Aalto University
School of Electrical Engineering

Stochastic (Partial) Differential Equation Methods for Gaussian Processes

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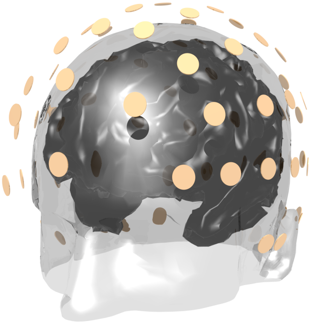
- Observed: Electromagnetic field (potential / flux).



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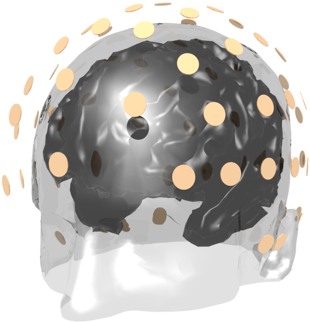

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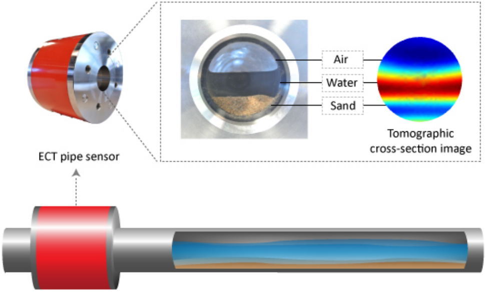

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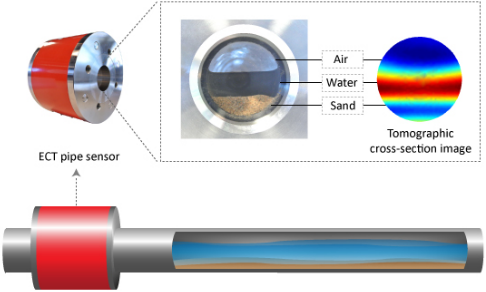

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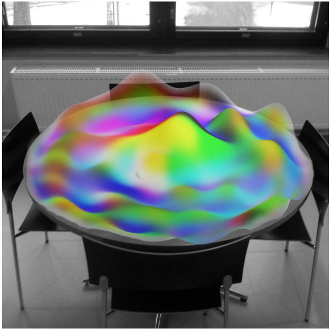

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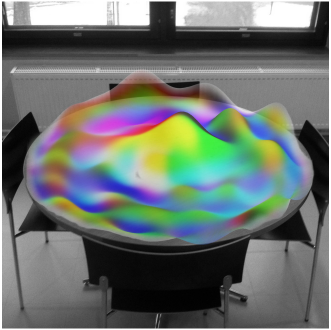

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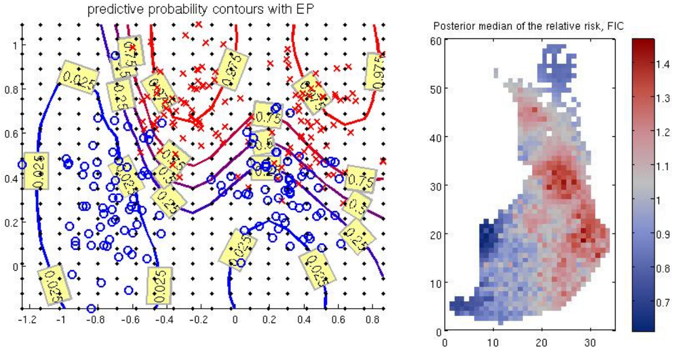

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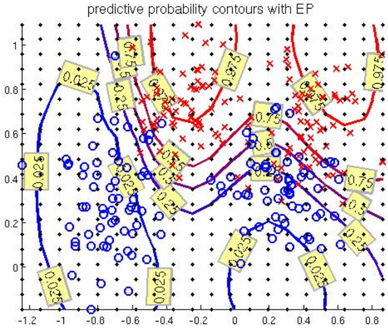

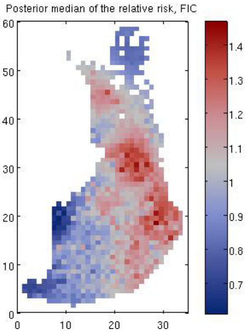

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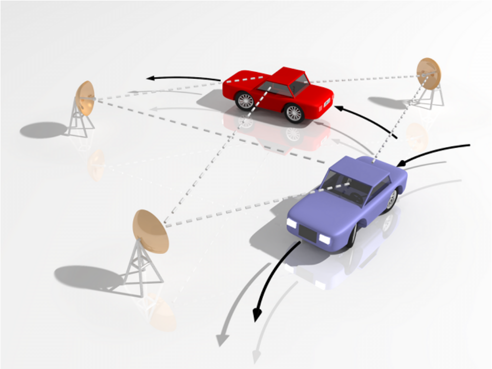

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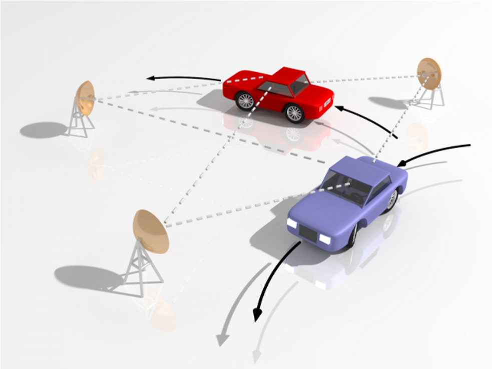

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Gaussian process regression models

- A typical GP regression problem:

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f(\mathbf{x}) &\sim \mathrm{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')) \\
\mathbf{y} &= \mathcal{H}\, f(\mathbf{x}) + \varepsilon
\end{aligned}
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- In plain Gaussian process regression we have

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\mathcal{H}\, f(\mathbf{x}) = \begin{pmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_n)) \end{pmatrix}
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- In inverse problems the operator matrix $\mathcal{H}$ encodes physics into the model.
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Gaussian process regression models (cont.)

- Temporal models (models with single input):

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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.
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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 $$\partial_t \mathbf{f}(\mathbf{x}, t) = \mathcal{A}_x\,\mathbf{f}(\mathbf{x}, t)\,dt + \mathbf{L}\,dW(\mathbf{x}, t)$$

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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.

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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:
  1. Finite-differences/FEM methods lead to sparse precision approximations.
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  3. Spectral factorization leads to state-space (Kalman) methods which are time-recursive (or sparse in precision).

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Finite-differences/FEM – sparse precision

- Basic idea:

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

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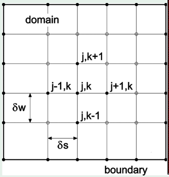

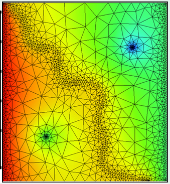

- We get an SPDE approximation $\mathcal{L} \approx \mathbf{L}$, where $\mathbf{L}$ is sparse
- The precision operator approximation is then sparse:

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

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

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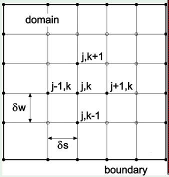

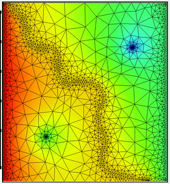

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Finite-differences/FEM – sparse precision

- Basic idea:

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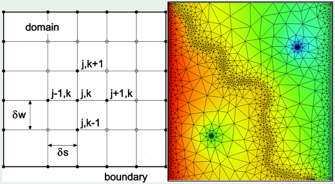

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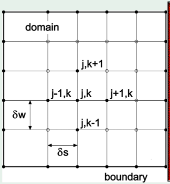

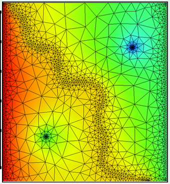

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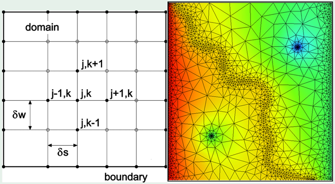

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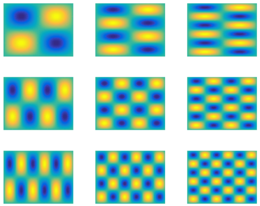
Classical and random Fourier methods – reduced rank approximations and FFT

- Approximation:

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

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



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

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

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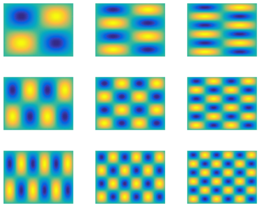

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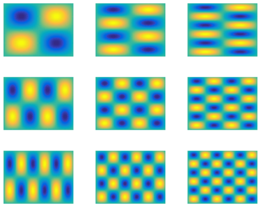

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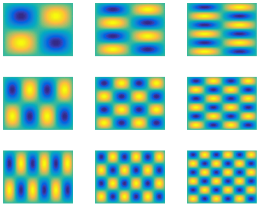

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Hilbert-space/Galerkin methods – reduced rank approximations

- Approximation:

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

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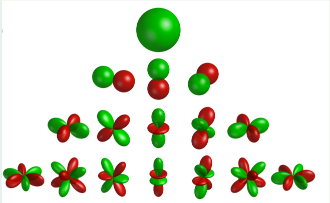

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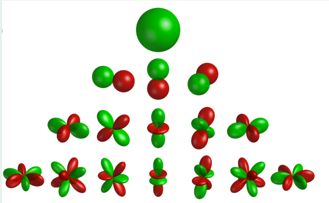

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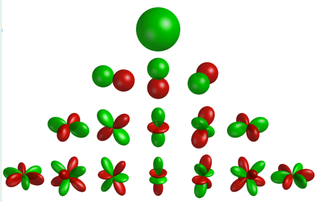

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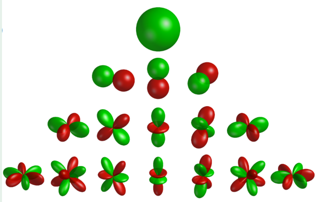

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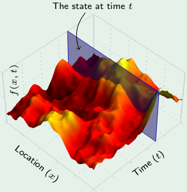
State-space methods – Kalman filters and sparse precision

- Approximation:

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



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

- More generally stochastic evolution equations.
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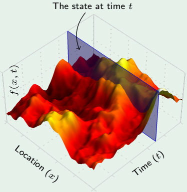

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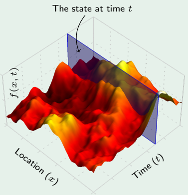

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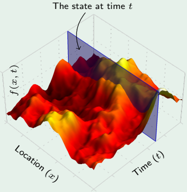

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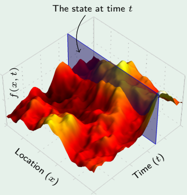

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State-space methods – Kalman filters and sparse precision (cont.)

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

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

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

Example (2D Matérn covariance function)

- Consider a space-time Matérn covariance function

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

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