Time-Dependent Statistical Finite Element Problems: Unstructured Data, Unknown Observation Operators, and Inversion

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Collaborators and References

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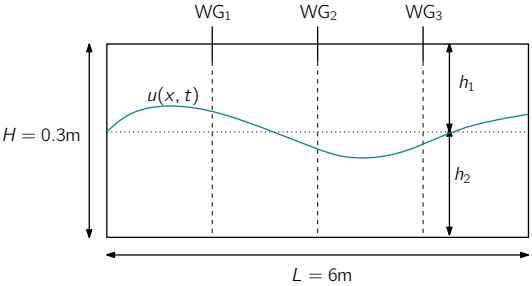
1. Connor Duffin et al. "Statistical Finite Elements for Misspecified Models". *Proceedings of the National Academy of Sciences* (Jan. 2021).
2. Alex Glyn-Davies et al. *Φ-DVAE: Physics-Informed Dynamical Variational Autoencoders for Unstructured Data Assimilation*, July 2023. arXiv: `2209.15609 [physics, stat]`.

Talk Structure

1. Problem Motivation.
2. Statistical Finite Element Methodology.
3. Case Study: Internal Waves Experimental Data.
4. Extending statFEM for Unstructured Data: Φ-DVAE.
5. Case Studies: Φ-DVAE inversion.

Motivation



- Internal waves flow between layers of density-varying water (mean depths h_1, h_2), in a tank of length L and total depth $H = h_1 + h_2$.
- KdV equation models the internal wave profile $u(s,t)$ (deviations from rest):

$$\partial_t u + \alpha u u_s + \beta u_{sss} + c u_s = 0.$$

- Can we synthesise this PDE with measurements $\mathbf{y}_{1:n} = (\mathbf{y}_1, \ldots, \mathbf{y}_n)$ obtained at wave gauges (labelled above)?

Motivation and Goals

However, the KdV equation,

$$\partial_t u + \alpha u u_s + \beta u_{sss} + c u_s = 0,$$

is an idealised model of reality, and may not match the data.

- Parameters: α drives nonlinear advection, β drives dispersion, and c is latent advection: well-known and able to be calculated!
- How to use the data to correct for model mismatch?
- Let $u_n = u(s, n\Delta_t)$ (the model at some discretised time n). To correct for this mismatch we will estimate the posterior $p(u_n \mid \mathbf{y}_{1:n}, \Lambda)$.
- How can we construct this filtering distribution?

Underlying dynamical process

- Use stochastic dynamics. Take the KdV equation:

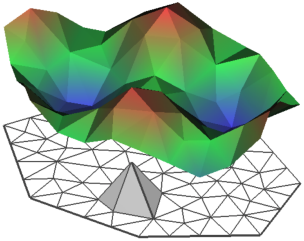
$$\partial_t u + \alpha u u_s + \beta u_{sss} + c u_s = \xi_\theta,$$

  we have $u := u(s,t)$, $s \in \Omega$, $t \in [0,T]$.
- Model uncertainty with a Gaussian process (with θ known):

$$\xi_\theta(s,t) \sim \mathcal{GP}(0, \delta(t-t') \cdot k_\theta(s,s')), \quad k_\theta(s,s') = \rho^2 \exp(-\|s-s'\|^2/(2\ell^2)).$$

In practise we need to discretize: we use FEM.

- Construct a mesh, Ω_h, with mesh-size h: discrete approximation to Ω.
- Use finite elements on the mesh Ω_h, $u(s, n\Delta_t) \approx \sum_{i=1}^{n_u} u_i \phi_i(s)$.
- Hat-functions $\implies \phi_i(s_j) = \delta_{ij}$.
- FEM coefficients $\mathbf{u}(t) = (u_1(t), \ldots, u_{n_u}(t))$.



FEM (from Bakka, H. (2019), arXiv:1803.03765).

Underlying dynamical process: an (implied) prior distribution

- Time discretization: let $\mathbf{u}_n = (u_1(n\Delta_t), \ldots, u_{n_u}(n\Delta_t))$; use Crank-Nicolson for stability.
- Important! We conduct inference over the *basis function coefficients* $\implies$ discrete representation of the process.
- So, on the basis function coefficients we have a Markov process:

$$\mathcal{M}(\mathbf{u}_n, \mathbf{u}_{n-1}) = \mathbf{e}^n, \quad \mathbf{e}^n \sim \mathcal{N}(0, \Delta_t \mathbf{G}),$$

  for $\mathbf{G}_{ij} = \langle \phi_i, \langle k_\theta(\cdot,\cdot), \phi_j \rangle \rangle$. This is our discretized version of KdV!
- This provides the transition densities $p(\mathbf{u}_n \mid \mathbf{u}_{n-1}, \Lambda)$, which in turn provides the prior distribution $p(\mathbf{u}_n \mid \Lambda)$.

This begs the question: how to embed data within this model structure? Nonlinear filtering methods...

Underlying dynamical process: an (implied) prior distribution

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Model-data synthesis

With data $\mathbf{y}_n \in \mathbb{R}^{n_y}$, we write $\mathbf{y}_n = \mathbf{H}\mathbf{u}_n + \varepsilon_n$.

- Observation operator $\mathbf{H} : \mathbb{R}^{n_u} \to \mathbb{R}^{n_y}$.
- Noisy measurements $\varepsilon_n \sim \mathcal{N}(\mathbf{0}, \sigma_n^2 \mathbf{I})$.

And this gives the state-space model

$$\begin{aligned} \mathcal{M}(\mathbf{u}_n, \mathbf{u}_{n-1}) = \mathbf{e}^n, \quad \mathbf{e}^n \sim \mathcal{N}(\mathbf{0}, \Delta_t \mathbf{G}), \quad &\text{(Transition)} \\ \mathbf{y}_n = \mathbf{H}\mathbf{u}_n + \varepsilon_n, \quad \varepsilon_n \sim \mathcal{N}(\mathbf{0}, \sigma_n^2 \mathbf{I}). \quad &\text{(Observation)} \end{aligned}$$

Compute the posterior $p(\mathbf{u}_n \mid \mathbf{y}_{1:n}, \Lambda)$ using nonlinear filtering methods: extended Kalman filter (ExKF).

Extended Kalman filtering

Let's start with $p(\mathbf{u}_{n-1} \mid \mathbf{y}_{1:n-1}, \Lambda) = \mathcal{N}(\mathbf{m}_{n-1}, \mathbf{C}_{n-1})$. Then:

1. Prediction step:

$$\hat{\mathbf{m}}_n \text{ solves } \mathcal{M}(\hat{\mathbf{m}}_n, \mathbf{m}_{n-1}) = 0,$$

$$\hat{\mathbf{C}}_n = \mathbf{J}_n^{-1} \left(\mathbf{J}_{n-1} \mathbf{C}_{n-1} \mathbf{J}_{n-1}^\top + \Delta_t \mathbf{G} \right) \mathbf{J}_n^{-\top},$$

   where $\mathbf{J}_n = \frac{\partial \mathcal{M}}{\partial \mathbf{u}_n}(\hat{\mathbf{m}}_n, \mathbf{m}_{n-1})$. So $p(\mathbf{u}_n \mid \mathbf{y}_{1:n-1}, \Lambda) = \mathcal{N}(\hat{\mathbf{m}}_n, \hat{\mathbf{C}}_n)$.

2. Update step:

$$\mathbf{m}_n = \hat{\mathbf{m}}_n + \left(\mathbf{H}\hat{\mathbf{C}}_n \right)^\top \left(\mathbf{H}\hat{\mathbf{C}}_n \mathbf{H}^\top + \sigma_n^2 \mathbf{I} \right)^{-1} (\mathbf{y}_n - \mathbf{H}\hat{\mathbf{m}}_n)$$

$$\mathbf{C}_n = \hat{\mathbf{C}}_n - \left(\mathbf{H}\hat{\mathbf{C}}_n \right)^\top \left(\mathbf{H}\hat{\mathbf{C}}_n \mathbf{H}^\top + \sigma_n^2 \mathbf{I} \right)^{-1} \mathbf{H}\hat{\mathbf{C}}_n.$$

   Then $p(\mathbf{u}_n \mid \mathbf{y}_{1:n}, \Lambda) = \mathcal{N}(\mathbf{m}_n, \mathbf{C}_n)$.

Aside: scaling to high dimensions

ExKF works for low-dimensional systems but is not scalable! How to scale the method?

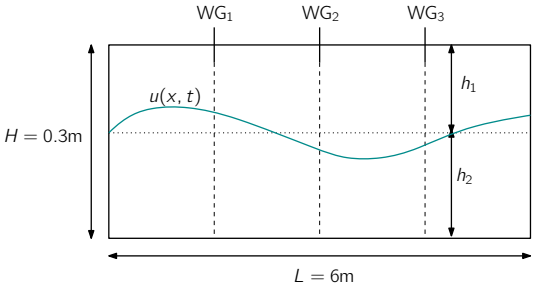
- To compute posterior $p(\mathbf{u}_n \mid \mathbf{y}_{1:n}, \Lambda)$ we use a low-rank Extended Kalman filter (LR-ExKF).
- Idea: $\mathcal{GP}$ covariance matrices (typically) only need a few dominant modes (eigenvector/value pairs) to describe the system. Leverage this inside of ExKF.
- LR-ExKF constructs approximate measure $p(\mathbf{u}_n \mid \mathbf{y}_{1:n}, \Lambda) = \mathcal{N}(\mathbf{m}_n, \mathbf{L}_n\mathbf{L}_n^\top)$, $\mathbf{m}_n \in \mathbb{R}^{n_u}$, $\mathbf{L}_n \in \mathbb{R}^{n_u \times k}$, $k \ll n_u$[1].
- Low-rank approximation is optimal in the ℓ^2 sense so UQ is sensible (not the case with, e.g., EnKF).

[1] Connor Duffin et al. "Low-Rank Statistical Finite Elements for Scalable Model-Data Synthesis". *Journal of Computational Physics* (Aug. 2022).

Case study: KdV experimental data

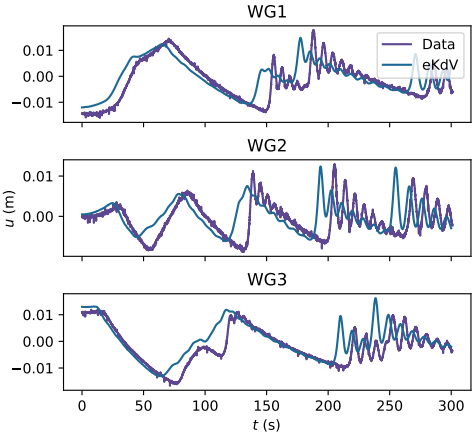
Case study: experimental data

Recall the experimental setup introduced in the first slide:

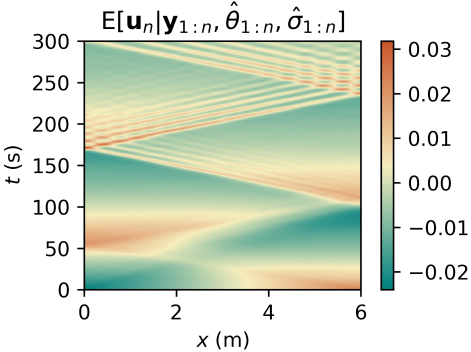


Apply statFEM to compute posterior $p(\mathbf{u}_n \mid \mathbf{y}_{1:n}, \Lambda)$ given the observations at each timestep. Observations $y_n = (u_n^{\mathrm{WG}_1}, u_n^{\mathrm{WG}_2}, u_n^{\mathrm{WG}_3})$, taking each of the $n_T = 1001$ timesteps for $0 \leq t \leq 300$ s.

Case Study: internal waves

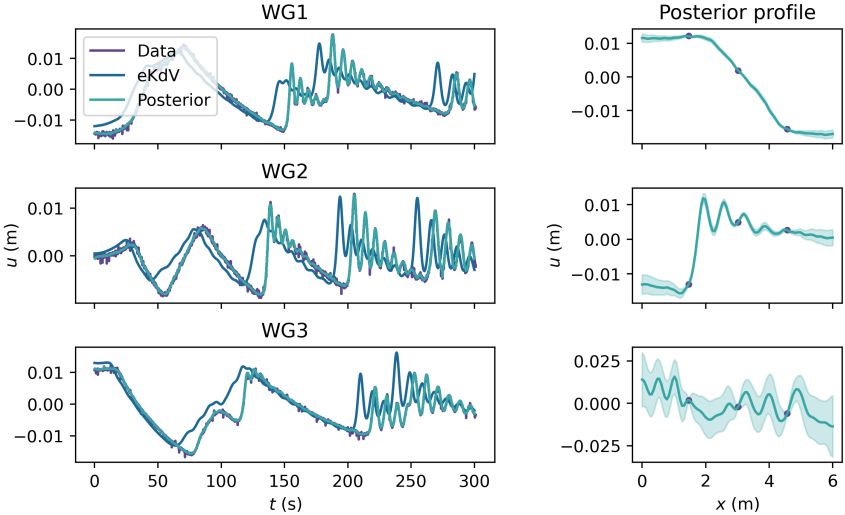


Experimental data and prior mean, up to time $t = 300$s.



KdV posterior mean across space-time grid.

Case study: internal waves



StatFEM posterior measure $p(\mathbf{u}_n \mid \mathbf{y}_{1:n}, \Lambda)$ for the KdV equation: posterior at WG locations (left); posterior wave profile $u(s,t)$ for $t = \{75, 150, 225\}$ s (right).

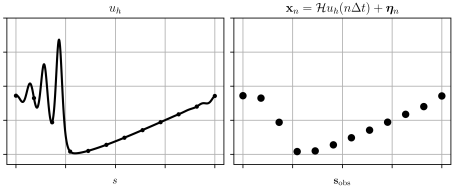
Case Study: Review and Conclusions

- Assimilated data with KdV equation: allows for physics-informed interpolator, with an interpretable posterior distribution.
- Uncertainty quantification is sensible and enables the calibration of simpler physical models with potentially sparse data.
- Next question: what if we don't know the observation operator?

Extending statFEM to Unkown Observation Operators

Known Observation Operator

Phenomena



Known observation operator for KdV

Mechanistic Model

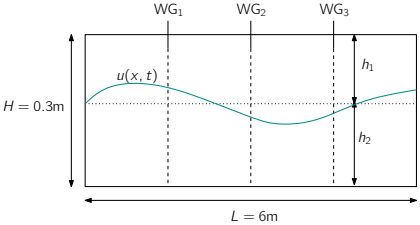
- We know that statFEM gives us transition densities of the form $p(\mathbf{u}_n \mid \mathbf{u}_{n-1}, \Lambda)$.
- These are derived from mechanistic descriptions (PDEs).

- Classical, known observation model.
- Can synthesise observed data with physical model

Observation Model

$$p(\mathbf{x}_n|\mathbf{u}_n) = \mathcal{N}(\mathbf{H}\mathbf{u}_n, \mathbf{R}),$$

$$\mathbf{H} : \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}.$$



Unknown Indirect Observation Operator

What if observation operator is unknown?

- That is, what if $\mathbf{y}_n = \mathcal{G}_\theta(\mathbf{u}_n) + \varepsilon_n$, for some learnable function $\mathcal{G}_\theta(\cdot)$.
- Use neural nets to learn this embedding from unstructured data into known mechanistic description.
- Mechanistic information used to identify the embedding: not to learn approximations to solution fields.
- Example: process is recorded with video camera, multi-channel recordings are taken (e.g., audio data).

How can we synthesise the phenomena with the mechanistic representation when we do not have an observation model?

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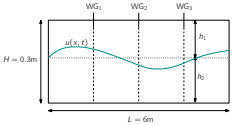
Unknown observation operator: some examples

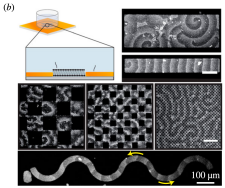
Measurement | **Phenomena** | **Mechanistic Representation**



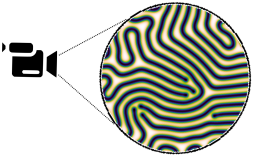
Observed internal wave.

Example: Korteweg-de Vries equation:

$$\partial_t u + \alpha u u_s + \beta u_{sss} + c u_s = 0.$$



Observed species concentrations.

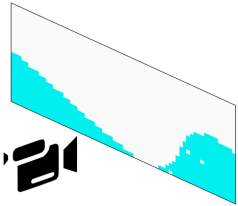


Example: Gray-Scott equation:

$$\partial_t u = D_u \nabla^2 u - uv^2 + F(1-u),$$
$$\partial_t v = D_v \nabla^2 v + uv^2 - (F+k)v.$$

Unknown Observation Operator

Phenomena



Mechanistic Representation

KdV equation:

$$\partial_t u + \alpha u u_s + \beta u_{sss} + c u_s = 0.$$

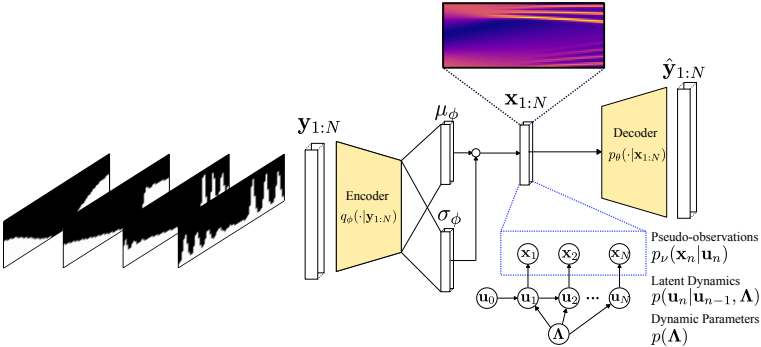
- Observation operator can be approximated with deep neural networks.
- We *posit* an observation operator of the form:

$$p(\mathbf{y}_n | \mathbf{u}_n) = \mathcal{N}(\mathcal{G}_\phi(\mathbf{u}_n), \mathbf{R}), \quad \mathcal{G} : \mathbb{R}^{n_u} \to \mathbb{R}^{n_y \times n_c}.$$

- Learn this embedding of the data to observations of the mechanistic system in a variational inference framework.

Φ-DVAE

- Phenomenological data received through time: $\mathbf{y}_{1:N}$ (e.g., video feeds).
- Encoded to latent mechanistic observations $\mathbf{x}_{1:N}$ using a variational autoencoder (VAE).
- Mechanistic representation embedded into latent space, driving latent stochastic dynamics with statFEM.



Φ-DVAE: Probabilistic Model Structure

We propose the following hierarchical probabilistic model:

- Parameter prior: $\Lambda \sim p(\Lambda)$.
- Transition density: $\mathbf{u}_n \mid \mathbf{u}_{n-1}, \Lambda \sim p(\mathbf{u}_n \mid \mathbf{u}_{n-1}, \Lambda)$ (assumed known form).
- Pseudo-observations: $\mathbf{x}_n \mid \mathbf{u}_n \sim p(\mathbf{x}_n \mid \mathbf{u}_n)$ (assumed known form).
- Decoder distribution: $\mathbf{y}_n \mid \mathbf{x}_n \sim p_\theta(\mathbf{y}_n \mid \mathbf{x}_n)$.

Following VAEs, we also introduce the "encoder" variational approximation, $q_\phi(\mathbf{x}_{1:N} | \mathbf{y}_{1:N}) = \mathcal{N}(\mu_\phi, \sigma_\phi)$, and the parameter posterior $p(\Lambda \mid \mathbf{y}_{1:N}) \approx q_\lambda(\Lambda)$.

How can we conduct joint parameter inference over $\{\Lambda, \theta, \phi\}$?

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Φ-DVAE: Variational Lower Bound

- Encoding, decoding, and model parameters are all jointly learnt through optimising a variational lower bound.
- Evidence lower bound provides a tractable target for optimisation:

$$\log p(\mathbf{y}_{1:N}) \geq \mathbb{E}_{q_\phi(\mathbf{x}_{1:N}|\mathbf{y}_{1:N})}\left[\log \frac{p_\theta(\mathbf{y}_{1:N}|\mathbf{x}_{1:N})}{q_\phi(\mathbf{x}_{1:N}|\mathbf{y}_{1:N})} + \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x}_{1:N} \mid \Lambda) + \log \frac{p(\Lambda)}{q_\lambda(\Lambda)}\right]\right].$$

- First term: encoder/decoder. Second term: pseudo-observations

$$p(\mathbf{x}_{1:N} \mid \Lambda) = \int p(\mathbf{u}_{1:N}, \mathbf{x}_{1:N} \mid \Lambda)\, d\mathbf{u}_{1:N}.$$

Marginalising over the dynamics acts as a "physics informed regulariser". Third term: variational parameter posterior KL divergence.

Φ-DVAE: Case studies

Φ-DVAE: Simulation Studies

- We now go through a selection of simulation studies using Φ-DVAE.
- We look at (variational) parameter inference and filtering inference, $p(\mathbf{u}_{1:n}|\mathbf{x}_{1:n})$.
- We look at 2 particular systems: the classic Lorenz-63 system, and the (hopefully, now-familiar) KdV equation.
- We simulate synthetic data consisting of velocity fields, for the Lorenz-63 case, and video data, for the KdV case. These are our $\mathbf{y}_{1:N}$.
- We aim to learn the mapping from $\mathbf{y}_{1:N} \to \mathbf{x}_{1:N}$, thus inferring the latent state $\mathbf{u}_n$, conditioned on $\mathbf{y}_{1:n}$.

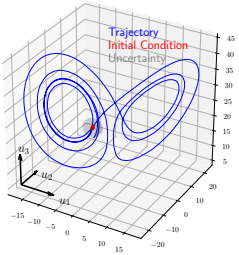
Lorenz-63 Dynamical System: Illustrative Example

Data $\mathbf{y}_{1:N}$ are simulated velocity field measurements, which are modulated by the first dimension of a latent stochastic Lorenz-63 system:

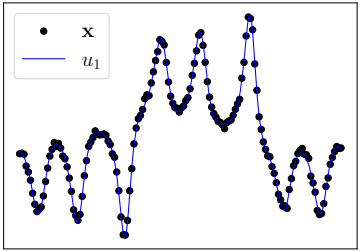
$$du_1 = -\sigma u_1 + \sigma u_2 + dw_1, \quad du_2 = -u_1 u_3 + r u_1 - u_2 + dw_2, \quad du_3 = u_1 u_2 - b u_3 + dw_3,$$

so now $\Lambda = \sigma$, $p(\Lambda) = \mathcal{N}(30, 5^2)$, and $q_\lambda(\Lambda) = \mathcal{N}(\mu_\lambda, \sigma_\lambda^2)$.

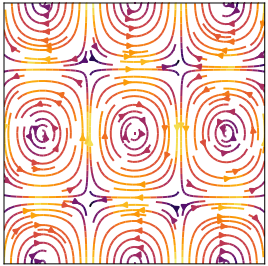
Latent Dynamics: $\mathbf{u}_{1:N}$



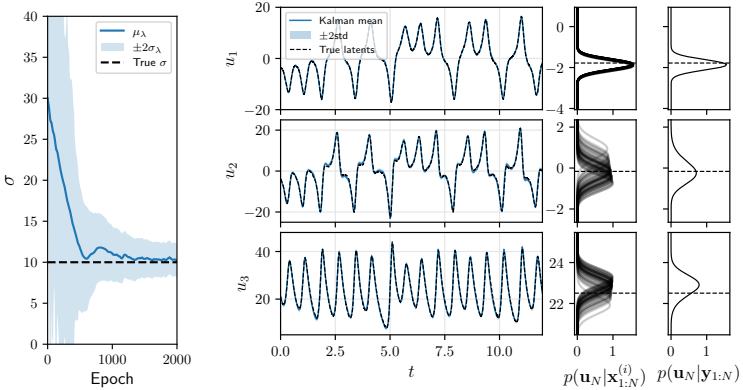
Pseudo-Observations: $\mathbf{x}_{1:N}$



Velocity Field: $\mathbf{y}_N$

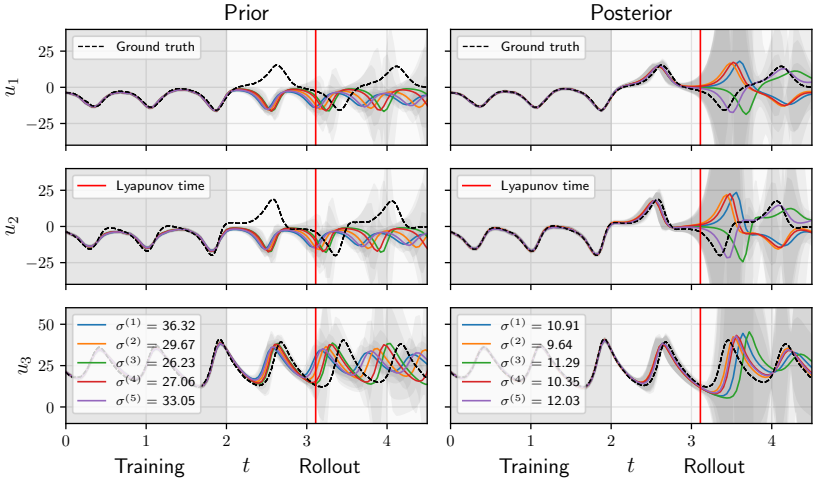


Lorenz-63: State and Parameter Inference



Left: "trace plot" of parameter variational distribution $q_\lambda(\mathbf{\Lambda}) = \mathcal{N}(\mu_\lambda, \sigma^2_\lambda)$, with mean (blue) and ± 2 standard deviations (blue fill). Right: filtering inference for latent states $\mathbf{u}_{1:N}$, where the filtering distribution $p(\mathbf{u}_n|\mathbf{x}_{1:n})$ is plotted with the ground truth $\mathbf{u}_n^{\text{true}}$.

Lorenz-63: Rolling Out Beyond Training



"Rollout": training time indicated with grey-fill, with (left) showing samples generated with the prior (left), and the posterior (right) variational distribution $q_\lambda(\cdot)$.

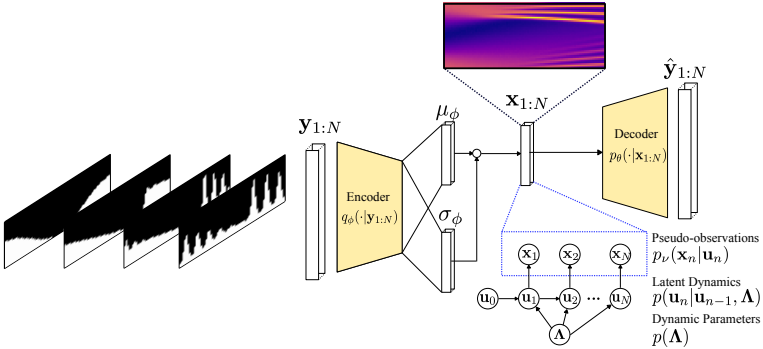
KdV: Learning the Observation Operator and Drag Coefficient

- In this final example we return to KdV: we generate synthetic video data (a sequence of images), giving our $\mathbf{y}_{1:N}$, from a governing KdV equation:

$$\partial_t u + \alpha u u_x + \beta u_{xxx} + \nu u = \xi_\theta.$$

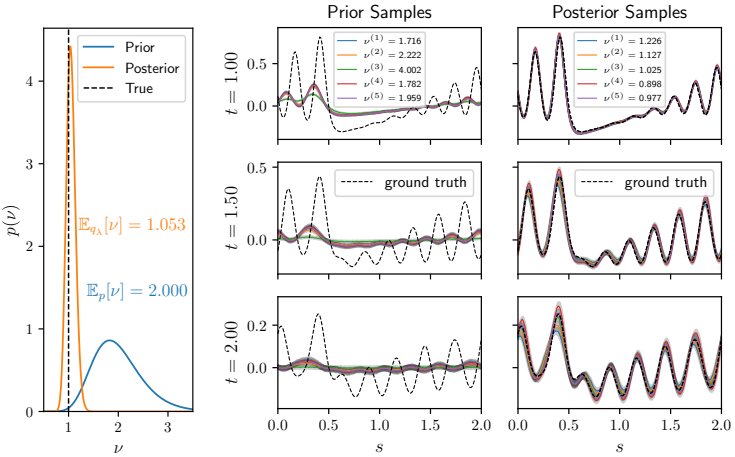
  We jointly estimate the embedding and the drag coefficient ν, so $\Lambda = \nu$, $p(\Lambda) = \mathcal{LN}(2, 0.5^2)$, $q_\lambda(\Lambda) = \mathcal{LN}(\mu_\lambda, \sigma_\lambda^2)$.
- Weakly-informative log-normal prior for the drag coefficient as $\nu > 0$.
- Encoding and decoding networks are MLPs with 3 hidden layers of width 128.

KdV: Learning the Observation Operator and Drag Coefficient



A reminder: video frames $\mathbf{y}_{1:N}$ are encoded to pseudo-observations $\mathbf{x}_{1:N}$ of a latent dynamical system with a known transition density $p(\mathbf{u}_n \mid \mathbf{u}_{n-1}, \Lambda)$. Φ-DVAE infers the encoder $q_\phi(\cdot)$, the decoder $p_\theta(\cdot \mid \mathbf{y}_{1:N})$, *and* parameters $q_\lambda(\cdot)$.

KdV: Results with drag coefficient estimation



Results for KdV with drag: (left) comparison of prior and variational posterior for model parameter $\nu = 1$. Right: latent filtering distribution for prior and posterior parameter estimates.

Conclusions

- Statistical FEM construction allows for the construction of physics-informed interpolators which naturally include nonstationarity.
- Enables interpolation and inference in sparse data settings.
- Interpretable and relatively robust framework to conduct inference with some latent dynamical process.
- Φ-DVAE enables the use of such methods when the mapping to observations is not known, and, when the parameters may be uncertain.
- Additional work on Langevin dynamics samplers for static problems (Akyildiz et al.).
- Current work focusses on applications (shallow water flows) and on generalising the framework to enable parameter estimation.

Thanks!

References I

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References II

Glyn-Davies, Alex, et al. *Φ-DVAE: Physics-Informed Dynamical Variational Autoencoders for Unstructured Data Assimilation*, arXiv:2209.15609, July 2023. https://doi.org/10.48550/arXiv.2209.15609. arXiv: 2209.15609 [physics, stat].