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Stochastic (Partial) Differential Equations and Gaussian Processes

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Why use S(P)DE solvers for GPs?

- The $O(n^3)$ computational complexity is always a challenge.
- Latent force models combine PDE/ODEs with GPs.
- What do we get:
  - Sparse approximations developed for SPDEs.
  - Reduced rank Fourier/basis function approximations.
  - The use of Markov properties and Markov approximations.
  - State-space methods for SDEs/SPDEs.
  - Path to non-Gaussian processes.
- Downsides:
  - Approximations of non-parametric models with parametric models.
  - Approximations of a non-Markovian models as Markovian.
  - Mathematics can become messy.

Kernel vs. SPDE representations of GPs

GP model $\mathbf{x} \in \mathbb{R}^d$, $t \in \mathbb{R}$	Equivalent Static SPDE model
Homogenous $k(\mathbf{x}, \mathbf{x}')$	SPDE model $$\mathcal{L}\, f(\mathbf{x}) = w(\mathbf{x})$$
Stationary $k(t, t')$	State-space/Itô-SDE model $$d\mathbf{f}(t) = \mathbf{A}\, \mathbf{f}(t)\, dt + \mathbf{L}\, dW(t)$$
Homogenous/stationary $k(\mathbf{x}, t; \mathbf{x}', t')$	Stochastic evolution equation $$\partial_t \mathbf{f}(\mathbf{x}, t) = \mathcal{A}_x\, \mathbf{f}(\mathbf{x}, t)\, dt + \mathbf{L}\, dW(\mathbf{x}, t)$$

Basic idea of SPDE inference on GPs [1/2]

- Consider e.g. the stochastic partial differential equation:

$$\frac{\partial^2 f(x,y)}{\partial x^2} + \frac{\partial^2 f(x,y)}{\partial y^2} - \lambda^2 f(x,y) = w(x,y)$$

- Fourier transforming gives the spectral density:

$$S(\omega_x, \omega_y) \propto \left(\lambda^2 + \omega_x^2 + \omega_y^2\right)^{-2}.$$

- Inverse Fourier transform gives the covariance function:

$$k(x,y;x',y') = \frac{\sqrt{(x-x')^2 + (y-y')^2}}{2\lambda} K_1(\lambda \sqrt{(x-x')^2 + (y-y')^2})$$

- But this is just the Matérn covariance function.
- The corresponding RKHS is actually a Sobolev space.

Basic idea of SPDE inference on GPs [2/2]

- More generally, SPDE for some linear operator $\mathcal{L}$:

$$\mathcal{L}\, f(\mathbf{x}) = w(\mathbf{x})$$

- Now f is a GP with precision and covariance operators:

$$\mathcal{K}^{-1} = \mathcal{L}^* \, \mathcal{L}$$
$$\mathcal{K} = (\mathcal{L}^* \, \mathcal{L})^{-1}$$

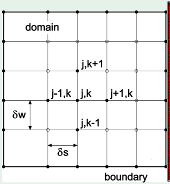
- Idea: approximate $\mathcal{L}$ or $\mathcal{L}^{-1}$ using PDE/ODE methods:
  1. Finite-differences/FEM methods lead to sparse precision approximations.
  2. Fourier/basis-function methods lead to reduced rank covariance approximations.
  3. Spectral factorization leads to state-space (Kalman) methods which are time-recursive (or sparse in precision).

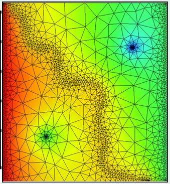
Finite-differences/FEM – sparse precision

- Basic idea:

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x+h) - f(x)}{h}$$

$$\frac{\partial^2 f(x)}{\partial x^2} \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$





- We get an SPDE approximation $\mathcal{L} \approx \mathbf{L}$, where $\mathbf{L}$ is sparse
- The precision operator approximation is then sparse:

$$\mathcal{K}^{-1} \approx \mathbf{L}^{\mathsf{T}} \mathbf{L} = \text{sparse}$$

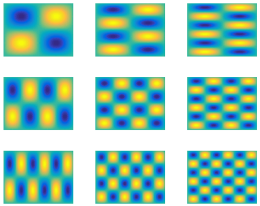
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

Classical and random Fourier methods – reduced rank approximations and FFT

- Approximation:

$$f(\mathbf{x}) \approx \sum_{\mathbf{k} \in \mathbb{N}^d} c_{\mathbf{k}} \exp\left(2\pi\,\mathrm{i}\,\mathbf{k}^\mathsf{T}\,\mathbf{x}\right)$$

$$c_{\mathbf{k}} \sim \text{Gaussian}$$



- We use less coefficients $c_{\mathbf{k}}$ than the number of data points.
- Leads to reduced-rank covariance approximations

$$k(\mathbf{x}, \mathbf{x}') \approx \sum_{|\mathbf{k}| \le N} \sigma_{\mathbf{k}}^2 \exp\left(2\pi\,\mathrm{i}\,\mathbf{k}^\mathsf{T}\,\mathbf{x}\right) \exp\left(2\pi\,\mathrm{i}\,\mathbf{k}^\mathsf{T}\,\mathbf{x}'\right)^*$$

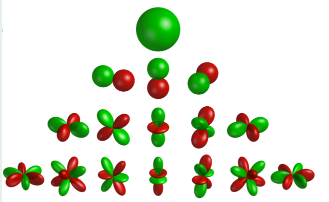
- Truncated series, random frequencies, FFT, ...

Hilbert-space/Galerkin methods – reduced rank approximations

- Approximation:

$$f(\mathbf{x}) \approx \sum_i c_i \, \phi_i(\mathbf{x})$$

$$\langle \phi_i, \phi_j \rangle_H \approx \delta_{ij}, \text{ e.g. } \nabla^2 \phi_i = -\lambda_i \, \phi_i$$



- Again, use less coefficients than the number of data points.
- Reduced-rank covariance approximations such as

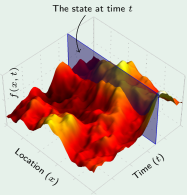
$$k(\mathbf{x}, \mathbf{x}') \approx \sum_{i=1}^{N} \sigma_i^2 \, \phi_i(\mathbf{x}) \, \phi_i(\mathbf{x}').$$

- Wavelets, Galerkin, finite elements, . . .

State-space methods – Kalman filters and sparse precision

- Approximation:

$$S(\omega) \approx \frac{b_0 + b_1\,\omega^2 + \cdots + b_M\,\omega^{2M}}{a_0 + a_1\,\omega^2 + \cdots + a_N\,\omega^{2N}}$$



- Results in a linear stochastic differential equation (SDE)

$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- More generally stochastic evolution equations.
- $O(n)$ GP regression with Kalman filters and smoothers.
- Parallel block-sparse precision methods $\longrightarrow O(\log n)$.

State-space methods – Kalman filters and sparse precision (cont.)

Example (Matérn class 1d)

The Matérn class of covariance functions is

$$k(t,t') = \sigma^2 \, \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{\ell} |t-t'| \right)^{\nu} K_\nu \left(\frac{\sqrt{2\nu}}{\ell} |t-t'| \right).$$

When, e.g., $\nu = 3/2$, we have

$$\begin{aligned} d\mathbf{f}(t) &= \begin{pmatrix} 0 & 1 \\ -\lambda^2 & -2\lambda \end{pmatrix} \mathbf{f}(t)\, dt + \begin{pmatrix} 0 \\ q^{1/2} \end{pmatrix} dW(t), \\ f(t) &= \begin{pmatrix} 1 & 0 \end{pmatrix} \mathbf{f}(t). \end{aligned}$$

State-space methods – Kalman filters and sparse precision (cont.)

Example (2D Matérn covariance function)

- Consider a space-time Matérn covariance function

$$k(x,t;x',t') = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\,\frac{\rho}{l}\right)^{\nu} K_{\nu}\left(\sqrt{2\nu}\,\frac{\rho}{l}\right).$$

  where we have $\rho = \sqrt{(t-t')^2 + (x-x')^2}$, $\nu = 1$ and $d = 2$.

- We get the following representation:

$$d\mathbf{f}(x,t) = \begin{pmatrix} 0 & 1 \\ \frac{\partial^2}{\partial x^2} - \lambda^2 & -2\sqrt{\lambda^2 - \frac{\partial^2}{\partial x^2}} \end{pmatrix} \mathbf{f}(x,t)\,dt + \begin{pmatrix} 0 \\ 1 \end{pmatrix} dW(x,t).$$

What then?

- Inducing point methods = basis function methods
- Inference on the basis functions/point-locations/etc.
- Non-Gaussian processes, non-Gaussian likelihoods.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in measurement model.
- State-space stochastic control in Gaussian processes and LFMs.
- SPDE methods for SVMs
- Kernel embedding of S(P)DEs
- Deep S(P)DE models