Gaussian Processes for time-series

Vincent Adam

Secondmind

Senior Machine Learning researcher

@vincentadam87

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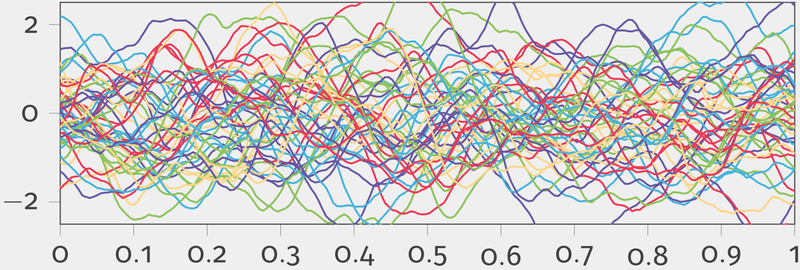
Outline

- Recap on Gaussian Processes
- 3 views of Gaussian processes
- Gaussian processes as SDE
- Inference and learning
- Examples

Inspired by Arno Solin's ICML 2020 tutorial



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Gaussian Process Regression

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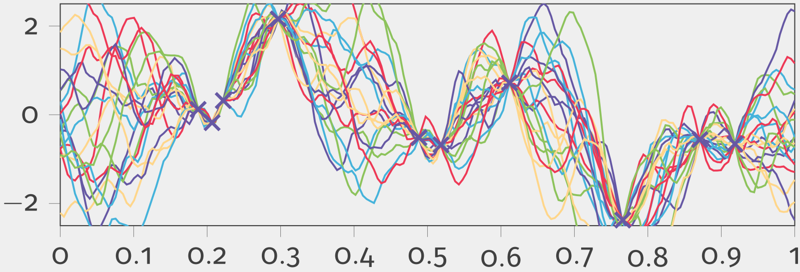
$$p(\mathbf{y}|f(\cdot)) = \prod_{i=1}^{n} p(y_i|f(t_i))$$



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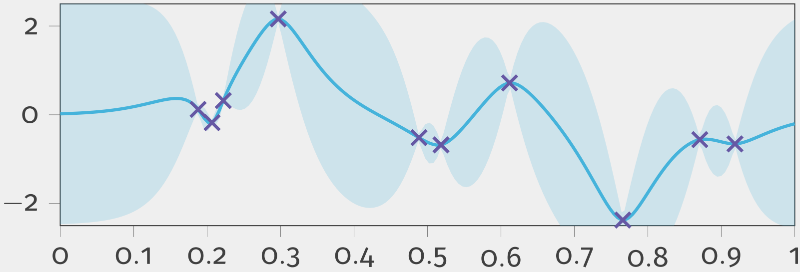

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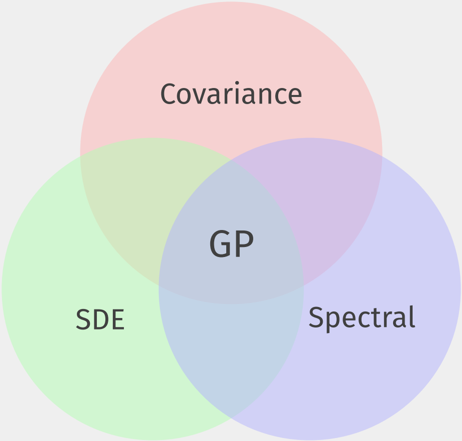
Three views of GPs [1]



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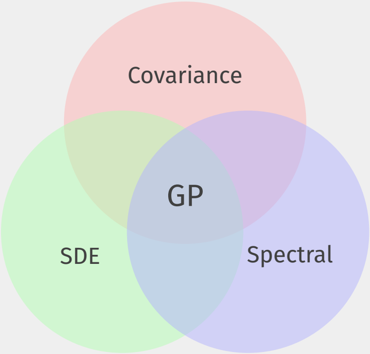

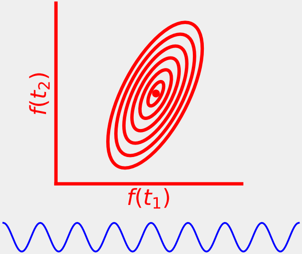

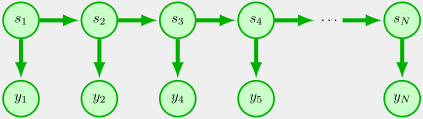

Parameterization through mean μ and covariance function k

$$
\begin{aligned}
f &\sim \mathcal{GP}(\mu(\cdot), k(\cdot,\cdot)) \\
y \,|\, f &\sim \prod_n p(y_n \,|\, f(t_n))
\end{aligned}
$$

Parameterization through mean μ and covariance function k

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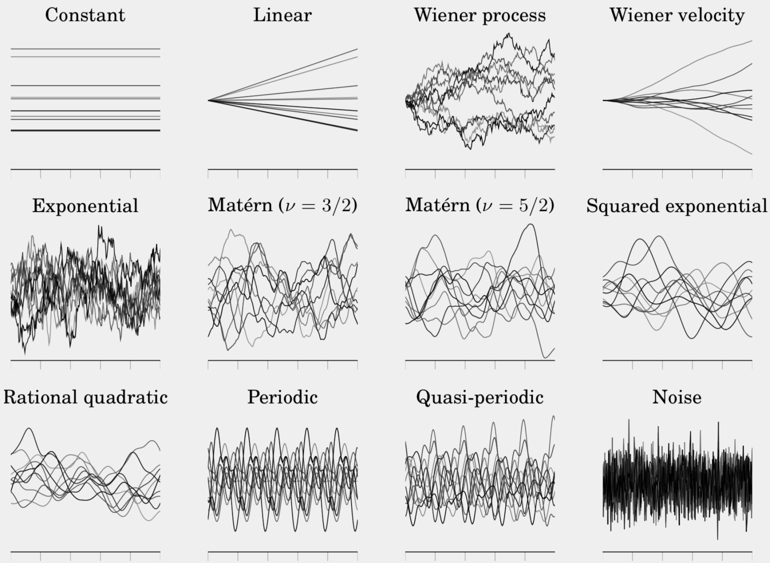
Noting $\mathbf{t} = (t_1, \ldots, t_N)$ and $\mathbf{f} = f(\mathbf{t})$, we have $\mathbf{f} \sim \mathcal{N}(\mu(\mathbf{t}), k(\mathbf{t}, \mathbf{t}))$

$$\begin{aligned} \mu(\mathbf{t}) &= \mathbb{E}[f(\mathbf{t})] \\ k(\mathbf{t}, \mathbf{t}) &= \mathbb{E}[(f(\mathbf{t}) - \mu(\mathbf{t}))(f(\mathbf{t}) - \mu(\mathbf{t}))^\top] \end{aligned}$$

Covariance view



Bochner theorem for stationary kernels

$$S(\omega) = \int e^{-i\omega\tau} k(\tau) d\tau$$

Power of Fourier components

$$s(i\omega) = \mathcal{F}[\omega](f) = \int e^{-i\omega t} f(t) dt$$
$$S(\omega) = \mathbb{E}[s(i\omega)\bar{s}(i\omega)^\top]$$

Example: Design through spectral density [2]

$$S(\omega) = \sum_i a_i \mathcal{N}(\omega \mid \mu_i, \sigma_i^2)$$

$$k(\tau) = \sum_i a_i \exp(-2\pi^2 \sigma_i^2 \tau^2) \cos(2\pi\tau\mu_i)$$

Gaussian Processes as SDE [3]

For Gaussian Process on the line (1d input), one can rewrite

$$f \sim GP(0, k(t,t')) \leftrightarrow \begin{cases} \frac{d\mathbf{s}(t)}{dt} = \mathbf{F}\,\mathbf{s}(t) + \mathbf{L}w(t) \\ f(t) = \mathbf{H}\,\mathbf{s}(t) \end{cases} \qquad (SDE)$$

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This can be discretized on $\mathbf{t} = [t_1, ..., t_T]$

$$\mathbf{f} \sim GP(0, K_{\mathbf{tt}}) \leftrightarrow \begin{cases} \mathbf{s}_{t+1} = \mathbf{A}_t\mathbf{s}_t + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, \mathbf{Q}_t) \\ f_t = \mathbf{H}\,\mathbf{s}_t \end{cases} \qquad (SSM)$$

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with

$$\mathbf{A}_i = e^{\Delta t_i \mathbf{F}} \quad \text{and} \quad \mathbf{Q}_i = \int_0^{\Delta t_i} e^{(\Delta t_i - \tau)\mathbf{F}}\,\mathbf{L}\,\mathbf{Q}_c\,\mathbf{L}^T\,e^{(\Delta t_i - \tau)\mathbf{F}^T} d\tau$$

$$\begin{cases} \mathbf{s}_{t+1} = \mathbf{A}_t \mathbf{s}_t + \epsilon_t, & \epsilon_t \sim \mathcal{N}(0, \mathbf{Q}_t) \\ f_t = \mathbf{H}\,\mathbf{s}_t \end{cases} \qquad (SSM)$$

Markov property

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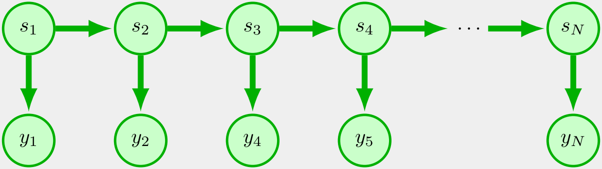

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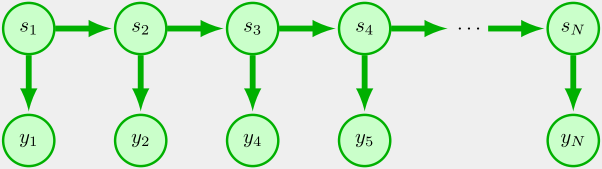

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\mathbf{s}_{t+1} \,\big|\, \mathbf{s}_0, \ldots, \mathbf{s}_t = \mathbf{s}_{t+1} \,\big|\, \mathbf{s}_t
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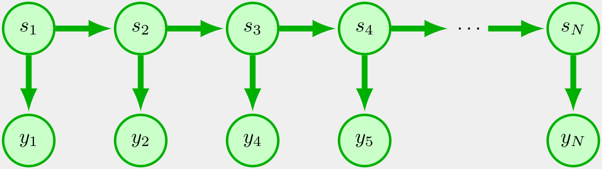


Markov Property

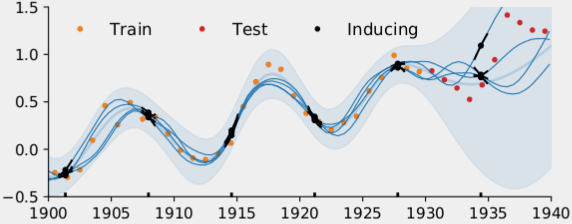
$$\mathbf{s}_{t+1} \,\big|\, \mathbf{s}_0, \ldots, \mathbf{s}_t = \mathbf{s}_{t+1} \,\big|\, \mathbf{s}_t$$

$$\mathbf{s}_t \,\big|\, \mathbf{s}_{\neg t} = \mathbf{s}_t \,\big|\, \mathbf{s}_{t-1}, \mathbf{s}_{t+1}$$

Gaussian Processes as SDE: Example

$$f \sim GP(0, k(t,t')) \leftrightarrow \begin{cases} \frac{d\mathbf{s}(t)}{dt} = \mathbf{F}\,\mathbf{s}(t) + \mathbf{L}w(t) \\ f(t) = \mathbf{H}\,\mathbf{s}(t) \end{cases} \qquad (SDE)$$

with $\mathbf{s} = [f, f', \ldots, f^{(d)}]$



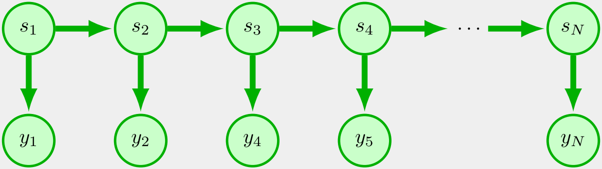
Inference in State Space Models [4]

$$\mathbf{f} \sim GP(0, K_{\mathbf{tt}}) \leftrightarrow \begin{cases} \mathbf{s}_{t+1} = \mathbf{A}_t \mathbf{s}_t + \epsilon_t, & \epsilon_t \sim \mathcal{N}(0, \mathbf{Q}_t) \\ f_t = \mathbf{H}\, \mathbf{s}_t \end{cases} \tag{SSM}$$

$$\mathbf{y} \,|\, \mathbf{f} \sim \prod_n p(\mathbf{y}_n \,|\, \mathbf{f}_n)$$

Inference and learning $\rightarrow$ **Kalman** filtering and smoothing

- both $p(\mathbf{f} \,|\, \mathbf{y})$ and $p(\mathbf{y})$ available in time $\mathcal{O}(Nd^3)$
- Sequential computation



Approximate Filtering $\mathcal{O}(N)$

- Sampling [5]
- Expectation Propagation (EP) [6, 7]
- Variational Inference (VI) [7, 8]
- ...
- (Sparse $\mathcal{GP}$) $\cap$ ($\mathcal{GP}$ as SDE) [9]

Kernel Combination

- Sum of kernels: $(d_1, d_2) \rightarrow d_1 + d_2$
- Product of kernels: $(d_1, d_2) \rightarrow d_1 \times d_2$

Model design [3]

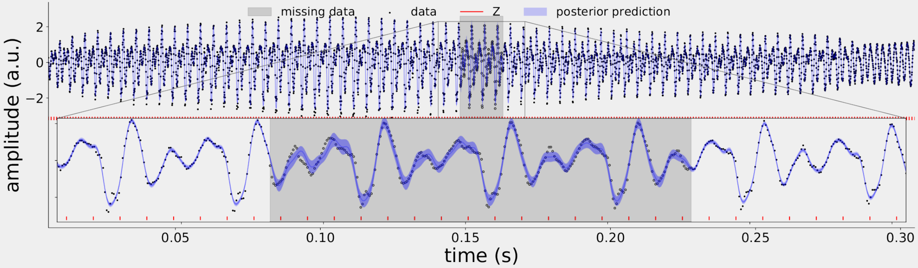
Kernel Combination

- Sum of kernels: $(d_1, d_2) \to d_1 + d_2$
- Product of kernels: $(d_1, d_2) \to d_1 \times d_2$

Multi-output Gaussian Processes

- o outputs: $\mathbf{f}_t = \mathbf{H}\,\mathbf{s}_t$, with $\mathbf{H} \in \mathbb{R}^{o \times d}$

Imputing missing segment in speech signal

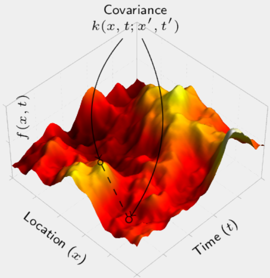


Harmonic kernel, Gaussian noise.

Spatio-Temporal Gaussian Processes [10]

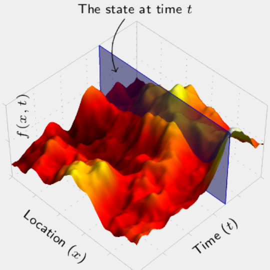
Kernel Formalism

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



Stochastic *partial* differential equation

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

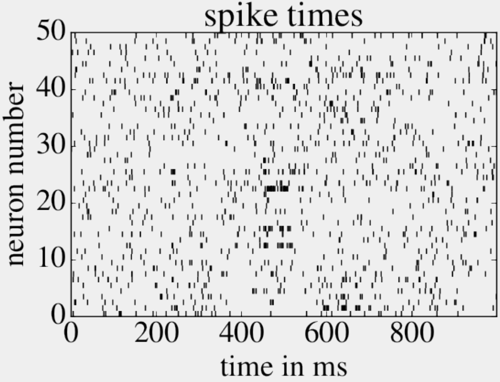


Scalar

- Classic Regression $y \mid \mathbf{f} = \mathcal{N}(y \mid \mathbf{f}_1, \sigma^2)$
- Heteroskedastic $y \mid \mathbf{f} = \mathcal{N}(y \mid \mathbf{f}_1, e^{\mathbf{f}_2})$

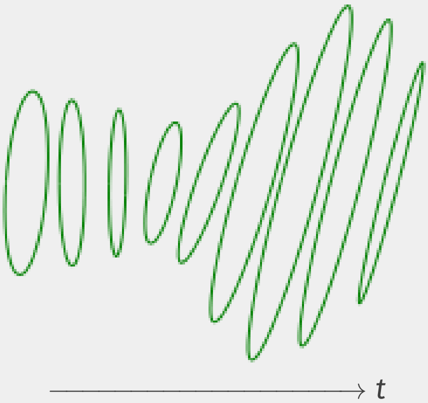
Multi-output (shared signal)

- $\mathbf{f}_t = \mathbf{H}\,\mathbf{s}_t$, with $\mathbf{H} \in \mathbb{R}^{o \times d}$



Multi-output (shared noise)

- Wishart: $\mathbf{y} \mid \mathbf{f} = \mathcal{N}(\mathbf{y} \mid 0, \mathbf{W}(\mathbf{f}))$



Summary

- 3 views of Gaussian processes
- Gaussian processes as SDE
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Thanks !

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