Correcting for Error in Reduced-Order Modeling Using Experimental Partial Observations and Bayesian System Identification

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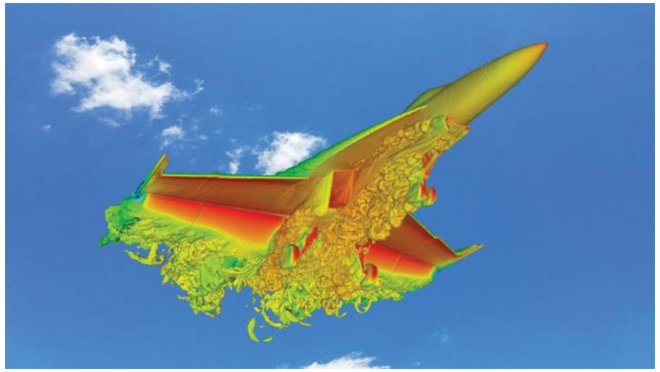
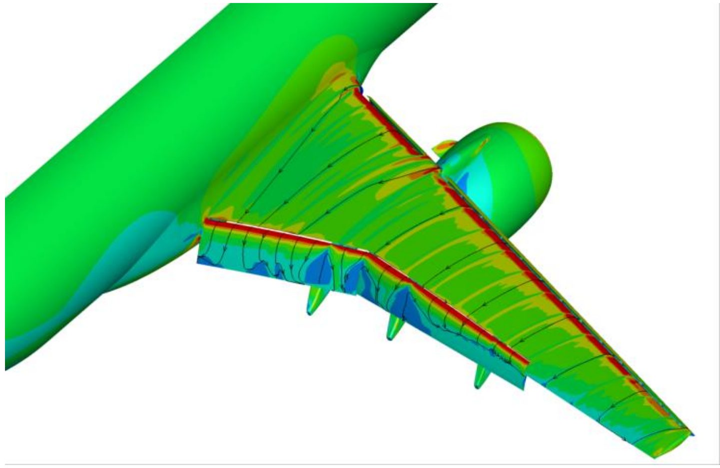
Motivation

- High-dimensional systems are ubiquitous within science and engineering
- Models often have unknown problem-dependent parameter values
  - For example, turbulence model coefficients
- Traditional parameter estimation and sampling methods do not scale well for expensive forward models

Goals:

1. Use an inexpensive model to infer parameter values of the expensive high-dimensional model
2. Embed prior physics knowledge within the learning process





https://hiliftpw.larc.nasa.gov/index.html

Highlights

We present an algorithm that:

- Leverages reduced-order modeling to efficiently perform parameter estimation of high-dimensional systems
- Accounts for various sources of uncertainty to yield robust estimation under high multiplicative measurement noise
- Enforces physical knowledge of Hamiltonian systems within the estimation procedure

Outline

1. Probabilistic inference
2. Dimension reduction
3. Structure preservation
4. Results
5. Conclusions and future work

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Introduction

Probabilistic inference

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High-level problem formulation

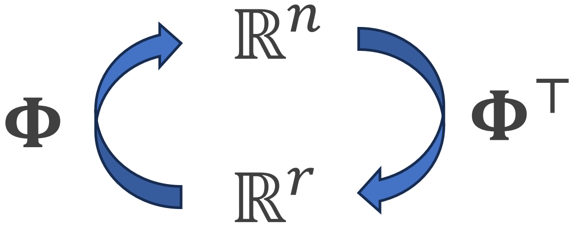
System of interest
$\{\mathbf{x}_k \in \mathbb{R}^n \mid k = 1, \dots, N\}$

$$\mathbf{y}_k = h(\mathbf{x}_k) + \eta_k$$

Data
$\mathcal{Y}_N = \{\mathbf{y}_k \in \mathbb{R}^m \mid k = 1, \dots, N\}$

η_k can represent either:
- Model uncertainty (simulation data)
- Sensor noise (experimental data)

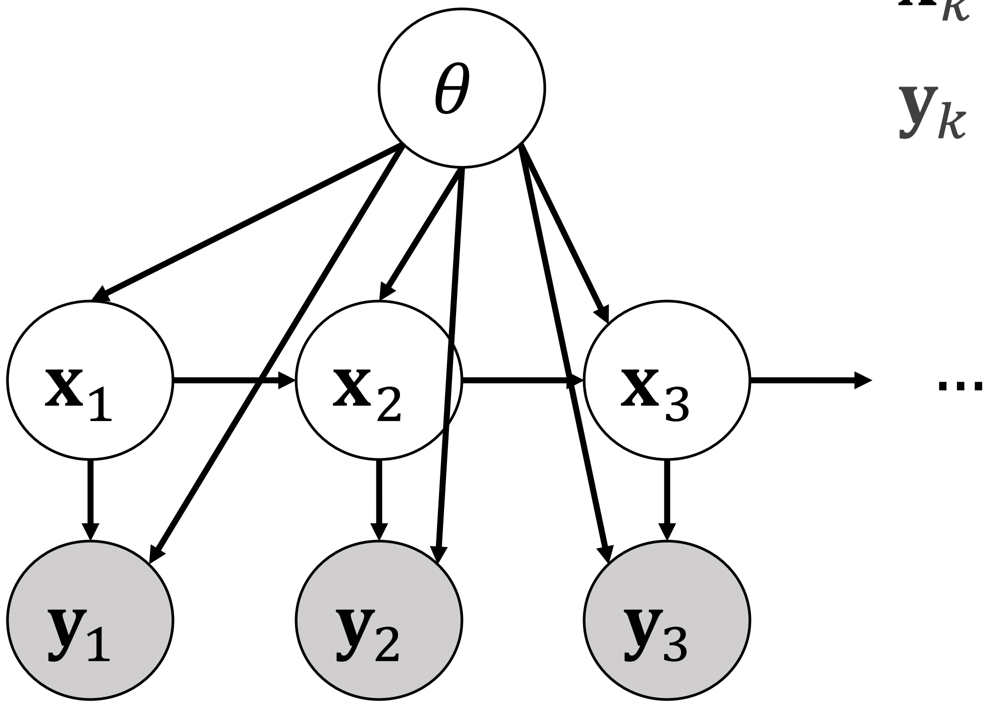
Step 1: Learn a mapping between full- and reduced-dimensional spaces



Step 2: Learn dynamics in the reduced-dimensional space

$$\tilde{\mathbf{x}}_k = \Psi(\tilde{\mathbf{x}}_{k-1}, \theta)$$
$$\mathbf{y}_k = h(\tilde{\mathbf{x}}_k, \theta)$$

Bayesian system identification



$$\mathbf{x}_k = \Psi(\mathbf{x}_{k-1}, \theta) + \xi_{k-1}, \quad \xi_{k-1} \sim \big(0, \Sigma(\theta)\big)$$
$$\mathbf{y}_k = h(\mathbf{x}_k, \theta) + \eta_k, \quad \eta_k \sim \big(0, \Gamma(\theta)\big)$$

Sources of error/uncertainty

ξ: Model uncertainty

η: Measurement uncertainty

θ: Parameter uncertainty

- Modeled by $\pi(\theta|\mathcal{Y}_N)$

Galioto, Nicholas, and Alex Arkady Gorodetsky. "Bayesian system ID: optimal management of parameter, model, and measurement uncertainty." *Nonlinear Dynamics* 102.1 (2020): 241-267.

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Bayesian system identification algorithm

MCMC

for $i = 1, \dots, M$

Propose sample θ

Evaluate posterior: $\pi(\theta|\mathcal{Y}_N) = \pi(\theta)\prod_{k=1}^{n}\mathcal{L}_k(\theta;\mathcal{Y}_k)$

Bayesian filtering

for $k = 0, \dots, N-1$

Predict: $\pi(\mathbf{x}_{k+1}|\mathcal{Y}_k,\theta) = \int \pi(\mathbf{x}_{k+1}|\mathbf{x}_k,\theta)\pi(\mathbf{x}_k|\mathcal{Y}_k,\theta)\mathrm{d}\mathbf{x}_k$

Marginalize: $\mathcal{L}_{k+1}(\theta;\mathcal{Y}_{k+1}) = \int \pi(\mathbf{y}_{k+1}|\mathbf{x}_{k+1},\theta)\pi(\mathbf{x}_{k+1}|\mathcal{Y}_k,\theta)\mathrm{d}\mathbf{x}_{k+1}$

Update: $\pi(\mathbf{x}_{k+1}|\mathcal{Y}_{k+1},\theta) = \dfrac{\pi(\mathbf{y}_{k+1}|\mathbf{x}_{k+1},\theta)\pi(\mathbf{x}_{k+1}|\mathcal{Y}_k,\theta)}{\pi(\mathbf{y}_{k+1}|\mathcal{Y}_k,\theta)}$

end for

Accept θ with Metropolis-Hastings probability; otherwise reject

end for

Särkkä, S. (2013). *Bayesian filtering and smoothing* (No. 3). Cambridge University Press.

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Probabilistic inference

Dimension reduction

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Challenge of high dimensions

Filtering algorithms have a computational complexity of

$$\mathcal{O}\left(N(n^3 + m^3)\right)$$

- N: number of data
- n: state dimension
- m: measurement dimension

For computational feasibility, we must reduce the dimensions of:

- the state $\mathbf{x}$
- the measurements $\mathbf{y}$

Projection introduces additional uncertainty

Stochastic uncertainty

$$\eta_k = \bar{\mathbf{y}}_k - \mathbf{y}_k$$

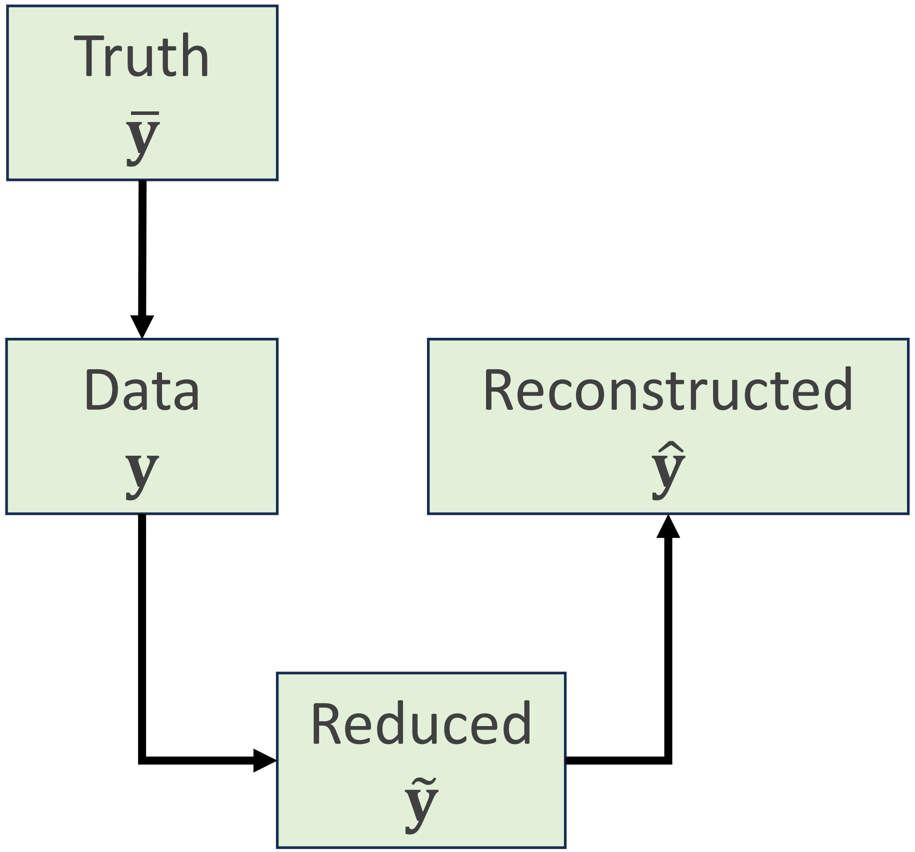
Deterministic uncertainty

$$\varepsilon_k = \hat{\mathbf{y}}_k - \mathbf{y}_k$$
$$= (\mathbf{\Phi}\mathbf{\Phi}^\top - \mathbf{I})\mathbf{y}_k$$

Projection error

$$\hat{\mathbf{y}}_k - \bar{\mathbf{y}}_k = \varepsilon_k + \eta_k$$

Projection $\mathbf{\Phi}$ introduces uncertainty dependent on ε and η



Modeling uncertainty in the reduced-order system

Dynamics:

1. Define a low-dimensional state

$$\tilde{\mathbf{x}}_{k+1} = \mathbf{\Phi}^\top(\varepsilon,\eta)\mathbf{x}_k$$

2. Model dynamics in the low-dimensional space

$$\tilde{\mathbf{x}}_{k+1} = \widetilde{\Psi}(\tilde{\mathbf{x}}_k(\varepsilon,\eta),\theta) + \xi_k$$

- ξ_k represents model-form uncertainty

3. Simplify uncertainty form

$$\boxed{\tilde{\mathbf{x}}_{k+1} = \widetilde{\Psi}(\tilde{\mathbf{x}}_k,\theta) + \tilde{\xi}_k}$$

Measurements:

1. Define low-dimensional measurements

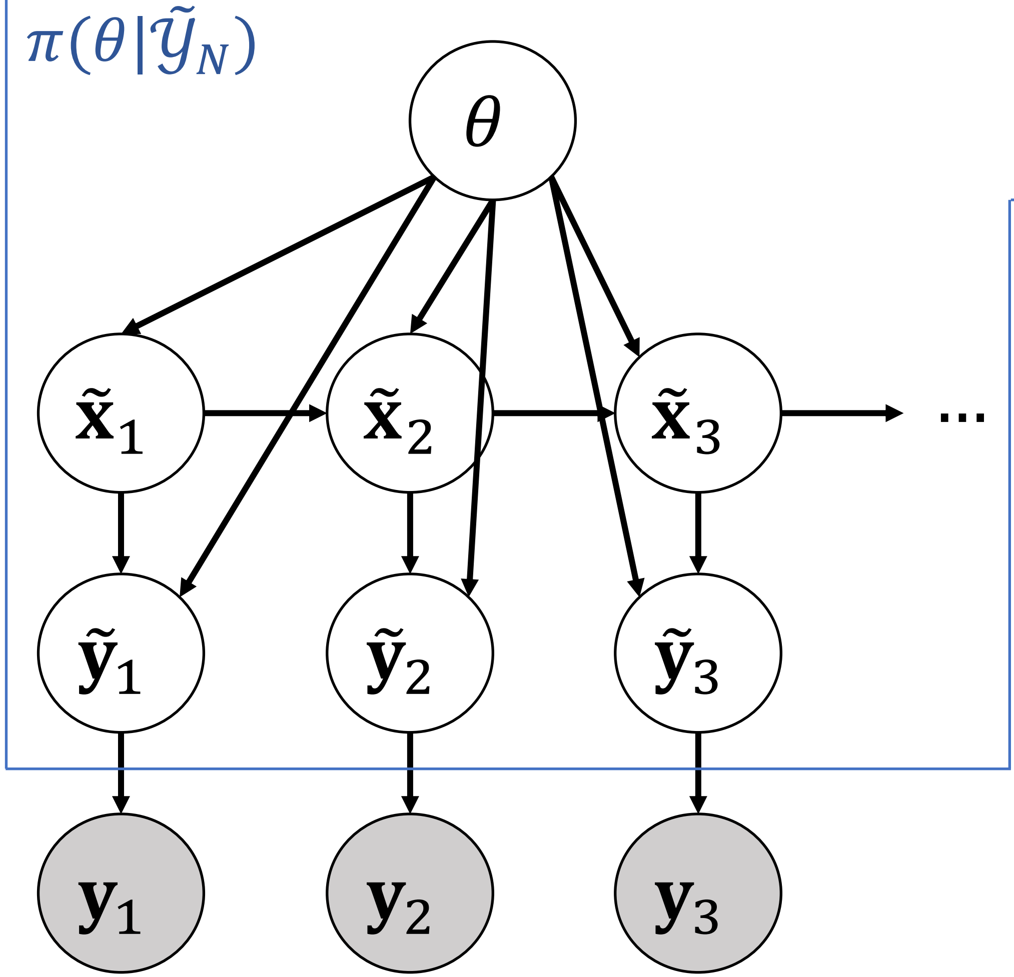
$$\begin{aligned}\tilde{\mathbf{y}}_k &= \mathbf{\Phi}^\top(\varepsilon,\eta)\mathbf{y}_k \\ &= \mathbf{\Phi}^\top(\varepsilon,\eta)(\mathbf{x}_k + \eta_k) \\ &= \tilde{\mathbf{x}}_k(\varepsilon,\eta) + \mathbf{\Phi}^\top(\varepsilon,\eta)\eta_k\end{aligned}$$

2. Simplify uncertainty form

$$\boxed{\tilde{\mathbf{y}}_k = \tilde{\mathbf{x}}_k + \tilde{\eta}_k}$$

$\tilde{\xi}_k$ and $\tilde{\eta}_k$ represent the *effective* noise

Inference in reduced dimensions



$$\tilde{\mathbf{x}}_k = \widetilde{\Psi}(\tilde{\mathbf{x}}_{k-1}, \theta) + \tilde{\xi}_{k-1}, \quad \tilde{\xi}_{k-1} \sim \left(0, \Sigma(\theta)\right)$$

$$\tilde{\mathbf{y}}_k = \tilde{h}(\tilde{\mathbf{x}}_k, \theta) + \tilde{\eta}_k, \quad \tilde{\eta}_k \sim \left(0, \Gamma(\theta)\right)$$

$$\mathbf{y}_k = \mathbf{\Phi}^\top \tilde{\mathbf{y}}_k$$

Sources of error/uncertainty

- ε: Projection error
- ξ: Model uncertainty
- η: Measurement uncertainty

⇩

- $\tilde{\xi}$: *effective* model uncertainty
- $\tilde{\eta}$: *effective* measurement uncertainty

⇩

- θ: Parameter uncertainty
  - Modeled by $\pi(\theta|\tilde{\mathcal{Y}}_N)$

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Hamiltonian systems

Hamiltonian is a scalar-valued function

$$H(\mathbf{q}, \mathbf{p}) = T(\mathbf{q}, \mathbf{p}) + V(\mathbf{q}, \mathbf{p})$$

Time derivatives are derived from Hamiltonian

$$\dot{\mathbf{q}} = \frac{\partial H(\mathbf{q}, \mathbf{p})}{\partial \mathbf{p}} \qquad \dot{\mathbf{p}} = -\frac{\partial H(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}}$$

$\mathbf{q} \in \mathbb{R}^d$: generalized position

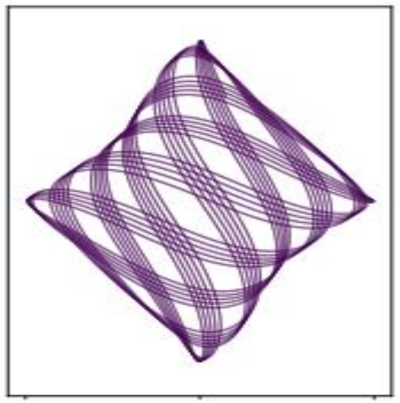
$\mathbf{p} \in \mathbb{R}^d$: generalized momentum

T: kinetic energy

V: potential energy

Properties of Hamiltonian systems

- Conservation
- Reversibility
- Symplecticity



Objective: Design $\widetilde{\Psi}$ to enforce these physical phenomena

Cotangent lift: symplectic model reduction

Form snapshot matrix

$$\mathbf{Y} = [\mathbf{q}_1 \quad \mathbf{q}_2 \quad \cdots \quad \mathbf{q}_N \quad \mathbf{p}_1 \quad \mathbf{p}_2 \quad \cdots \quad \mathbf{p}_N] \in \mathbb{R}^{d \times 2N}$$

Compute the truncated SVD

$$\mathbf{Y} \approx$$

Construct the symplectic projection matrix

$$\boldsymbol{\Phi} = \begin{bmatrix} \mathbf{U} & \mathbf{0} \\ \mathbf{0} & \mathbf{U} \end{bmatrix} \in \mathbb{R}^{2d \times 2r}$$

Peng, Liqian, and Kamran Mohseni. "Symplectic model reduction of Hamiltonian systems." *SIAM Journal on Scientific Computing* 38.1 (2016): A1-A27.

Hamiltonian operator inference (H-OpInf)

Given a parameterized form of a high-dimensional Hamiltonian

$$H(\mathbf{q}, \mathbf{p}, \theta) = H_{quad}(\mathbf{q}, \mathbf{p}, \mathbf{q}_z, \mathbf{p}_z, \dots) + H_{nl}(\mathbf{q}, \mathbf{p}, \theta_{nl})$$

H-OpInf yields the reduced-order Hamiltonian using $\mathbf{\Phi}$

$$\widetilde{H}(\widetilde{\mathbf{q}}, \widetilde{\mathbf{p}}, \theta) = \widetilde{\mathbf{q}}^\top \mathbf{D}_q(\theta_{quad})\widetilde{\mathbf{q}} + \widetilde{\mathbf{p}}^\top \mathbf{D}_p(\theta_{quad})\widetilde{\mathbf{p}} + \mathbf{\Phi}^\top H_{nl}(\mathbf{\Phi}\widetilde{\mathbf{q}}, \mathbf{\Phi}\widetilde{\mathbf{p}}, \theta_{nl})$$

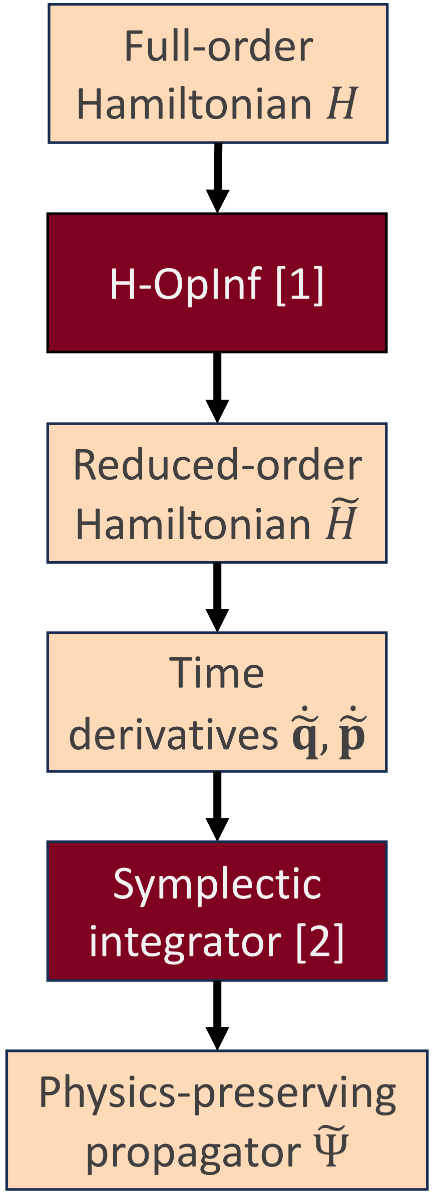
The time derivatives are derived as

$$\dot{\widetilde{\mathbf{q}}} = \mathbf{D}_p(\theta_{quad})\widetilde{\mathbf{p}} + \mathbf{\Phi}^\top \frac{\partial H_{nl}}{\partial \mathbf{p}}(\mathbf{\Phi}\widetilde{\mathbf{q}}, \mathbf{\Phi}\widetilde{\mathbf{p}}, \theta_{nl})$$

$$\dot{\widetilde{\mathbf{p}}} = -\mathbf{D}_q(\theta_{quad})\widetilde{\mathbf{q}} - \mathbf{\Phi}^\top \frac{\partial H_{nl}}{\partial \mathbf{q}}(\mathbf{\Phi}\widetilde{\mathbf{q}}, \mathbf{\Phi}\widetilde{\mathbf{p}}, \theta_{nl})$$

A symplectic integrator is used to complete the symplectic propagator

$$\widetilde{\Psi}(\widetilde{\mathbf{q}}, \widetilde{\mathbf{p}}) \coloneqq \text{SymplecticIntegrator}\big(\widetilde{\mathbf{q}}, \widetilde{\mathbf{p}}, \dot{\widetilde{\mathbf{q}}}, \dot{\widetilde{\mathbf{p}}}, \Delta t\big)$$



[1] Sharma, Harsh, Zhu Wang, and Boris Kramer. "Hamiltonian operator inference: Physics-preserving learning of reduced-order models for canonical Hamiltonian systems." *Physica D: Nonlinear Phenomena* 431 (2022): 133122.

[2] Tao, Molei. "Explicit symplectic approximation of nonseparable Hamiltonians: Algorithm and long time performance." *Physical Review E* 94.4 (2016): 043303.

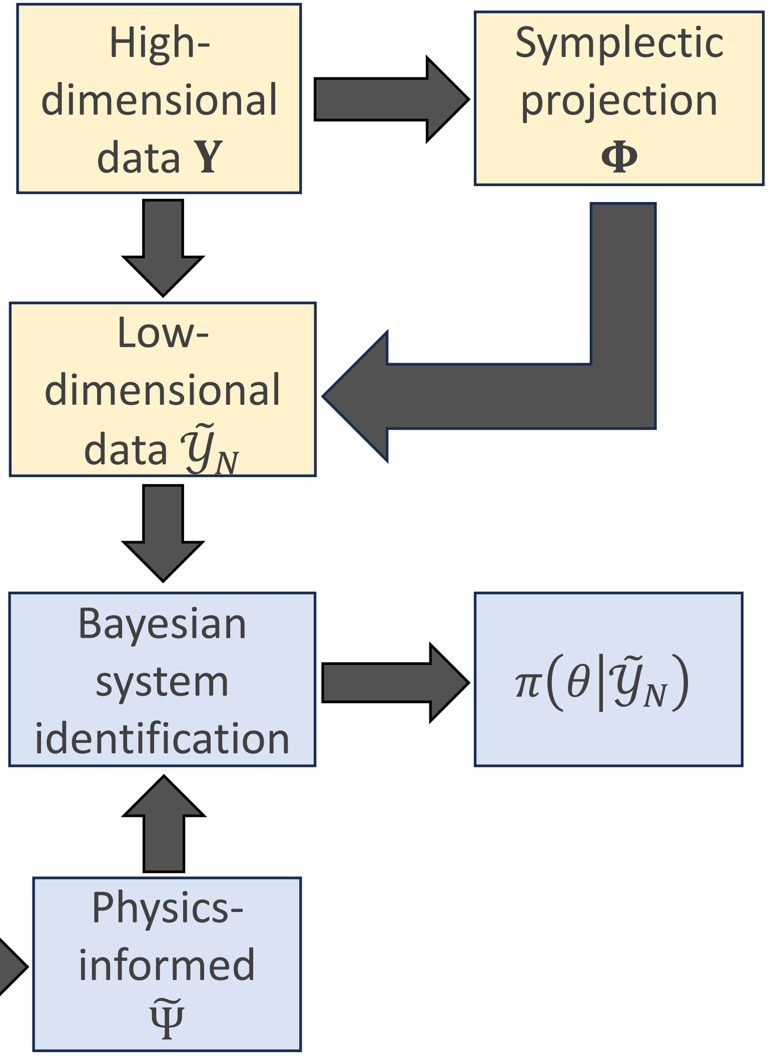
Reduced-dimensional likelihood evaluation of a high-dimensional Hamiltonian system

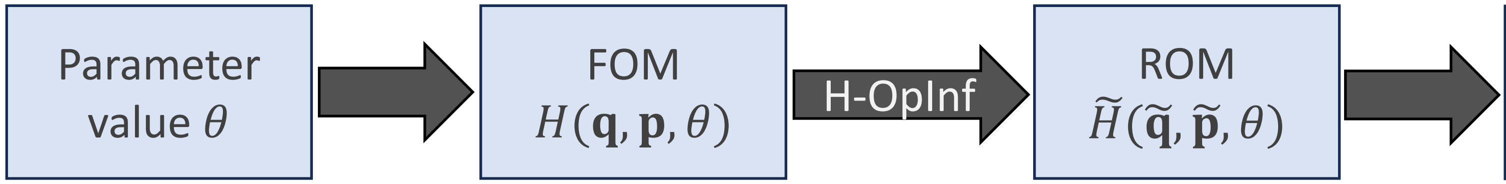
Pre-processing

1. Form the snapshot matrix $\mathbf{Y} = [\mathbf{q}_1 \quad \mathbf{q}_2 \quad \cdots \quad \mathbf{q}_n \quad \mathbf{p}_1 \quad \mathbf{p}_2 \quad \cdots \quad \mathbf{p}_n]$
2. Compute the symplectic projection matrix $\mathbf{\Phi}$ with cotangent lift
3. Define the low-dimensional data $\tilde{\mathcal{Y}}_N = \{\mathbf{\Phi}^\top \mathbf{y}_k | k = 1, \dots, N\}$

Evaluation

4. Estimate Hamiltonian reduced-order model with H-OpInf
5. Define low-dimensional symplectic dynamics $\tilde{\Psi}(\tilde{\mathbf{q}}, \tilde{\mathbf{p}})$
6. Define low-dimensional observations $\tilde{h}(\tilde{\mathbf{q}}, \tilde{\mathbf{p}})$
7. Evaluate the posterior $\pi(\theta | \tilde{\mathcal{Y}})$ using filtering algorithm





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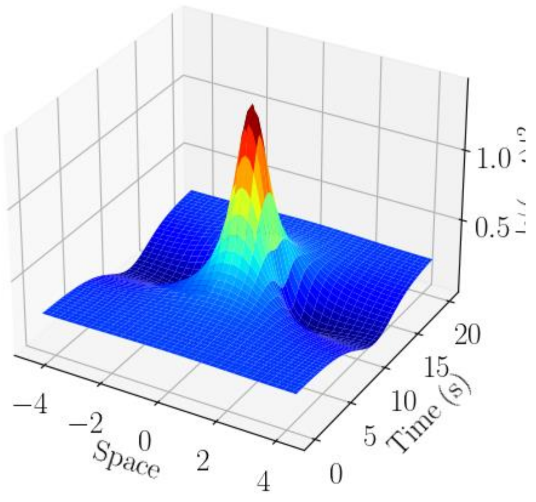
Nonlinear Schrodinger Equation (NLSE)

$$\mathcal{H}(q,p) = \frac{1}{2}\int \left(p_z^2 + q_z^2 - \frac{\gamma}{2}(p^2+q^2)^2\right) \mathrm{d}z$$

Additionally conserves mass $\mathcal{Q}_1$ and momentum $\mathcal{Q}_2$

$$\mathcal{Q}_1(q,p) = \int (p^2+q^2)\mathrm{d}z, \qquad \mathcal{Q}_2(q,p) = \int (p_z q - q_z p)\mathrm{d}z$$



We attempt to learn γ

$$H_{nl}(q,p,\theta) = -\frac{\theta_\gamma}{2}(p^2+q^2)^2$$

True $\gamma = 2$

Periodic boundary conditions with initial conditions:

$q(z,0) = 0$ and $p(z,0) = 0.5\left(1 + 0.01\cos\left(\frac{2\pi z}{L}\right)\right)$, $\quad z \in \left[-\frac{L}{2}, \frac{L}{2}\right]$, $L = 2\pi\sqrt{2}$

Spatial discretization $d = 64$

NLSE: Data generation

Measurement function: $h(\mathbf{q}_k, \mathbf{p}_k) = [\mathbf{q}_k^\top \quad \mathbf{p}_k^\top]^\top$

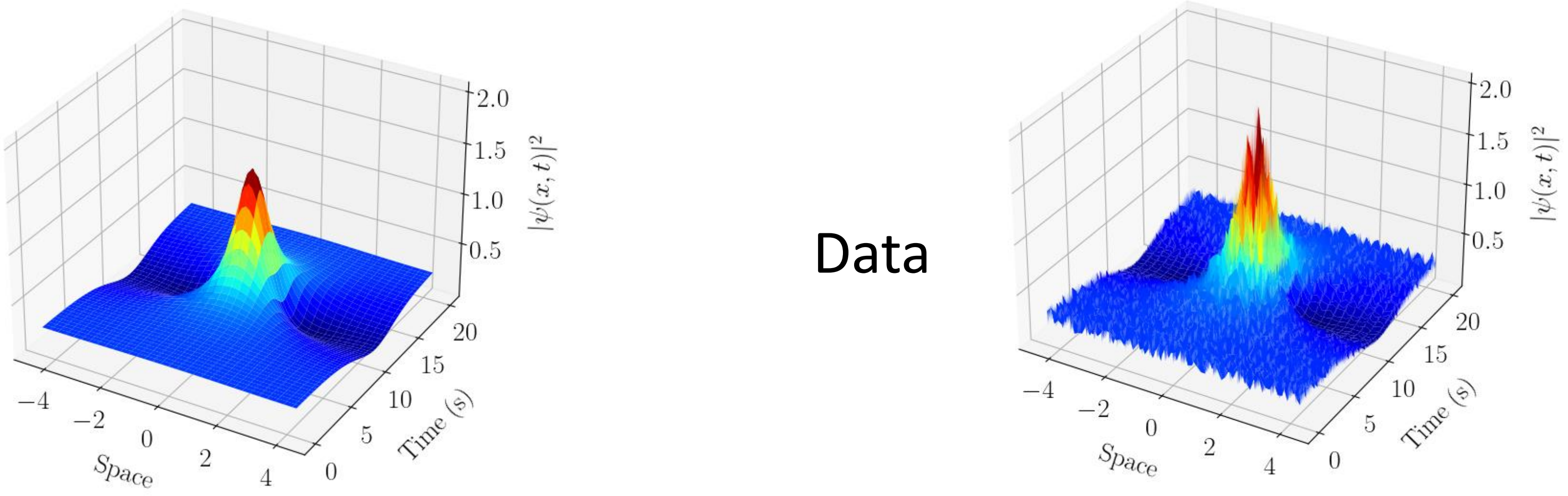
Data: $\mathbf{y}_k = h(\mathbf{q}_k, \mathbf{p}_k)(1 + u_k), \quad u_k \sim \mathcal{U}[-0.2 \quad 0.2]$

Model: $\tilde{h}(\tilde{\mathbf{q}}_k, \tilde{\mathbf{p}}_k) = [\tilde{\mathbf{q}}_k^\top \quad \tilde{\mathbf{p}}_k^\top]^\top$, $r = 8$

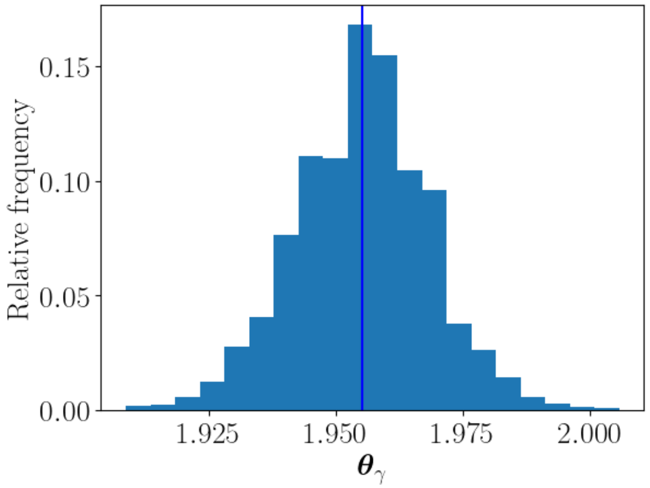
Collect $N = 4000$ with timestep $\Delta t = 0.005$

True

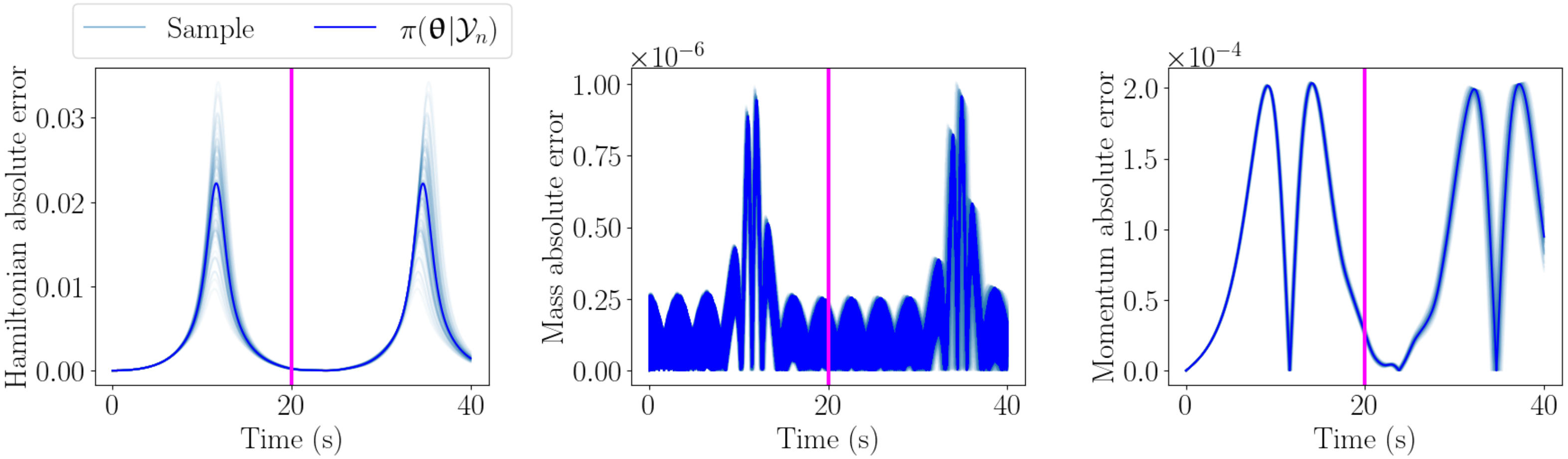
Data



The algorithm learns an accurate model under high measurement uncertainty



Parameter marginal



Conserved quantities

Average relative noise:

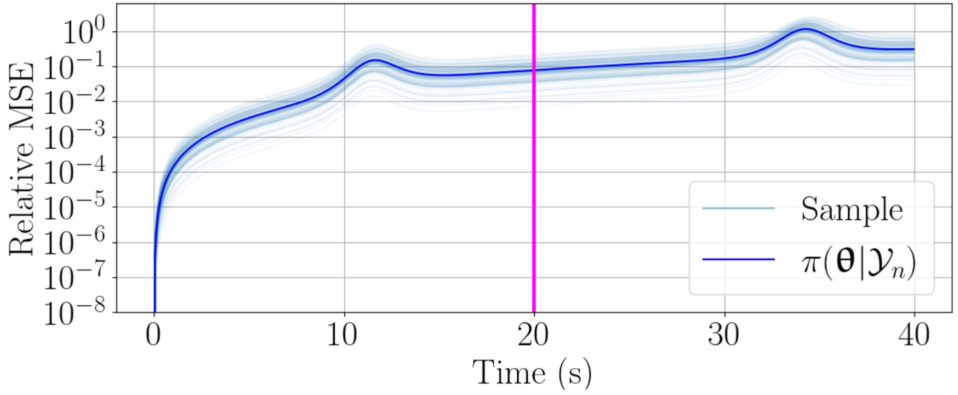
$$\frac{\|\mathbf{Y}-\bar{\mathbf{Y}}\|_F^2}{\|\bar{\mathbf{Y}}\|_F^2} = 2.11$$

Relative deterministic projection error:

$$\frac{\|(\mathbf{\Phi}\mathbf{\Phi}^\top - \mathbf{I})\mathbf{Y}\|_F}{\|\mathbf{Y}\|_F} = 1.19 \times 10^{-7}$$

Relative MSE formula:

$$\frac{\|\hat{\mathbf{y}}_k - \mathbf{y}_k\|_2^2}{\|\mathbf{y}_k\|_2^2}$$



Relative state MSE

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Conclusions

- Reduced-order modeling allows for efficient parameter estimation of high-dimensional models
- Working in reduced dimensions introduces additional uncertainty
- Modeling this added uncertainty with stationary effective noise terms can yield accurate model estimates

Future work

- Correcting inaccurate projection mappings with experimental data
- More precise tracking of uncertainty

Publications

Galioto, Nicholas, et al. "Bayesian identification of nonseparable Hamiltonians with multiplicative noise using deep learning and reduced-order modeling." *arXiv preprint arXiv:2401.12476* (2024).

Galioto, Nicholas, and Alex Arkady Gorodetsky. "Bayesian system ID: optimal management of parameter, model, and measurement uncertainty." *Nonlinear Dynamics* 102.1 (2020): 241-267.

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