Gaussian processes – theory and applications:

State space representations of GPs

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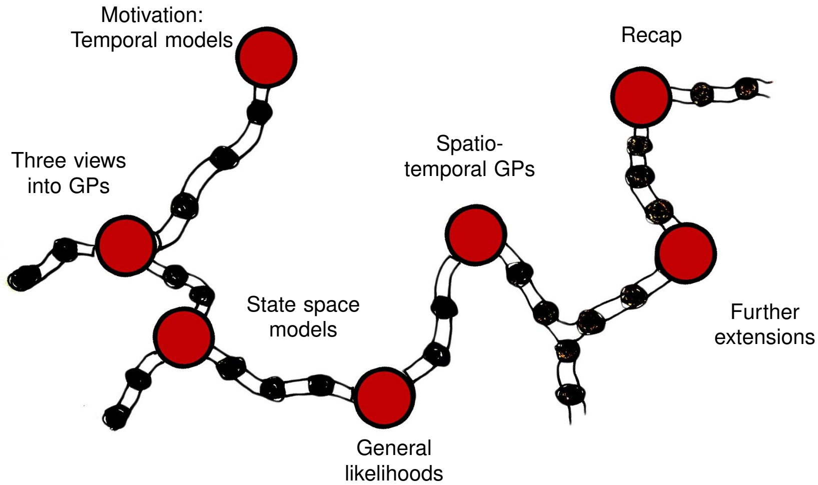
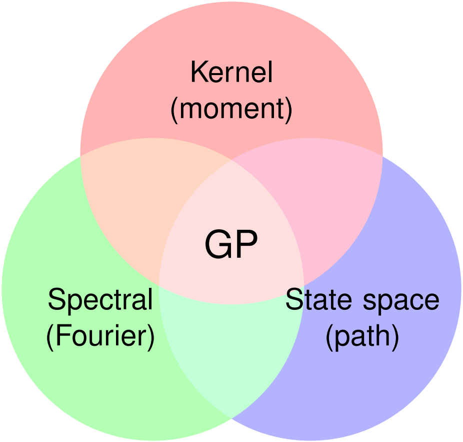
Lecture 6: Outline



Motivation: Temporal models

- **One-dimensional problems**
  (the data has a natural ordering)
- **Spatio-temproal models**
  (something developing over time)
- **Long / unbounded data**
  (sensor data streams, daily observations, etc.)

Three views into GPs



Kernel (moment) representation

$$f(t) \sim \mathrm{GP}(\mu(t), \kappa(t,t')) \qquad \textit{GP prior}$$

$$\mathbf{y} \mid \mathbf{f} \sim \prod_i p(y_i \mid f(t_i)) \qquad \textit{likelihood}$$

- Let's focus on the GP prior only.
- A temporal Gaussian process (GP) is a random function $f(t)$, such that joint distribution of $f(t_1), \ldots, f(t_n)$ is always Gaussian.
- Mean and covariance functions have the form:

$$\mu(t) = \mathbb{E}[f(t)],$$

$$\kappa(t,t') = \mathbb{E}[(f(t) - \mu(t))(f(t') - \mu(t'))^\mathsf{T}].$$

- Convenient for model specification, but expanding the kernel to a covariance matrix can be problematic (the notorious $\mathcal{O}(n^3)$ scaling).

Spectral (Fourier) representation

- The Fourier transform of a function $f(t) : \mathbb{R} \to \mathbb{R}$ is

$$\mathcal{F}[f](\mathrm{i}\,\omega) = \int_{\mathbb{R}} f(t)\,\exp(-\mathrm{i}\,\omega\,t)\,\mathrm{d}t$$

- For a stationary GP, the covariance function can be written in terms of the difference between two inputs:

$$\kappa(t, t') \triangleq \kappa(t - t')$$

- Wiener–Khinchin: If $f(t)$ is a stationary Gaussian process with covariance function $\kappa(t)$ then its spectral density is $S(\omega) = \mathcal{F}[\kappa]$.
- Spectral representation of a GP in terms of spectral density function

$$S(\omega) = \mathbb{E}[\tilde{f}(\mathrm{i}\,\omega)\,\tilde{f}^{\mathsf{T}}(-\mathrm{i}\,\omega)]$$

State space (path) representation [1/3]

- Path or state space representation as solution to a linear time-invariant (LTI) stochastic differential equation (SDE):

$$\mathrm{d}\mathbf{f} = \mathbf{F}\,\mathbf{f}\,\mathrm{d}t + \mathbf{L}\,\mathrm{d}\boldsymbol{\beta},$$

  where $\mathbf{f} = (f, \mathrm{d}f/\mathrm{d}t, \ldots)$ and $\boldsymbol{\beta}(t)$ is a vector of Wiener processes.

- Equivalently, but more informally

$$\frac{\mathrm{d}\mathbf{f}(t)}{\mathrm{d}t} = \mathbf{F}\,\mathbf{f}(t) + \mathbf{L}\,\mathbf{w}(t),$$

  where $\mathbf{w}(t)$ is white noise.

- The model now consists of a drift matrix $\mathbf{F} \in \mathbb{R}^{m \times m}$, a diffusion matrix $\mathbf{L} \in \mathbb{R}^{m \times s}$, and the spectral density matrix of the white noise process $\mathbf{Q}_\mathrm{c} \in \mathbb{R}^{s \times s}$.

- The scalar-valued GP can be recovered by $f(t) = \mathbf{H}\,\mathbf{f}(t)$.

State space (path) representation [2/3]

- The initial state is given by a stationary state $\mathbf{f}(0) \sim \mathrm{N}(\mathbf{0}, \mathbf{P}_\infty)$ which fulfills

$$\mathbf{F}\,\mathbf{P}_\infty + \mathbf{P}_\infty\,\mathbf{F}^\mathsf{T} + \mathbf{L}\,\mathbf{Q}_\mathrm{c}\,\mathbf{L}^\mathsf{T} = \mathbf{0}$$

- The covariance function at the stationary state can be recovered by

$$\kappa(t,t') = \begin{cases} \mathbf{P}_\infty \exp((t'-t)\mathbf{F})^\mathsf{T}, & t' \geq t \\ \exp((t'-t)\mathbf{F})\,\mathbf{P}_\infty & t' < t \end{cases}$$

where $\exp(\cdot)$ denotes the matrix exponential function.

- The spectral density function at the stationary state can be recovered by

$$S(\omega) = (\mathbf{F} + \mathrm{i}\,\omega\,\mathbf{I})^{-1}\,\mathbf{L}\,\mathbf{Q}_\mathrm{c}\,\mathbf{L}^\mathsf{T}\,(\mathbf{F} - \mathrm{i}\,\omega\,\mathbf{I})^{-\mathsf{T}}$$

State space (path) representation [3/3]

- Similarly as the kernel has to be evaluated into covariance matrix for computations, the SDE can be solved for discrete time points $\{t_i\}_{i=1}^n$.
- The resulting model is a discrete state space model:

$$\mathbf{f}_i = \mathbf{A}_{i-1}\,\mathbf{f}_{i-1} + \mathbf{q}_{i-1}, \quad \mathbf{q}_i \sim \mathrm{N}(\mathbf{0}, \mathbf{Q}_i),$$

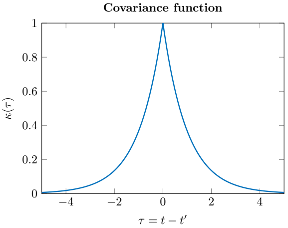
  where $\mathbf{f}_i = \mathbf{f}(t_i)$.
- The discrete-time model matrices are given by:

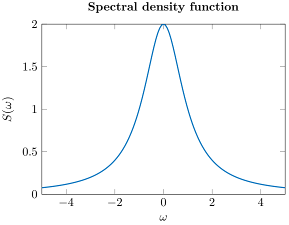
$$\mathbf{A}_i = \exp(\mathbf{F}\,\Delta t_i),$$
$$\mathbf{Q}_i = \int_0^{\Delta t_i} \exp(\mathbf{F}\,(\Delta t_i - \tau))\,\mathbf{L}\,\mathbf{Q}_\mathrm{c}\,\mathbf{L}^\mathsf{T} \exp(\mathbf{F}\,(\Delta t_i - \tau))^\mathsf{T}\,\mathrm{d}\tau,$$

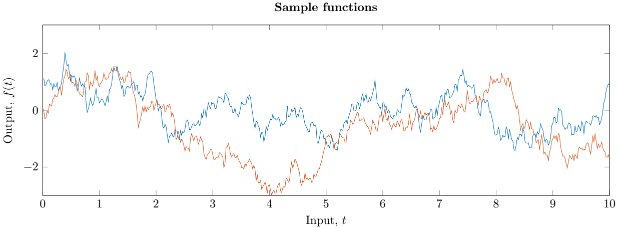
  where $\Delta t_i = t_{i+1} - t_i$
- If the model is stationary, $\mathbf{Q}_i$ is given by

$$\mathbf{Q}_i = \mathbf{P}_\infty - \mathbf{A}_i\,\mathbf{P}_\infty\,\mathbf{A}_i^\mathsf{T}$$

Three views into GPs







Example: Exponential covariance function

- Exponential covariance function (Ornstein-Uhlenbeck process):

$$\kappa(t, t') = \exp(-\lambda\,|t - t'|)$$

- Spectral density function:

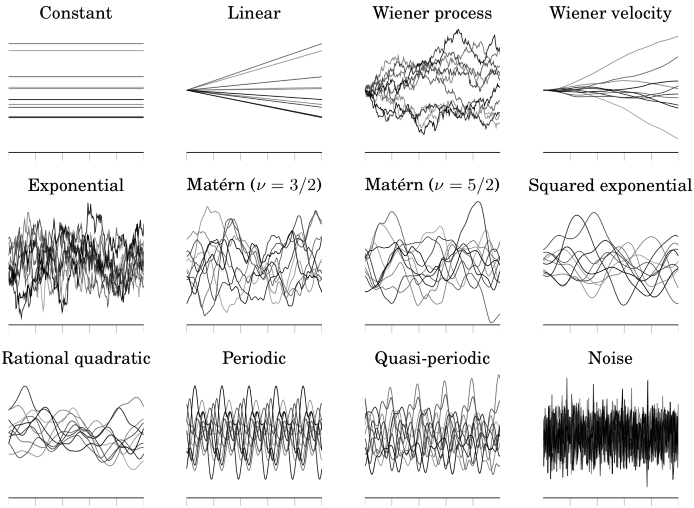
$$S(\omega) = \frac{2}{\lambda + \omega^2/\lambda}$$

- Path representation: Stochastic differential equation (SDE)

$$\frac{\mathrm{d}f(t)}{\mathrm{d}t} = -\lambda\, f(t) + w(t),$$

or using the notation from before:
$F = -\lambda$, $L = 1$, $Q_\mathrm{c} = 2$, $H = 1$, and $P_\infty = 1$.

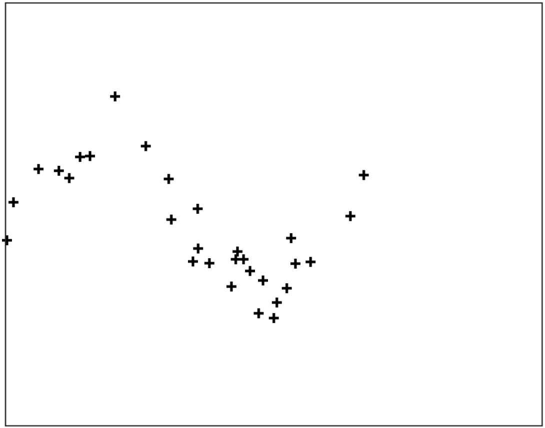
Applicable GP priors



Applicable GP priors

- The covariance function needs to be Markovian (or approximated as such).
- Covers many common stationary and non-stationary models.
- Sums of kernels: $\kappa(t, t') = \kappa_1(t, t') + \kappa_2(t, t')$
  - Stacking of the state spaces
  - State dimension: $m = m_1 + m_2$
- Product of kernels: $\kappa(t, t') = \kappa_1(t, t')\, \kappa_2(t, t')$
  - Kronecker sum of the models
  - State dimension: $m = m_1\, m_2$

Example: GP regression, $\mathcal{O}(n^3)$



Example: GP regression, $\mathcal{O}(n^3)$

- Consider the GP regression problem with input–output training pairs $\{(t_i, y_i)\}_{i=1}^{n}$:

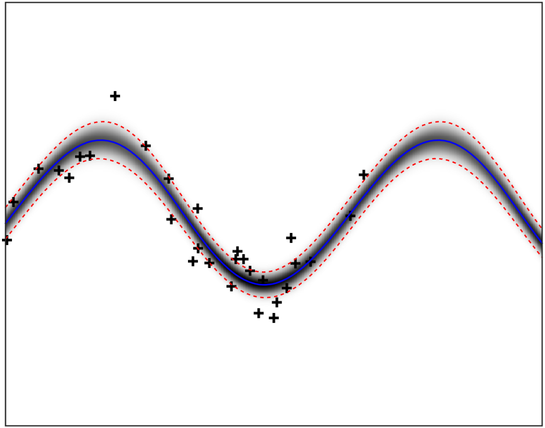
$$f(t) \sim \mathrm{GP}(0, \kappa(t, t')),$$
$$y_i = f(t_i) + \varepsilon_i, \quad \varepsilon_i \sim \mathrm{N}(0, \sigma_\mathrm{n}^2)$$

- The posterior mean and variance for an unseen test input t_* is given by (see previous lectures):

$$\mathbb{E}[f_*] = \mathbf{k}_* \, (\mathbf{K} + \sigma_\mathrm{n}^2 \, \mathbf{I})^{-1} \, \mathbf{y},$$
$$\mathbb{V}[f_*] = \mathbf{k}_* \, (\mathbf{K} + \sigma_\mathrm{n}^2 \, \mathbf{I})^{-1} \, \mathbf{k}_*^\mathsf{T}$$

- Note the inversion of the $n \times n$ matrix.

Example: GP regression, $\mathcal{O}(n^3)$



Example: GP regression, $\mathcal{O}(n)$

- The sequential solution (goes under the name 'Kalman filter') considers one data point at a time, hence the linear time-scaling.
- Start from $\mathbf{m}_0 = \mathbf{0}$ and $\mathbf{P}_0 = \mathbf{P}_\infty$ and for each data point iterate the following steps.
- Kalman prediction:

$$\begin{aligned}
\mathbf{m}_{i|i-1} &= \mathbf{A}_{i-1}\,\mathbf{m}_{i-1|i-1}, \\
\mathbf{P}_{i|i-1} &= \mathbf{A}_{i-1}\,\mathbf{P}_{i-1|i-1}\,\mathbf{A}_{i-1}^{\mathsf{T}} + \mathbf{Q}_{i-1}.
\end{aligned}$$

- Kalman update:

$$\begin{aligned}
\mathbf{v}_i &= y_i - \mathbf{H}\,\mathbf{m}_{i|i-1}, \\
\mathbf{S}_i &= \mathbf{H}_i\,\mathbf{P}_{i|i-1}\,\mathbf{H}^{\mathsf{T}} + \sigma_\mathrm{n}^2, \\
\mathbf{K}_i &= \mathbf{P}_{i|i-1}\,\mathbf{H}^{\mathsf{T}}\,\mathbf{S}_i^{-1}, \\
\mathbf{m}_{i|i} &= \mathbf{m}_{i|i-1} + \mathbf{K}_i\,\mathbf{v}_i, \\
\mathbf{P}_{i|i} &= \mathbf{P}_{i|i-1} - \mathbf{K}_i\,\mathbf{S}_i\,\mathbf{K}_i^{\mathsf{T}}.
\end{aligned}$$

Example: GP regression, $\mathcal{O}(n)$

- To condition all time-marginals on all data, run a backward sweep (Rauch–Tung–Striebel smoother):

$$
\begin{aligned}
\mathbf{m}_{i+1|i} &= \mathbf{A}_i \, \mathbf{m}_{i|i}, \\
\mathbf{P}_{i+1|i} &= \mathbf{A}_i \, \mathbf{P}_{i|i} \, \mathbf{A}_i^\mathsf{T} + \mathbf{Q}_i, \\
\mathbf{G}_i &= \mathbf{P}_{i|i} \, \mathbf{A}_i^\mathsf{T} \, \mathbf{P}_{i+1|i}^{-1}, \\
\mathbf{m}_{i|n} &= \mathbf{m}_{i|i} + \mathbf{G}_i \, (\mathbf{m}_{i+1|n} - \mathbf{m}_{i+1|i}), \\
\mathbf{P}_{i|n} &= \mathbf{P}_{i|i} + \mathbf{G}_i \, (\mathbf{P}_{i+1|n} - \mathbf{P}_{i+1|i}) \, \mathbf{G}_i^\mathsf{T},
\end{aligned}
$$

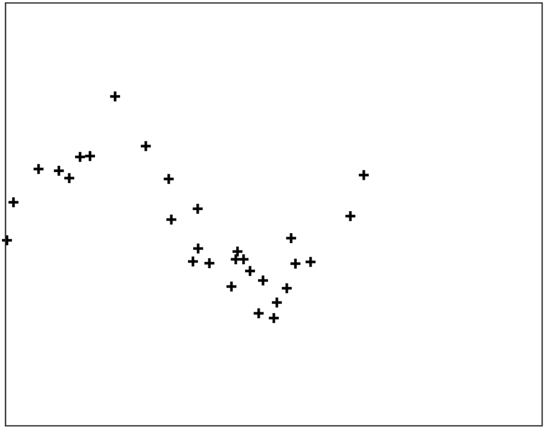
- The marginal mean and variance can be recovered by:

$$
\begin{aligned}
\mathbb{E}[f_i] &= \mathbf{H} \, \mathbf{m}_{i|n}, \\
\mathbb{V}[f_i] &= \mathbf{H} \, \mathbf{P}_{i|n} \, \mathbf{H}^\mathsf{T}
\end{aligned}
$$

- The log marginal likelihood can be evaluated as a by-product of the Kalman update:

$$
\log p(\mathbf{y}) = -\frac{1}{2} \sum_{i=1}^{n} \log |2\pi \, \mathbf{S}_i| + \mathbf{v}_i^\mathsf{T} \, \mathbf{S}_i^{-1} \mathbf{v}_i
$$

Example: GP regression, $\mathcal{O}(n)$



Example

- Number of births in the US
- Daily data between 1969–1988 ($n = 7305$)
- GP regression with a prior covariance function:

$$\kappa(t,t') = \kappa_{\text{Mat.}}^{\nu=5/2}(t,t') + \kappa_{\text{Mat.}}^{\nu=3/2}(t,t') \\ + \kappa_{\text{Per.}}^{\text{year}}(t,t')\,\kappa_{\text{Mat.}}^{\nu=3/2}(t,t') + \kappa_{\text{Per.}}^{\text{week}}(t,t')\,\kappa_{\text{Mat.}}^{\nu=3/2}(t,t')$$

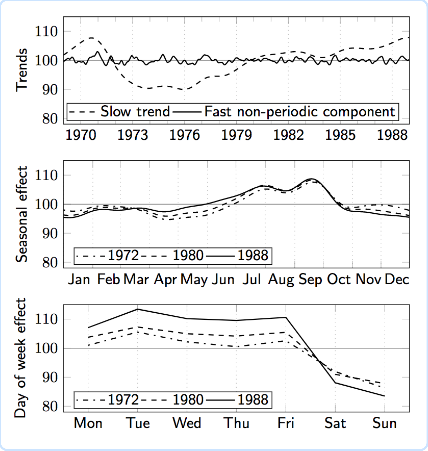
- Learn hyperparameters by optimizing the marginal likelihood

Example

- Number of
- Daily data
- GP regress ... on:

$\kappa(t, t') = \kappa$ ... $t, t')\, \kappa^{\nu=3/2}_{\text{Mat.}}(t, t')$

- Learn hype ... arginal likelihood



Explaining changes in number of births in the US

General likelihoods

Non-Gaussian likelihoods

- The observation model might not be Gaussian

$$f(t) \sim \mathrm{GP}(0, \kappa(t, t'))$$
$$\mathbf{y} \mid \mathbf{f} \sim \prod_i p(y_i \mid f(t_i))$$

- There exists a multitude of great methods to tackle general likelihoods with approximations of the form

$$\mathbb{Q}(\mathbf{f} \mid \mathcal{D}) = \mathrm{N}(\mathbf{f} \mid \mathbf{m} + \mathbf{K}\boldsymbol{\alpha}, (\mathbf{K}^{-1} + \mathbf{W})^{-1})$$

- Use those methods, but deal with the latent using state space models

Inference

- Laplace approximation
  (both inner-loop and outer-loop)
- Variational Bayes
- Direct KL minimization
- Assumed denisty filtering / Single-sweep EP
  (only requires one-pass through the data)
- Can be evaluated in terms of a (Kalman) filter forward and backward pass, or by iterating them

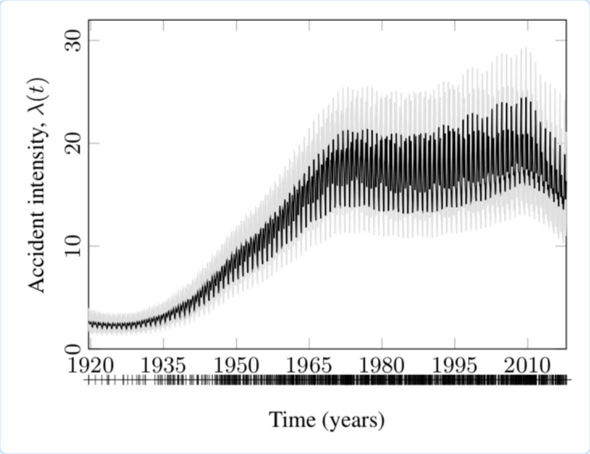
Example

- Commercial aircraft accidents 1919–2017
- Log-Gaussian Cox process (Poisson likelihood) by ADF/EP
- Daily binning, $n = 35{,}959$
- GP prior with a covariance function:

$$\kappa(t,t') = \kappa_{\text{Mat.}}^{\nu=3/2}(t,t') + \kappa_{\text{Per.}}^{\text{year}}(t,t')\,\kappa_{\text{Mat.}}^{\nu=3/2}(t,t') + \kappa_{\text{Per.}}^{\text{week}}(t,t')\,\kappa_{\text{Mat.}}^{\nu=3/2}(t,t')$$

- Learn hyperparameters by optimizing the marginal likelihood

Example



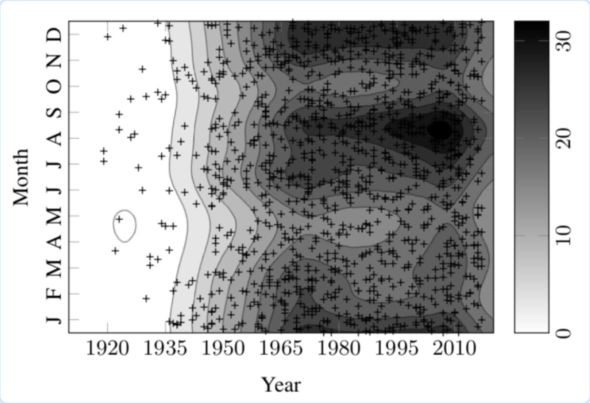
▶ Com
▶ Log- ADF/EP
▶ Daily
▶ GP
$\kappa(t,$ $\nu=3/2$ Mat. (t, t')
▶ Lear likeli

Example

- Com
- Log- ... ADF/EP
- Daily
- GP ...

$\kappa(t, t$ ... $^{\nu=3/2}_{\text{Mat.}}(t, t')$

- Lear ... likeli



Spatio-temporal Gaussian processes

Spatio-temporal GPs

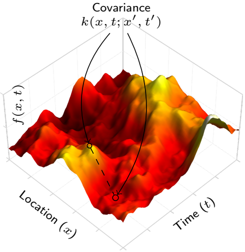
$$f(\mathbf{x}) \sim \mathrm{GP}(0, \kappa(\mathbf{x}, \mathbf{x}'))$$
$$\mathbf{y} \mid \mathbf{f} \sim \prod_i p(y_i \mid f(\mathbf{x}_i))$$

$$f(\mathbf{r}, t) \sim \mathrm{GP}(0, \kappa(\mathbf{r}, t; \mathbf{r}', t'))$$
$$\mathbf{y} \mid \mathbf{f} \sim \prod_i p(y_i \mid f(\mathbf{r}_i, t_i))$$

Spatio-temporal Gaussian processes

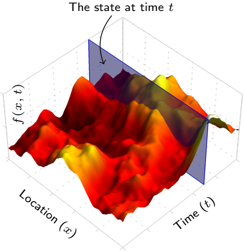
GPs under the kernel formalism

$$f(\mathbf{x}, t) \sim \mathrm{GP}(0, k(\mathbf{x}, t; \mathbf{x}', t'))$$
$$y_i = f(\mathbf{x}_i, t_i) + \varepsilon_i$$

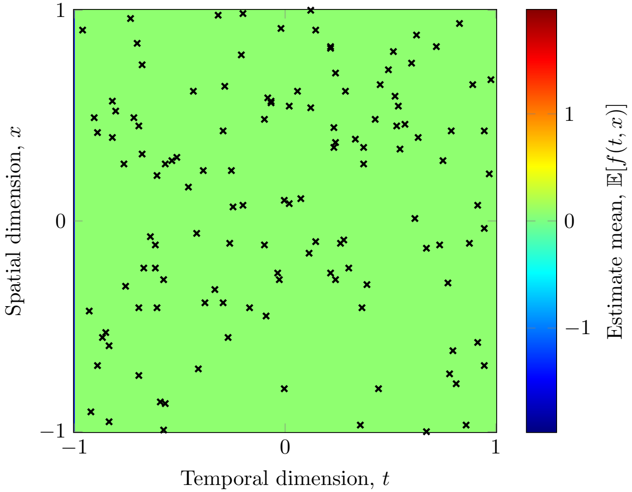


Stochastic partial differential equations

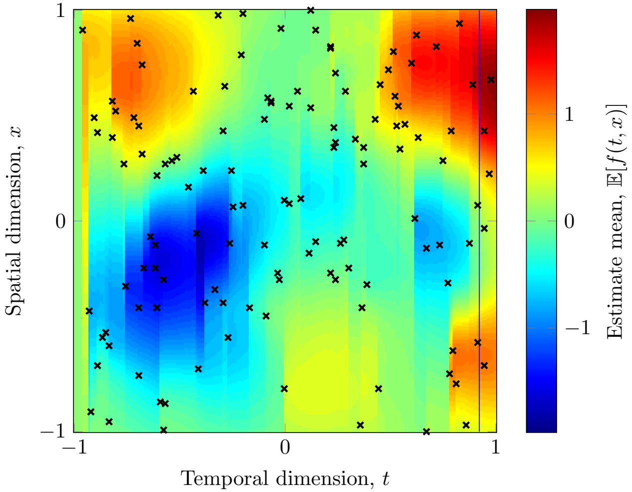
$$\frac{\partial \mathbf{f}(\mathbf{x}, t)}{\partial t} = \mathcal{F}\, \mathbf{f}(\mathbf{x}, t) + \mathcal{L}\, w(\mathbf{x}, t)$$
$$y_i = \mathcal{H}_i\, \mathbf{f}(\mathbf{x}, t) + \varepsilon_i$$



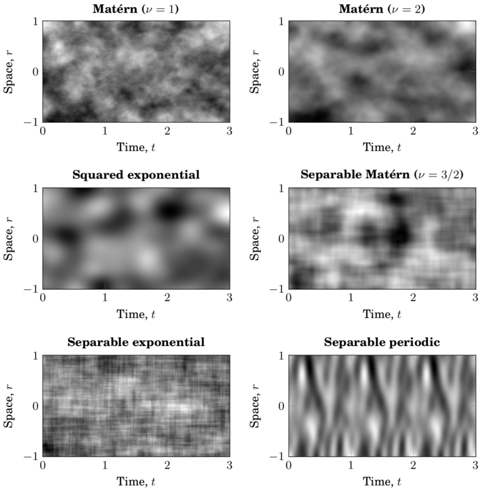
Spatio-temporal GP regression



Spatio-temporal GP regression

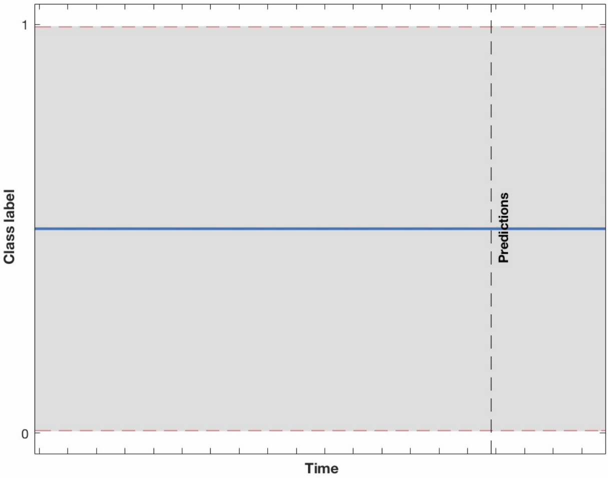


Spatio-temporal GP priors

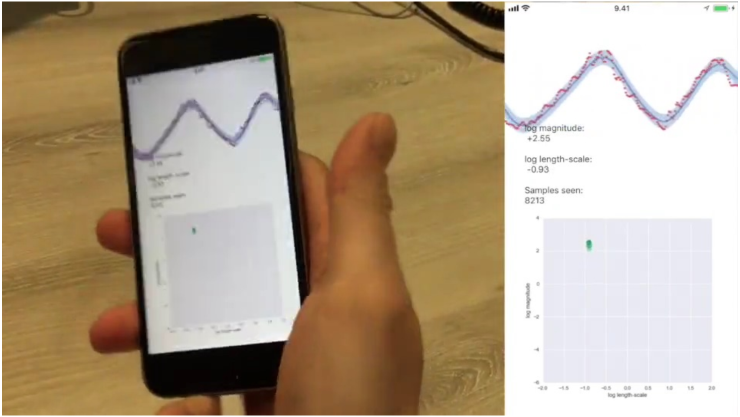


Further extensions

What if the data really is infinite?



Adapting the hyperparameters online



https://youtu.be/myCvUT3XGPc

Recap

Gaussian processes ❤ SDEs

GPs under the kernel formalism

$$f(t) \sim \mathrm{GP}(0, \kappa(t, t'))$$

$$\mathbf{y} \mid \mathbf{f} \sim \prod_i p(y_i \mid f(t_i))$$

Flexible model specification

Inference / First-principles

Stochastic differential equations

$$\mathrm{d}\mathbf{f}(t) = \mathbf{F}\,\mathbf{f}(t) + \mathbf{L}\,\mathrm{d}\beta(t)$$

$$y_i \sim p(y_i \mid \mathbf{h}^\mathsf{T}\mathbf{f}(t_i))$$

Recap

- Gaussian processes have different representations:
  • Covariance function • Spectral density • State space
- Temporal (single-input) Gaussian processes
  $\iff$ stochastic differential equations (SDEs)
- Conversions between the representations can make model building easier
- (Exact) inference of the latent functions, can be done in $\mathcal{O}(n)$ time and memory complexity by Kalman filtering

Bibliography

The examples and methods presented on this lecture are presented in greater detail in the following works:

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