Aalto University
School of Electrical Engineering

Stochastic (partial) differential equations and Gaussian processes

Simo Särkkä

Aalto University, Finland

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Kernel vs. SPDE representations of GPs

GP model $\mathbf{x} \in \mathbb{R}^d, t \in \mathbb{R}$	Equivalent S(P)DE model
Spatial $k(\mathbf{x}, \mathbf{x}')$	SPDE model ($\mathcal{L}$ is an operator) $$\mathcal{L} \, f(\mathbf{x}) = w(\mathbf{x})$$
Temporal $k(t, t')$	State-space/SDE model $$\frac{d\mathbf{f}(t)}{dt} = \mathbf{A} \, \mathbf{f}(t) + \mathbf{L} \, w(t)$$
Spatio-temporal $k(\mathbf{x}, t; \mathbf{x}', t')$	Stochastic evolution equation $$\frac{\partial}{\partial t} \mathbf{f}(\mathbf{x}, t) = \mathcal{A}_x \, \mathbf{f}(\mathbf{x}, t) + \mathbf{L} \, w(\mathbf{x}, t)$$

Why use S(P)DE solvers for GPs?

- The $O(n^3)$ computational complexity is a challenge.
- What do we get:
  - $O(n)$ state-space methods for SDEs/SPDEs.
  - Sparse approximations developed for SPDEs.
  - Reduced rank Fourier/basis function approximations.
  - Path to non-Gaussian processes.
- Downsides:
  - We often need to approximate.
  - Mathematics can become messy.

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Ornstein-Uhlenbeck process

- The mean and covariance functions:

$$m(x) = 0$$
$$k(x, x') = \sigma^2 \exp(-\lambda |x - x'|)$$

- This has a *path representation* as a stochastic differential equation (SDE):

$$\frac{df(t)}{dt} = -\lambda f(t) + w(t).$$

where $w(t)$ is a white noise process with x relabeled as t.

- Ornstein–Uhlenbeck process is a Markov process.
- What does this actually mean $\Longrightarrow$ white board.

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FT: $(i\omega)\hat{f} = -\lambda \hat{f} + \hat{w}$

$\hat{f} = \frac{\hat{w}}{\lambda + i\omega}$

$$\frac{df(t)}{dt} = -\lambda f(t) + w(t).$$

Spectral Density:

$S(\omega) = \frac{E[|\hat{w}|^2]}{\omega^2 + \lambda^2} = \frac{q}{\omega^2 + \lambda^2}$

where $w(t)$ is a white noise process with x relabeled as t.

$h(\tau) = \frac{1}{2\pi} \int \frac{q}{\omega^2 + \lambda^2} \exp(i\omega\tau) \, d\omega$

$\tau = t - t'$

$= \frac{q}{2\lambda} \exp(-\lambda|\tau|)$

Residual Transform.

$=$

- Ornstein–Uhlenbeck process is a Markov process.
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Ornstein-Uhlenbeck process (cont.)

- Consider a Gaussian process regression problem

$$
\begin{aligned}
f(x) &\sim \mathrm{GP}(0, \sigma^2 \exp(-\lambda |x - x'|)) \\
y_k &= f(x_k) + \varepsilon_k
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- This is equivalent to the state-space model

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f_{k+1} &\sim p(f_{k+1} \mid f_k) \\
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- Solvable in $O(n)$ time using Kalman filter/smoother.

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$$\frac{df(t)}{dt} = -\lambda\, f(t) + w(t)$$
$$y_k = f(t_k) + \varepsilon_k$$

$\times e^{\lambda T}$ (integrating factor)

$e^{\lambda T} \cdot \frac{df(t)}{dt} + \lambda f(t) e^{\lambda t} = w \cdot e^{\lambda t}$

$\frac{d}{dt}(e^{\lambda t} \cdot f) = e^{\lambda t} \cdot w \quad \Big| \int_{t_0}^{t}$

$e^{\lambda t} f(t) - e^{\lambda t_0} f(t_0) = \int_{t_0}^{t} e^{\lambda s} w\, ds$

that is, with $f_k = f(t_k)$ we have a Gauss-Markov model

$\Rightarrow f(t) = \underbrace{e^{-\lambda(t-t_0)}}_{\to A} f(t_0) + \underbrace{\int_{t_0}^{t} e^{-\lambda(t-s)} w(s)\, ds}_{\to Q}$

$$f_{k+1} \sim p(f_{k+1} \mid f_k)$$
$$y_k \sim p(y_k \mid f_k)$$

KF.

- Solvable in $O(n)$ time using Kalman filter/smoother.

$\boxed{f(t_{k+1}) = A \cdot f_k + q \qquad q \sim N(0, Q)}$

$\cancel{\frac{q}{2\lambda}(1 - e^{-2\lambda(t-t_0)})}$

$\Rightarrow p(f(t) \mid f(t_0)) = N(f(t) \mid A f(t_0), Q)$

$A = e^{-\lambda(t-t_0)}$

$Q = \int_{t_0}^{t} e^{-2\lambda(t-s)} q\, ds$

State Space Form of Linear Time-Invariant SDEs

- Consider a Nth order LTI SDE of the form

$$\frac{d^N f}{dt^N} + a_{N-1} \frac{d^{N-1} f}{dt^{N-1}} + \cdots + a_0 f = w(t).$$

- If we define $\mathbf{f} = (f, \ldots, d^{N-1} f / dt^{N-1})$, we get a state space model:

$$\frac{d\mathbf{f}}{dt} = \underbrace{\begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ -a_0 & -a_1 & \ldots & -a_{N-1} \end{pmatrix}}_{\mathbf{A}} \mathbf{f} + \underbrace{\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}}_{\mathbf{L}} w(t)$$

$$f(t) = \underbrace{\begin{pmatrix} 1 & 0 & \cdots & 0 \end{pmatrix}}_{\mathbf{H}} \mathbf{f}.$$

- The vector process $\mathbf{f}(t)$ is Markovian although $f(t)$ isn't.

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Spectra of Linear Time-Invariant SDEs

- By taking the Fourier transform of the LTI SDE, we can derive the spectral density which has the form:

$$S(\omega) = \frac{\text{(constant)}}{\text{(polynomial in } \omega^2)} \qquad \frac{q}{\omega^2 + \lambda^2}$$

- We can also do this conversion to the other direction:
  - With certain parameter values, the Matérn has the form:

$$S(\omega) \propto (\lambda^2 + \omega^2)^{-(p+1)}.$$

  - Many non-rational spectral densities can be approximated:

$$S(\omega) = \sigma^2 \sqrt{\frac{\pi}{\kappa}} \exp\left(-\frac{\omega^2}{4\kappa}\right) \approx \frac{\text{(const)}}{N!/0!(4\kappa)^N + \cdots + \omega^{2N}}$$

- For the conversion of a rational spectral density to a Markovian (state-space) model, we can use the spectral factorization.

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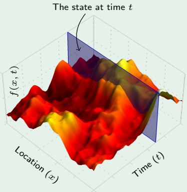
State-space methods for Gaussian processes

- 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 $\longrightarrow O(\log n)$.

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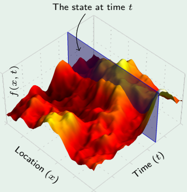

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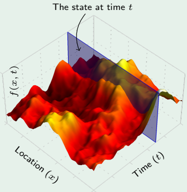

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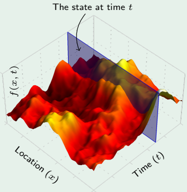

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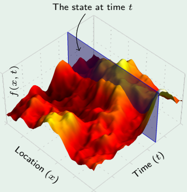

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State-space methods – temporal example

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 – spatio-temporal example

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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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 [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.

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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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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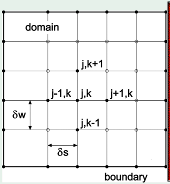

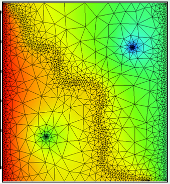

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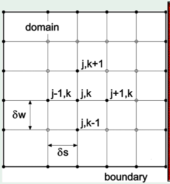

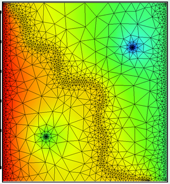

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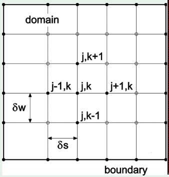

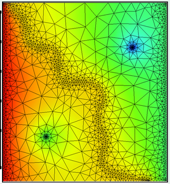

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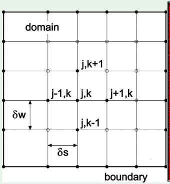

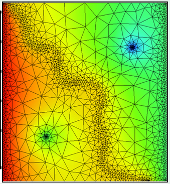

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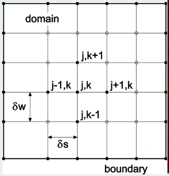

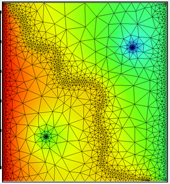

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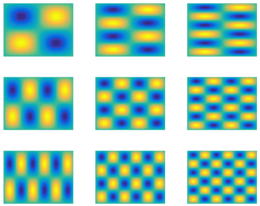
Classical and random Fourier methods – reduced rank approximations and FFT

- 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

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

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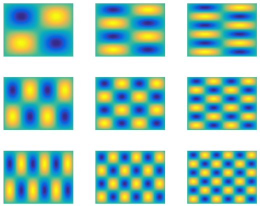

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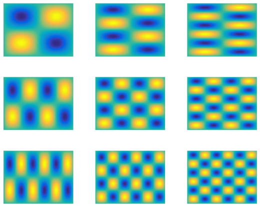

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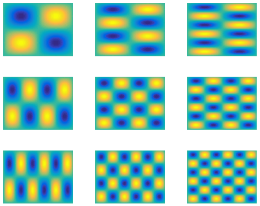

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Hilbert-space/Galerkin methods – reduced rank approximations

- Approximation:

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

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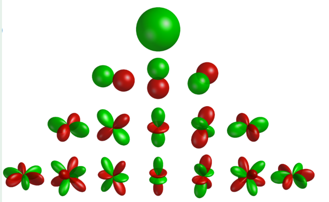

- Again, use less coefficients than the number of data points.
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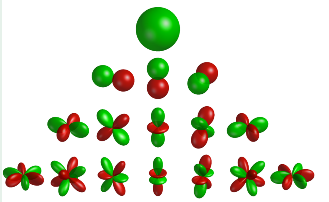

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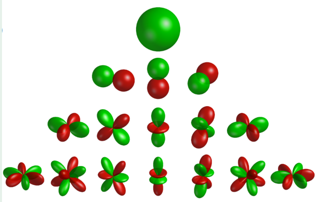

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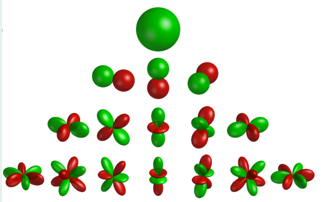

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Back to SPDE representations of GPs

GP model $\mathbf{x} \in \mathbb{R}^d$, $t \in \mathbb{R}$	Equivalent S(P)DE model
Spatial $k(\mathbf{x}, \mathbf{x}')$	SPDE model ($\mathcal{L}$ is an operator) $$\mathcal{L}\, f(\mathbf{x}) = w(\mathbf{x})$$
Temporal $k(t, t')$	State-space/SDE model $$\frac{d\mathbf{f}(t)}{dt} = \mathbf{A}\,\mathbf{f}(t) + \mathbf{L}\,w(t)$$
Spatio-temporal $k(\mathbf{x}, t; \mathbf{x}', t')$	Stochastic evolution equation $$\frac{\partial}{\partial t}\mathbf{f}(\mathbf{x}, t) = \mathcal{A}_x\,\mathbf{f}(\mathbf{x}, t) + \mathbf{L}\,w(\mathbf{x}, t)$$

What then?

- Exchange and map approximations between the fields:
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Useful references

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