, K<|k-l|\le 2K}} \widetilde{u}_l^{n-1} \widetilde{u}_{k-l}^{n-j}$$



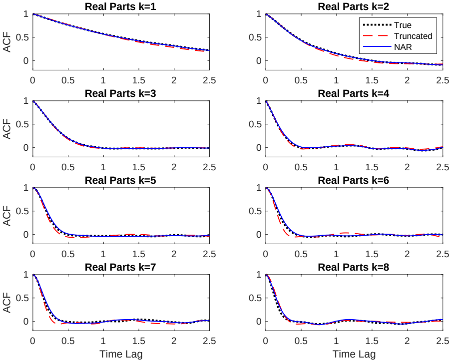
Energy spectrum



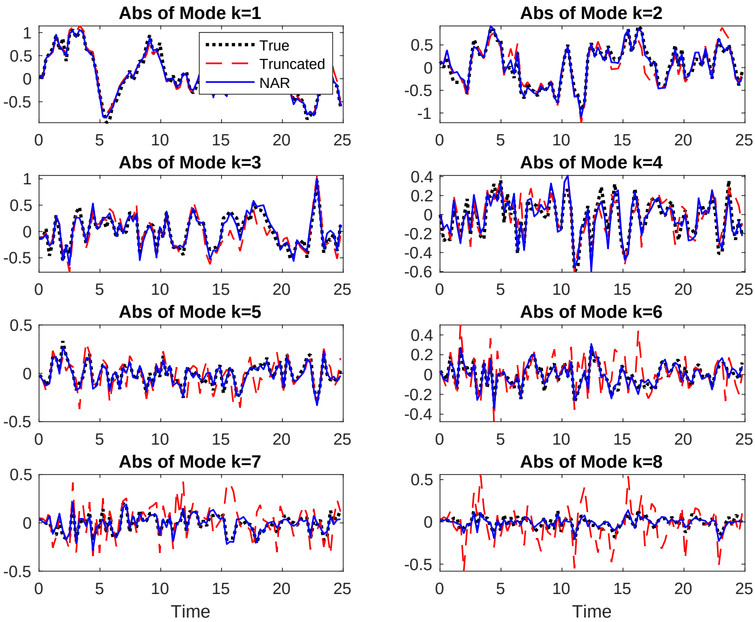
Cross-ACF of ernergy



probability density function



auto-correlation function



Prediction in response to force

Several questions:

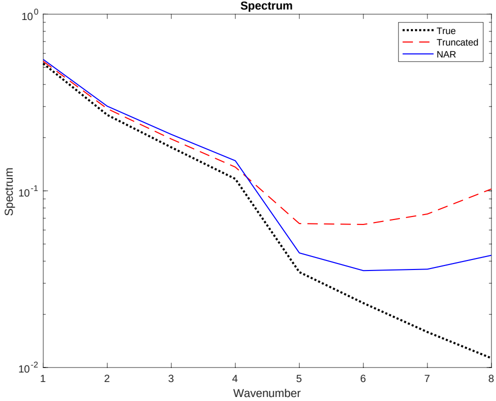
- How to determine Lag length? ($e^{-QA(t-s)}$ not good)

$$w(t) = e^{-QAt}w(0) + \int_0^t e^{-QA(t-s)}[QB(u(s) + w(s))]ds$$

$$w^n \approx c_0 QB(u^n) + c_1 QB(u^{n-1}) + \cdots + c_p QB(u^{n-p})$$

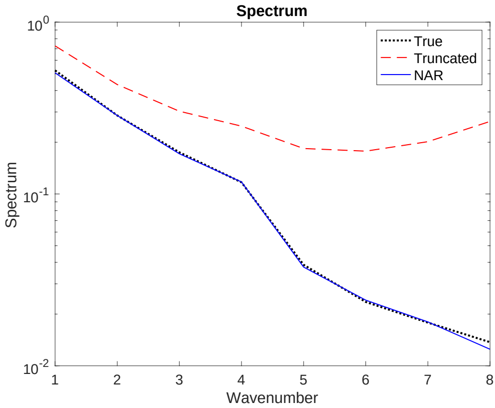
- Larger observation gap?
- Smaller ν?
- The role of $(w^2)_x$?
- Memory kernel? Correlated noise?
- Generalization to other dissipative systems?

When observe gap = 80 time steps:



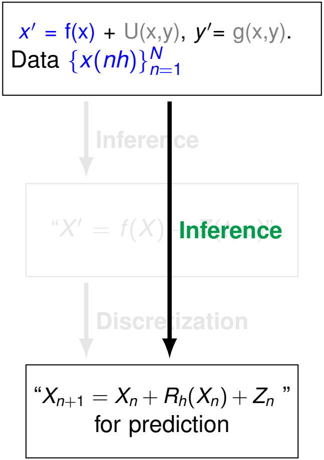
Energy spectrum

When viscosity becomes smaller $\nu = 0.02$ (more Burgulent)



Energy spectrum

Summary and ongoing work



- Stochastic model reduction by
  Discrete-time stochastic parametrization
  - simplifies the inference from data
  - incorporates memory flexibly
  - effective reduced model (**NARMA**)
    - capture key statistical-dynamical features
    - make medium-range forecasting
- Improves performance of Data assimilation

Open problems:

- model reduction
  - model selection
  - scaling of the discrete system? (With A. Chorin)
  - 2D N-S equation?
- noisy data: state estimation and model inference
  - data assimilation with non-Markovian models
  - inference for hidden non-Markovian models
- theoretical understanding of the approximation
  - distance between the two stochastic processes?
  - discrete-time Mori-Zwanzig formalism (With K. Lin)

    A Winer filter implementation (instead of the likelihood)

References

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  - Lu-Lin-Chorin: Comparison of continuous and discrete-time data-based modeling for hypoelliptic systems. **CAMCoS, 11 (2016)**, no. 8, 4227–4246.
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Thank you!

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