Physics-Constrained, Structure-Preserving Machine Learning for Structural Health Assessment of As-Built, As-Deployed Structures

Prepared for: MLDL Workshop

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Motivation: Representation of the as-built, as-deployed state

- SNL is interested in monitoring systems that are constantly evolving, and that may have deviated from original design specification due to upgrades, or the fact that they are legacy systems with unknown design pedigree.
- These requirements motivate the use of a data-driven approach since the physics-based models may not always be available.
- This requirement combined with the need for understanding the physical behavior of the as-built, as-deployed system in order to perform physically interpretable structural health monitoring motivate the use of physics constraints and/or structure preservation in our data-driven approach.
- **Objectives:**
  - i. Establish a general family of physics-constrained and structure-preserving data-driven methods for SHM
  - ii. Address practical challenges associated with physics-constrained data-driven methods
  - iii. Propose an SHM workflow that enables the development of physically-interpretable models

Bias-Variance Trade-Off in Machine Learning

- “The most fundamental lesson of ML is the bias-variance tradeoff: when you have sufficient data, you do not need to impose a lot of human generated inductive bias on your model. You can “let the data speak”. However, when you do not have sufficient data available you will need to use human-knowledge to fill the gaps.” [1]
- In physics, data generation is expensive and therefore we cannot simply “let the data speak”, so we need to impose structure and domain knowledge for generalization.

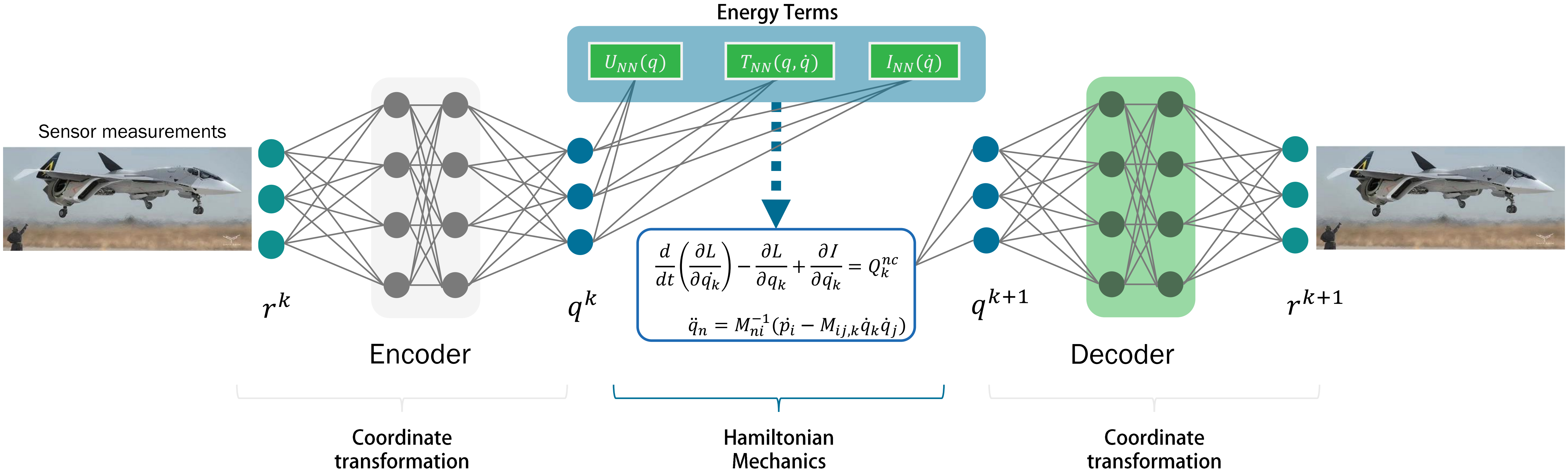
[1]. “Do we still need models or just more data and compute?” Article by Prof. Max Welling (University of Amsterdam), 2019

Physics/Data Trade-Offs

1. Physics-informed: the goal is to solve a known partial differential equation (PDE) with ML (least amount of data, max amount of physics knowledge)
2. **Structure preservation**: the goal is to preserve the underlying geometric structure of the physical system through the use of architectural constraints or inductive biases (low amount of data, medium amount of physics knowledge)
3. **Physics constraints**: the goal is to constrain the ML model to obey certain physical laws (more amount of data, low amount of physics knowledge)
4. Purely data-driven: no physical constraints, the ML model has maximum flexibility to learn from data (most amount of data, no physics knowledge)

Structure-Preserving Hamiltonian Neural Differential Operator

Ensemble of neural networks



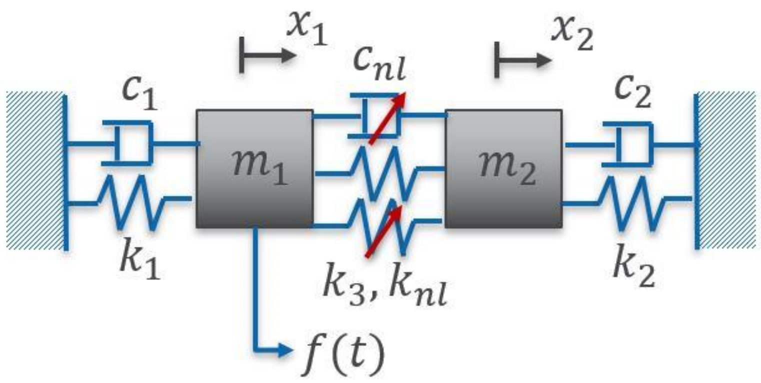
No assumptions of linearity anywhere

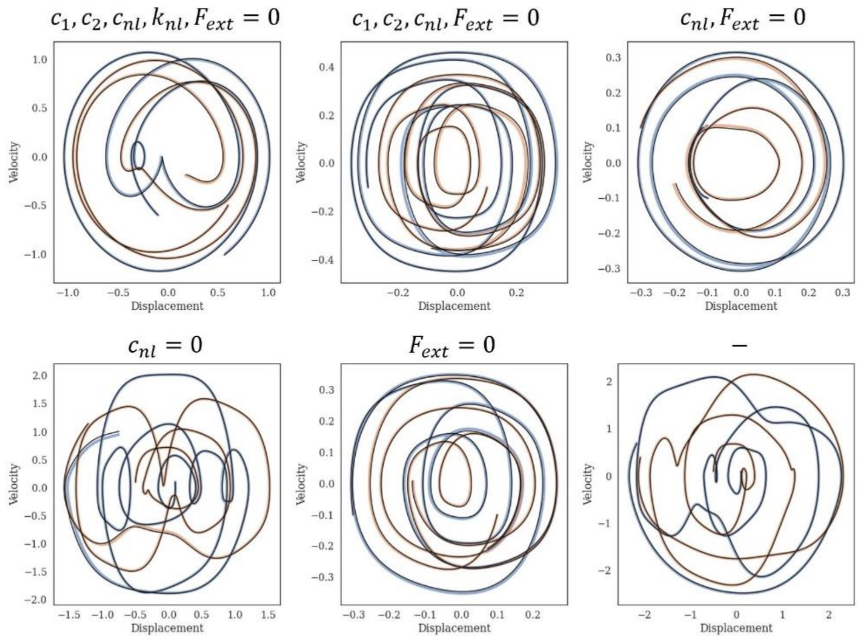
Application of structure-preserving, data-driven digital twins

- Oscillator with nonlinear damping and stiffness.
- Trained with a single realization, and tested with different initial conditions and/or boundary conditions.

$m_1 = 1.1, m_2 = 1.5, k_1 = 1.0, k_2 = 1.3, k_3 = 0.8, c_1 = 0.01, c_2 = 0.08$

$k_{nl} = 10.0, c_{nl} = 0.095$





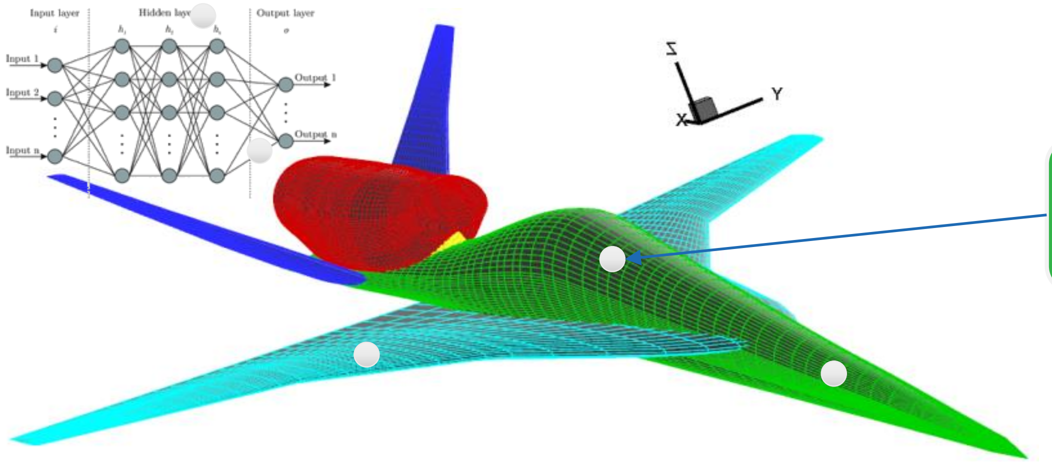
Terms set to 0.0	Runtime per evaluation (s)	Displacement MSE
$c_1,\ c_2,\ c_{nl},\ k_{nl},\ F_{ext}$	9.24e−9	0.22e−3
$c_1,\ c_2,\ c_{nl},\ F_{ext}$	1.29e−5	1.19e−3
$c_{nl},\ F_{ext}$	2.12e−5	1.15e−3
c_{nl}	6.76e−6	2.11e−3
F_{ext}	1.01e−5	0.58e−3
–	1.38e−5	2.19e−3

Najera-Flores, D. A., and Todd, M. D., 2023, “A structure-preserving neural differential Operator with embedded Hamiltonian constraints for modeling structural dynamics,” Computational Mechanics, 3.

How to reconcile realistic measurements techniques with data-driven methods?

The challenge of reconstructing the state-space from partial measurements

- A consequence of choosing Hamiltonian mechanics is that the **system must be solved in generalized coordinates**. An autoencoder is used to perform coordinate transformation from some arbitrary coordinate set to the generalized coordinates.
- **CHALLENGE:** typically, observable data (i.e., measured) does not represent a complete set of generalized coordinates.

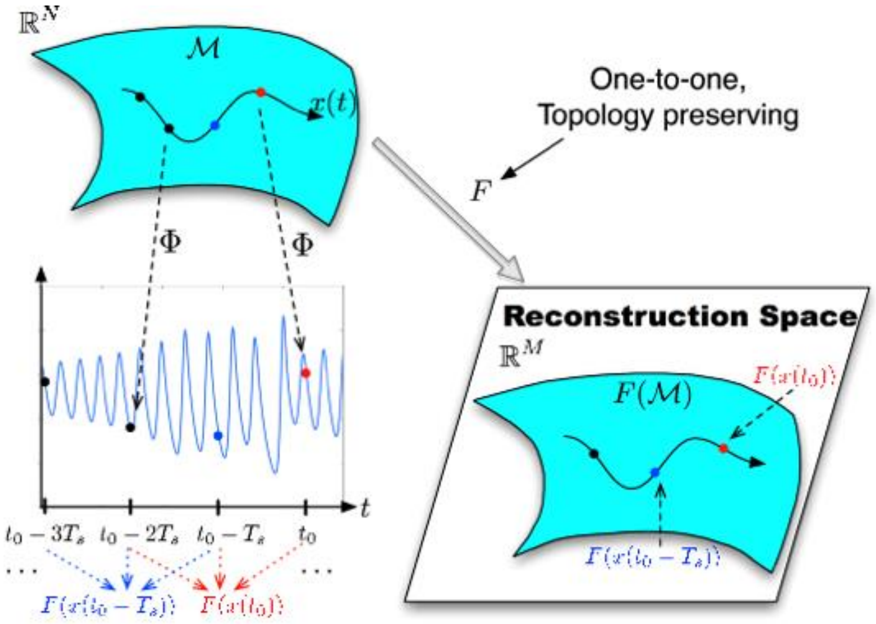


Typically, only sparse measurements are available.

Addressing partial observability challenge

Taken’s embedding theorem

- Taken’s theorem [1] implies that state space reconstruction is possible via time-delay embeddings of observable data (under certain conditions).
- Formally, it is stated that **there exists a diffeomorphism** between time-delay embeddings of data and its underlying state space (or manifold).
- Challenges:
  - Determining the time delays and the number of delayed time series to use.
  - Finding the diffeomorphic mapping between the time-delay embeddings and the appropriate manifold.



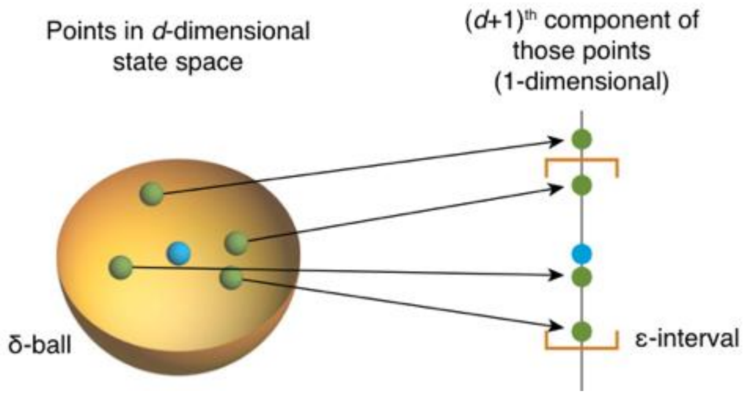
https://cnx.org/contents/k57_M8Tw@2/Takens-Embedding-Theorem

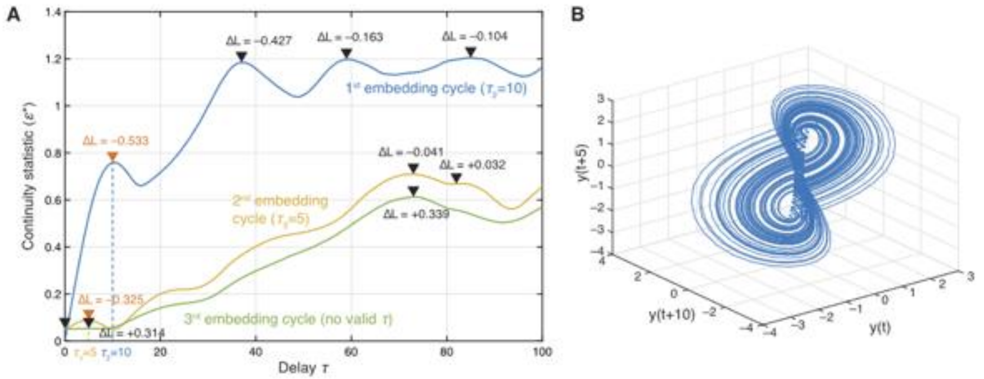
[1]. Takens, F.: Detecting strange attractors in turbulence. In: Rand, D., Young, L.-S. (eds.) Dynamical Systems and Turbulence, Warwick 1980, pp. 366–381. Springer, Berlin, Heidelberg (1981)

Kraemer's automated & unified embedding recipe

Leveraging embeddology algorithms

- Continuity statistic by Pecora et al [1].:
  - Continuity statistic is used to test whether a new proposed embedded component can be reconstructed from existing components, thus testing its redundancy and irrelevance.
- L-statistic by Uzal et al [2]:
  - L-statistic quantifies the goodness of a reconstruction and is used to select the candidate components indicated by the continuity statistic.
- Kraemer et al. [3] combined these ideas into an algorithm called PECUZAL, which is used in this work.





[1]. Pecora, L.M., Moniz, L., Nichols, J., Carroll, T.L.: A unified approach to attractor reconstruction. Chaos: An Interdisciplinary Journal of Nonlinear Science 17(1), 013110 (2007) https://doi.org/10.1063/1.2430294.

[2]. Uzal, L.C., Grinblat, G.L., Verdes, P.F.: Optimal reconstruction of dynamical systems: A noise amplification approach. Phys. Rev. E 84, 016223 (2011). https://doi.org/10.1103/PhysRevE.84.016223

[3]. Kraemer, K.H., Datseris, G., Kurths, J., Kiss, I.Z., Ocampo-Espindola, J.L., Marwan, N.: A unified and automated approach to attractor reconstruction. New Journal of Physics 23(3), 033017 (2021). https://doi.org/10.1088/1367-2630/abe336

Normalizing flow autoencoder

Learning bijective autoencoders

- In order to find a the diffeomorphic mapping, a bijective neural network is used.
- A well-known bijective architecture is the normalizing flow network (also know as an invertible neural network).
- However, the normalizing flow network cannot change dimensions, limiting any dimensionality compression.
- To overcome this limitation, a singular value decomposition is used on the original time-delay embeddings, and a reduced number of dimensions is kept.
- The reduced-order vectors are then linearly "mixed" to avoid any biases when the NF network splits the data in two.

$$\tilde{\mathbf{z}} = \mathbf{V}^{\mathbf{T}}\mathbf{x}$$ SVD projection

$$\mathbf{z} = \mathbf{T}\tilde{\mathbf{z}}$$ Linear mixing, learned

$$\mathbf{q}_A = \mathbf{z}_A \odot \exp\big(s_B(\mathbf{z}_B)\big) + t_B(\mathbf{z}_B)$$

$$\mathbf{q}_B = \mathbf{z}_B \odot \exp\big(s_A(\mathbf{z}_A)\big) + t_A(\mathbf{z}_A)$$

Normalizing flow

$$\mathbf{z}_B = \big(\mathbf{q}_B - t_A(\mathbf{q}_A)\big) \odot \exp(-s_A(\mathbf{q}_A))$$

$$\mathbf{z}_A = \big(\mathbf{q}_A - t_B(\mathbf{q}_B)\big) \odot \exp(-s_B(\mathbf{q}_B))$$

$$\tilde{\mathbf{z}} = \mathbf{T}^{-1}\mathbf{z}$$

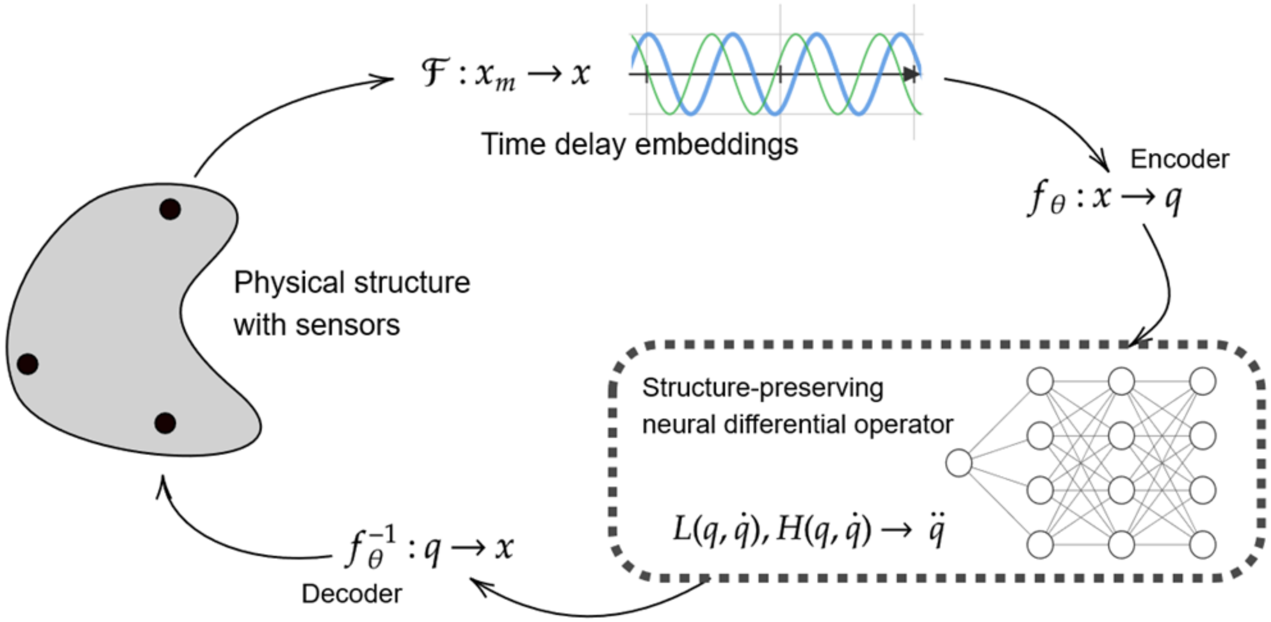
$$\mathbf{x} = \mathbf{V}\tilde{\mathbf{z}}$$

Dinh, L., Sohl-Dickstein, J., Bengio, S.: Density estimation using Real NVP (2017)

Proposed workflow

Integration of bijective autoencoder with structure-preserving neural differential operator

- The PECUZAL time-delay algorithm is integrated with the normalizing flow autoencoder and then passed to the structure-preserving neural differential operator.
- The autoencoder and the structure-preserving neural differential operator are all trained simultaneously.



Najera-Flores, D.A., Todd, M.D. State-space reconstruction from partial observables using an invertible neural network with structure-preserving properties for nonlinear structural dynamics. *Nonlinear Dyn* (2024). https://doi.org/10.1007/s11071-024-09642-4.

Demonstration: Half Brake-Reuss Beam

Experimental example

- The Half Brake-Reuss beam was used to demonstrate the proposed approach.
- The nonlinearities in this beam are due to the three bolt lap joint used to join two beams.
- The beam was tested by exciting the beam at the frequency of interest with a fixed sinusoidal signal and then detaching the shaker.
    - Although this test is meant to isolate a single model, modal coupling occurs due to the nonlinearities
    - It was excited with enough energy to excite the nonlinearities
- Digital image correlation (DIC) was used to obtain full field displacement response but in this work, only three locations were assumed to be measured.

Experimental setup courtesy of [1].

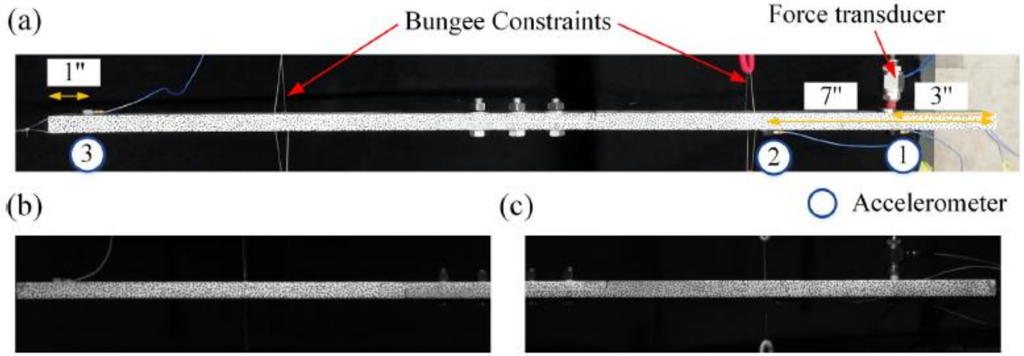
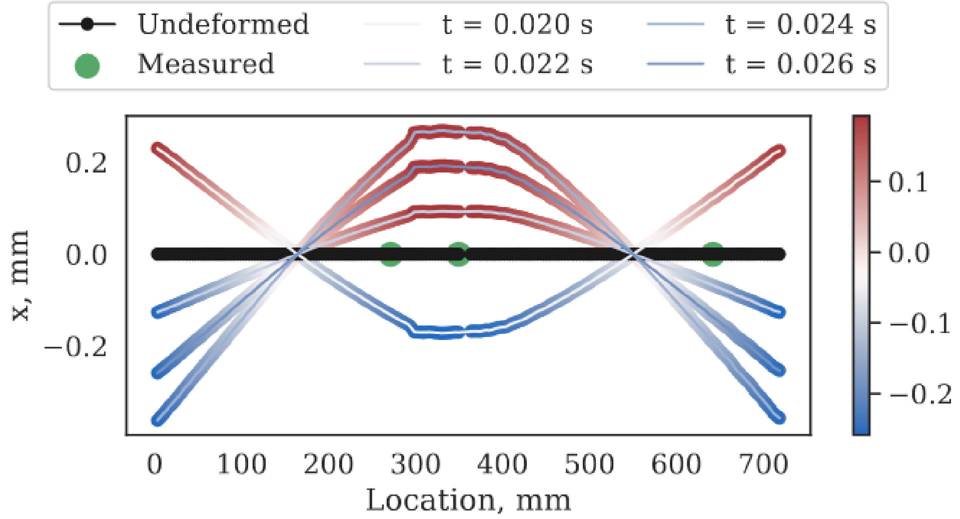


Fig. 5. The images of the test beam, shown are (a) the top view of the HBRB, (b) the image from the left camera, and (c) the image from the right camera. The blue circles with numbers inside in (a) refer to the accelerometers.



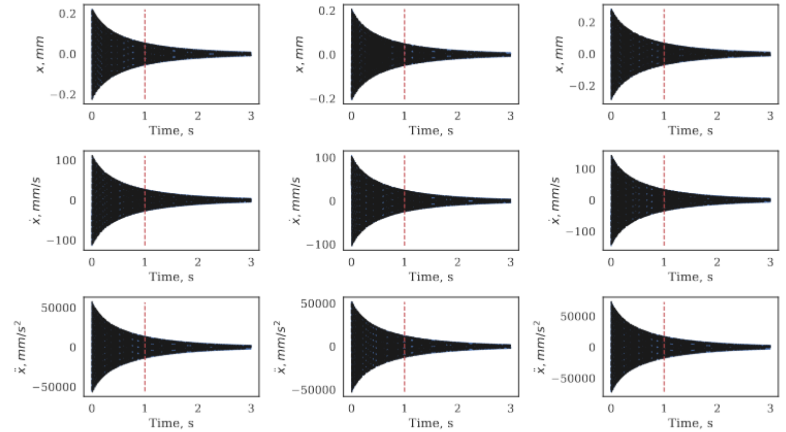
[1]. Wei Chen et al. Measurement and identification of the nonlinear dynamics of a jointed structure using full-field data, part i: Measurement of nonlinear dynamics. *Mechanical Systems and Signal Processing*, 166:108401, 2022

Demonstration: Half Brake-Reuss Beam

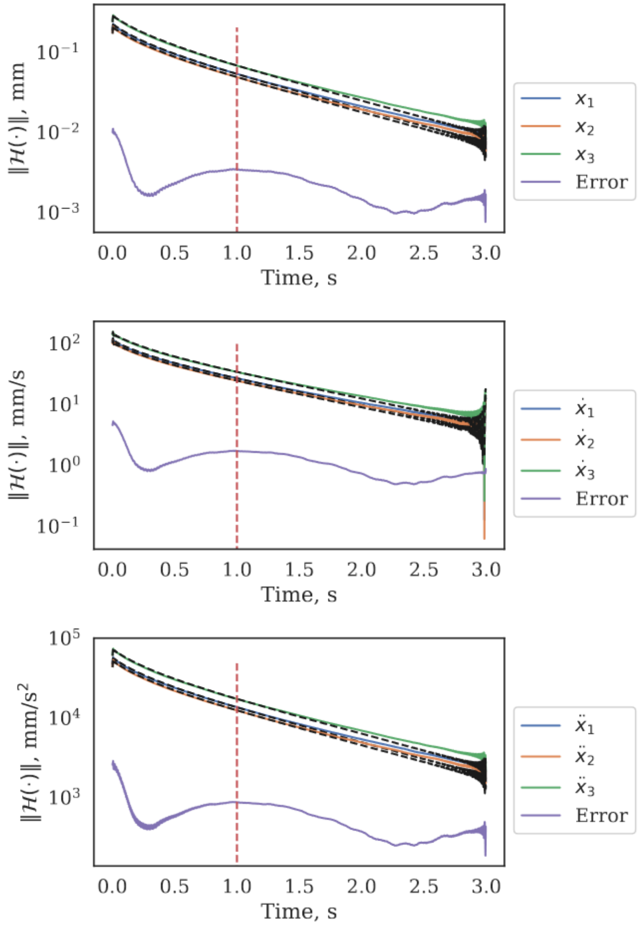
Accurate predictions past 300% of training region. Accurate representation of nonlinear frequency and damping.

Experimental Example

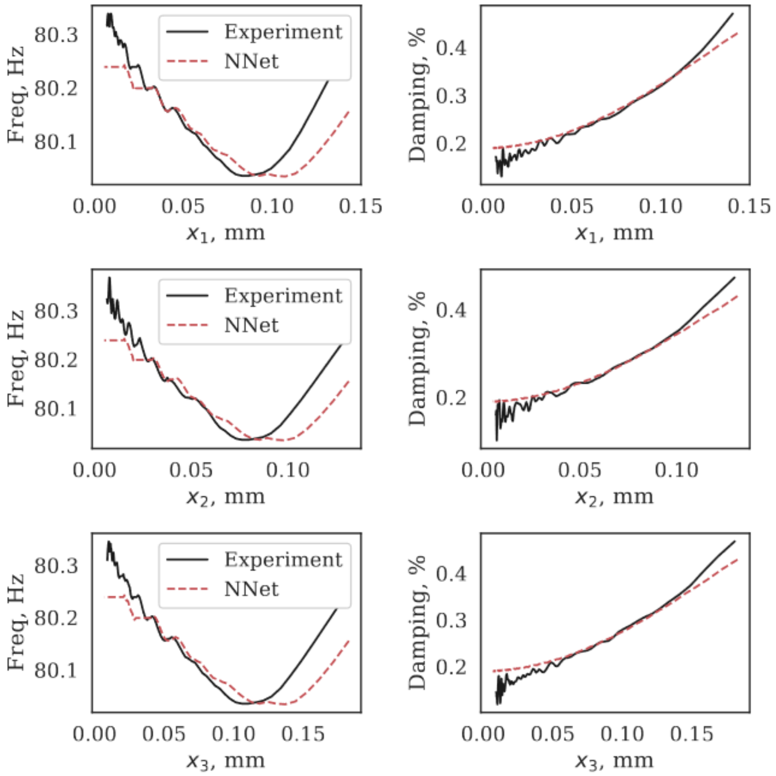
- The PECUZAL algorithm determined that only two dimensions were required for state-space reconstruction.
    - Physically, this result made sense given the descriptions provided by the authors of the original experimental paper, which showed that there was coupling between two modes.



Hilbert Transform of three response measurements



Amplitude-dependent frequency and damping backbone curves



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How can we use the trained model to detect damage or changes in the system?

Identifying domain shift when confronted with new data

- Once trained, the digital twin is meant to be used to detect changes in the system. This problem is difficult because the healthy/baseline state may be nonlinear, so a nonlinearity test is insufficient. Furthermore, because of its nonlinear behavior, bifurcations may not necessarily indicate damage.
- We need a strategy for detection that is robust to “normative” changes, such as variability in initial conditions.
- Idea: **encode distance awareness in the hidden feature space in a physically-meaningful way.**

Uncertainty-aware models, courtesy of [1]:

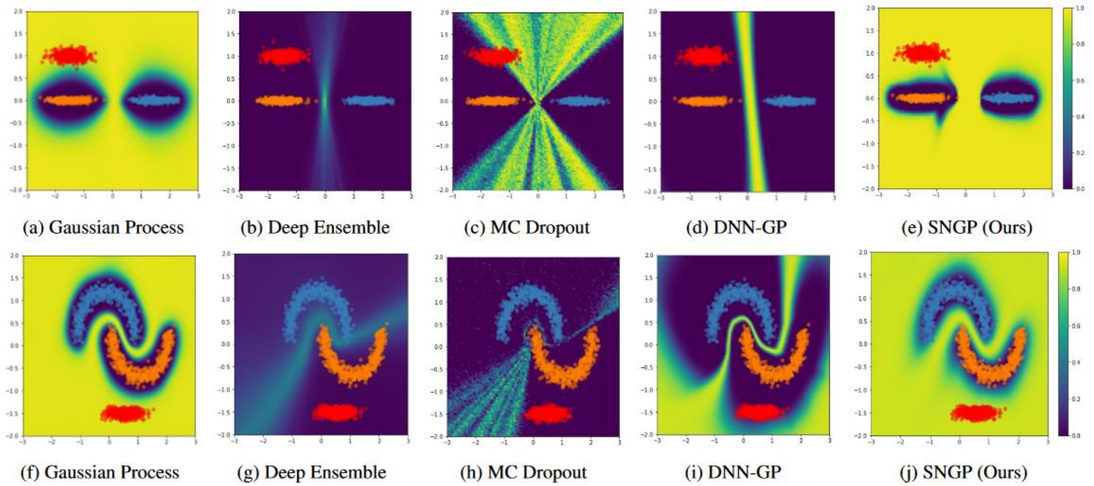
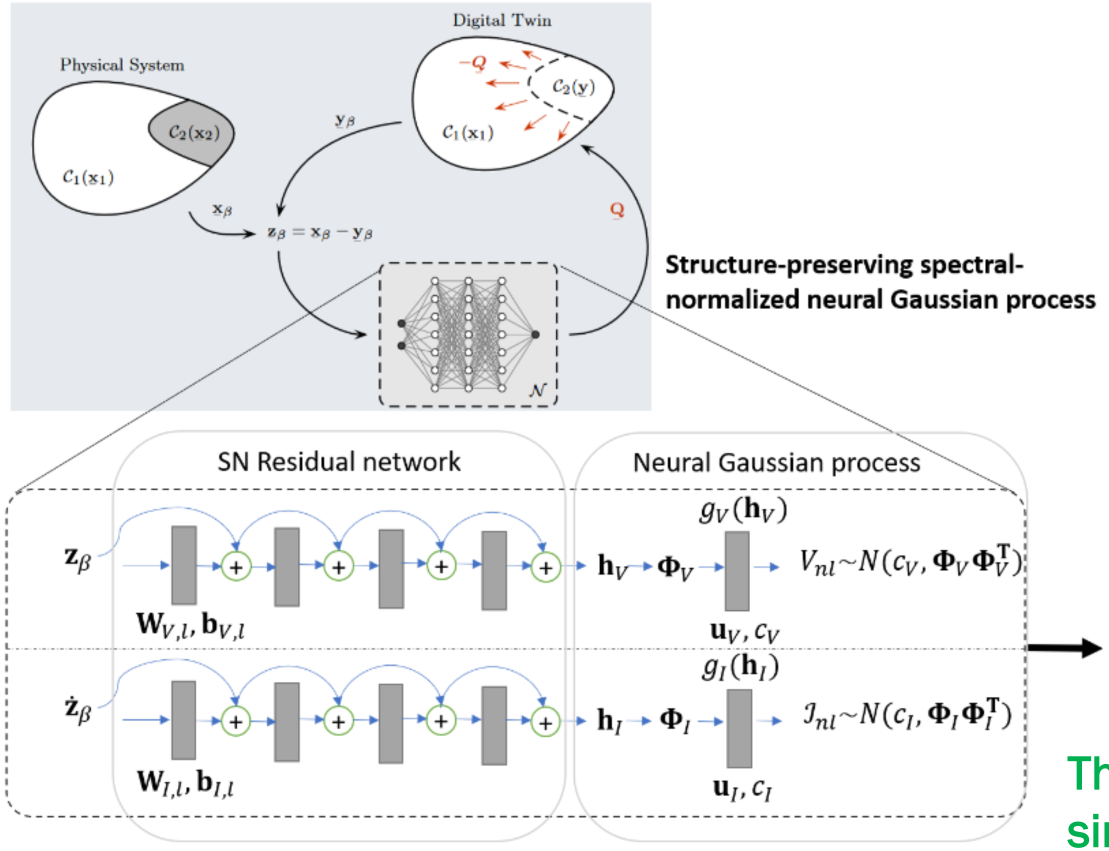


Figure 1: The uncertainty surface of a GP and different DNN approaches on the *two ovals* (Top Row) and *two moons* (Bottom Row) 2D classification benchmarks. SNGP is the only DNN-based approach achieving a distance-aware uncertainty similar to the gold-standard GP. Training data for positive (**Orange**) and negative classes (**Blue**). OOD data (**Red**) not observed during training. Background color represents the estimated model uncertainty (See 1e and 1j for color map). See Section 5.1 for details.

[1]. Liu, J. Z., Lin, Z., Padhy, S., Tran, D., Bedrax Weiss, T., and Lakshminarayanan, B., 2020, Simple and principled uncertainty estimation with deterministic deep learning via distance awareness. *34th Conference on Neural Information Processing Systems (NeurIPS 2020), Vancouver, Canada*

Improving neural network's distance-awareness

Spectral normalization Gaussian process networks



$$\mathbf{Q}_* = \frac{\partial V_{nl}(\mathbf{z}_\beta)}{\partial \mathbf{z}_\beta} + \frac{\partial \mathcal{I}_{nl}(\dot{\mathbf{z}}_\beta)}{\partial \dot{\mathbf{z}}_\beta}$$

David Najera-Flores, Justin Jacobs, D. Dane Quinn, Anthony Garland, and Michael Todd. Uncertainty-aware, structure-preserving machine learning approach for domain shift detection from nonlinear dynamic responses of structural systems. Manuscript submitted for publication to the *Journal of Risk and Uncertainty in Engineering Systems Part B: Mechanical Engineering*, 2024

Neural network's hidden features **h** are used to compute $\boldsymbol{\Phi}$

$$\boldsymbol{\Phi}_i = \sqrt{2\sigma^2/d_L}\cos(-\mathbf{W}_L\mathbf{h}_i + \mathbf{b}_L)$$

$$g(h_i) = \boldsymbol{\Phi}_i^T\mathbf{u} + c$$

$$V_{\text{nl}}(\mathbf{z}) = g_V(\mathbf{h}_V) \sim N(c_V, \boldsymbol{\Phi}_V^T\boldsymbol{\Phi}_V^T)$$

$$\mathscr{I}_{\text{nl}}(\dot{\mathbf{z}}) = g_I(\mathbf{h}_I) \sim N(c_I, \boldsymbol{\Phi}_I^T\boldsymbol{\Phi}_I^T),$$

$$\mathbf{K}_{\text{GP}} = \boldsymbol{\Phi}\boldsymbol{\Phi}^T$$

$$\mathbf{K}_{\text{GP},ij} = \exp\left(-\|\mathbf{h}_i - \mathbf{h}_j\|_2^2/2\right)$$

The kernel matrix captures the distance in the hidden space and since the inputs to the network represent the state space, the distance is then measured in a transformed state space manifold.

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$$V_{\mathrm{nl}}(\mathbf{z}) = g_V(\mathbf{h}_V) \sim N(c_V, \Phi_V^T \Phi_V^T)$$

$$\mathscr{I}_{\mathrm{nl}}(\dot{\mathbf{z}}) = g_I(\mathbf{h}_I) \sim N(c_I, \Phi_I^T \Phi_I^T),$$

Nonlinear damping prediction variance

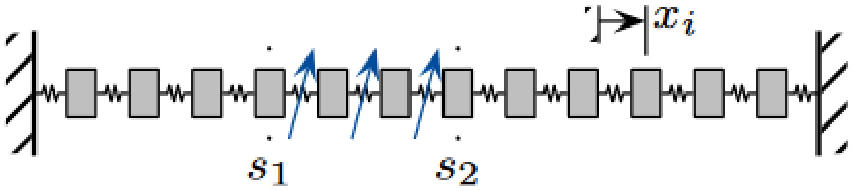
Gradual cubic stiffness example

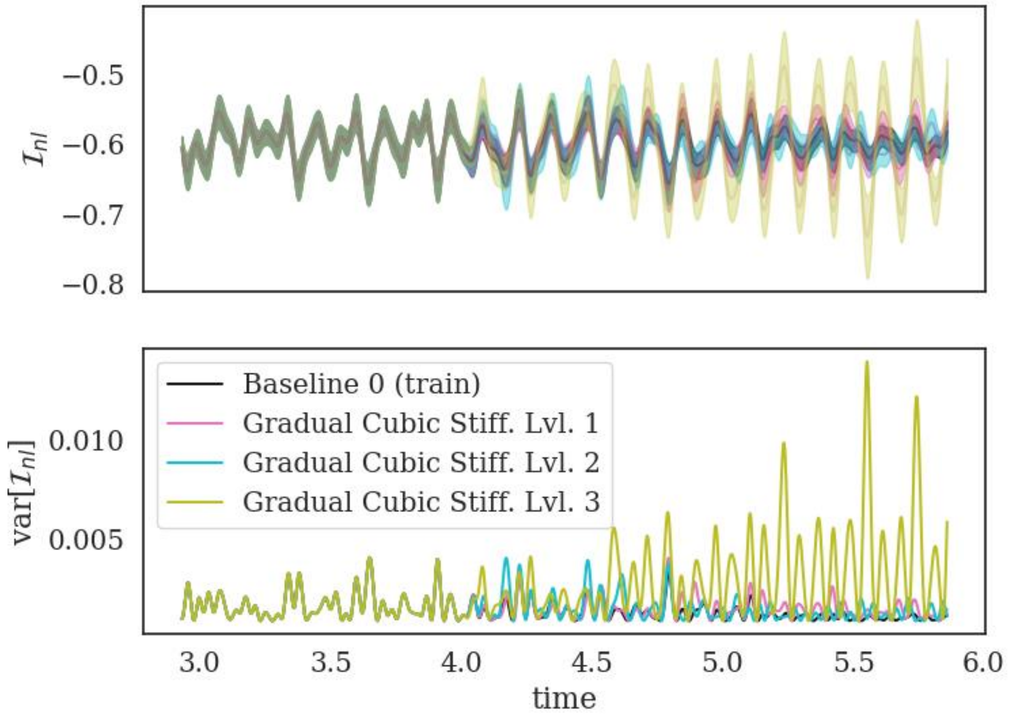
- As an example, damage was simulated by gradually changing the cubic stiffness coefficient

$$f_{\mathrm{nl},i} = \eta_i (x_{i+1} - x_i)^3 + \eta_{\mathrm{d},i} (t - t_{\mathrm{d}})^2 (x_{i+1} - x_i)^3$$

$$\begin{cases} \eta_{\mathrm{d}} = 0.6944, & \text{if } t \geq t_{\mathrm{d}} = 4 \\ 0 & \text{otherwise,} \end{cases}$$

- This damage model is simulating a self-accelerating degradation mechanism.

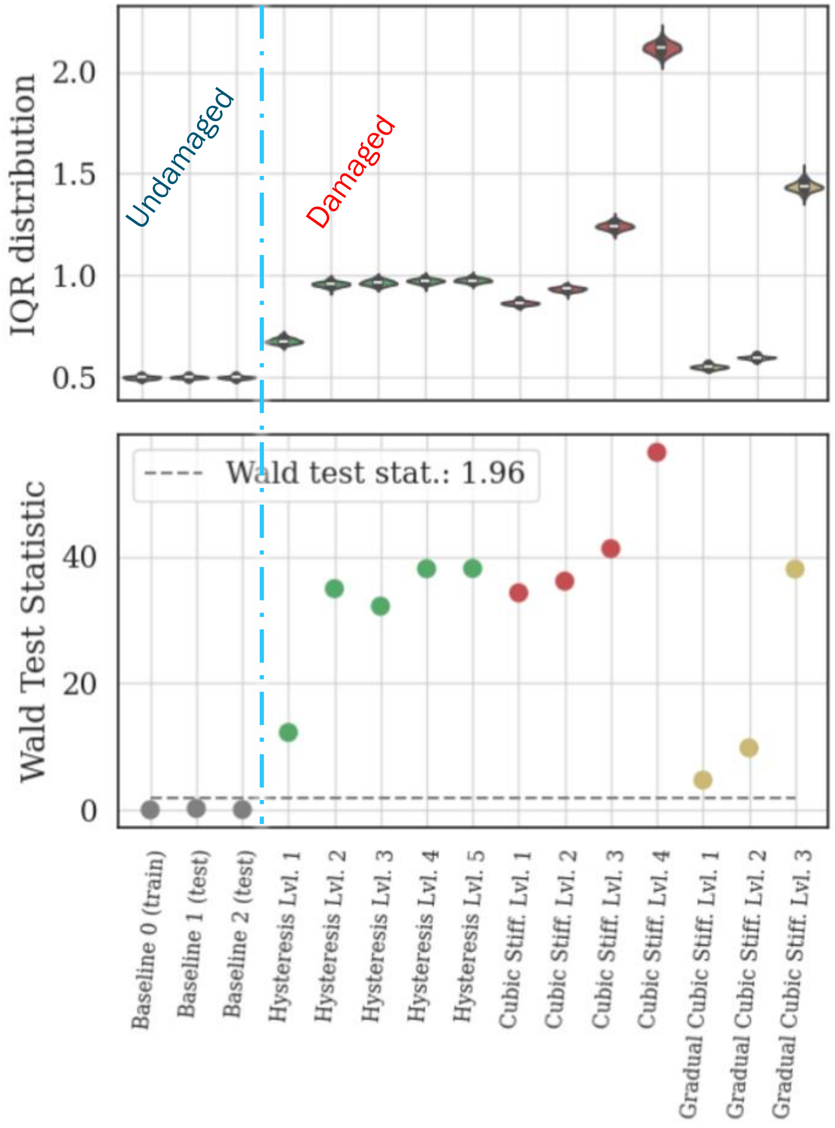




Testing for damage

Comparing test statistic and p-value

- Given the dispersion distributions of the nonlinear damping prediction variance, a hypothesis test was performed.
- The results showed that the p-value for the normative cases (i.e., variation of initial conditions) was below 0.05, while it was greater than 0.05 for the cases with a structural change (i.e., damaged).
- This result indicates that the hypothesis test was successful at detecting damage while being robust to normative changes.

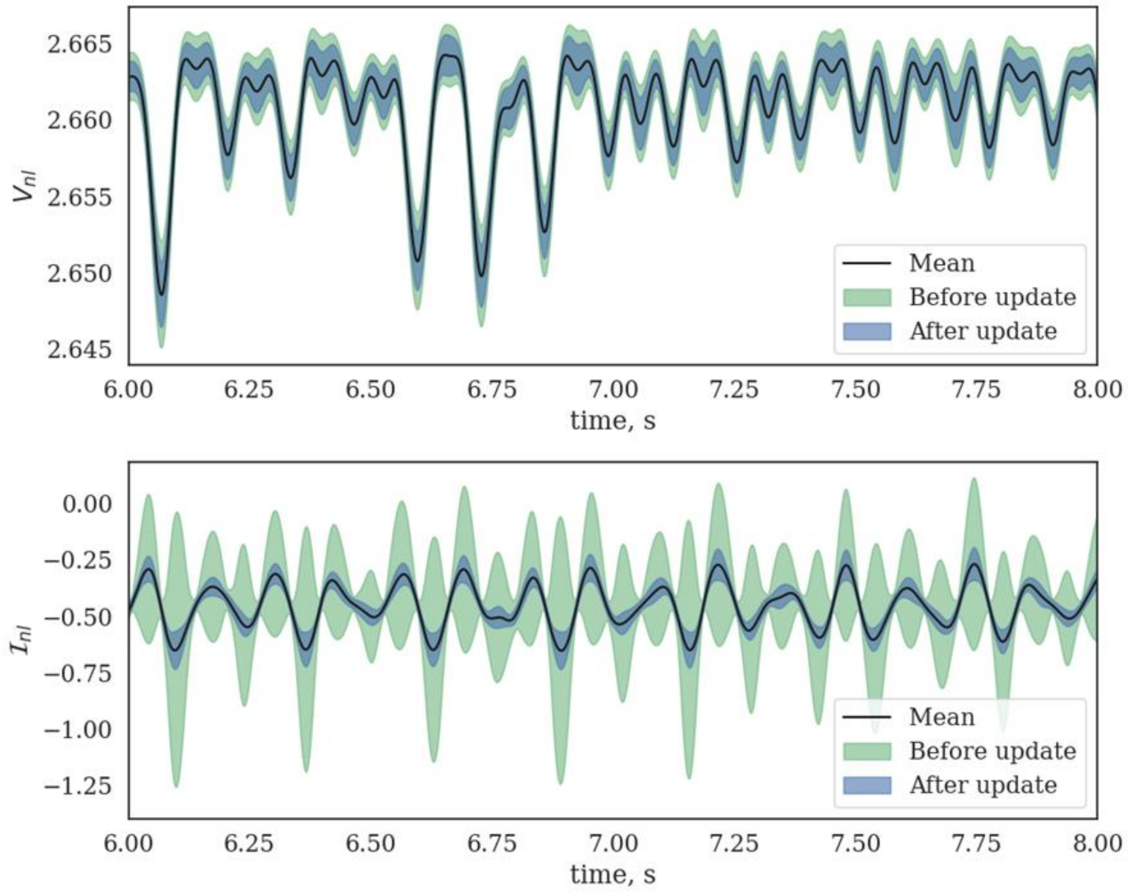


Model updates after having detected damage

Updated variance after re-training

- After having detected damage, one could simply take the system offline and stop monitoring. But depending on the severity of damage, model updating may be desired so that continuous forecasting can continue.
- The model updates were performed by re-training the models with a WS = 3500 time steps for 10,000 epochs (15 minutes). Classical backpropagation methods were used, leveraging the interpretation of stochastic gradient descent as a proper posterior sampler (thus re-training is akin to performing Bayesian inference).

Prediction variance was significantly reduced after model update.



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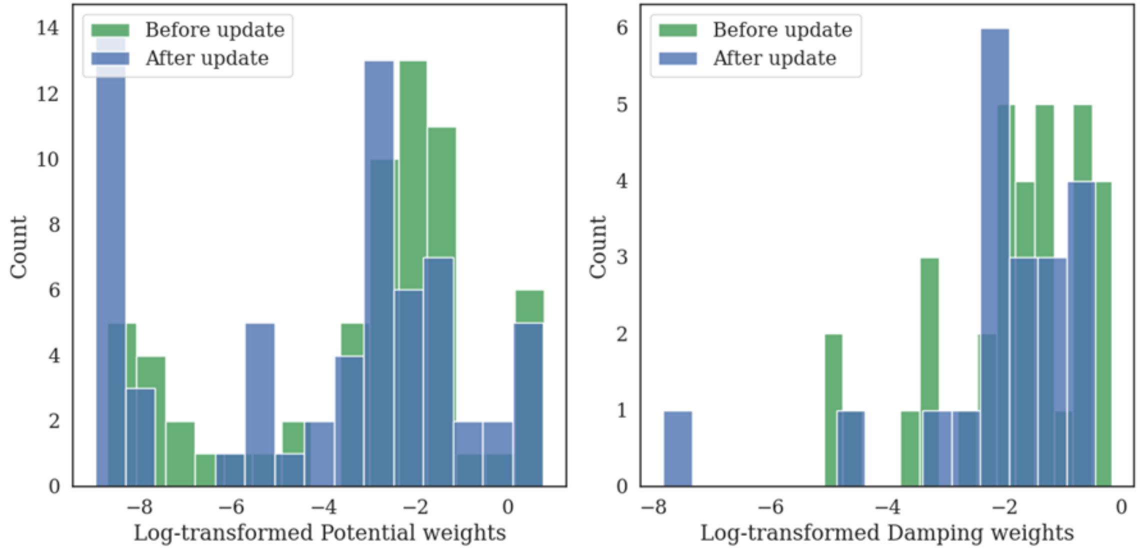
Can we leverage the updated parameters to say something about the type of damage?

Inferring structural change type based on updated parameters

- The neural network weights were updated, so we can explore their statistical distributions to see if we can say something about the nature of the damage or structural change that triggered the update.
- A Kolmogorov-Smirnov two-sample test was performed to compare the two statistical distributions.

$$V_{\mathrm{nl}}(\mathbf{z}) = g_V(\mathbf{h}_V) \sim N(c_V, \Phi_V^T \Phi_V^T)$$

$$\mathscr{I}_{\mathrm{nl}}(\dot{\mathbf{z}}) = g_I(\mathbf{h}_I) \sim N(c_I, \Phi_I^T \Phi_I^T),$$



NL Potential weights p-value: 0.030 < 0.05
NL Damping weights p-value: 0.626 > 0.05

Therefore, the differences in the statistical distribution of NL potential weights are statistically significant while they are not for the damping. We can infer that the structural change is affecting the stiffness rather than the damping, which is correct.

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Conclusions

- We developed a structure-preserving approach for modeling nonlinear structural dynamics while enabling uncertainty quantification for domain shift and damage detection.
- The approach addressed the challenge of partial observability.
- Many more applications of the work not presented here.
- And many more opportunities for extensions and other applications.

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Questions or Comments?

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