Gaussian process models for Combining GCM Output

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Overview

Section 1

A Motivating Problem

Motivating Problem

- Consider estimating some interesting function of climate e.g. heatwave frequency
- Try with single climate model.
- Try with multiple (average?) of climate models.
- What goes wrong?
- What if we try with corrected marginal statistics?
- What goes wrong?

Motivating Problem

Desiderata

A statistical spatio-temporal model which:

1. has the ability to utilise many sources of information
2. is grid agnostic / can do downscaling
3. is able to model multi-timestep events e.g. heatwaves
4. can handle uncertainty
5. is computationally tractable

Section 2

Types of Uncertainty

Types of Uncertainty
UQ

- Multiple sources of uncertainty
- Some more tractable than others

Types of Uncertainty
[Kennedy and O'Hagan, 2001]

- Parameter uncertainty (eg. unknown parametrisation settings)

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- Parametric variability (eg. unknown forcing inputs)
- Observation error
- Code uncertainty (eg. unknown output at certain locations)

Section 3

Gaussian Processes

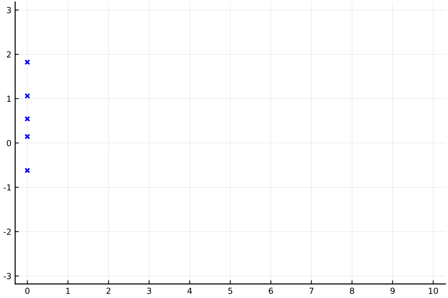
Gaussian processes

Interesting properties of GPs / why bother?

- Flexible, interpretable, uncertainty-aware, probabilistic models for functions
- Combine simple GPs to construct complicated GPs
- Natural data-efficient way to infer hyperparameters
- Exact Bayesian inference tractable for small-medium data sets
- Good / excellent approximations available for large data sets
- See GPML textbook [Rasmussen and Williams, 2006] for a thorough (ML-centric) introduction

Gaussian processes

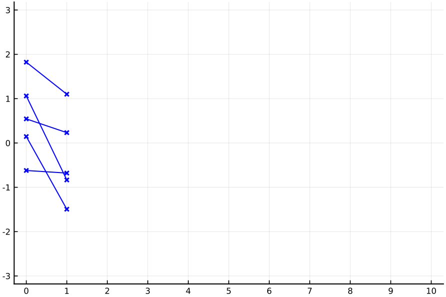
Multivariate Gaussians



$$\begin{bmatrix} 1.0 \end{bmatrix}$$

Gaussian processes

Multivariate Gaussians



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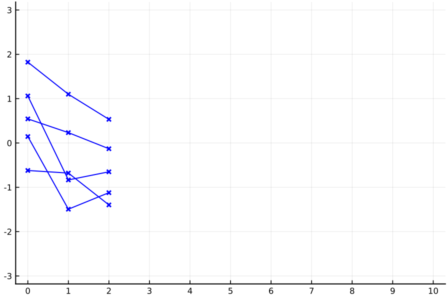
Gaussian processes

Multivariate Gaussians



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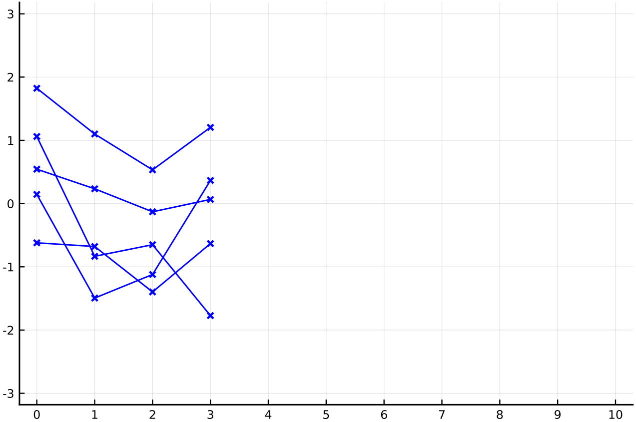
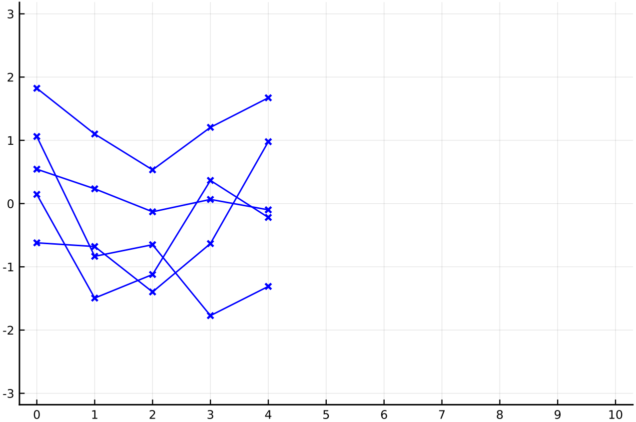
Gaussian processes
Multivariate Gaussians



Gaussian processes

Multivariate Gaussians



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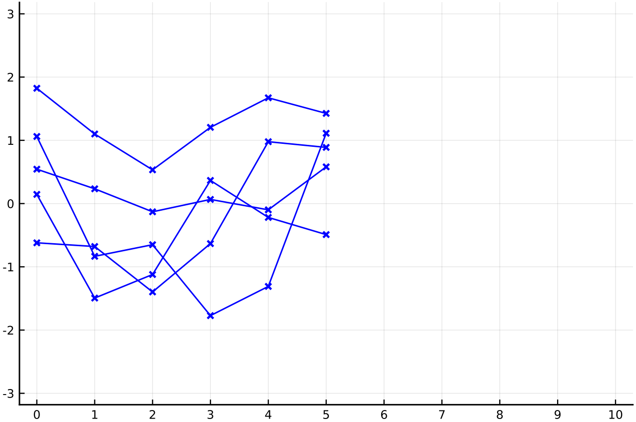
Multivariate Gaussians



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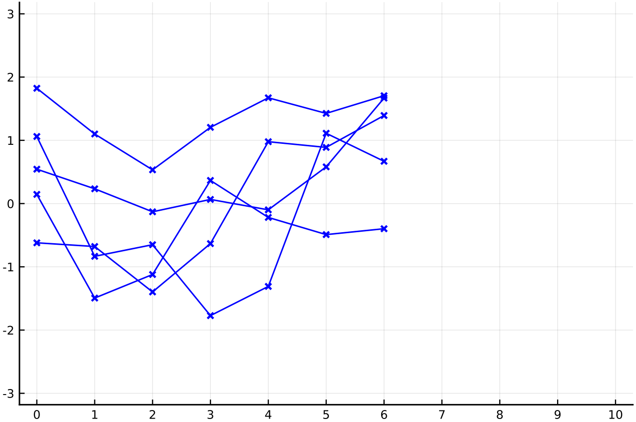

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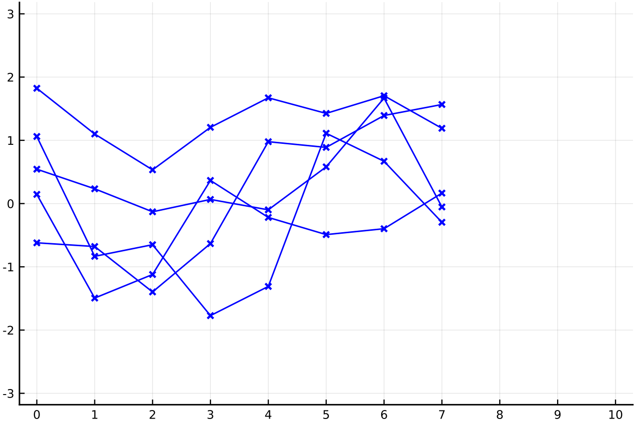

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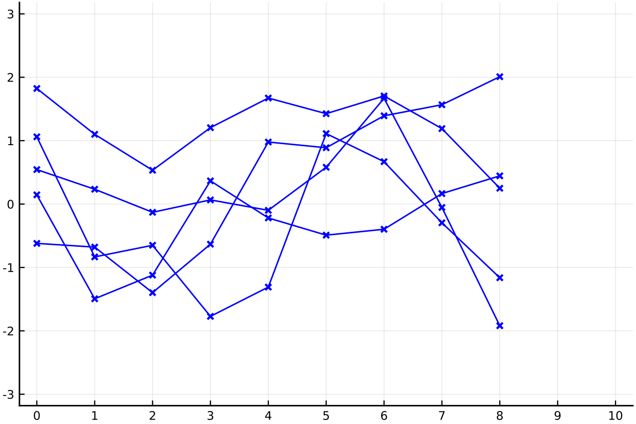

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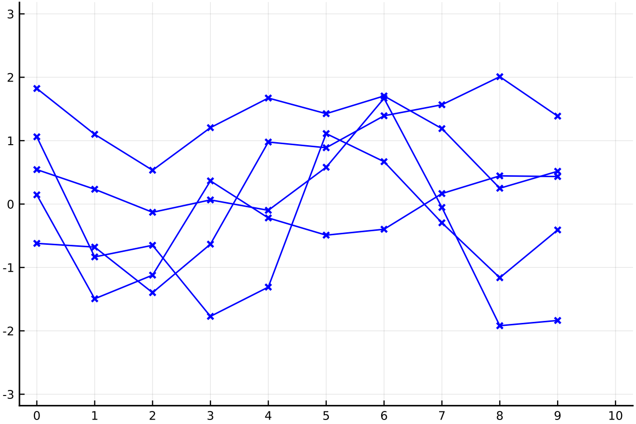

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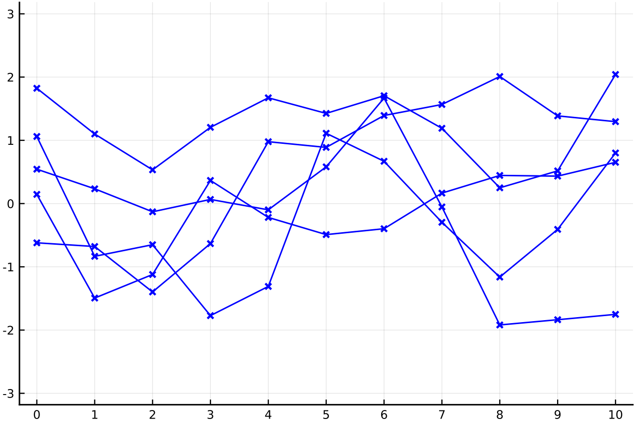

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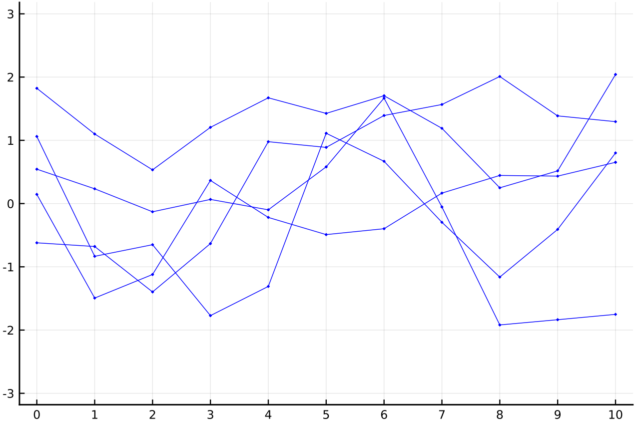

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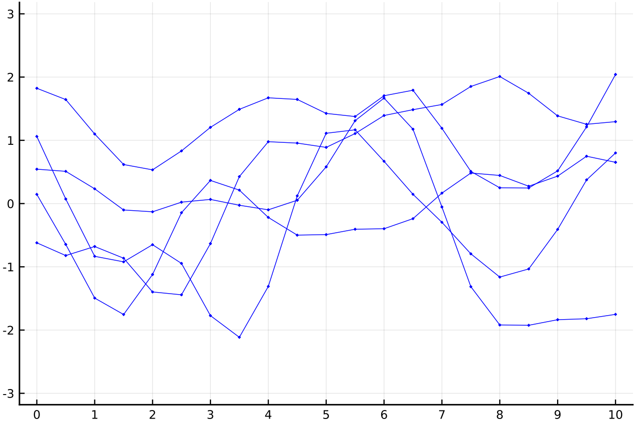

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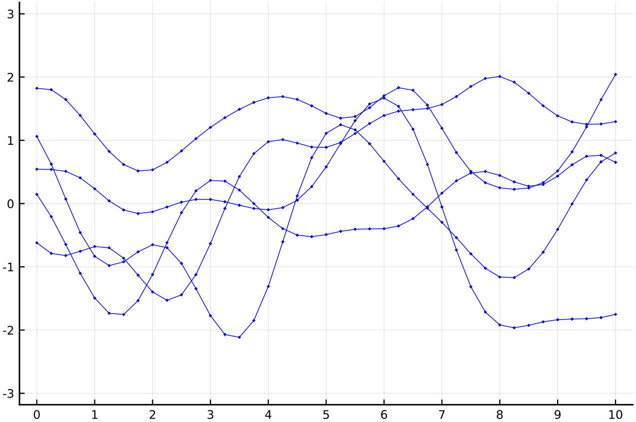

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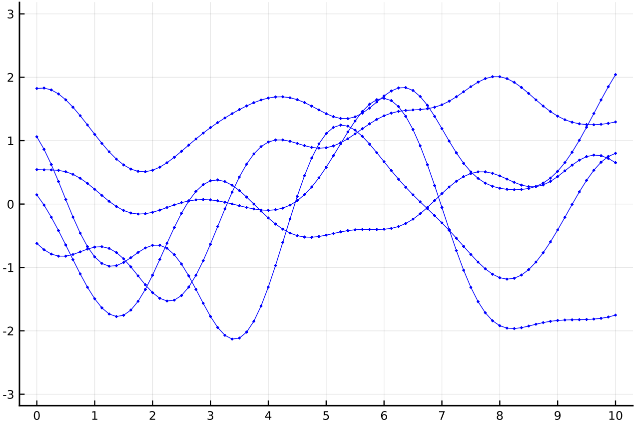

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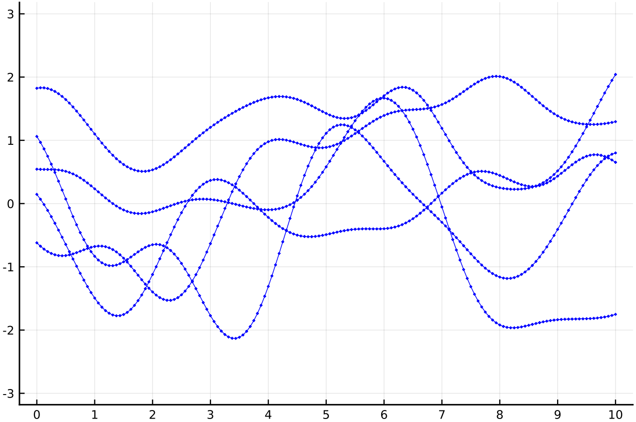

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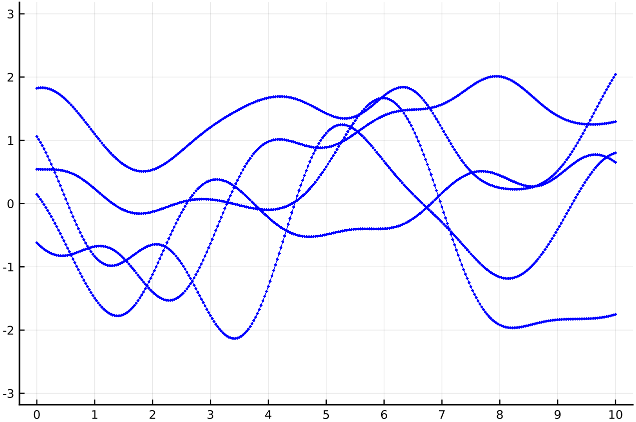


Gaussian processes

From Multivariate Gaussians to Gaussian Processes - Construction

Multivariate Gaussian

$$\mathsf{f} \sim \mathcal{N}(\mu, \Sigma)$$

$$\mu \in \mathbb{R}^D$$
$$\Sigma \in \mathbb{R}^{D \times D}$$

Gaussian Process

$$f \sim \mathcal{GP}(m, \kappa)$$

$$m : \mathbb{R} \to \mathbb{R}$$
$$\kappa : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$$

Gaussian processes

From Multivariate Gaussians to Gaussian Processes - Construction

Let $\mathbf{x} \in \mathbb{R}^N$ be a vector of input locations, then

$$f(\mathbf{x}) \sim \mathcal{N}(\mathbf{m}, \mathbf{C})$$

where

$$\begin{aligned} \mathbf{m}_n &:= m(\mathbf{x}_n) \\ \mathbf{C}_{nm} &:= \kappa(\mathbf{x}_n, \mathbf{x}_m) \end{aligned}$$

(Follows from the marginalisation property of Gaussians)

Gaussian processes

From Multivariate Gaussians to Gaussian Processes - Conditioning

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_{\mathbf{f}} \\ \mu_{\mathbf{g}} \end{bmatrix}, \begin{bmatrix} \Sigma_{\mathbf{ff}} & \Sigma_{\mathbf{fg}} \\ \Sigma_{\mathbf{gf}} & \Sigma_{\mathbf{gg}} \end{bmatrix} \right)$$

Gaussian processes

From Multivariate Gaussians to Gaussian Processes - Conditioning

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_{\mathbf{f}} \\ \mu_{\mathbf{g}} \end{bmatrix}, \begin{bmatrix} \Sigma_{\mathbf{ff}} & \Sigma_{\mathbf{fg}} \\ \Sigma_{\mathbf{gf}} & \Sigma_{\mathbf{gg}} \end{bmatrix} \right)$$

$$\implies \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} | \mathbf{f} \sim \mathcal{N}(\mu', \Sigma')$$

Gaussian processes

From Multivariate Gaussians to Gaussian Processes - Conditioning

$$f \sim \mathcal{GP}(m, \kappa)$$

Gaussian processes

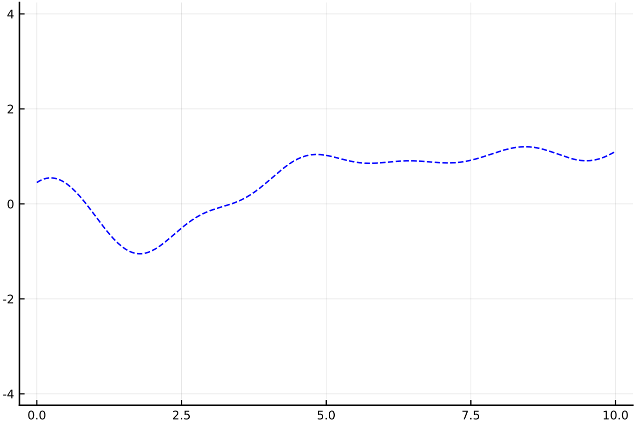
From Multivariate Gaussians to Gaussian Processes - Conditioning

$$f \sim \mathcal{GP}(m, \kappa)$$

$$\implies f | f(\mathbf{x}) \sim \mathcal{GP}\big(m', \kappa'\big)$$

Gaussian processes

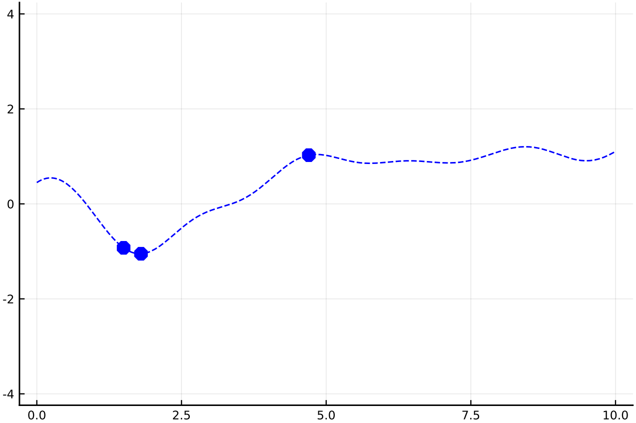
Non-Linear Regression



$$m(x) := 0, \quad \kappa\big(x, x'\big) := \exp\big(-(x - x')^2/2\big)$$

Gaussian processes

Non-Linear Regression



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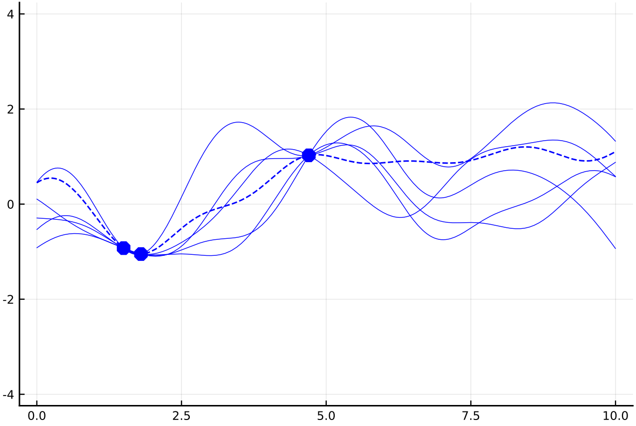

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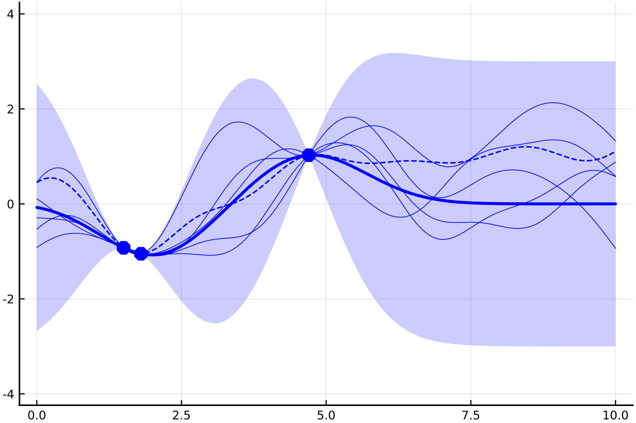

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Transformations of GPs

Linear (and affine) transformations of GPs yield GPs e.g.

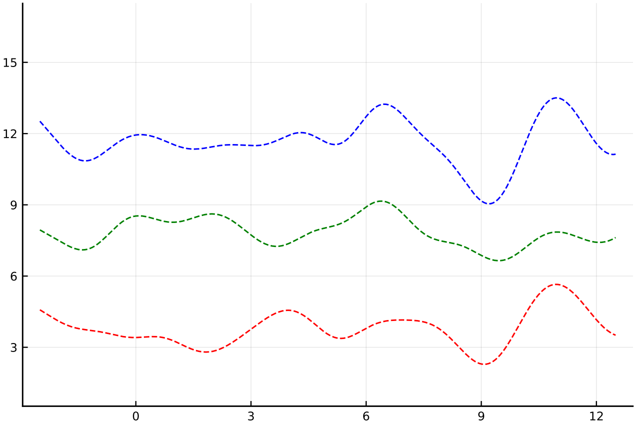
$$\begin{aligned} \text{addition:}\quad & f_3(x) := f_1(x) + f_2(x) \\ \text{scaling:}\quad & f_2(x) := a f_1(x) \\ \text{differentiation:}\quad & f_2(x) := \mathrm{d} f_1(x) \, / \mathrm{d} x \\ \text{integration:}\quad & f_2(x) := \int_l^x f_1(s) \, \mathrm{d} s \end{aligned}$$

Also conditioning, indexing, convolution, composition with deterministic functions, translation, etc

Transformations of GPs

Worked Example: Addition

$$f_3 = f_1 + f_2$$



Transformations of GPs

Worked Example: Addition

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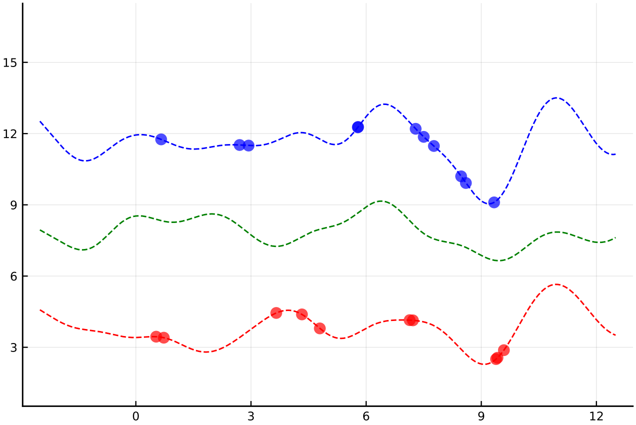

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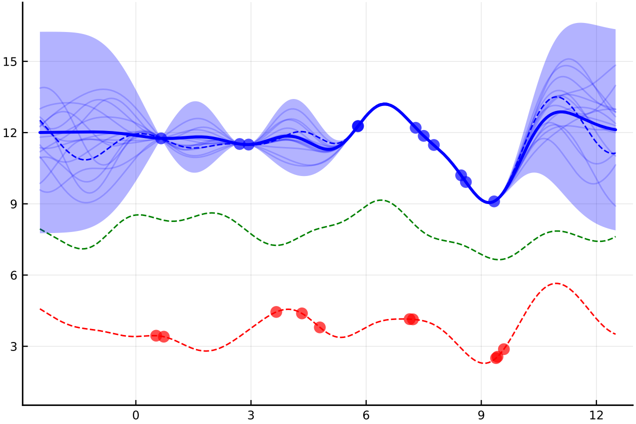

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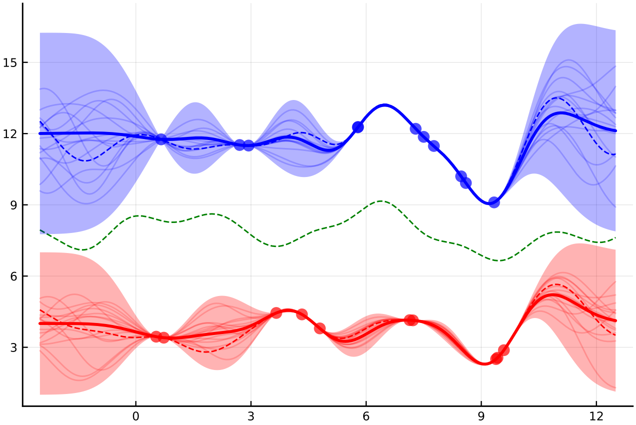

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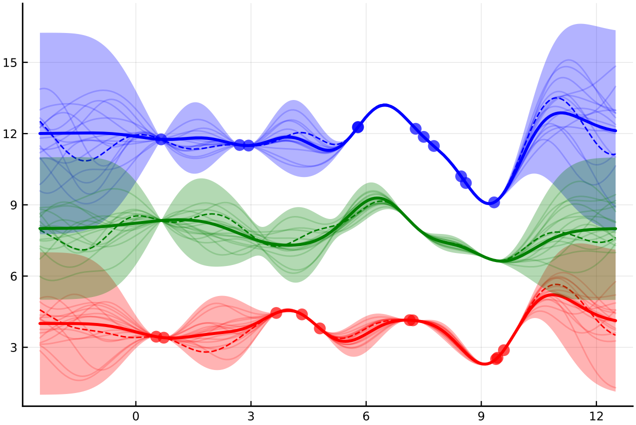


Section 4

A Model for GCM Combination

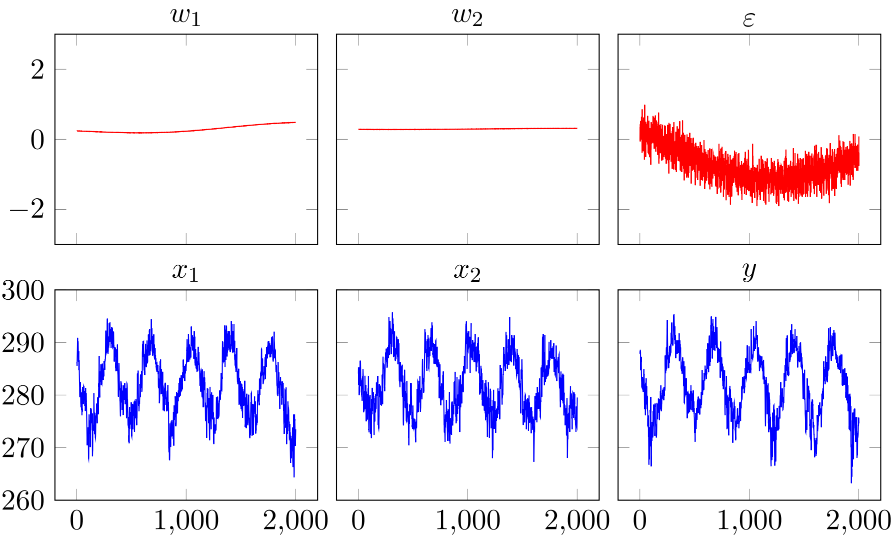
A Model for GCM Combination

Probabilistic Model

$$
\begin{aligned}
x_p &:= \text{Output of } p^{\text{th}} \text{ GCM} \\
w_p &\sim \mathcal{GP}\left(0, \kappa_p^{\mathrm{w}}\right), \quad p \in \{1, ..., P\} \\
f(t) &:= \sum_{p=1}^{P} w_p(t)\, x_p(t)
\end{aligned}
$$

$$
\begin{aligned}
\varepsilon &\sim \mathcal{GP}(0, \kappa^{\varepsilon}) \\
y(t) &:= f(t) + \varepsilon(t)
\end{aligned}
$$

A Model for GCM Combination



A Model for GCM Combination

Concrete Set Up

- Observe $\mathbf{x}_p := [x_p(t_1), ..., x_p(t_N)]^\top$
- Observe $\mathbf{y} := [y(t_1), ..., y(t_N)]^\top$
- Infer w_1, ..., w_P, and ε
- Learn kernel parameters

$$\underset{\theta}{\operatorname{argmax}} \quad \log p(\mathbf{y} \,|\, \mathbf{x}_{1:P}, \theta)$$

A Model for GCM Combination

Comments

- Correlated weather
- Allows for time-varying weights
- Jointly Gaussian, so inference tractable

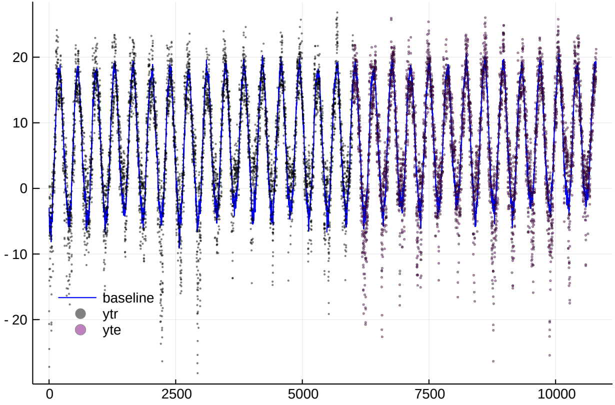
Section 5

Results

Results

- 28 GCMs, CMIP5, AMIP
- Era Interim
- Roughly 30 year's worth of data (10800 days)
- 6000 train, 4800 test

Results



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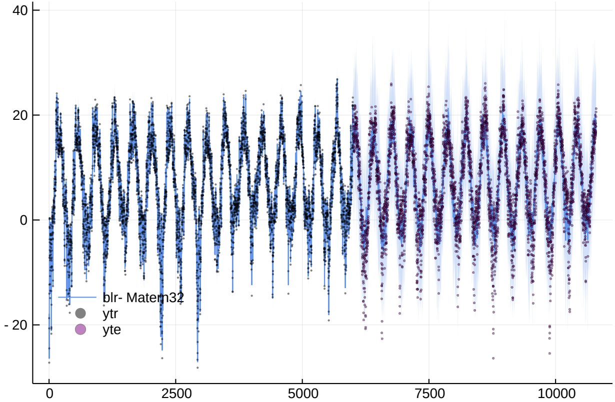

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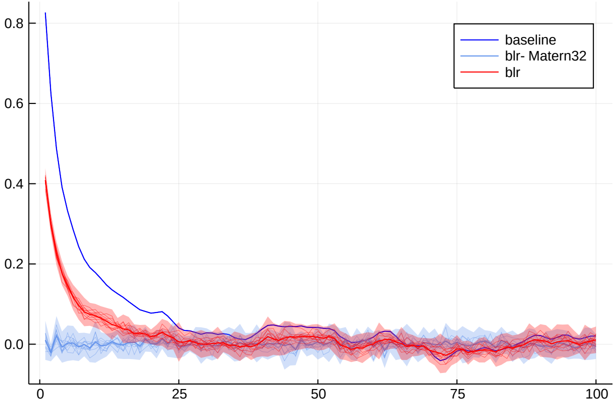

Results

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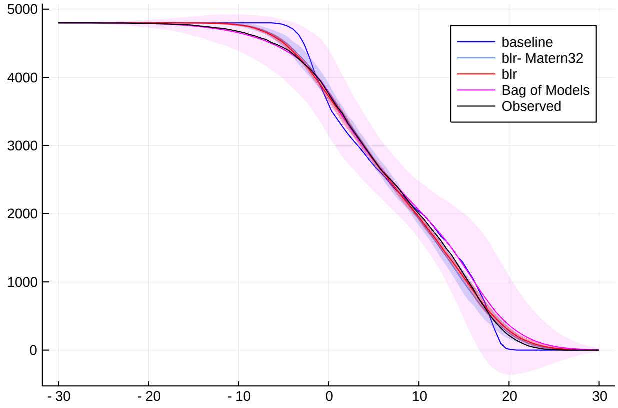

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Results

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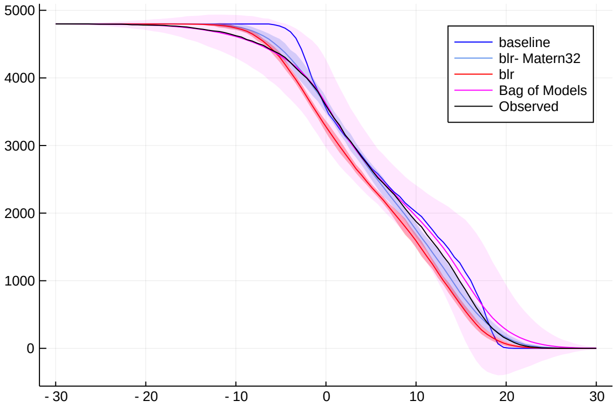
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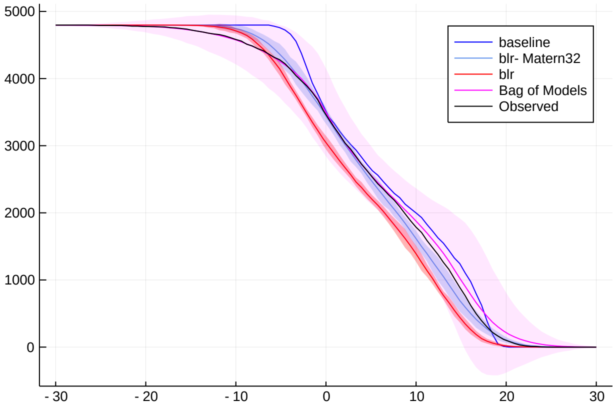

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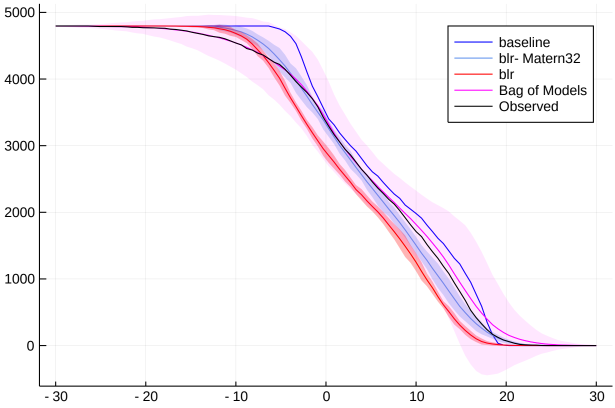

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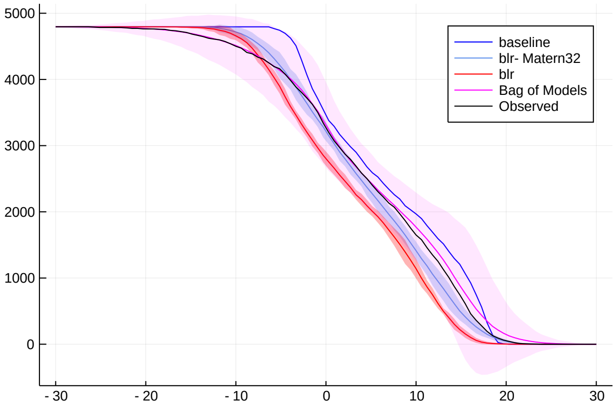
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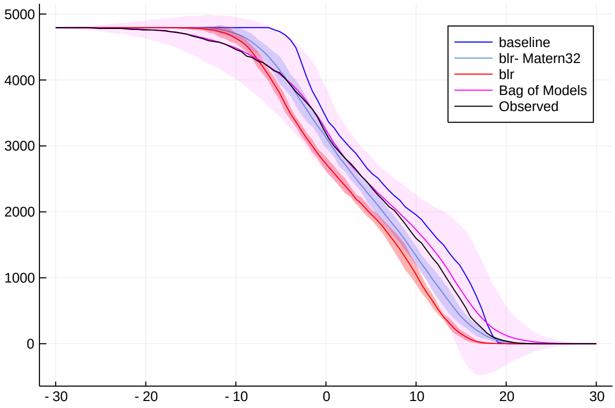

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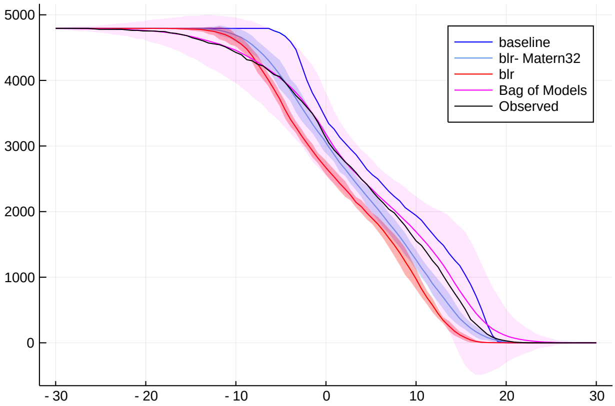
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Results

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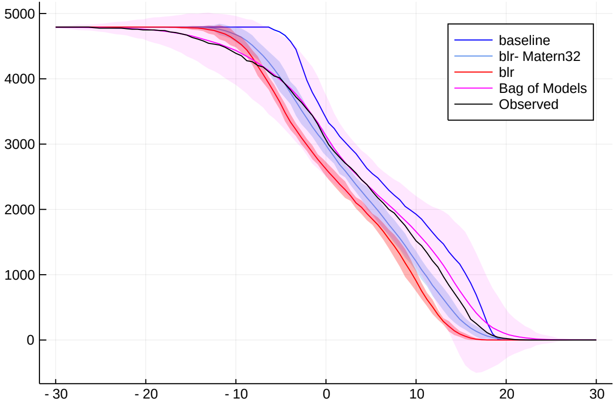

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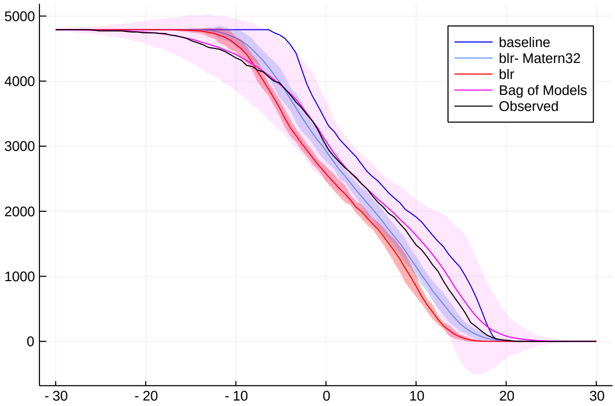
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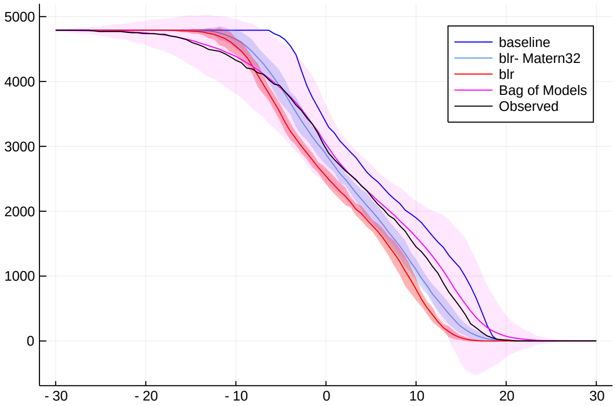

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Section 6

Conclusion

Conclusion

- Certain aspects of GCM uncertainty can be addressed with machine learning / statistical techniques
- Gaussian processes are a possible candidate for temperature - fine-tuning required for optimal performance
- Quite efficient inference for time-series
- Open problem to scale to very large spatio-temporal problems
- Hierarchical models containing GPs needed for eg. precipitation
- Side information?

Conclusion

- Model ensembling
- Downscaling
- Statistical weather modelling
- Single statistical model for all three?

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Section 7

Bibliographic Notes

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]

Bibliographic Notes

Combining GCM Predictions

- [Stainforth et al., 2007]: provides strong (not unreasonable) objections this entire line of work. [Chandler, 2013] provides a pragmatic alternative view. This pair of papers are the most important to read in my opinion. They elucidate all of the things that can go wrong, and that you therefore need to be aware of.
- Early work: [Krishnamurti et al., 1999], [Giorgi and Mearns, 2002], [Nychka and Tebaldi, 2003].
- [Monteleoni et al., 2011] - an interesting approach, the first (to my knowledge) with a time-varying combination of models. [McQuade and Monteleoni, 2012] extends to time + space varying.

Bibliographic Notes

Foundational Work on Simulators

Work on ways to "correct" the output of simulators has a long history. Some

- [McKay et al., 1979] - the earliest work I could find on the matter
- [Sacks et al., 1989] - very influential early work.
- [Kennedy and O'Hagan, 2001] - early uncertainty quantification work. A must read to get a good understanding of the issues.

Section 8

Gaussian processes for Time Series

GPs for Time Series

Preliminaries

GPs for Time Series
Preliminaries

$$f \sim \mathcal{GP}(0, \kappa)$$

GPs for Time Series

Preliminaries

$$
\begin{aligned}
& f \sim \mathcal{GP}(0, \kappa) \\
& \mathbf{f} := [f(t_1), ..., f(t_N)]^\top \sim \mathcal{N}(0, \mathbf{C})
\end{aligned}
$$

GPs for Time Series

Preliminaries

$$f \sim \mathcal{GP}(0, \kappa)$$
$$\mathbf{f} := [f(t_1), ..., f(t_N)]^\top \sim \mathcal{N}(0, \mathbf{C})$$
$$\text{where } \mathbf{C}_{nm} := \kappa(t_n, t_m)$$

GPs for Time Series

Preliminaries

$$f \sim \mathcal{GP}(0, \kappa)$$

$$\mathbf{f} := [f(t_1), ..., f(t_N)]^\top \sim \mathcal{N}(0, \mathbf{C})$$

where $\mathbf{C}_{nm} := \kappa(t_n, t_m)$

$\varepsilon \sim \mathcal{N}(0, \Sigma)$, assume Σ is diagonal

GPs for Time Series

Preliminaries

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$$\mathbf{f} := [f(t_1), ..., f(t_N)]^\top \sim \mathcal{N}(0, \mathbf{C})$$

where $\mathbf{C}_{nm} := \kappa(t_n, t_m)$

$\varepsilon \sim \mathcal{N}(0, \Sigma)$, assume Σ is diagonal

$$\mathbf{y} = \mathbf{f} + \varepsilon \sim \mathcal{N}(0, \mathbf{C} + \Sigma)$$

GPs for Time Series

Asymptotic Complexity

GPs for Time Series
Asymptotic Complexity

$\mathcal{O}(N^3)$ temporal complexity

GPs for Time Series

Asymptotic Complexity

$\mathcal{O}(N^3)$ temporal complexity

$\mathcal{O}(N^2)$ spatial complexity

GPs for Time Series

Ooooo that takes a while

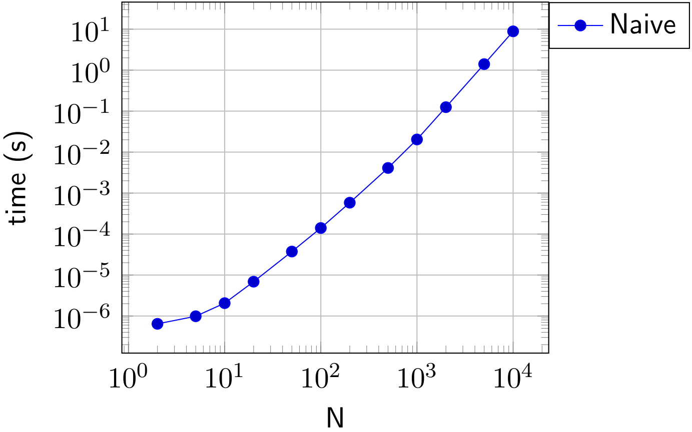


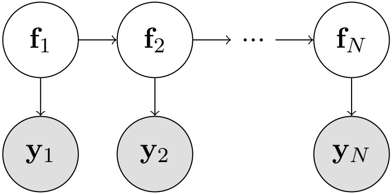
Figure 2: Naive log marginal likelihood computation requires $\mathcal{O}(N^3)$ time. Single thread.

Section 9

State Space Inference for Gaussian Processes

Linear Gaussian SSMs

What are they?

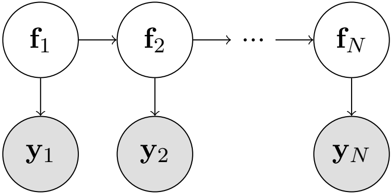


$$\mathbf{f}_n, \mathbf{q}_n \in \mathbb{R}^{D_{\text{lat}}}$$
$$\mathbf{y}_n, \mathbf{r}_n \in \mathbb{R}^{D_{\text{obs}}}$$

$$\mathbf{q}_n \sim \mathcal{N}(0, \mathbf{Q}_n)$$
$$\mathbf{f}_n = \mathbf{A}_n \mathbf{f}_{n-1} + \mathbf{q}_n$$
$$\mathbf{r}_n \sim \mathcal{N}(0, \mathbf{R}_n)$$
$$\mathbf{y}_n = \mathbf{H}_n \mathbf{f}_n + \mathbf{r}_n$$

Linear Gaussian SSMs

What are they?



- Specified by $(\mathbf{A}_n, \mathbf{Q}_n, \mathbf{H}_n, \mathbf{R}_n)_{n=1}^N$

$$\mathbf{f}_n, \mathbf{q}_n \in \mathbb{R}^{D_{\text{lat}}}$$
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Linear Gaussian SSMs

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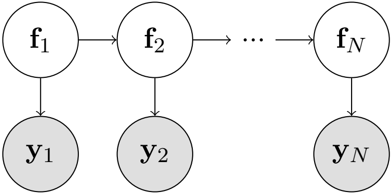

- Specified by $(\mathbf{A}_n, \mathbf{Q}_n, \mathbf{H}_n, \mathbf{R}_n)_{n=1}^N$
- $p(\mathbf{f}_{1:N}, \mathbf{y}_{1:N})$ jointly Gaussian

$$\mathbf{f}_n, \mathbf{q}_n \in \mathbb{R}^{D_{\text{lat}}}$$
$$\mathbf{y}_n, \mathbf{r}_n \in \mathbb{R}^{D_{\text{obs}}}$$

$$\mathbf{q}_n \sim \mathcal{N}(0, \mathbf{Q}_n)$$
$$\mathbf{f}_n = \mathbf{A}_n \mathbf{f}_{n-1} + \mathbf{q}_n$$
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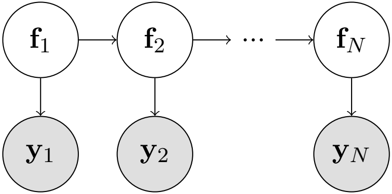
$$\mathbf{y}_n = \mathbf{H}_n \mathbf{f}_n + \mathbf{r}_n$$

Linear Gaussian SSMs

What are they?



- Specified by $(\mathbf{A}_n, \mathbf{Q}_n, \mathbf{H}_n, \mathbf{R}_n)_{n=1}^N$
- $p(\mathbf{f}_{1:N}, \mathbf{y}_{1:N})$ jointly Gaussian
- Inference tractable, $\log p(\mathbf{y}_{1:N})$ has

$$\mathbf{f}_n, \mathbf{q}_n \in \mathbb{R}^{D_{\text{lat}}}$$
$$\mathbf{y}_n, \mathbf{r}_n \in \mathbb{R}^{D_{\text{obs}}}$$

$$\mathbf{q}_n \sim \mathcal{N}(0, \mathbf{Q}_n)$$
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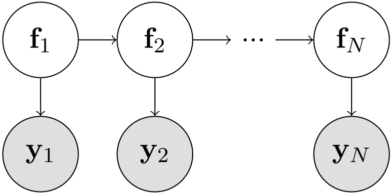
Linear Gaussian SSMs

What are they?



- Specified by $(\mathbf{A}_n, \mathbf{Q}_n, \mathbf{H}_n, \mathbf{R}_n)_{n=1}^N$
- $p(\mathbf{f}_{1:N}, \mathbf{y}_{1:N})$ jointly Gaussian
- Inference tractable, $\log p(\mathbf{y}_{1:N})$ has
  - $\mathcal{O}\big(N {D_{\text{obs}}}^3 {D_{\text{lat}}}^3\big)$ temporal complexity

$$\mathbf{f}_n, \mathbf{q}_n \in \mathbb{R}^{D_{\text{lat}}}$$
$$\mathbf{y}_n, \mathbf{r}_n \in \mathbb{R}^{D_{\text{obs}}}$$

$$\mathbf{q}_n \sim \mathcal{N}(0, \mathbf{Q}_n)$$
$$\mathbf{f}_n = \mathbf{A}_n \mathbf{f}_{n-1} + \mathbf{q}_n$$
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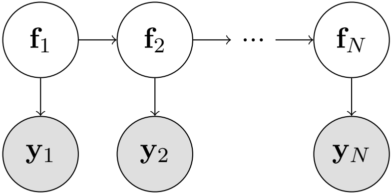
Linear Gaussian SSMs

What are they?



- Specified by $(\mathbf{A}_n, \mathbf{Q}_n, \mathbf{H}_n, \mathbf{R}_n)_{n=1}^N$
- $p(\mathbf{f}_{1:N}, \mathbf{y}_{1:N})$ jointly Gaussian
- Inference tractable, $\log p(\mathbf{y}_{1:N})$ has
  - $\mathcal{O}\left(N {D_{\text{obs}}}^3 {D_{\text{lat}}}^3\right)$ temporal complexity
  - $\mathcal{O}\left(N {D_{\text{obs}}}^2 {D_{\text{lat}}}^2\right)$ spatial complexity

$$\mathbf{f}_n, \mathbf{q}_n \in \mathbb{R}^{D_{\text{lat}}}$$
$$\mathbf{y}_n, \mathbf{r}_n \in \mathbb{R}^{D_{\text{obs}}}$$

$$\mathbf{q}_n \sim \mathcal{N}(0, \mathbf{Q}_n)$$
$$\mathbf{f}_n = \mathbf{A}_n \mathbf{f}_{n-1} + \mathbf{q}_n$$
$$\mathbf{r}_n \sim \mathcal{N}(0, \mathbf{R}_n)$$
$$\mathbf{y}_n = \mathbf{H}_n \mathbf{f}_n + \mathbf{r}_n$$

The Main Idea

- Convert GP f into a linear SDE
- 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

State Space Inference Techniques

Compute the log marginal likelihood

- Inputs:
  - f: a GP in terms of a kernel κ_θ
  - $t_{1:N}$: input locations
  - $\mathbf{y}_{1:N}$: corresponding observations
  - Σ: observation model covariance matrix
- Procedure:
  - Compute Linear Gaussian SSM $(\mathbf{A}_n, \mathbf{Q}_n, \mathbf{H}_n, \mathbf{R}_n)_{n=1}^{N}$ from κ_θ, $t_{1:N}$ and Σ
  - Compute $\log p(\mathbf{y}_{1:N})$ using Linear Gaussian SSM

Upshot

Properties

- Exact or almost exact inference
- $\mathcal{O}\left(ND^3\right)$ temporal complexity
- $\mathcal{O}\left(ND^2\right)$ spatial complexity
- D is reasonable in lots of interesting cases. Governed by smoothness of samples from the GP.

Upshot

Benchmarks

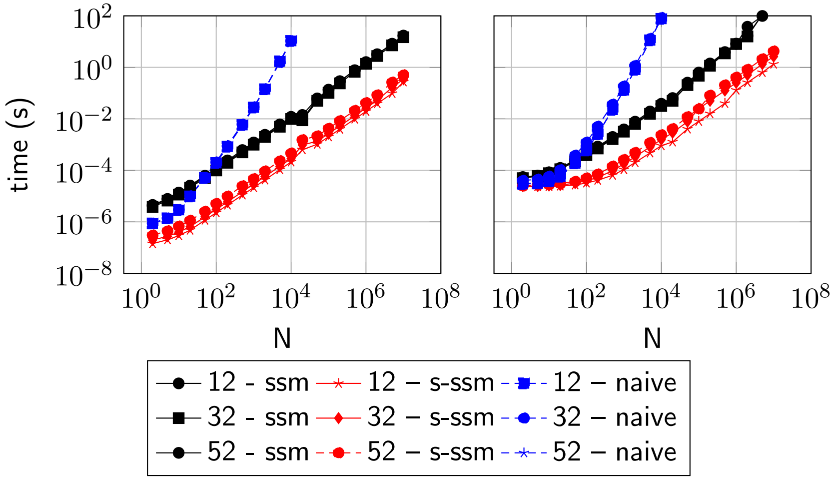
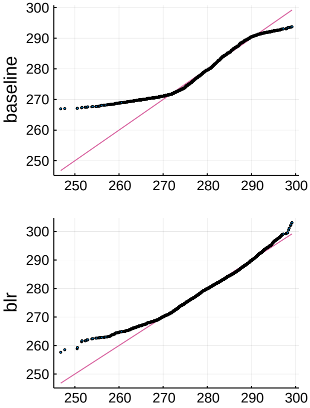


Figure 3: The total time to compute the log marginal likelihood (left) and log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