Fast Gaussian Processes for Time Series

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Slides: https://willtebbutt.github.io

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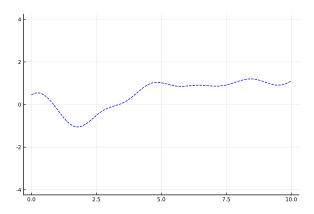


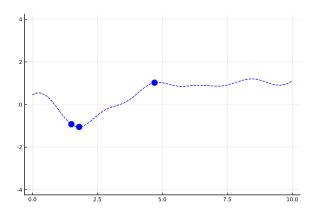
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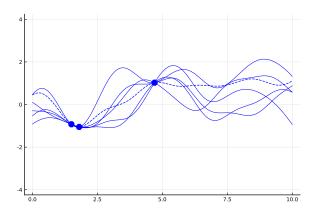
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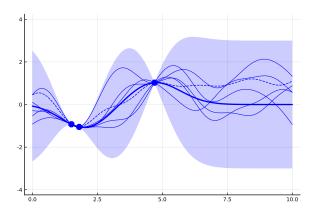
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Scalability Issues

- $ightharpoonup \mathcal{O}(N^3)$ temporal complexity
- $ightharpoonup \mathcal{O}(N^2)$ spatial complexity

Scaling Ooooo that takes a while

 10^{-6}

 10^{0}

 10^{1}

 $\begin{array}{c|c} & 10^1 \\ 10^0 \\ 10^{-1} \\ 10^{-2} \\ & 10^{-3} \\ 10^{-4} \\ 10^{-5} \\ \end{array}$

Figure: Naive log marginal likelihood computation requires $\mathcal{O}(N^3)$ time. Single thread. Uses Stheno.jl.

N

 10^{2}

 10^{3}

 10^{4}

GPs as SDEs in a Nutshell

- Convert GP f into a linear SDE
- lacktriangle Convert linear SDE into Linear Gaussian SSM at times $t_{1:N}$
- ▶ Do inference e.g. compute $\log p(\mathbf{y}_{1:N})$

See [Särkkä and Solin, 2019] for details

TemporalGPs.jl Scaling

- Exact or almost exact inference
- $ightharpoonup \mathcal{O}(ND^3)$ temporal complexity
- $ightharpoonup \mathcal{O}(ND^2)$ spatial complexity
- ▶ D is reasonably small in lots of interesting cases.

TemporalGPs.jl Scaling

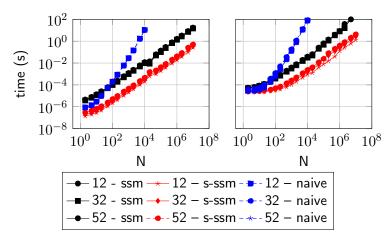


Figure: Time to compute log marginal likelihood (left) and log marginal likelihood + gradient (right). Naive uses Stheno.jl.

GPs as SDEs in a Nutshell

Use TemporalGPs.jl

```
using Stheno, TemporalGPs
# Specify a Stheno.jl GP as usual
f_naive = GP(Matern32(), GPC())
# Wrap it in an object that TemporalGPs knows how to handle.
f = to_sde(f_naive)
# Project onto finite-dimensional distribution as usual.
x = range(-5.0, 5.0; length=10 000 000)
fx = f(x, 0.1)
# Sample from the prior as usual.
y = rand(fx)
# Compute the log marginal likelihood of the data as usual.
logpdf(fx, y)
```

Features of TemporalGPs.jl

- ► Accelerate inference and learning in GPs from Stheno.jl
- Reverse-mode AD
- Checkpointing for memory-intensive problems (e.g. AD)
- ▶ Utilise StaticArrays.jl when D is small
- Spatio-temporal problems (small-medium space)

The Future

- ► Tidy up some of the API / types for prediction
- ▶ Integration with AbstractGPs.jl
- ► Further integration with Stheno.jl
- ► Non-Gaussian prediction problems

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Summary

- ► GPs scale poorly to large data
- ► TemporalGPs.jl makes them scale well for time-series.

Bibliography I



Hartikainen, J. et al. (2013).

Sequential inference for latent temporal gaussian process models.



Särkkä, S. and Solin, A. (2019).

Applied stochastic differential equations, volume 10. Cambridge University Press.



Solin, A. et al. (2016).

Stochastic differential equation methods for spatio-temporal gaussian process regression.

Bibliographic Notes GPs as Linear SDEs

- ► Final chapter of [Särkkä and Solin, 2019]
- ► Arno's these [Solin et al., 2016]
- ▶ Jouni Hartikainen's thesis: [Hartikainen et al., 2013]