The Statistical Finite Element Method: A Theoretical Foundation for Digital Twins

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- 1. Digital Twin Modelling: what is it?
- 2. Examples of Digital Twin Modelling.
- 3. Finite Elements: The Backbone of Digital Twins.
- 4. Extending Finite Elements to Handle Model Misspecification.
- 5. The Statistical Finite Element Method (statFEM).
- 6. Convergence & Theoretical Guarantees of statFEM.
- 7. Methodology: Nonlinear problems, high dimensions.
- 8. Examples in Oceanography, Structural Mechanics, Nonlinear Oscillators.
- 9. Extensions: Machine Learning methods for unstructured data.
- 10. Conclusions.

Digital Twins: Not Just Hype

- Digital twins are a powerful step forward, following the computational modelling revolution of the 20th century.
- They allow for us to combine powerful mechanistic descriptions of reality with data, with massive impact across engineering and healthcare (among other fields).
- A lot of attention has been focussed on digital twins in the last decade, but there still remains ambiguity as to what they are.
- So what is a digital twin?

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- So what is a digital twin?



- A digital twin is virtual duplicate of a real system, coupling a mathematical model to observations.
- Simple paradigm common in science and engineering, which is highly versatile and universal.
- However, building a DT in practice is complex and challenging.
- Require knowledge of mechanistic models underlying the system, and the relations of these to data.

- 1. Time evolving; ideally over the complete lifecycle of the asset, from design through to end of life.
- 2. Continued connectivity; data, and information passed between the physical and digital twin continuously.
- 3. Versatility; enables highly context dependent digital twins: Entirely bespoke to each individual asset considered.
- 4. Universality; can be applied to all fields of human activity.
- 5. New functionalities; prediction; learning; management; autonomy.
- 6. Reduces uncertainty; can quantify the uncertainties present using the digital twin so decisions can more readily be supported.

Digital Twins: Application Areas



Digital Twins are driving innovation across health, environment, and infrastructure (see, e.g., the Turing Research and Innovation Cluster in Digital Twins).

Digital Twins: Health Examples



Current Cohorts of 20 hearts



The Alan Turing Institute





Digital Twins: Environment Examples in EU





Digital Twins: Infrastructure Examples in UK



Finite Element Simulation: The Workhorse of DTs

Hawk Aircraft Digital Twin Structure



In the Digital Twin of the Hawk aircraft, a core component of the model is Finite Element Simulation.

- Underneath FEM simulations are partial differential equations which describe the physical processes which are occuring within the domain of interest.
- These transcribe physical laws into mathematical objects which we can use and realise analytically, or, computationally.
- For example, conservation of momentum and conservation of mass of fluids gives us the famous Navier-Stokes equations.
- Often numerical methods are the only recourse to interacting with these systems; the most popular being the Finite Element Method.

To illustrate FEM, consider the Poisson equation:

$$-\nabla \cdot (a(x,\Lambda)\nabla u) = f(x), x \in \Omega$$
$$u(x) = 0, x \in \partial \Omega.$$

Note: Ω can be an arbitrary shape, but for a 2D square, the setup looks like:

$$-\nabla \cdot (a(x,\Lambda)\nabla u) = f(x)$$

$$u = 0$$

$$\overline{\Omega}$$

- Now we want to look for solutions u ∈ H¹₀(Ω), and we assume a ∈ L[∞](Ω) and f ∈ L²(Ω). To do so we introduce the weak form.
- Weak form of PDE enables "weak solutions" which lower differentiability requirements and ease solving.
- Letting v ∈ V(Ω) := {v ∈ H¹(Ω) : v = 0 on ∂Ω}, we multiply and integrate to give the weak form:

$$\int_{\Omega} \left(a(x, \Lambda) \nabla u \right) \cdot \nabla v \, \mathrm{d}x = \int_{\Omega} f \cdot v \, \mathrm{d}x, \quad \forall v \in \mathcal{V}(\Omega).$$

Which we can write as the shorthand bilinear form $\mathcal{A}_{\Lambda}(u, v) = \langle f, v \rangle$.

• This is the beginning of our discretization of the PDE.

Introduce degree-*r* polynomial basis functions $\{\phi_i(x)\}_{i=1}^M$, parameterized by a mesh refinement parameter *h*. Subsequently, $\mathcal{V}_h(\Omega) := \operatorname{span}\{\phi_i(x)\}_{i=1}^M$; the space we "look" for solutions in.

Noting that $\mathcal{V}_h(\Omega) \subset \mathcal{V}(\Omega)$, then the variational problem becomes finite-dimensional, $u_h = \sum_{i=1}^{M} u_{h,i}\phi_i(x)$, and so

$$\mathcal{A}_{\Lambda}(u_h,\phi_j)=\langle f,\phi_j\rangle,\quad\forall j=1,\ldots,M.$$

Theorem (FEM convergence)

Let $\|\cdot\|_s$ be the Sobolev norm of degree s. Under technical assumptions for degree-1 polynomial bases $\{\phi_i\}_{i=1}^M$ (i.e. piecewise continuous)

 $||u - u_h||_{L^2(\Omega)} \le Ch^2 ||f||_{L^2(\Omega)}.$

FEM: Solving

The finite-dimensional weak form defines a linear system to solve:

$$Au = b$$
,

$$\mathbf{A}_{ji} = \mathcal{A}_{\Lambda}(\phi_i, \phi_j), \ \mathbf{u}_i = u_{h,i}, \ \mathbf{b}_i = \langle f, \phi_i \rangle.$$

- Deterministic system of equations to solve for the solution vector $\mathbf{u} = \mathbf{A}^{-1}\mathbf{b}$.
- Powerful framework to turn PDE descriptions of physical systems to linear or nonlinear — deterministic systems of equations.
- Advanced numerical linear algebra to solve these systems: for example, Krylov methods, multigrid methods/preconditioners.

FEM: Classical Simulation Examples



FEM is widely used across all engineering, physics, and biomechanics.¹

¹Figures from https://link.springer.com/article/10.1007/s00784-018-2671-z, https://www.mdpi.com/2073-8994/13/2/254/htm, https://www.twscon.com/en/fem_analysis.html

Requirement for Statistical Construction of FEM

- However we know that models are often idealized representations of reality. There is inherent uncertainty due to possible misspecification.
- Roughly, our models should be of the form (see, e.g., Kennedy and O'Hagan)

$$\mathbf{u} pprox \mathbf{A}^{-1}\mathbf{b} + \mathbf{\xi},$$

where $\boldsymbol{\xi}$ describes structural, stochastic, model error.

- This allows for uncertainty quantification, through the admission of possibly misspecified model parameters, enabling:
 - 1. The assimilation of data;
 - 2. The solving of the inverse problem;
 - 3. The combination of deep learning approaches with physical systems.

How do we construct such statistical descriptions of FEM? We will now go through one such approach.

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The Statistical Finite Element Method (statFEM) Construction

statFEM Prior Measure

Consider a stochastically forced elliptic PDE,

$$\begin{aligned} \mathcal{L}u &= -\nabla \cdot (a(x,\Lambda)\nabla u(x)) = \xi, \quad x \in \Omega\\ u &= 0, \quad x \in \partial \Omega, \end{aligned}$$

where $\xi \sim \mathcal{GP}(f, k_{\theta}(x, x'))$, and $\Omega \subset \mathbb{R}^d$ is open and bounded.

We shall assume that a has no unknown parameters and is thus fully deterministic, so $a(x, \Lambda) := a(x)$. It is also assumed $a(\cdot) \in C(\overline{\Omega}) \cap C^1(\Omega)$ and $a(x) > a_0 > 0$ for $x \in \Omega$.

Because \mathcal{L} is linear and deterministic, we have, formally that

$$u \sim \mathcal{GP}(\mathcal{L}^{-1}f, k_{\mathcal{L},\theta}),$$

where

$$k_{\mathcal{L},\theta}(x,y) = (-\mathcal{L})_x^{-1} (-\mathcal{L})_y^{-1} k_{\theta}(x,y).$$

Gaussian process ξ induces hierarchical prior distribution on the space of fields u.

From the Gaussian process we can look at the associated Gaussian measure on $L^2(\Omega)$. Via the weak interpretation of elliptic example we have \mathcal{L}^{-1} : $L^2(D) \to L^2(D)$, and thus

$$u \sim \mu_0 = \mathcal{N}(\mathcal{L}^{-1}f, \mathcal{L}^{-1}C_{\theta}\mathcal{L}^{-*}),$$

where C_{θ} is the covariance operator with kernel $k_{\theta}(\cdot, \cdot)$.

In the function-space setting Gaussian measure provides an appropriate prior measure μ_0 , which can be updated to give the posterior measure μ^y .

Next suppose that data, $\mathbf{y} \in \mathbb{R}^{n_y}$, is observed via $\mathbf{y} = \mathcal{H}u + \eta$, where \mathcal{H} is the continuous observation operator, and $\eta \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$. From this we can define

$$rac{d\mu^y}{d\mu_0}(u)\propto \exp\left(-\Phi(u;\mathbf{y})
ight), \quad \Phi(u;\mathbf{y})=rac{1}{2\sigma^2}\|\mathbf{y}-\mathcal{H}u\|_2^2.$$

The Radon-Nikodym derivative

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defines the posterior Gaussian measure μ^{y} , on the $L^{2}(\Omega)$ function space.

This posterior is absolutely continuous with respect to the prior, $\mu_0 \ll \mu$, inheriting "information" from the prior distribution. The prior defines the starting point for inference and should be well-specified!

Using statFEM, data can update our prior beliefs in the model solution.

Now, when discretised, can we be sure that this prior is converging to something sensible?

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Given a triangulated mesh Ω_h with mesh-size h > 0 we can introduce a finite element approximation with M degrees of freedom.

This leads to approximate prior:

$$u_h(x) \sim \mathcal{GP}(\mathbf{\Phi}_h(x)\mathbf{A}^{-1}\mathbf{b}, \mathbf{\Phi}_h(x)\mathbf{C}_u\mathbf{\Phi}_h(y)^*),$$

where $\Phi_h : \Omega \to \mathbb{R}^M$ is the basis-to-coordinate map. This is an intrinsically finite dimensional distribution as

$$u_h(\cdot) \sim \mathbf{\Phi}_h(\cdot) \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{C}_u),$$

where **A** is the stiffness matrix and C_u is the induced covariance by the FEM basis.

The random fields u and u_h are two Gaussian processes on the same compact domain Ω .

We expect that $u_h \rightarrow u$ as $h \rightarrow 0$ in an appropriate sense. Can we quantify the discretisation error?

For risk-assessment applications, it is important that we can control the error over all aspects of the distributions, i.e. we should be able to control the error in:

- mean
- covariance
- quantiles
- extrema (spatial maximum, spatial minimum distributions)
- other appropriate quantities of interest.

What is the appropriate metric/distance in which to assess the discrepancy between fields u and u_h which captures all of the above?

Challenge: We have no guarantees that the measures u_h and u are not mutually singular on the Hilbert space on which they are both supported.

This precludes analysis based on KL, Fisher, Hellinger or related distances/divergences.

Proposed Approach: Analyse error in p-Wasserstein distance, for $p \ge 2$.

To upper-bound the Wasserstein distance, we exploit a connection between the Wasserstein distance between Gaussian measures and the Procrustes Metric on the respective covariance operators (Masarotto, Panaretos, and Zemel)².

Theorem (Vastly simplified main result)

Suppose that $f \in L^2(\Omega)$ where Ω is open and bounded with Lipshitz boundary and the covariance operator k_{θ} satisfies some technical conditions. Then for given a regular triangulation Ω_h of Ω with mesh size h sufficiently small, there exists $\gamma > 0$ independent of h such that:

$$W_2(\mathcal{D}[u], \mathcal{D}[u_h]) \leq \gamma h^2,$$

where $\mathcal{D}[u]$ is the measure associated with the Gaussian random field u.

²Yanni Papandreou et al. "Theoretical Guarantees for the Statistical Finite Element Method". *SIAM/ASA Journal on Uncertainty Quantification* (Dec. 2023): 1278–1307.

This bound is consistent with $L^2(\Omega)$ a-priori error estimates for deterministic finite element approximations obtained via Aubin-Nitche. In particular, as the variance of the noisy forcing goes to zero, we have that

$$\mathcal{D}[u] \to \delta_{\mathcal{L}^{-1}f}, \text{ and } \mathcal{D}[u_h] \to \delta_{\mathcal{L}_h^{-1}f_h},$$

and

$$W_{2}(\delta_{\mathcal{L}^{-1}f}, \delta_{\mathcal{L}_{h}^{-1}f_{h}}) = \|\mathcal{L}^{-1}f - \mathcal{L}_{h}^{-1}f_{h}\|_{L^{2}(\Omega)} = O(h^{2})$$

Realizing statFEM

Of course, to work with these measures they must be realized in practice. We can write our discretized (stochastic) weak form as

$$\mathcal{A}_{\Lambda}(u_h,\phi_j)=\langle \xi,\phi_j\rangle,\quad \forall j=1,\ldots,M.$$

Which gives the Gaussian law

$$(\mathbf{u} \mid \Lambda, \theta) \sim \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1}\mathbf{G}_{\theta}\mathbf{A}^{-\top}),$$

where $\mathbf{b}_{j} = \langle f, \phi_{j} \rangle$, $\mathbf{A}_{jk} = \mathcal{A}_{\Lambda}(\phi_{j}, \phi_{k})$, $\mathbf{G}_{\theta, jk} = \langle \phi_{j}, \langle k_{\theta}(\cdot, \cdot)\phi_{k} \rangle \rangle$.

- Now suppose that we have observed some data $\mathbf{y} \in \mathbb{R}^N$. Observed on a grid $\mathbf{X} = (\mathbf{x}_1^{\mathrm{obs}}, \dots, \mathbf{x}_N^{\mathrm{obs}})$, with some measurement error.
- Measurement process could be described if full knowledge of true process available.
- Data is a linear combination of the measurement error and the response of the true unknown generating process.
- Define H : ℝ^M → ℝ^N, the discrete observation operator which maps from the domain of the FEM solution: Hu = (u_h(x₁^{obs}),..., u_h(x_N^{obs})).

To deal with possible model misspecification we posit the following data generating process (DGP): $\mathbf{y} = \rho \mathbf{H} \mathbf{u} + \mathbf{d} + \boldsymbol{\varepsilon}$,

- $\mathbf{y} \in \mathbb{R}^N$: observations observed on $\mathbf{X} \in \Omega$.
- $\mathbf{u} \in \mathbb{R}^{M}$: statFEM model, $p(\mathbf{u} \mid \Lambda, \theta) \sim \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1}\mathbf{G}_{\theta}\mathbf{A}^{-\top})$.
- $\mathbf{H} : \mathbb{R}^M \to \mathbb{R}^N$: observation operator.
- d ~ GP(0, K_d): systematic model bias/discrepancy/mismatch (similar ideas from Kennedy-O'Hagan type models — models the functional difference between FEM and observed data).
- $\varepsilon \sim \mathcal{N}(0, \sigma_y^2 \mathbf{I})$: observation noise, could be known from measurement devices or able to be inferred using e.g. marginal likelihood.
- Denote any hyperparameters of **d**, ε as **w**, and assumed **u** \perp **d** \perp ε .

This gives the likelihood $(\mathbf{y} | \mathbf{u}, \mathbf{w}) \sim \mathcal{N}(\mathbf{H}\mathbf{u}_h, \mathbf{K}_d + \sigma^2 \mathbf{I})$, which can be combined with the prior $p(\mathbf{u}_h | \mathbf{f}, \Lambda, \theta)$ to give the posterior

 $p(\mathbf{u} \mid \mathbf{y}, \mathbf{w}, \Lambda, \theta) \propto p(\mathbf{y} \mid \mathbf{u}, \mathbf{w}) \cdot p(\mathbf{u}_h \mid \Lambda, \theta).$

Statistically coherent combination of prior physical knowledge *and* observed data, taking into account model mismatch.

Allows for known information from the physics of the problem to be rigorously incorporated in the inference procedure.

Marginal likelihood:

$$p(\mathbf{y} \mid \mathbf{w}, \Lambda, \theta) = \mathcal{N}(\mathbf{H}\mathbf{m}_u, \mathbf{H}\mathbf{C}_u\mathbf{H}^\top + \mathbf{K}_d + \sigma^2\mathbf{I}).$$

We optimize the marginal likelihood to learn the mismatch hyperparameters.

Characterise the statFEM measures through sampling methods which avoid computing matrix square-roots: unadjusted Langevin methods. Let $\Psi(\mathbf{u}) = \frac{1}{2} \|\mathbf{A}\mathbf{u} - \mathbf{b}\|_{\mathbf{G}^{-1}}^2$, $\nabla_{\mathbf{u}}\Psi(\mathbf{u}) = \mathbf{A}^{\top}\mathbf{G}^{-1}(\mathbf{A}\mathbf{u} - \mathbf{b})$ and³

$$\mathrm{d}\mathbf{u} = -\nabla_{\mathbf{u}}\Psi(\mathbf{u})\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}\mathbf{B}_t,$$

where $(\mathbf{B}_t)_{t\geq 0}$ is a SBM.

The asymptotic law is $(\mathbf{u} | \Lambda, \theta)$, samples $\{\mathbf{u}^{(k)}\}$ generated using the Euler-Maruyama step:

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} - \eta \nabla_{\mathbf{u}} \Psi(\mathbf{u}^{(k)}) + \sqrt{2\eta} \mathbf{Z}^{(k)}.$$

Under Lipschitz gradients this also extends to nonlinear forward models i.e. $\Psi(\textbf{u}) = \frac{1}{2} \|\textbf{A}(\textbf{u}) - \textbf{b}\|_{\textbf{G}^{-1}}^2.$

³Ömer Deniz Akyildiz et al. "Statistical Finite Elements via Langevin Dynamics". *SIAM/ASA Journal on Uncertainty Quantification* (Dec. 2022): 1560–1585.
Denoting the law of the unadjusted Langevin algorithm as $p_k(\mathbf{u} \mid \Lambda, \theta)$, we can provide guarantees for the convergence to the conditional target measure $p(\mathbf{u} \mid \Lambda, \theta)$:

$$\mathsf{KL}(p_k||p) \leq \mathcal{O}(e^{-\eta mk}) + \mathcal{O}(\eta),$$

for some m > 0 (due to strong convexity) and η is the step-size of the ULA.

The bias can be made arbitrarily small with small $\eta > 0$ and $k \to \infty$.

More precisely, we obtain guarantees for the convergence to the conditional target measure $p(\mathbf{u} \mid \Lambda, \theta)$:

$$\mathsf{KL}(p_k||p) \leq e^{-\lambda_{\min}(\mathbf{A}^{\top}\mathbf{G}^{-1}\mathbf{A})\eta k} \mathsf{KL}(p_0,p) + 8\eta d \frac{\lambda_{\max}(\mathbf{A}^{\top}\mathbf{G}^{-1}\mathbf{A})^2}{\lambda_{\min}(\mathbf{A}^{\top}\mathbf{G}^{-1}\mathbf{A})},$$

where $\lambda_{\max}(\cdot)$ and $\lambda_{\min}(\cdot)$ denote the maximum and minimum eigenvalue of a given matrix, respectively.

The same scheme can be used to sample from the posterior, giving a similar convergence rate:

$$\mathsf{KL}(p_k||p) \leq e^{-\lambda_{\min}(\mathbf{C}_y)\eta k}\mathsf{KL}(p_0,p) + 8\eta drac{\lambda_{\max}(\mathbf{C}_y^{-1})^2}{\lambda_{\min}(\mathbf{C}_y^{-1})}.$$

Powerful sampling methodology can be used to generate samples and characterise the prior and posterior statFEM measures.

statFEM Numerical Results: Samplers

For our experiments, we consider the Poisson problem

$$\begin{aligned} -\nabla \cdot (a(x)\nabla u(x)) &= f(x) + \xi(x), \qquad & x \in \Omega, \\ u &= 0, \qquad & x \in \partial\Omega, \end{aligned}$$

where $\Omega = [0,1] \times [0,1]$ and $f(x) \equiv 1$. Stochasticity is defined as

$$\xi \sim \mathcal{GP}(0, \beta^2 \delta(x - x')), \beta = 0.05,$$

log $a(x) \sim \mathcal{GP}(\log(1 + 0.3 \sin(\pi(x_0 + x_1)), k_{\theta}(x, x')))$

where

$$k_{ heta} = 0.1^2 \exp\left(-\frac{\|x - x'\|^2}{2 \cdot 0.2^2}
ight).$$

Upon discretization we have conditional Gaussian

$$p(\mathbf{u}|\theta) = \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1}\mathbf{G}\mathbf{A}^{-\top}).$$

We construct \mathbf{G} by noting that

$$\begin{split} \tilde{G}_{ij} &= \beta^2 \int_{\Omega} \phi_i(x) \int \delta(x - x') \phi_j(x') \, \mathrm{d}x' \, \mathrm{d}x \\ &= \beta^2 \int_{\Omega} \phi_i(x) \phi_j(x) \, \mathrm{d}x' \, \mathrm{d}x = \beta^2 \mathbf{M}_{ij}, \end{split}$$

for the mass matrix **M**. We next make a diagonal approximation such that $\mathbf{G}_{ii} = \sum_{j} \tilde{\mathbf{G}}_{ij}$ (*lumping*).



Prior results for state dimension d = 1089, plotting the sampled values of the log-target (a), and the relative errors on the mean (b). For ULA, the stepsize offers a tradeoff between bias and rate of convergence.

Consider the prior of the previous examples, and now suppose that the data are observed according to a nonlinear observational model:

$$\mathbf{y}_i = \mathbf{H}(\mathbf{u}) + arepsilon_i, \quad arepsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{R}).$$

We take $\mathbf{H}(\cdot)$ to be a sigmoid function to mimic sensor "saturation" past a certain level.

Take n_{obs} observations in total, so the potential for $p(\mathbf{u}|\mathbf{y}, \theta)$ is given by

$$\Psi(\mathbf{u}) = \frac{1}{2} \sum_{i=1}^{n_{obs}} (\mathbf{y}_i - \mathbf{H}(\mathbf{u}))^\top \mathbf{R}^{-1} (\mathbf{y}_i - \mathbf{H}(\mathbf{u})) + \frac{1}{2} (\mathbf{A}\mathbf{u} - \mathbf{b})^\top \mathbf{G}^{-1} (\mathbf{A}\mathbf{u} - \mathbf{b}).$$

Compare MALA, pMALA, ULA, pULA, and pCN.



Nonlinear likelihood: posterior results. The ACF plot is shown for the samples from the FEM coefficient $\mathbf{u}^{(100)}$. All samplers are accurate in the mean, but preconditioning captures the variance.

Time-varying, Nonlinear Dynamics

Use stochastic dynamics. Take a nonlinear, time-evolving system:

$$\partial_t u + \mathcal{L} u + \mathcal{N}(u) = \xi_{\theta},$$

we have $u := u(\mathbf{x}, t)$, $\mathbf{x} \in \Omega$, $t \in [0, T]$. Model uncertainty with a GP (with known θ):

$$\xi_{\theta}(\mathbf{x}, t) \sim \mathcal{GP}(\mathbf{0}, \delta(t - t') \cdot k_{\theta}(\mathbf{x}, \mathbf{x}')).$$

Making a spatial discretisation with FEM, and time-discretisation gives a transition model over the FEM coefficients $\mathbf{u}_n := \mathbf{u}(n\Delta_t)$:

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

Nonlinear dynamics encoded in $\mathcal{M}(\cdot, \cdot)$, implied transition densities $p(\mathbf{u}_n | \mathbf{u}_{n-1}, \Lambda, \theta)$.

Time-dependent data synthesis

With data $\mathbf{y}_n \in \mathbb{R}^{n_y}$, we write $\mathbf{y}_n = \mathbf{H}\mathbf{u}_n + \boldsymbol{\varepsilon}_n$. 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 $p(\mathbf{u}_n | \mathbf{y}_{1:n}, \Lambda, \theta)$ using nonlinear filtering methods such as the extended Kalman filter (ExKF)⁴.

⁴Connor Duffin et al. "Statistical Finite Elements for Misspecified Models". *Proceedings of the National Academy of Sciences* (Jan. 2021).

With the observation model this gives a nonlinear Gaussian state-space model. Assuming $p(\mathbf{u}_{n-1}|\mathbf{y}_{1:n-1}) = \mathcal{N}(\mathbf{m}_{n-1}, \mathbf{C}_{n-1})$ we compute the posterior $p(\mathbf{u}_n|\mathbf{y}_{1:n})$ via filtering:

- 1. Prediction: $p(\mathbf{u}_n | \mathbf{y}_{1:n-1}) = \int p(\mathbf{u}_n | \mathbf{u}_{n-1}, \mathbf{y}_{1:n-1}) p(\mathrm{d}\mathbf{u}_{n-1} | \mathbf{y}_{1:n-1}).$
- 2. Update: $p(\mathbf{u}_n | \mathbf{y}_{1:n}) \propto p(\mathbf{y}_n | \mathbf{u}_n) p(\mathbf{u}_n | \mathbf{y}_{1:n-1}).$

This gives the Gaussian $p(\mathbf{u}_n | \mathbf{y}_{1:n}) = \mathcal{N}(\mathbf{m}_n, \mathbf{C}_n) \implies$ describes uncertainty with solution given all information up to and including current time $n\Delta_t$. Scaled with low-rank approaches.

Conditioning procedure for time-dependent problems

The ExKF is given by, if one assumes that $p(\mathbf{u}_{n-1} | \mathbf{y}_{1:n-1}, \theta) \sim \mathcal{N}(\mathbf{m}_{n-1}, \mathbf{C}_{n-1})$:

1. (*Prediction step*) Solve for $\hat{\mathbf{m}}_n$, $\mathcal{M}_{\Lambda}(\hat{\mathbf{m}}_n, \mathbf{m}_{n-1}) = \mathbf{0}$, and update the covariance matrix

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

 ${f J}_{\cdot}$ is the Jacobian of the the nonlinear ${\cal M}(\cdot,\cdot).$

2. (Update step) Set the observed marginal likelihood covariance $\mathbf{S}_n = \mathbf{H}_n \hat{\mathbf{C}}_n \mathbf{H}_n^\top + \sigma_n^2 \mathbf{I}$, and compute a standard Kalman update on the mean

$$\mathbf{m}_n = \hat{\mathbf{m}}_n + \hat{\mathbf{C}}_n \mathbf{H}_n^\top \mathbf{S}_n^{-1} (\mathbf{y}_n - \mathbf{H}_n \hat{\mathbf{m}}_n).$$

and the covariance

$$\mathbf{C}_n = \hat{\mathbf{C}}_n - \hat{\mathbf{C}}_n \mathbf{H}_n^\top \mathbf{S}_n^{-1} \mathbf{H}_n \hat{\mathbf{C}}_n$$

Note that this general procedure is exact for linear models - the Jacobians J_n just become the appropriate linear combiations of FEM matrices (e.g. the mass/stiffness matrices).

Aside: scaling to high dimensions

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

- To compute posterior p(u_n | y_{1:n}, Λ) we use a low-rank Extended Kalman filter (LR-ExKF).
- Idea: *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 $p(\mathbf{u}_n | \mathbf{y}_{1:n}, \Lambda) = \mathcal{N}(\mathbf{m}_n, \mathbf{L}_n \mathbf{L}_n^{\top}),$ $\mathbf{m}_n \in \mathbb{R}^{n_u}, \ \mathbf{L}_n \in \mathbb{R}^{n_u \times k}, \ k \ll n_u^{-5}.$
- Low-rank approximation is optimal in the ℓ^2 sense so UQ is sensible (not the case with, e.g., EnKF).

⁵Connor Duffin et al. "Low-Rank Statistical Finite Elements for Scalable Model-Data Synthesis". *Journal of Computational Physics* (Aug. 2022).

Examples



• Digital twin of Staffordshire bridge: how to combine sensor data with FEM model, acknowledging model misspecification and wanting UQ?⁶.

⁶Eky Febrianto et al. "Digital Twinning of Self-Sensing Structures Using the Statistical Finite Element Method". *Data-Centric Engineering* (2022): e31.

- Use FEM model with subdivision surfaces, to arrive at the usual Gaussian prior: $p(\mathbf{u}) = \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1}\mathbf{G}\mathbf{A}^{-\top})$. In this example there are no unknown parameters Λ , θ , so uncertainty in the prior only comes in stochastic forcing.
- Posit the same DGP: $\mathbf{y} = \rho \mathbf{H} \mathbf{u} + \mathbf{d} + \eta$, assuming as previous $\mathbf{d} \sim \mathcal{N}(0, \mathbf{K}_d)$, and $\eta \sim \mathcal{N}(0, \sigma_e^2 \mathbf{I})$.
- Covariance K_d is given from a squared-exponential kernel, with parameters σ_d, and ℓ_d, so hyperparameters that need to be estimated are w = {ρ, σ_d, ℓ_d}.
- Data Y = [y₁, y₂,..., y_{n_o}] ∈ ℝ<sup>n_y×n_o consists of n_o = 501 observations at n_y = 40 sensors over a two-second observation window t ∈ [1,3] s, in which a T1-type train with four carriages passes over the bridge.
 </sup>
- MCMC estimates \mathbf{w} , setting them to fixed $\mathbf{w}^* = \mathbb{E}[\mathbf{w} | \mathbf{Y}]$, using prior $p(\mathbf{w}) \propto 1$.
- Qol: posterior measure $p(\mathbf{Hu} | \mathbf{y}, \mathbf{w}^*)$, at times t = 1 s, t = 2 s, and t = 3 s.

Staffordshire bridge



Simulated bridge displacements, using the FEM forward model.



FEM strain results with experimental data, across all observation times.



Hyperparameter w estimates from MCMC, $w^* = \mathbb{E}[w]$ shown as a dashed red line.



Posterior results for the statFEM posterior, shown as the projected measure $p(Hu | Y, w^*)$. 51/80

Staffordshire Bridge Example: Takeaways

- Statistically coherent FEM model of Staffordshire railway bridge, with complete uncertainty quantification, via statFEM
- Acknowledgement of misspecification enables inference, model hyperparameters calibrated with data.
- Sensible UQ with models calibrated with data.

Case Study: Nonlinear Internal Waves



- 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(x, t) (deviations from rest):

$$\partial_t u + \alpha u u_x + \beta u_{xxx} + c u_x + \nu u = \dot{\xi}.$$

Can we synthesise this PDE with measurements y_{1:n} = (y₁,..., y_n) obtained at wave gauges (labelled above)?

Case Study: Nonlinear Internal Waves



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

Case Study: internal waves



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



KdV posterior mean across space-time grid.

Case study: internal waves



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

Internal Waves: Takeaways

- 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.
- Conjecture: physically sensible way of incorporating nonstationarity into GP-type models → nonstationarity driven by dynamics.

Apply the statFEM methodology to the Oregonator system of equations:⁷

$$u_t = \frac{1}{\varepsilon} \left(u(1-u) - fv \frac{u-q}{u+q} \right) + D_u \nabla^2 u + \dot{\xi}^u,$$
$$v_t = u - v + D_v \nabla^2 v + \dot{\xi}^v,$$
$$u := u(x, t), \ v := v(x, t), \ x \in [0, L] \times [0, L], \ t \in [0, T],$$

using zero-flux boundary conditions.

Sparse measurements and misspecified initial conditions; "spiral-wave" regime: $(f, q, \varepsilon) = (2, 0.002, 0.02), (D_u, D_v) = (1, 0.6).$

Stochastic Oregonator system implicitly defines the prior distribution: set $\xi^u = 0$, induce uncertainty through *v*-component:

$$\mathcal{G}^{\mathsf{v}}(x,t)\sim \mathcal{GP}(0,\delta(t-t')\cdot k_{ heta}(x,x')), \quad k_{ heta}(x,x')=
ho^2\exp(-\|x-x'\|_2^2/(2\ell^2)).$$

⁷Connor Duffin et al. "Low-Rank Statistical Finite Elements for Scalable Model-Data Synthesis". *Journal of Computational Physics* (Aug. 2022).

Discretise to give u_n and v_n — the FEM coefficients at time n∆_t — and compute joint posterior with LR-ExKF:

$$p(\mathbf{u}_n, \mathbf{v}_n \mid \mathbf{y}_{1:n}, \Lambda, \theta) \sim \mathcal{N}(\mathbf{m}_n, \mathbf{L}_n \mathbf{L}_n^{\top}).$$

- StatFEM posterior mean has blurred initial condition: model is misspecified through incorrect initialisation.
- Noisy data, only single component observed: $\mathbf{y}_n = \mathbf{H}\mathbf{v}_n + \eta_n$, $\eta_n \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$.



Initial conditions: statFEM (left) and true (right). We observe the \mathbf{v}_n component only $\implies \mathbf{u}_n$ misspecified and unobserved.



Top: statFEM posterior means $(\mathbf{m}_n^u, \mathbf{m}_n^v)$ and observed data (\mathbf{y}_n) at time t = 5. Bottom: statFEM posterior variances $(\text{diag}(\mathbf{C}_n))$ on the u and v components, at time t = 5.



Leading-order covariance modes for the spiral-wave problem \implies variance decomposes surrounding the main spiral feature.

Relative errors show the data generating process is tracked:

$$\frac{\|\mathbf{m}_n^u - \mathbf{u}_n^{\mathsf{DGP}}\|_2}{\|\mathbf{u}_n^{\mathsf{DGP}}\|_2}, \quad \frac{\|\mathbf{m}_n^v - \mathbf{v}_n^{\mathsf{DGP}}\|_2}{\|\mathbf{v}_n^{\mathsf{DGP}}\|_2}.$$



Effective rank of covariance:

$$D_{\rm eff} = \frac{\sum_{j=1}^k \sqrt{\lambda_j}}{\sum_{j=1}^k \lambda_j}.$$



Reaction Diffusion: Takeaways

- Low-rank approximation scales the method to high dimensionalities, enabling application of the method to complex "real world" systems.
- Uncertainty quantification is again sensible, and initial condition misspecification is calibrated with data.
- Enables inference in systems which may be partially observed.

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



Observed internal wave.



Mechanistic Representation

Example: Korteweg-de Vries equation:

 $\partial_t u + \alpha u u_x + \beta u_{xxx} + c u_x = 0.$

Example: Gray-Scott equation:

$$\begin{split} \partial_t u &= D_u \nabla^2 u - u v^2 + F(1-u), \\ \partial_t v &= D_v \nabla^2 v + u v^2 - (F+k) v. \end{split}$$



Observed species concentrations.



Unknown Observation Operator

Phenomena



Mechanistic Representation

KdV equation:

$$\partial_t u + \alpha u u_x + \beta u_{xxx} + c u_x = 0.$$

- 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**⁸

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



⁸Alex Glyn-Davies et al. Φ-DVAE: Physics-Informed Dynamical Variational Autoencoders for Unstructured Data Assimilation, July 2023. arXiv: 2209.15609

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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: $\mathbf{x}_n | \mathbf{u}_n \sim p(\mathbf{x}_n | \mathbf{u}_n)$ (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 $p(\Lambda | \mathbf{y}_{1:N}) \approx q_{\lambda}(\Lambda)$.

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

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

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.

- 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 **y**_{1:N}.
- We aim to learn the mapping from y_{1:N} → x_{1:N}, thus inferring the latent state u_n, conditioned on 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:

 $du_1 = -\sigma u_1 + \sigma u_2 + dw_1, \quad du_2 = -u_1 u_3 + ru_1 - u_2 + dw_2, \quad du_3 = u_1 u_2 - bu_3 + dw_3,$

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: $\mathbf{x}_{1:N}$









Left: "trace plot" of parameter variational distribution $q_{\lambda}(\Lambda) = \mathcal{N}(\mu_{\lambda}, \sigma_{\lambda}^2)$, 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 $q_{\lambda}(\cdot)$.

In this final example we return to KdV: we generate synthetic video data (a sequence of images), giving our 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 $p(\mathbf{u}_n | \mathbf{u}_{n-1}, \Lambda)$. Φ -DVAE infers the encoder $q_{\phi}(\cdot)$, the decoder $p_{\theta}(\cdot | \mathbf{y}_{1:N})$, 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.

StatFEM synthesises data and FEM models via the posterior $p(\mathbf{u}_n \mid \mathbf{y}_{1:n}, \Lambda)$.

- Works in nonlinear, time-dependent models, enabling interpolation and inference in sparse data settings.
- Quantifies uncertainty and robust to model misspecification.



All code on Github!

• Demonstrated through structural mechanics, fluid dynamics, nonlinear oscillators, and machine learning extensions.

More broadly: statFEM broadly provides a fundamental methodology to underpin modern digital twin models; which is derived from a statistically coherent construction.

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