



Aalto University
School of Electrical
Engineering

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.
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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:

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

- 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.

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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:

- Finite-differences/FEM methods lead to sparse precision approximations.
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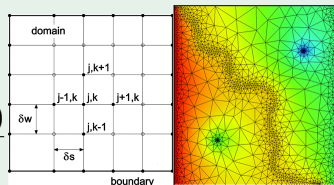
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Finite-differences/FEM – sparse precision

- 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:

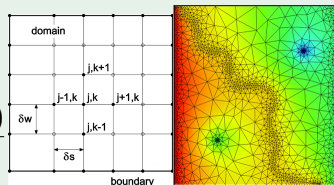
$$\mathcal{K}^{-1} \approx \mathbf{L}^T \mathbf{L} = \text{sparse}$$

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

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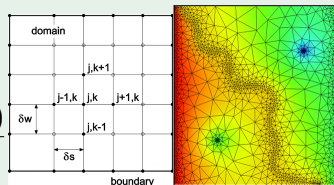
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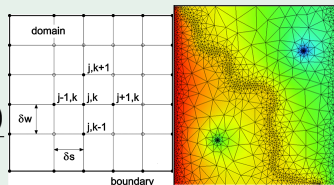
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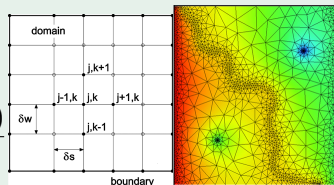
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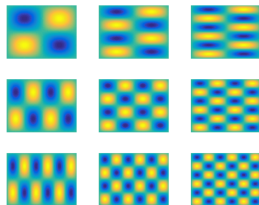
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Classical and random Fourier methods – reduced rank approximations and FFT

- Approximation:

$$f(\mathbf{x}) \approx \sum_{\mathbf{k} \in \mathbb{N}^d} \alpha_{\mathbf{k}} \exp(2\pi i \mathbf{k}^T \mathbf{x})$$

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



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

$$k(\mathbf{x}, \mathbf{x}') \approx \sum_{|\mathbf{k}| \leq N} \sigma_{\mathbf{k}}^2 \exp(2\pi i \mathbf{k}^T \mathbf{x}) \exp(2\pi i \mathbf{k}^T \mathbf{x}')^*$$

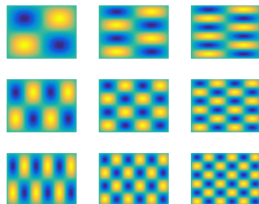
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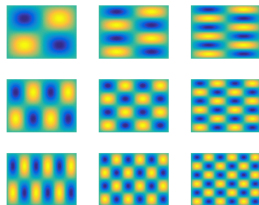
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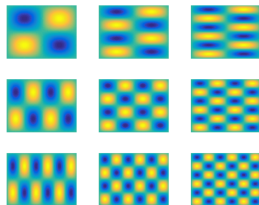
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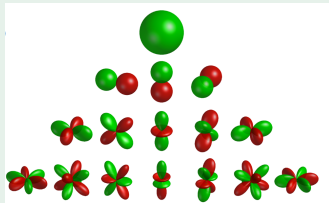
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Hilbert-space/Galerkin methods – reduced rank approximations

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

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



- Again, use less coefficients than the number of data points.
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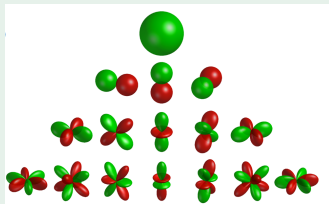
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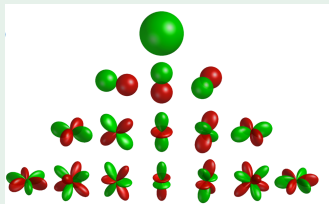
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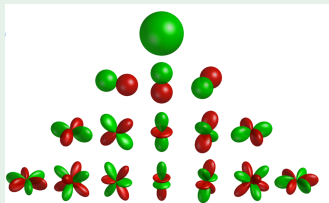
- Wavelets, Galerkin, finite elements, ...

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

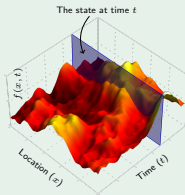
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State-space methods – Kalman filters and sparse precision

- Approximation:

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



- Results in a linear stochastic differential equation (SDE)

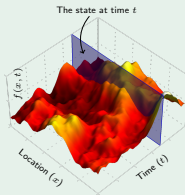
$$d\mathbf{f}(t) = \mathbf{A} \mathbf{f}(t) dt + \mathbf{L} d\mathbf{W}$$

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

State-space methods – Kalman filters and sparse precision

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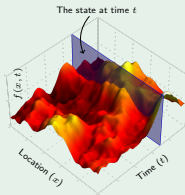
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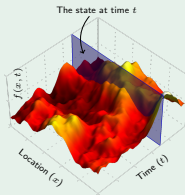
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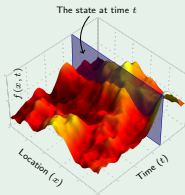
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State-space methods – Kalman filters and sparse precision (cont.)

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

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

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:

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

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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.
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- SPDE methods for SVMs
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