Aalto University
School of Electrical
Engineering

Stochastic (Partial) Differential Equation Methods for Gaussian Processes

Simo Särkkä

Aalto University, Finland

Contents

Contents

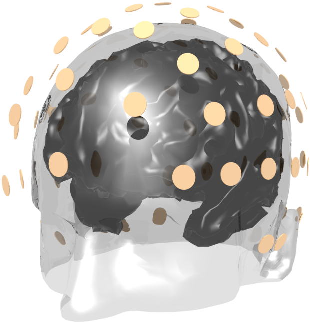
Contents

Contents

Contents

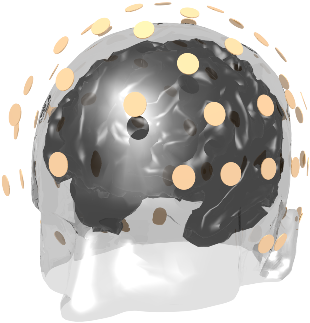
Magneto- and Electroencephalography (MEG & EEG)

- Unknown: Time course of amplitudes of dipole sources.
- Observed: Electromagnetic field (potential / flux).



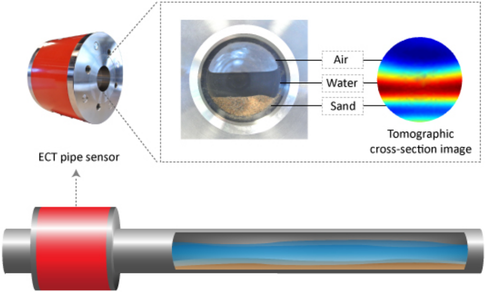
Magneto- and Electroencephalography (MEG & EEG)

- Unknown: Time course of amplitudes of dipole sources.
- Observed: Electromagnetic field (potential / flux).



Electrical Impedance and Capacitance Tomography (EIT & ECT)

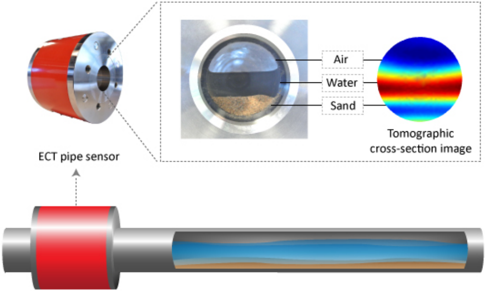
- Unknown: Conductivity/permittivity constants.
- Observed: Impedances on boundary.



Source: Rocsole Ltd. – www.rocsole.com

Electrical Impedance and Capacitance Tomography (EIT & ECT)

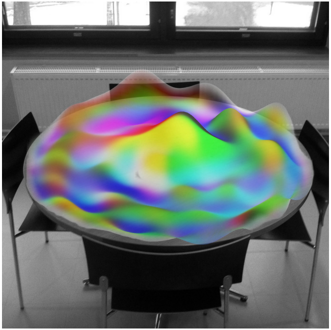
- Unknown: Conductivity/permittivity constants.
- Observed: Impedances on boundary.



Source: Rocsole Ltd. – www.rocsole.com

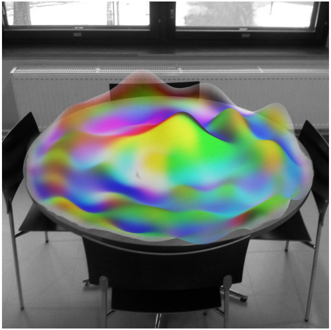
Magnetic field mapping

- Unknown: Magnetic field (or actually the corresponding potential).
- Observed: Point measurements of the magnetic field.



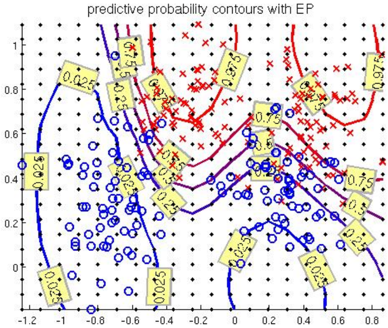
Magnetic field mapping

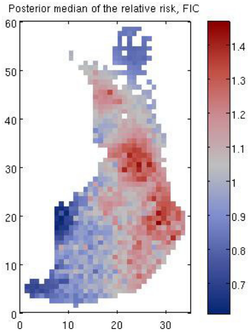
- Unknown: Magnetic field (or actually the corresponding potential).
- Observed: Point measurements of the magnetic field.



Machine learning and Kriging

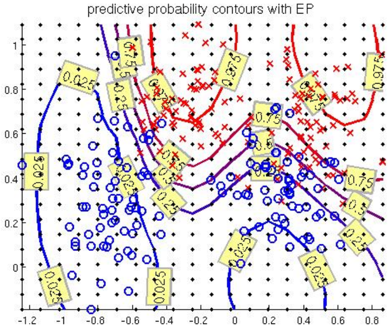
- Unknown: Class labels or missing spatial values.
- Observed: Subset (training set) of class labels, spatial values, and predictors.

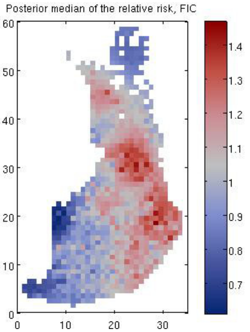




Machine learning and Kriging

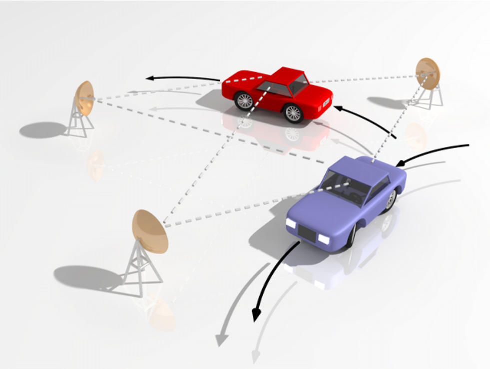
- Unknown: Class labels or missing spatial values.
- Observed: Subset (training set) of class labels, spatial values, and predictors.





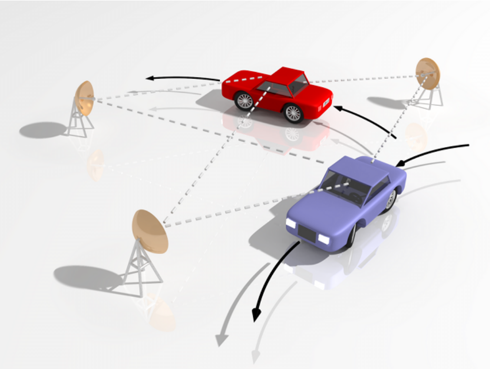
Target Tracking and Location Sensing

- Unknown: Target trajectories and velocities.
- Observed: Direction or inertial measurements.



Target Tracking and Location Sensing

- Unknown: Target trajectories and velocities.
- Observed: Direction or inertial measurements.



Contents

Gaussian process regression models

- A typical GP regression problem:

$$f(\mathbf{x}) \sim \mathrm{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$
$$\mathbf{y} = \mathcal{H}\, f(\mathbf{x}) + \varepsilon$$

- In plain Gaussian process regression we have

$$\mathcal{H}\, f(\mathbf{x}) = \begin{pmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_n)) \end{pmatrix}$$

- In inverse problems the operator matrix $\mathcal{H}$ encodes physics into the model.
- The mean $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$ encode the prior information on $f(\mathbf{x})$.

Gaussian process regression models

- A typical GP regression problem:

$$f(\mathbf{x}) \sim \mathrm{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$
$$\mathbf{y} = \mathcal{H}\, f(\mathbf{x}) + \varepsilon$$

- In plain Gaussian process regression we have

$$\mathcal{H}\, f(\mathbf{x}) = \begin{pmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_n)) \end{pmatrix}$$

- In inverse problems the operator matrix $\mathcal{H}$ encodes physics into the model.
- The mean $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$ encode the prior information on $f(\mathbf{x})$.

Gaussian process regression models

- A typical GP regression problem:

$$f(\mathbf{x}) \sim \mathrm{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$
$$\mathbf{y} = \mathcal{H}\, f(\mathbf{x}) + \varepsilon$$

- In plain Gaussian process regression we have

$$\mathcal{H}\, f(\mathbf{x}) = \begin{pmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_n)) \end{pmatrix}$$

- In inverse problems the operator matrix $\mathcal{H}$ encodes physics into the model.
- The mean $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$ encode the prior information on $f(\mathbf{x})$.

Gaussian process regression models

- A typical GP regression problem:

$$f(\mathbf{x}) \sim \mathrm{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$
$$\mathbf{y} = \mathcal{H}\, f(\mathbf{x}) + \varepsilon$$

- In plain Gaussian process regression we have

$$\mathcal{H}\, f(\mathbf{x}) = \begin{pmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_n)) \end{pmatrix}$$

- In inverse problems the operator matrix $\mathcal{H}$ encodes physics into the model.
- The mean $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$ encode the prior information on $f(\mathbf{x})$.

Gaussian process regression models (cont.)

- Temporal models (models with single input):

$$
\begin{aligned}
f(t) &\sim \mathrm{GP}(m(t), k(t, t')) \\
\mathbf{y} &= \mathcal{H}\, f(t) + \varepsilon
\end{aligned}
$$

- Spatio-temporal models:

$$
\begin{aligned}
f(\mathbf{x}, t) &\sim \mathrm{GP}(m(\mathbf{x}, t), k(\mathbf{x}, t; \mathbf{x}', t')) \\
\mathbf{y} &= \mathcal{H}\, f(\mathbf{x}, t) + \varepsilon
\end{aligned}
$$

- All of these can be recasted as statistical estimation on a stochastic partial differential equation (SPDE) model.

Gaussian process regression models (cont.)

- Temporal models (models with single input):

$$f(t) \sim \mathrm{GP}(m(t), k(t, t'))$$
$$\mathbf{y} = \mathcal{H}\, f(t) + \varepsilon$$

- Spatio-temporal models:

$$f(\mathbf{x}, t) \sim \mathrm{GP}(m(\mathbf{x}, t), k(\mathbf{x}, t; \mathbf{x}', t'))$$
$$\mathbf{y} = \mathcal{H}\, f(\mathbf{x}, t) + \varepsilon$$

- All of these can be recasted as statistical estimation on a stochastic partial differential equation (SPDE) model.

Gaussian process regression models (cont.)

- Temporal models (models with single input):

$$f(t) \sim \mathrm{GP}(m(t), k(t, t'))$$
$$\mathbf{y} = \mathcal{H}\, f(t) + \varepsilon$$

- Spatio-temporal models:

$$f(\mathbf{x}, t) \sim \mathrm{GP}(m(\mathbf{x}, t), k(\mathbf{x}, t; \mathbf{x}', t'))$$
$$\mathbf{y} = \mathcal{H}\, f(\mathbf{x}, t) + \varepsilon$$

- All of these can be recasted as statistical estimation on a stochastic partial differential equation (SPDE) model.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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

Contents

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 [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 [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 [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.
  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).

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).

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).

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).

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).

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:

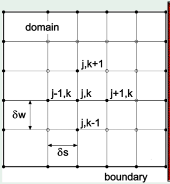
$$\begin{aligned} \mathcal{K}^{-1} &= \mathcal{L}^*\, \mathcal{L} \\ \mathcal{K} &= (\mathcal{L}^*\, \mathcal{L})^{-1} \end{aligned}$$

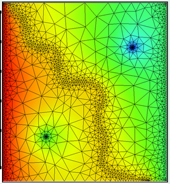
- Idea: approximate $\mathcal{L}$ or $\mathcal{L}^{-1}$ using PDE/ODE methods:
  1. Finite-differences/FEM methods lead to sparse precision approximations.
  2. Fourier/basis-function methods lead to reduced rank covariance approximations.
  3. Spectral factorization leads to state-space (Kalman) methods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

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

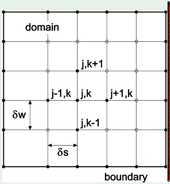
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

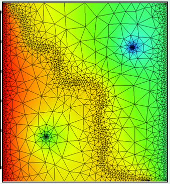
Finite-differences/FEM – sparse precision

- 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:

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

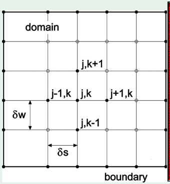
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

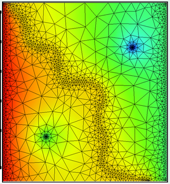
Finite-differences/FEM – sparse precision

- 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:

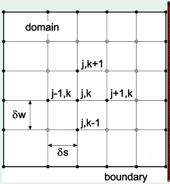
$$\mathcal{K}^{-1} \approx \mathbf{L}^\mathsf{T}\,\mathbf{L} = \text{sparse}$$

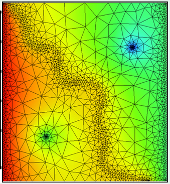
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

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:

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

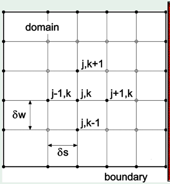
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

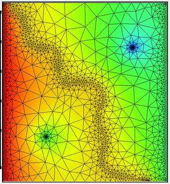
Finite-differences/FEM – sparse precision

- 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:

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

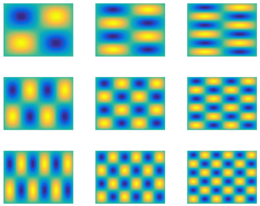
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

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

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

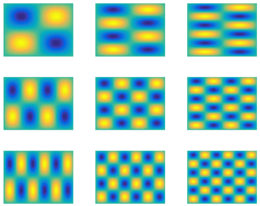
- Truncated series, random frequencies, FFT, ...

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

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

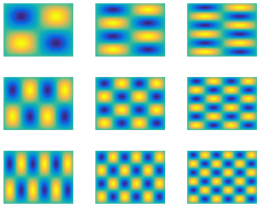
- Truncated series, random frequencies, FFT, ...

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

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

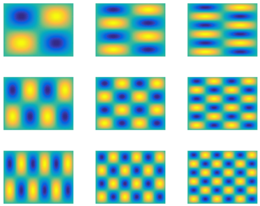
- Truncated series, random frequencies, FFT, ...

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

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

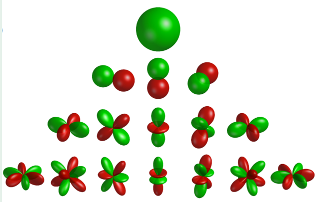
- Truncated series, random frequencies, FFT, . . .

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

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

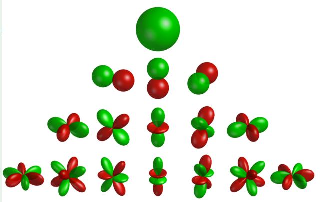
- Wavelets, Galerkin, finite elements, ...

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

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

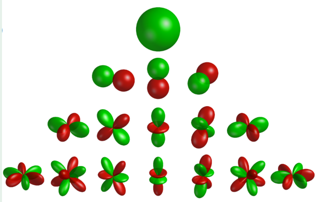
- Wavelets, Galerkin, finite elements, ...

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

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

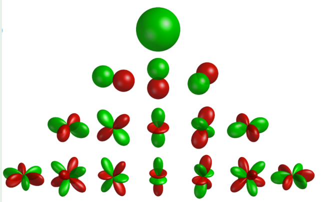
- Wavelets, Galerkin, finite elements, …

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

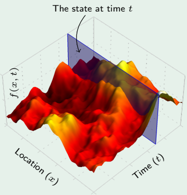
$$k(\mathbf{x}, \mathbf{x}') \approx \sum_{i=1}^{N} \sigma_i^2 \, \phi_i(\mathbf{x}) \, \phi_i(\mathbf{x}').$$

- 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)

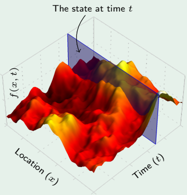
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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

- 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)

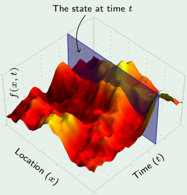
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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

- 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)

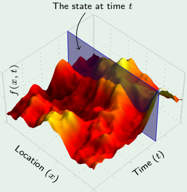
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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

- 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)

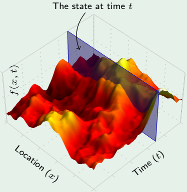
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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

- 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:

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

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:

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

Contents

What then?

- We can exchange and map approximations between the fields:
  - Inducing points $\leftrightarrow$ point-collocation; spectral methods $\leftrightarrow$ Galerkin methods; finite-differences $\leftrightarrow$ GMRFs;
  - EP $\leftrightarrow$ linearization; ...
- Non-Gaussian processes.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in the measurement model.

What then?

- We can exchange and map approximations between the fields:
  - Inducing points $\leftrightarrow$ point-collocation; spectral methods $\leftrightarrow$ Galerkin methods; finite-differences $\leftrightarrow$ GMRFs;
  - EP $\leftrightarrow$ linearization; ...
- Non-Gaussian processes.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in the measurement model.

What then?

- We can exchange and map approximations between the fields:
  - Inducing points $\leftrightarrow$ point-collocation; spectral methods $\leftrightarrow$ Galerkin methods; finite-differences $\leftrightarrow$ GMRFs;
  - EP $\leftrightarrow$ linearization; . . .
- Non-Gaussian processes.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in the measurement model.

What then?

- We can exchange and map approximations between the fields:
  - Inducing points $\leftrightarrow$ point-collocation; spectral methods $\leftrightarrow$ Galerkin methods; finite-differences $\leftrightarrow$ GMRFs;
  - EP $\leftrightarrow$ linearization; ...
- Non-Gaussian processes.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in the measurement model.

What then?

- We can exchange and map approximations between the fields:
  - Inducing points $\leftrightarrow$ point-collocation; spectral methods $\leftrightarrow$ Galerkin methods; finite-differences $\leftrightarrow$ GMRFs;
  - EP $\leftrightarrow$ linearization; ...
- Non-Gaussian processes.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in the measurement model.

What then?

- We can exchange and map approximations between the fields:
  - Inducing points $\leftrightarrow$ point-collocation; spectral methods $\leftrightarrow$ Galerkin methods; finite-differences $\leftrightarrow$ GMRFs;
  - EP $\leftrightarrow$ linearization; ...
- Non-Gaussian processes.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in the measurement model.

What then?

- We can exchange and map approximations between the fields:
  - Inducing points $\leftrightarrow$ point-collocation; spectral methods $\leftrightarrow$ Galerkin methods; finite-differences $\leftrightarrow$ GMRFs;
  - EP $\leftrightarrow$ linearization; ...
- Non-Gaussian processes.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- Inverse problems – operators in the measurement model.

Summary

- Gaussian processes (GPs) are nice, but the computational scaling is bad.
- Applications in e.g. brain imaging, tomography, positioning, and Kriging.
- GPs have representations as solutions to SPDEs.
- SPDE methods can be used to speed up GP inference.
- In temporal models we can use Kalman/Bayesian filters and smoothers.
- Opens up new paths towards non-linear GP models.

Summary

- Gaussian processes (GPs) are nice, but the computational scaling is bad.
- Applications in e.g. brain imaging, tomography, positioning, and Kriging.
- GPs have representations as solutions to SPDEs.
- SPDE methods can be used to speed up GP inference.
- In temporal models we can use Kalman/Bayesian filters and smoothers.
- Opens up new paths towards non-linear GP models.

Summary

- Gaussian processes (GPs) are nice, but the computational scaling is bad.
- Applications in e.g. brain imaging, tomography, positioning, and Kriging.
- GPs have representations as solutions to SPDEs.
- SPDE methods can be used to speed up GP inference.
- In temporal models we can use Kalman/Bayesian filters and smoothers.
- Opens up new paths towards non-linear GP models.

Summary

- Gaussian processes (GPs) are nice, but the computational scaling is bad.
- Applications in e.g. brain imaging, tomography, positioning, and Kriging.
- GPs have representations as solutions to SPDEs.
- SPDE methods can be used to speed up GP inference.
- In temporal models we can use Kalman/Bayesian filters and smoothers.
- Opens up new paths towards non-linear GP models.

Summary

- Gaussian processes (GPs) are nice, but the computational scaling is bad.
- Applications in e.g. brain imaging, tomography, positioning, and Kriging.
- GPs have representations as solutions to SPDEs.
- SPDE methods can be used to speed up GP inference.
- In temporal models we can use Kalman/Bayesian filters and smoothers.
- Opens up new paths towards non-linear GP models.

Summary

- Gaussian processes (GPs) are nice, but the computational scaling is bad.
- Applications in e.g. brain imaging, tomography, positioning, and Kriging.
- GPs have representations as solutions to SPDEs.
- SPDE methods can be used to speed up GP inference.
- In temporal models we can use Kalman/Bayesian filters and smoothers.
- Opens up new paths towards non-linear GP models.