Aalto University
School of Electrical
Engineering

Stochastic (Partial) Differential Equations and Gaussian Processes

Simo Särkkä

Aalto University, Finland

Contents

1. Motivating applications
2. Using SPDE solvers on Gaussian processes
3. What do the SPDE methods then look like?
4. Discussion and summary

Contents

1. Motivating applications
2. Using SPDE solvers on Gaussian processes
3. What do the SPDE methods then look like?
4. Discussion and summary

Contents

1. Motivating applications
2. Using SPDE solvers on Gaussian processes
3. What do the SPDE methods then look like?
4. Discussion and summary

Contents

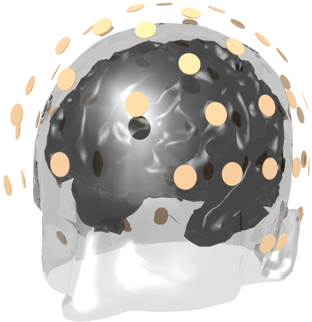
1. Motivating applications
2. Using SPDE solvers on Gaussian processes
3. What do the SPDE methods then look like?
4. Discussion and summary

Contents

1. Motivating applications
2. Using SPDE solvers on Gaussian processes
3. What do the SPDE methods then look like?
4. Discussion and summary

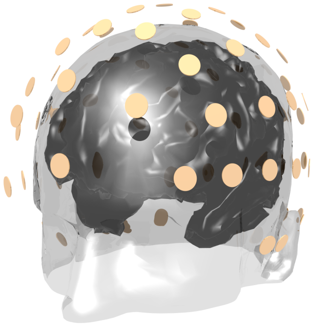
Magneto- and Electroencephalography (MEG & EEG)

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



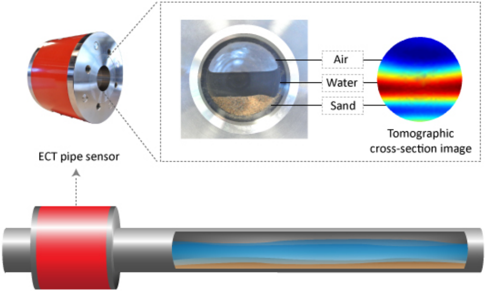
Magneto- and Electroencephalography (MEG & EEG)

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



Electrical Impedance and Capacitance Tomography (EIT & ECT)

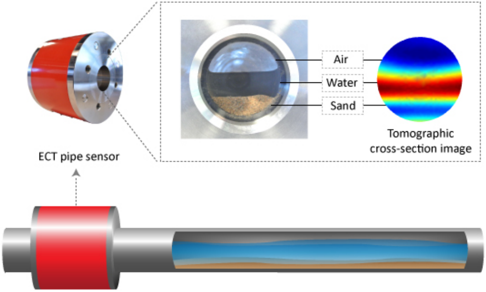
- Unknown: Conductivity/permittivity constants.
- Observed: Impedances on boundary.



Source: Rocsole Ltd. – www.rocsole.com

Electrical Impedance and Capacitance Tomography (EIT & ECT)

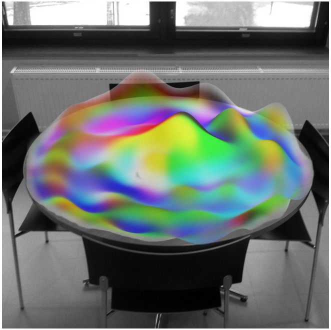
- Unknown: Conductivity/permittivity constants.
- Observed: Impedances on boundary.



Source: Rocsole Ltd. – www.rocsole.com

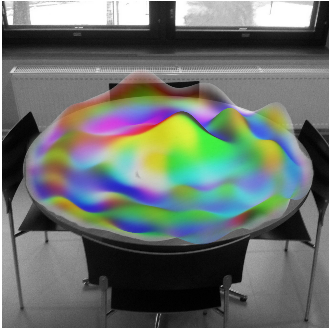
Magnetic field mapping

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



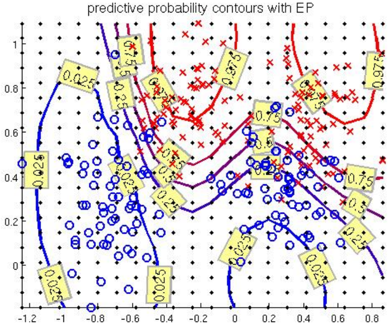
Magnetic field mapping

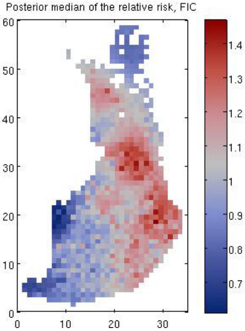
- Unknown: Magnetic field (or actually the corresponding potential).
- Observed: Point measurements of the magnetic field.



Machine learning and Kriging

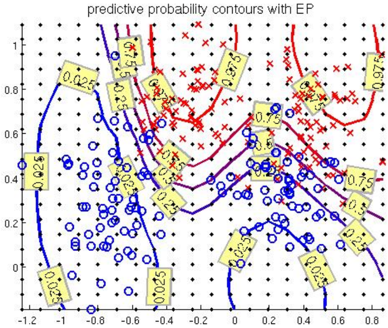
- Unknown: Class labels or missing spatial values.
- Observed: Subset (training set) of class labels, spatial values, and predictors.

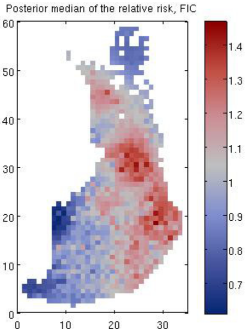




Machine learning and Kriging

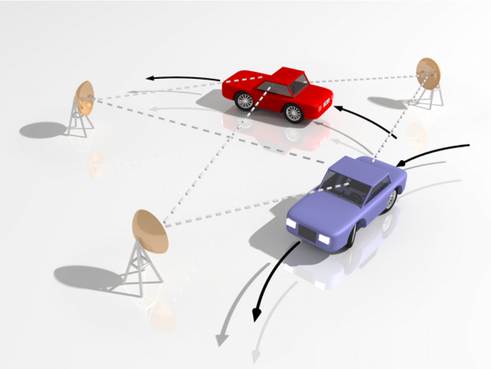
- Unknown: Class labels or missing spatial values.
- Observed: Subset (training set) of class labels, spatial values, and predictors.





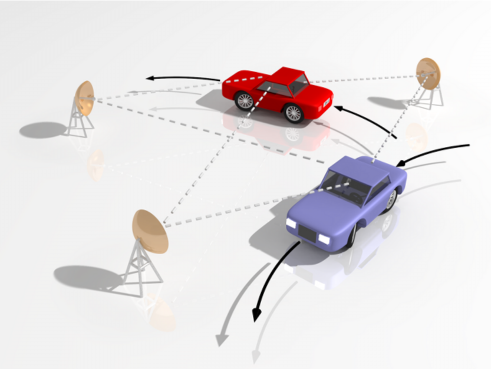
Target Tracking and Location Sensing

- 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

1 Motivating applications

2 Using SPDE solvers on Gaussian processes

3 What do the SPDE methods then look like?

4 Discussion and summary

Gaussian process regression models and inverse problems

- A typical statistical inverse problem:

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

- 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 $f(\mathbf{x})$.
- In plain Gaussian process regression we have

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

Gaussian process regression models and inverse problems

- A typical statistical inverse problem:

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

- 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 $f(\mathbf{x})$.
- In plain Gaussian process regression we have

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

Gaussian process regression models and inverse problems

- A typical statistical inverse problem:

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

- 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 $f(\mathbf{x})$.
- In plain Gaussian process regression we have

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

Gaussian process regression models and inverse problems

- A typical statistical inverse problem:

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

- 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 $f(\mathbf{x})$.
- In plain Gaussian process regression we have

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

Gaussian process regression models and inverse problems (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 and inverse problems (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 and inverse problems (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

1 Motivating applications

2 Using SPDE solvers on Gaussian processes

3 What do the SPDE methods then look like?

4 Discussion and summary

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 a Sobolev space.

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 a Sobolev space.

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 a Sobolev space.

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 a Sobolev space.

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 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).

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:

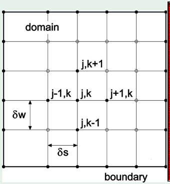
$$\mathcal{K}^{-1} = \mathcal{L}^*\, \mathcal{L}$$
$$\mathcal{K} = (\mathcal{L}^*\, \mathcal{L})^{-1}$$

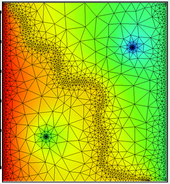
- Idea: approximate $\mathcal{L}$ or $\mathcal{L}^{-1}$ using PDE/ODE methods:
  1. Finite-differences/FEM methods lead to sparse precision approximations.
  2. Fourier/basis-function methods lead to reduced rank covariance approximations.
  3. Spectral factorization leads to state-space (Kalman) methods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

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:

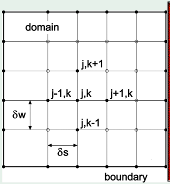
$$\mathcal{K}^{-1} \approx \mathbf{L}^{\mathsf{T}} \mathbf{L} = \text{sparse}$$

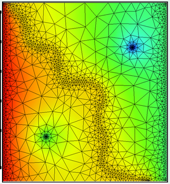
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

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:

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

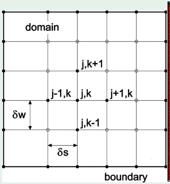
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

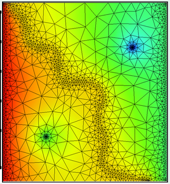
Finite-differences/FEM – sparse precision

- 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:

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

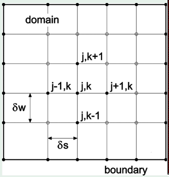
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

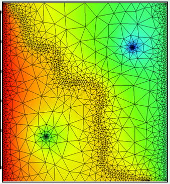
Finite-differences/FEM – sparse precision

- 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:

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

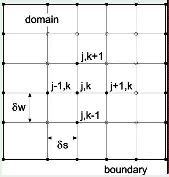
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

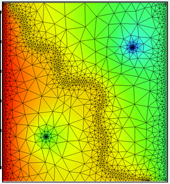
Finite-differences/FEM – sparse precision

- 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:

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

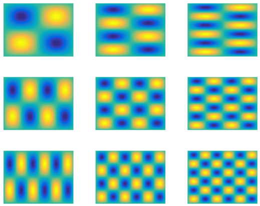
- $\mathcal{L}$ need to be approximated as integro-differential operator.
- Requires formation of a grid, but parallelizes well.

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

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

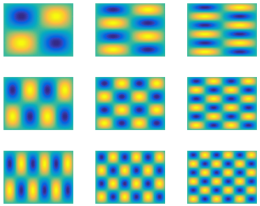
- Truncated series, random frequencies, FFT, ...

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

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

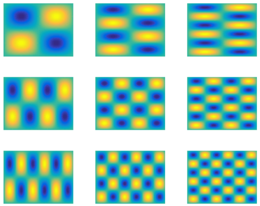
- Truncated series, random frequencies, FFT, ...

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

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

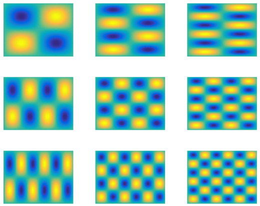
- Truncated series, random frequencies, FFT, ...

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

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

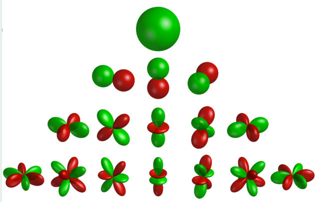
- Truncated series, random frequencies, FFT, ...

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

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

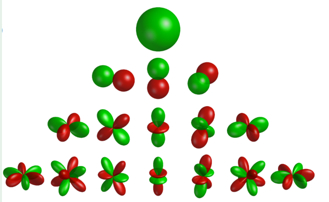
- Wavelets, Galerkin, finite elements, …

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

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

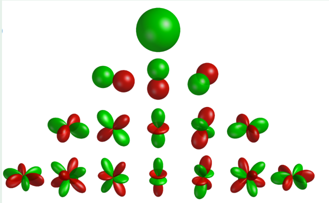
- Wavelets, Galerkin, finite elements, …

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

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

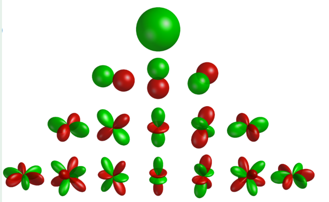
- Wavelets, Galerkin, finite elements, ...

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

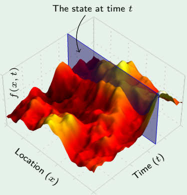
$$k(\mathbf{x}, \mathbf{x}') \approx \sum_{i=1}^{N} \sigma_i^2 \, \phi_i(\mathbf{x}) \, \phi_i(\mathbf{x}').$$

- 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)

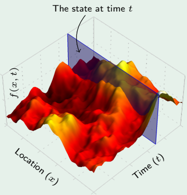
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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)

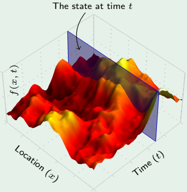
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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)

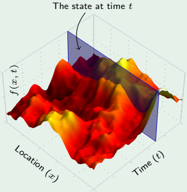
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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)

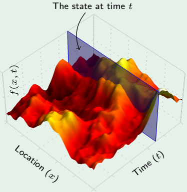
$$d\mathbf{f}(t) = \mathbf{A}\,\mathbf{f}(t)\,dt + \mathbf{L}\,d\mathbf{W}$$

- 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

1. Motivating applications
2. Using SPDE solvers on Gaussian processes
3. What do the SPDE methods then look like?
4. Discussion and summary

What then?

- We can exchange approximations between the fields.
- Inference on the basis functions/point-locations/etc.
- Non-Gaussian processes, non-Gaussian likelihoods.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- State-space stochastic control in Gaussian processes and LFMs.

What then?

- We can exchange approximations between the fields.
- Inference on the basis functions/point-locations/etc.
- Non-Gaussian processes, non-Gaussian likelihoods.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- State-space stochastic control in Gaussian processes and LFMs.

What then?

- We can exchange approximations between the fields.
- Inference on the basis functions/point-locations/etc.
- Non-Gaussian processes, non-Gaussian likelihoods.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- State-space stochastic control in Gaussian processes and LFMs.

What then?

- We can exchange approximations between the fields.
- Inference on the basis functions/point-locations/etc.
- Non-Gaussian processes, non-Gaussian likelihoods.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- State-space stochastic control in Gaussian processes and LFMs.

What then?

- We can exchange approximations between the fields.
- Inference on the basis functions/point-locations/etc.
- Non-Gaussian processes, non-Gaussian likelihoods.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- State-space stochastic control in Gaussian processes and LFMs.

What then?

- We can exchange approximations between the fields.
- Inference on the basis functions/point-locations/etc.
- Non-Gaussian processes, non-Gaussian likelihoods.
- Hierarchical (deep) SPDE models.
- Combined first-principles and nonparametric models – latent force models (LFM).
- State-space stochastic control in Gaussian processes and LFMs.

Summary

- Gaussian processes (GPs) can be used as priors in inverse problems.
- 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) can be used as priors in inverse problems.
- 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) can be used as priors in inverse problems.
- 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) can be used as priors in inverse problems.
- 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) can be used as priors in inverse problems.
- 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) can be used as priors in inverse problems.
- 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.