Paper Review of Data-assisted reduced-order modeling of extreme events in complex dynamical systems

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Problem Setup

- $\frac{du}{dt} = F(u) = Lu + h(u)$, $u(t) \in \mathbb{R}^n$, where n is a large number.
- We are specifically interested in systems whose dynamics results in a intrinsically low dimensional globally attracting manifold.

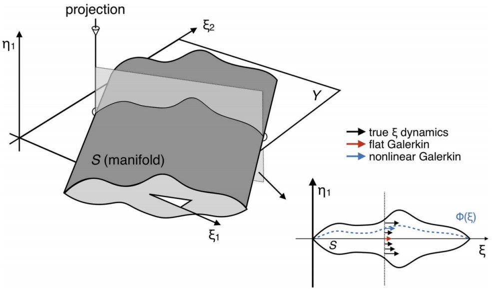

Figure: Example of a Globally Attracting Manifold

Problem Setup

Goal:

- Dimensionality Reduction of the ODE
- Derive an ODE in a low dimensional subspace, which preserves as much dynamical property of original ODE as possible.

Ansatz:

$$u = \mathbf{Y}\xi + \mathbf{Z}\eta + b \tag{1}$$

where the columns of matrix $\mathbf{Y} = [y_1, ..., y_m]$ form an orthonormal basis of Y, an m-dimensional subspace of $\mathbb{R}^d$, and the columns of $\mathbf{Z} = [z_1, ..., z_{d-m}]$ make up an orthonormal basis for the orthogonal complement $Z = \mathbb{R}^d \setminus Y$; ξ and η are the projection coordinates associated with $\mathbf{Y}$ and $\mathbf{Z}$.

Problem Setup

How to get **Y** and **Z**?

- Randomly sample 10000 points on the attractor, denoted as **X**.
- Do PCA on these datapoints:
  Let $C = X^T X$, then $\mathbf{Y} = [y_1, ..., y_m]$, where $[y_1, ..., y_m]$ are the eigenvectors of C corresponding to the m largest eigenvalues of C.
  $\mathbf{Z} = [z_1, ..., z_{d-m}]$, where $[z_, ..., z_{d-m}]$ are the rest of eigenvectors of C.

Back to equation (1), we know Y, Z and the ODE for u, can we have the ODE for ξ?

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Flat Galerkin Method

Plug (1) back to the ODE, we get

$$\frac{d\xi}{dt} = Y^T LY\xi + Y^T LZ\eta + Y^T h(Y\xi + Z\eta + b) + Y^T Lb \tag{2}$$

If $|\eta| << |\xi|$, then we may assume $\eta = 0$, leading to a m-dimensional system:

$$\frac{d\xi}{dt} = Y^T LY\xi + Y^T h(Y\xi + b) + Y^T Lb = F_\xi(\xi) \tag{3}$$

This is called the Flat Galerkin Method.

Nonlinear Galerkin Projection

Problems:

- $\eta = 0$ may be too strict.
- Z is derived merely based on statistical properties of the manifold without addressing the dynamics. This implies that even if η has small magnitude on average it may play a big role in the dynamics of the space.

Existing solution: Let $\eta = \Phi(\xi)$, then

$$\frac{d\xi}{dt} = Y^T L Y \xi + Y^T L Z \Phi(\xi) + Y^T h(Y\xi + Z\Phi(\xi) + b) + Y^T L b \tag{4}$$

This is called the Nonlinear Galerkin Projection Method.

Nonlinear Galerkin Projection

Problems:

- Φ has to be found empirically.
- Φ may not be well-defined!

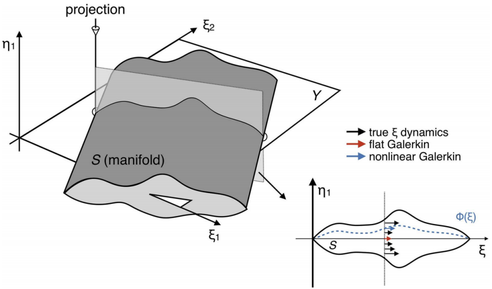

Figure: Example of a Globally Attracting Manifold

Data-driven Method

Proposed Data-driven solution:

$$\frac{d\xi}{dt} = Y^T L Y \xi + Y^T L Z \eta + Y^T h(Y\xi + Z\eta + b) + Y^T L b \tag{5}$$

rewritten as

$$\frac{d\xi}{dt} = F_\xi(\xi) + G(\xi, \eta) \tag{6}$$

Try to learn G from the data.
Assumption: $\Psi(t) = G(\xi(t), \eta(t)) \approx \hat{G}(\xi(t), \xi(t-\tau), \xi(t-2\tau), ...)$
What is $\hat{G}$? LSTM...

LSTM

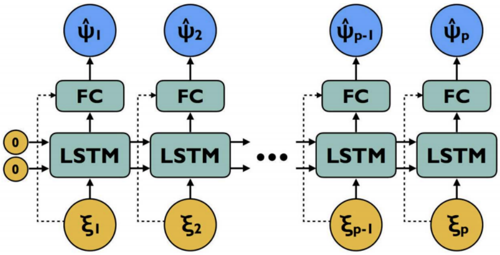

Figure: Architecture of the First Proposed Model

Loss: $L = \sum_{i=1}^{p} w_i ||\hat{\Psi}_i - \Psi_i||^2$, where $w_i = \begin{cases} w_0 & 0 < i \leq p_t \\ 1 & p_t < i \leq p \end{cases}$

LSTM

Problem:

- Input representing the ξ is always accurate regardless of any errors made in predicting the dynamics previously, i.e. the model only learns to predict one step ahead.
- This is undesirable especially for chaotic systems where errors tend to grow exponentially.

(II)

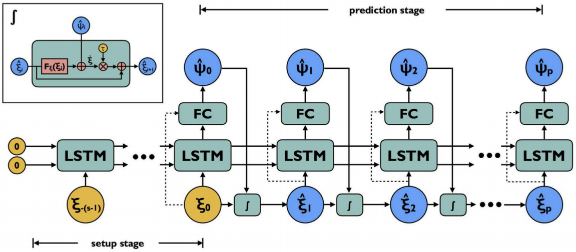

Figure: Architecture of the Second Proposed Model

LSTM

- Loss for the second model:
  $L = \sum_{i=1}^{p} w_i ||\hat{\Psi}_i + F_\xi(\hat{\xi}_i) - \dot{\xi}_i||^2$, where $w_i = \gamma^{i-1}$, $0 < \gamma < 1$.
- Use first model for pre-training, use second model for fine-tuning and prediction.

An alternative to the method proposed is fully data-driven modeling, which simply make predictions of ξ based on previous observed ξs. It is shown that this fully data-driven model is worse in the numerical experiments.

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CDV

$$\dot{x}_1 = \gamma_1^* x_3 - C(x_1 - x_1^*), \qquad \dot{x}_2 = -(\alpha_1 x_1 - \beta_1) x_3 - C x_2 - \delta_1 x_4 x_6,$$

$$\dot{x}_3 = (\alpha_1 x_1 - \beta_1) x_2 - \gamma_1 x_1 - C x_3 + \delta_1 x_4 x_5, \qquad \dot{x}_4 = \gamma_2^* x_6 - C(x_4 - x_4^*) + \varepsilon(x_2 x_6 - x_3 x_5),$$

$$\dot{x}_5 = -(\alpha_2 x_1 - \beta_2) x_6 - C x_5 - \delta_2 x_4 x_3, \qquad \dot{x}_6 = (\alpha_2 x_1 - \beta_2) x_5 - \gamma_2 x_4 - C x_6 + \delta_2 x_4 x_2,$$

where the model coefficients are given by

$$\alpha_m = \frac{8\sqrt{2} m^2 (b^2 + m^2 - 1)}{\pi (4m^2 - 1)(b^2 + m^2)}, \quad \beta_m = \frac{\beta b^2}{b^2 + m^2},$$

$$\delta_m = \frac{64\sqrt{2}}{15\pi} \frac{b^2 - m^2 + 1}{b^2 + m^2}, \quad \gamma_m^* = \gamma \frac{4\sqrt{2} m b}{\pi (4m^2 - 1)},$$

$$\varepsilon = \frac{16\sqrt{2}}{5\pi}, \quad \gamma_m = \gamma \frac{4\sqrt{2} m^3 b}{\pi (4m^2 - 1)(b^2 + m^2)},$$

Figure: CDV Equations

$(x_1^*, x_4^*, C, \beta, \gamma, b) = (0.95, -0.760955, 0.1, 1.25, 0.2, 0.5)$. Use 10000 trajectories, 80% for training, 10% for validation, 10% for test. $n_{LSTM} = 1$, $n_{FC} = 16$. Try to predict $p = 200$ time steps ahead, with $\delta t = 0.01$.

CDV

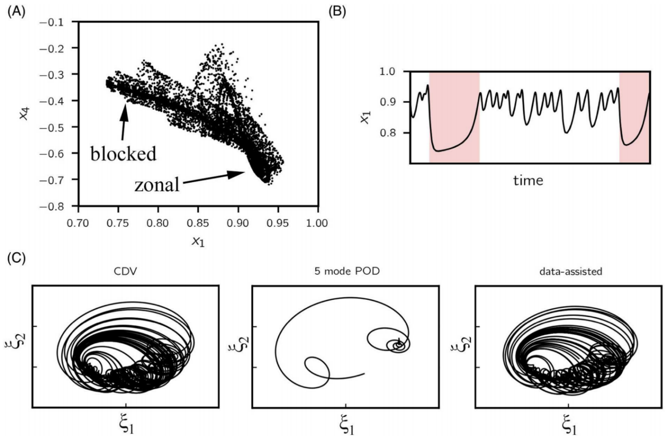


Fig 3. CDV system. (A) 10^4 points sampled from the CDV attractor, projected to (x_1, x_4) plane. (B) Example time series for x_1; *blocked* flow regime is shaded in red. (C) Length-2000 trajectory projected to the first two POD modes (normalized) integrated using the CDV model (left), 5-mode POD projected model (middle) and data-assisted model (right). Despite preserving 99.6% of the total variance, the 5-mode projected model has a single fixed point as opposed to a chaotic attractor. Data-assisted model, however, is able to preserve the geometric features of the original attractor.

Results

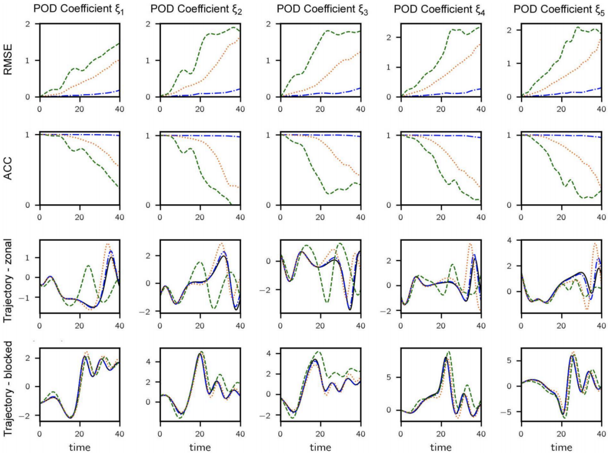


Fig 4. Results for CDV system. (Row 1) RMSE vs. lead time for 5-mode POD projected model (orange dotted), data-assisted model (blue dashdotted) and purely data-driven model (green dashed). (Row 2) ACC vs. lead time. (Row 3) A sample trajectory corresponding to zonal flow—true trajectory is shown (black solid). (Row 4) A sample trajectory involving regime transition (happening around $t = 20$). For rows 1, 3 and 4, plotted values are normalized by the standard deviation of each dimension.

Intermittent bursts of dissipation in Kolmogorov

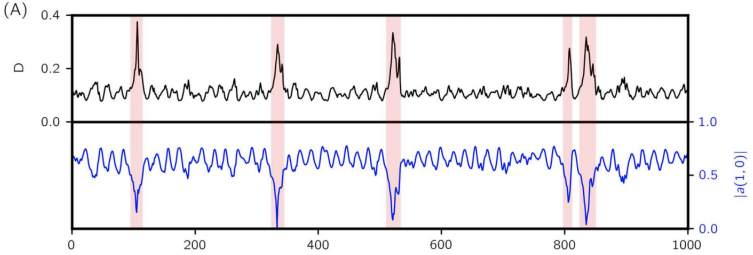
$$\begin{aligned} \partial_t \mathbf{u} &= -\mathbf{u} \cdot \nabla \mathbf{u} - \nabla p + \nu \Delta \mathbf{u} + \mathbf{f} \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned} \tag{17}$$

where $\mathbf{u} = (u_x, u_y)$ is the fluid velocity defined over the domain $(x, y) \in \Omega = [0, 2\pi] \times [0, 2\pi]$ with periodic boundary conditions, $\nu = 1/Re$ is the non-dimensional viscosity equal to reciprocal of the Reynolds number and p denotes the pressure field over Ω. We consider the flow driven by the monochromatic Kolmogorov forcing $\mathbf{f}(\mathbf{x}) = (f_x, f_y)$ with $f_x = \sin(k_f y)$ and $f_y = 0$. $\mathbf{k}_f = (0, k_f)$ is the forcing wavenumber.

$$\begin{aligned} E(\mathbf{u}) &= \frac{1}{|\Omega|} \int_\Omega \frac{1}{2} |\mathbf{u}|^2 \ d\Omega, \\ D(\mathbf{u}) &= \frac{\nu}{|\Omega|} \int_\Omega |\nabla u|^2 \ d\Omega, \\ I(\mathbf{u}) &= \frac{1}{|\Omega|} \int_\Omega \mathbf{u} \cdot \mathbf{f} \ d\Omega \end{aligned} \tag{18}$$

Intermittent bursts of dissipation in Kolmogorov

- The Kolmogorov flow admits a laminar solution $u_x = Re/k_f^2 \sin(k_f y)$, $u_y = 0$. For sufficiently large k_f and Re, this laminar solution is unstable, chaotic and exhibiting intermittent surges in energy input I and dissipation D.
- Study the flow under a particular set of parameters $Re = 40$ and $k_f = 4$ for which there is the occurrence of extreme events.



Due to spatial periodicity, it is natural to examine the velocity field in Fourier space. The divergence-free velocity field **u** admits the following Fourier series expansion:

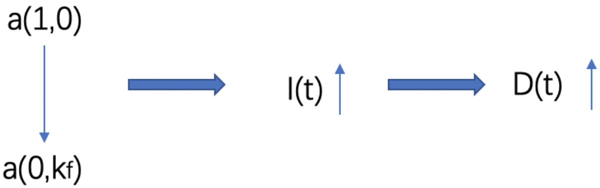
$$\mathbf{u}(\mathbf{x}, t) = \sum_{\mathbf{k}} \frac{a(\mathbf{k}, t)}{|\mathbf{k}|} \begin{pmatrix} k_2 \\ -k_1 \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{x}} \tag{19}$$

where $\mathbf{k} = (k_1, k_2)$ is the wavenumber and $a(\mathbf{k}, t) = -\overline{a(-\mathbf{k}, t)}$ for **u** to be real-valued. For notation clarity, we will not explicitly write out the dependence on t from here on. Substituting Eq (19) into the governing equations Eq (17) we obtain the evolution equations for a as (more details are presented in S1 Appendix)

$$\dot{a}(\mathbf{k}) = \sum_{\mathbf{p}+\mathbf{q}=\mathbf{k}} i \frac{(p_1 q_2 - p_2 q_1)(k_1 q_1 + k_2 q_2)}{|\mathbf{p}||\mathbf{q}||\mathbf{k}|} a(\mathbf{p}) a(\mathbf{q}) - \nu |\mathbf{k}|^2 a(\mathbf{k}) - \frac{1}{2} i(\delta_{\mathbf{k},\mathbf{k}_f} + \delta_{\mathbf{k},-\mathbf{k}_f}) \tag{20}$$

Intermittent bursts of dissipation in Kolmogorov

- In the reduced model,
  Let $\xi_1 = a(0, k_f)$, $\xi_2 = a(1, 0)$, $\xi_3 = a(1, k_f)$,
  ξ_4, ξ_5, ξ_6 are the conjugate pairs of ξ_1, ξ_2, ξ_3.
- This is because in the interest of predicting I and D, the most revealing interaction to observe is among these nodes.



- However, only 59% energy are contained in these nodes, so a simple linear projection could lead to a bad result.

Intermittent bursts of dissipation in Kolmogorov

- $n_{LSTM} = 70$, $n_{FC} = 38$. Number of time steps in setup stage $= 100$, progressively increase number of time steps in prediction stage from $\{10, 30, 50, 100\}$.
- 100000 trajectories, 80% training, 5% validation, 15% test.
- $n_{epochs} = 1000$, batch size $= 250$, $p_t = 60$, $w_0 = 0.01$, $\gamma = 0.98$.

Intermittent bursts of dissipation in Kolmogorov

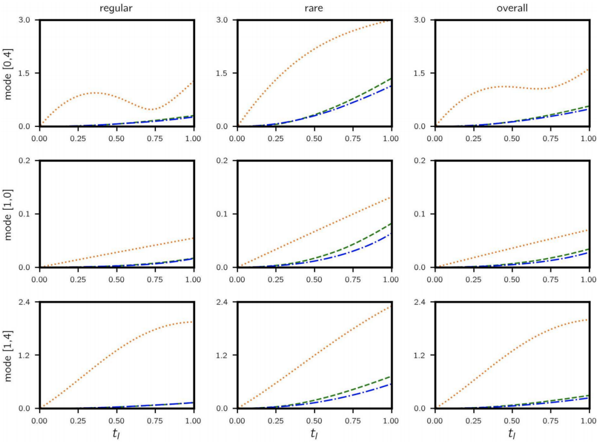


Fig 6. Kolmogorov flow—RMSE vs. time. Errors are computed for 10^4 test trajectories (legend: fully data-driven—green dashed; data-assisted—blue dashdotted; triad—orange dotted). The RMSE in each mode is normalized by the corresponding amplitude $E(\mathbf{k}) = \sqrt{\mathbb{E}[|a(\mathbf{k})|^2]}$. A test trajectory is classified as *regular* if $|a(1,0)| > 0.4$ at $t = 0$ and *rare* otherwise. Performance for regular, rare and all trajectories are shown in three columns. Data-assisted model has very similar errors to those of purely data-driven models for regular trajectories, but the performance is visibly improved for rare events.

Intermittent bursts of dissipation in Kolmogorov

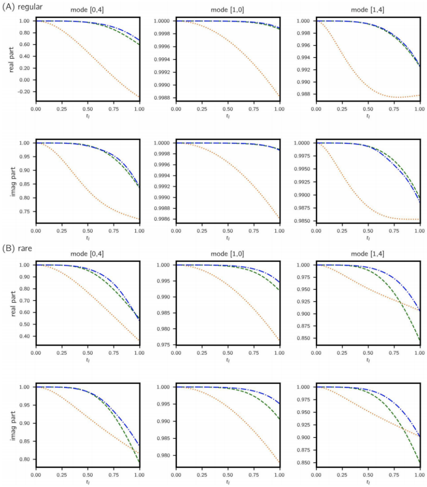


Fig 7. Kolmogorov flow: ACC vs. time. Values are computed for (A) regular and (B) rare trajectories classified from 10^4 test cases. Legend: fully data-driven—green dashed; data-assisted—blue dashdotted; triad dynamics—orange dotted. Real and imaginary parts are treated independently. Similarly to RMSE in Fig 6, improvements in predictions made by the data-assisted model are more prominent for rare events.

Intermittent bursts of dissipation in Kolmogorov

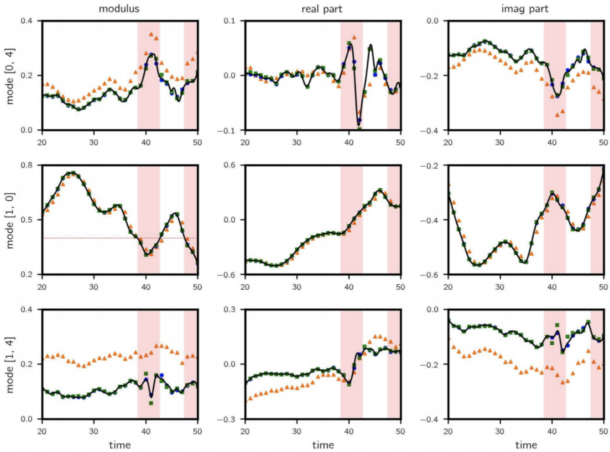


Fig 8. Kolmogorov flow: Predictions along a sample trajectory with lead time = 0.5. Results for the complex modulus (left column), real part (middle column) and imaginary part (right column) of the wavenumber triad are shown. Legend: truth—black solid line; data-assisted—blue circle; triad dynamics—orange triangle; purely data-driven—green square. Rare events are recorded when $|a(1, 0)|$ (left column, mid row) falls below 0.4 (shaded in red). Significant improvements are observed for wavenumbers (0, 4) and (1, 4).

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Conclusion

- Goal of the paper: Dimensionality Reduction of ODEs
- Approach: Data + ODE Prior (Physics-informed LSTM?)
- Testcases on CDV and Navier-Stokes Equations
  Also show the ability to predict rare events
- Possible future research: Singular perturbation?

The End