Probabilistic Programming with Gaussian Processes in Stheno.jl

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Slides: `https://willtebbutt.github.io`

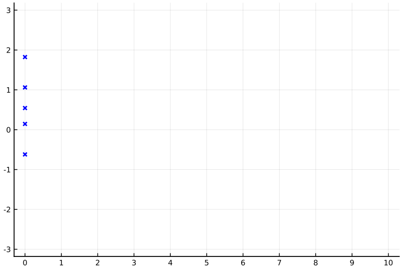
Introduction to GPs

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 introduction

Introduction to GPs

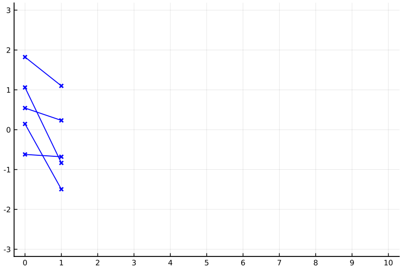
Multivariate Gaussians



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

Introduction to GPs

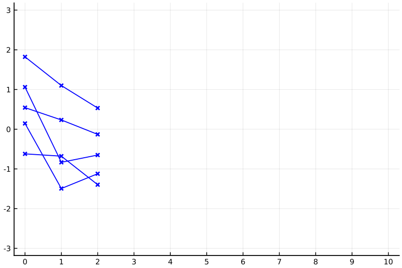
Multivariate Gaussians



$$\begin{bmatrix} 1.0 & 0.61 \\ 0.61 & 1.0 \end{bmatrix}$$

Introduction to GPs

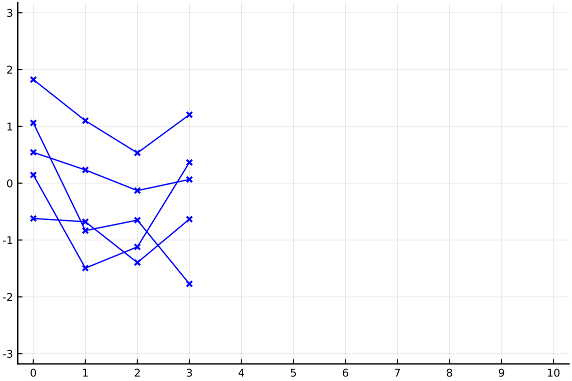
Multivariate Gaussians



$$\begin{bmatrix} 1.0 & 0.61 & 0.14 \\ 0.61 & 1.0 & 0.61 \\ 0.14 & 0.61 & 1.0 \end{bmatrix}$$

Introduction to GPs

Multivariate Gaussians



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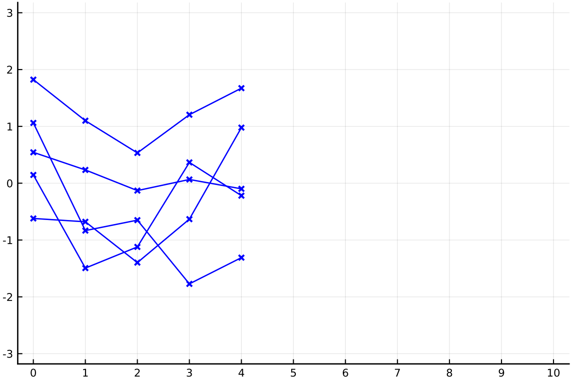

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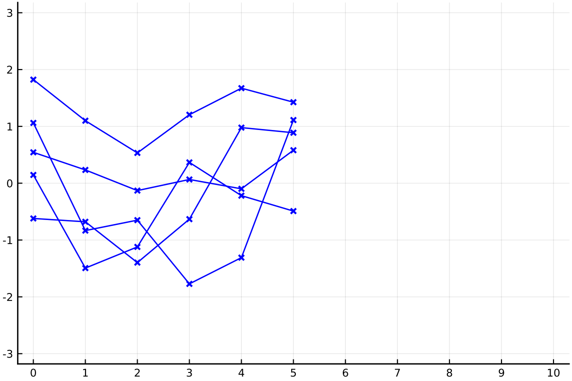

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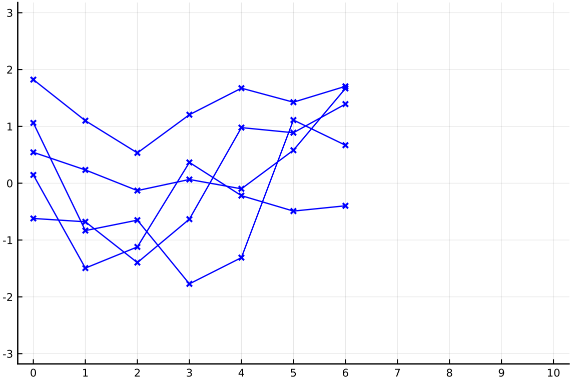

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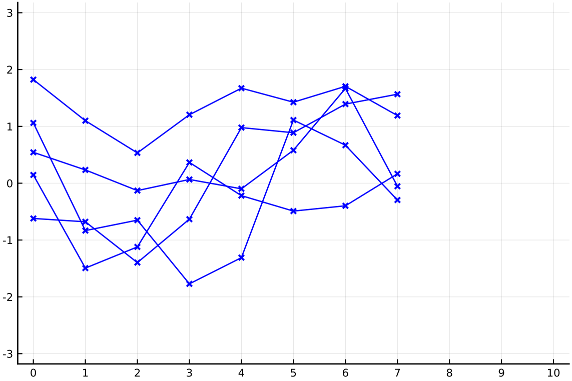

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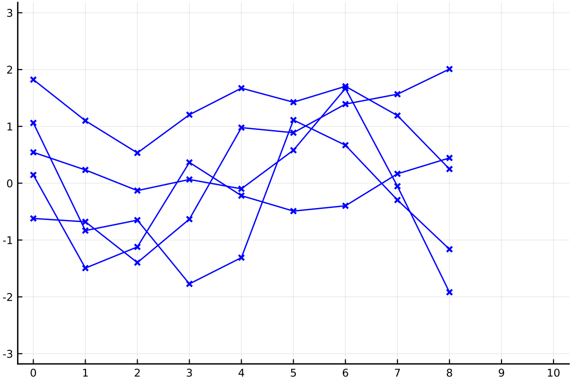

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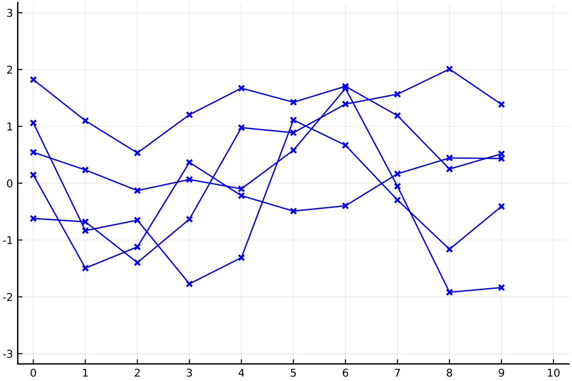

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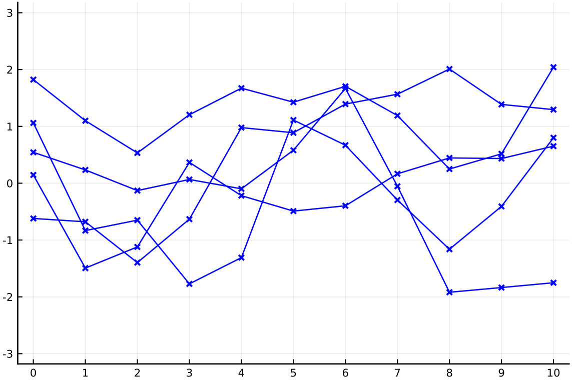
Multivariate Gaussians



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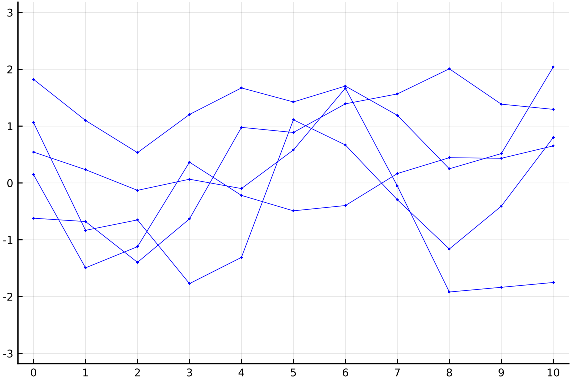

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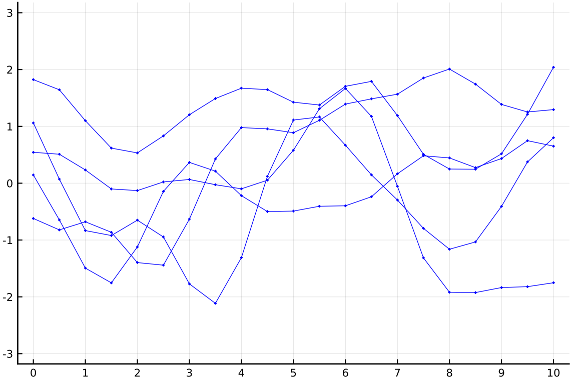

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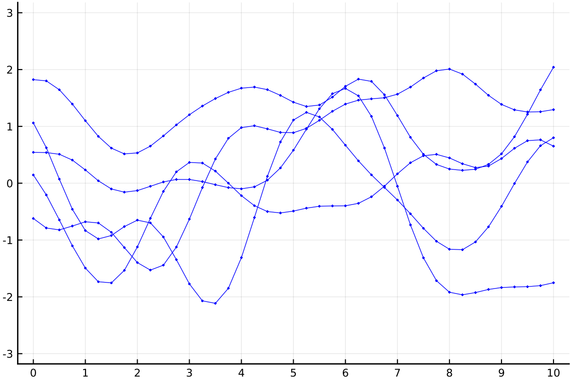

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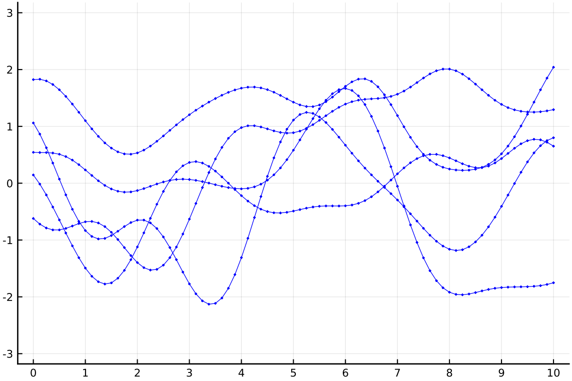

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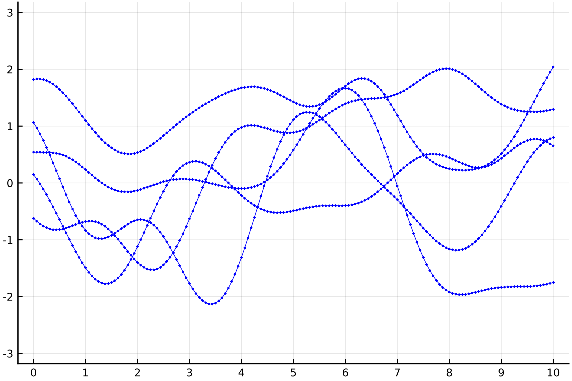

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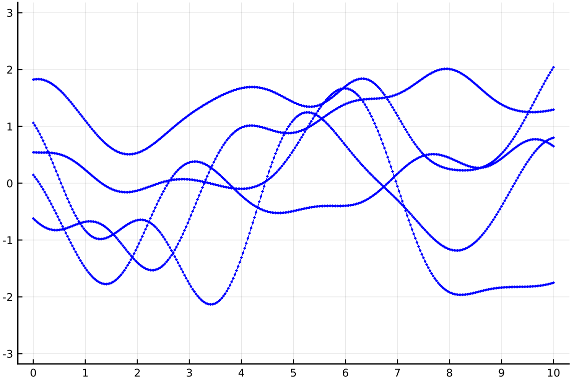


Multivariate Gaussian

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

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

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

Gaussian Process

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

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

$$c : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$$

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

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

(Follows from the marginalisation property of Gaussians)

Introduction to GPs

From Multivariate Gaussians to Gaussian Processes - Conditioning

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

Introduction to GPs

From Multivariate Gaussians to Gaussian Processes - Conditioning

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

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

Introduction to GPs

From Multivariate Gaussians to Gaussian Processes - Conditioning

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

Introduction to GPs

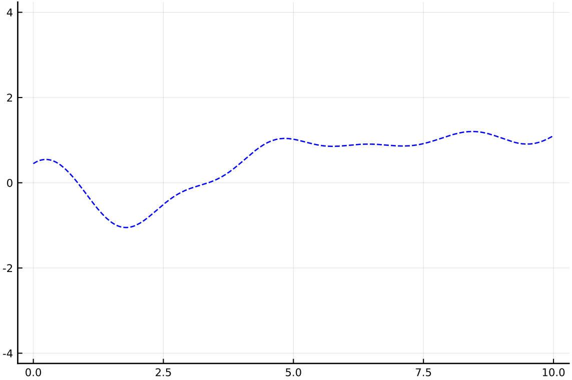
From Multivariate Gaussians to Gaussian Processes - Conditioning

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

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

Introduction to GPs

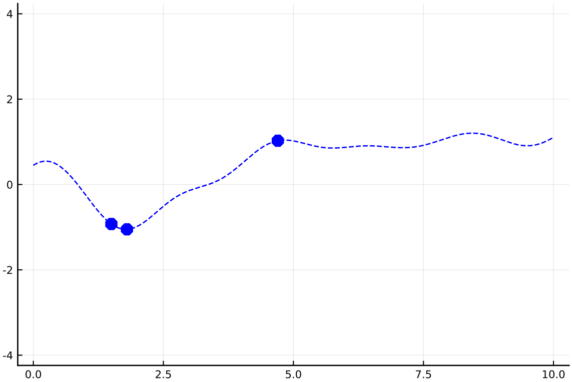
Non-Linear Regression



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

Introduction to GPs

Non-Linear Regression



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Introduction to GPs

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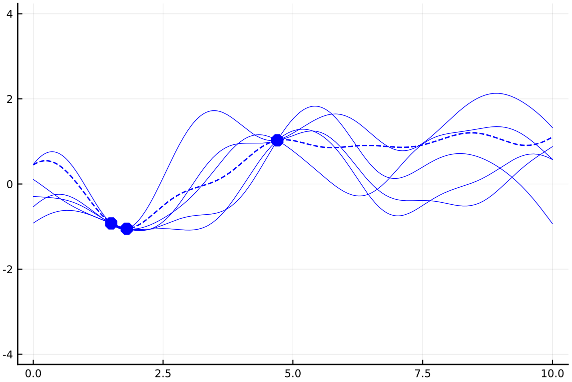

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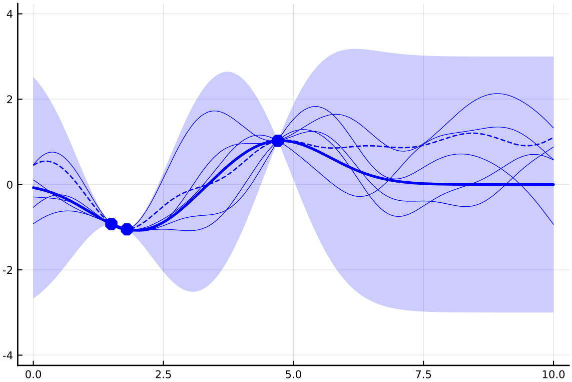
Introduction to GPs

Non-Linear Regression



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

Transformations of GPs

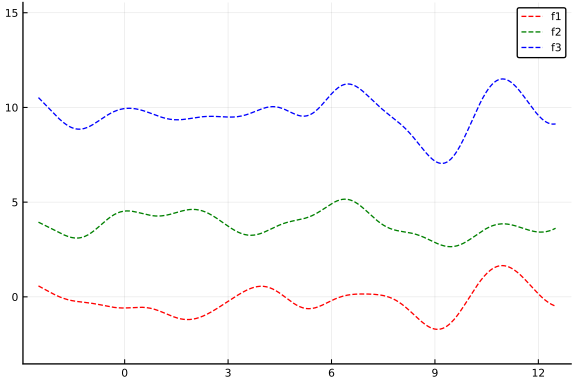
Linear (and affine) transformations of GPs yield GPs e.g.

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

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

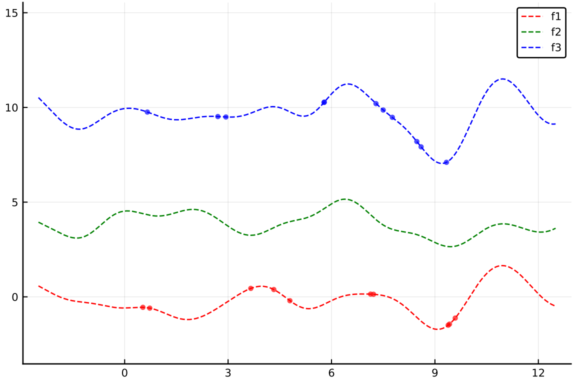
Transformations of GPs

Worked Example: Addition



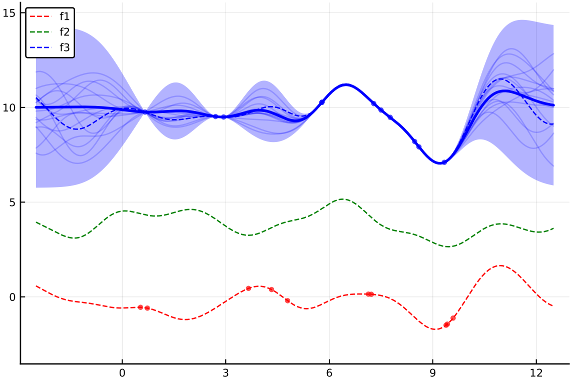
Transformations of GPs

Worked Example: Addition



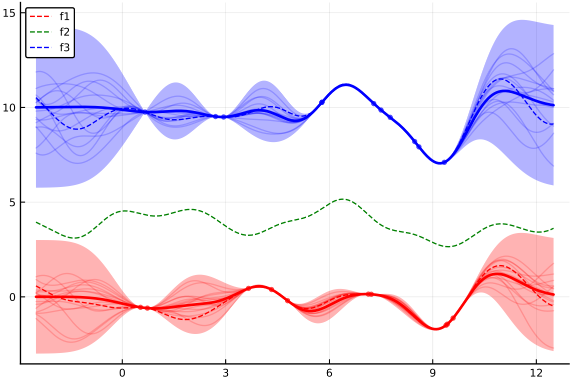
Transformations of GPs

Worked Example: Addition



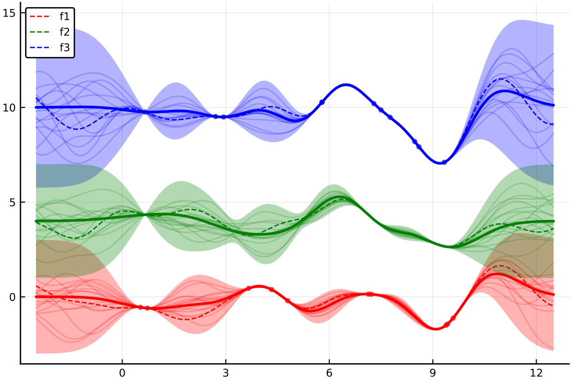
Transformations of GPs

Worked Example: Addition



Transformations of GPs

Worked Example: Addition



The GP Probabilistic Programme
What is it?

Gaussian Process Probabilistic Programmes (GPPPs)

A GPPP is a collection of independent atomic GPs, with known mean and covariance functions, and affine transformations thereof.

Properties

- A GPPP *is* a GP
- Conditioning is an affine transformation in a GPPP

The GP Probabilistic Programme

Example programme

$$f_1 \sim \mathcal{GP}(m_1, c_1)$$
$$f_2 \sim \mathcal{GP}(m_2, c_2)$$
$$f_3 = \mathcal{A}_3(f_1, f_2)$$
$$f_4 = \mathcal{A}_4(f_1, f_3)$$

```julia
@model function model()
    f₁ = GP(m₁, c₁)
    f₂ = GP(m₂, c₂)
    f₃ = f₁ + f₂
    f₄ = f₁ | (f₃(x) ← y)
end
```

where

- $\mathcal{A}_3(f_1, f_2) :=$ sum f_1 and f_2
- $\mathcal{A}_4(f_1, f_3) :=$ condition f_1 on observations of f_3

The GP Probabilistic Programme

What can you do with it?

- Generate samples jointly from any component processes
- Compute the log marginal likelihood of observations of any of the component processes
- Compute the posteriors of any component processes
- Specify non-standard "multi-output" models

Not straightforward to do these things using traditional GP software

The GP Probabilistic Programme

What is Stheno?

- Stheno.jl and Stheno (Python) are two concrete implementations of the GPPP
- Provides a collection of mean and covariance functions to construct atomic GPs
- Provides a collection of affine transformations to combine these GPs
- A framework to glue these things together
- rand, logpdf, conditioning

The GP Probabilistic Programme

What is Stheno?

```
rand(rng, [f₁(x₁), f₂(x₂)], N_samples)
```

The GP Probabilistic Programme

What is Stheno?

```
rand(rng, [f₁(x₁), f₂(x₂)], N_samples)
```

```
logpdf([f₁(x₁), f₂(x₂)], [y₁, y₂])
```

The GP Probabilistic Programme

What is Stheno?

```
rand(rng, [f₁(x₁), f₂(x₂)], N_samples)
```

```
logpdf([f₁(x₁), f₂(x₂)], [y₁, y₂])
```

```
g′ = g | (f₁(x₁) ← y₁, f₂(x₂) ← y₂)
```

Zygote + Stheno

Type II Maximum Likelihood

- Affine transformations often have unknown parameters
- Define function which computes the negative log marginal likelihood of the hyperparameters given some observations
- Use Zygote to compute gradients w.r.t. hyperparameters
- Use your favourite optimisation tool to find optimal hyperparameters

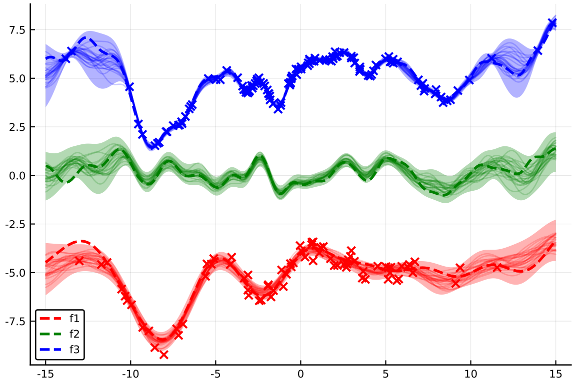
Zygote + Stheno

Type II Maximum Likelihood

```
function nlml(θ)
    f1, f2, f3 = model(θ)
    fx1, fx3 = f1(x1, exp(θ[1]) + 1e-6), f3(x3, exp(θ[3]) + 1e-6)
    return -logpdf(fx1 ← y1, fx3 ← y3)
end
```

Zygote + Stheno

Type II Maximum Likelihood



Zygote + Stheno

Bayesian Inference

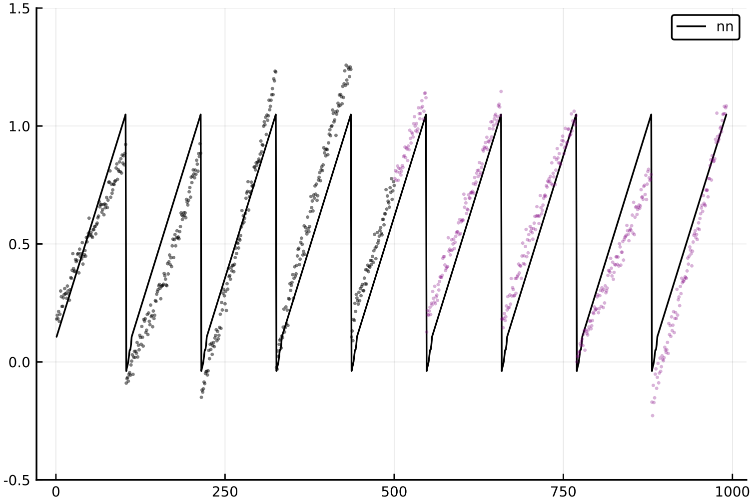
- Specify some priors over hyperparamters
- Using Zygote to compute gradient log joint probability density w.r.t. hyperparamaters
- Run HMC / NUTS using e.g. AdvancedHMC.jl

Flux + Stheno

Idea: transform inputs to a GP via a Neural Network

Flux + Stheno: Modulated Noisy Sawtooth

NN only



$$y_t := \phi(y_{t-\tau:t-1})$$

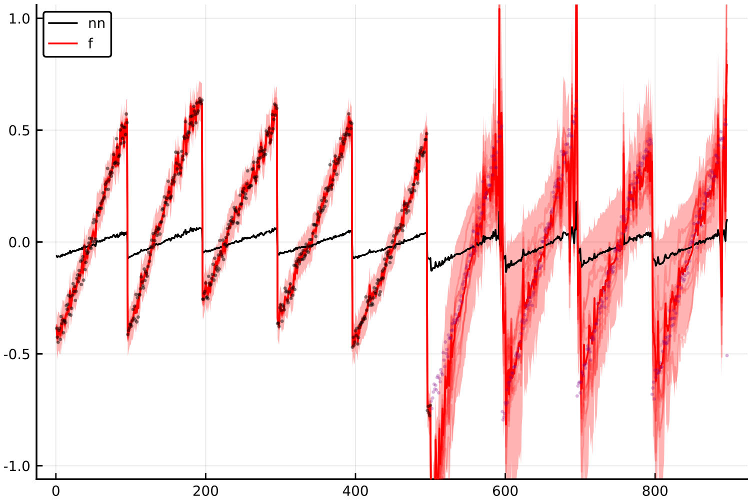
Flux + Stheno: Modulated Noisy Sawtooth

GP-modulated NN

```
w = σw * stretch(GP(mw, eq()), lw) + 1
b = σb * stretch(GP(mb, eq()), lb)
f = b + w * DataTransform(ϕ(θ, Y, relu))
```

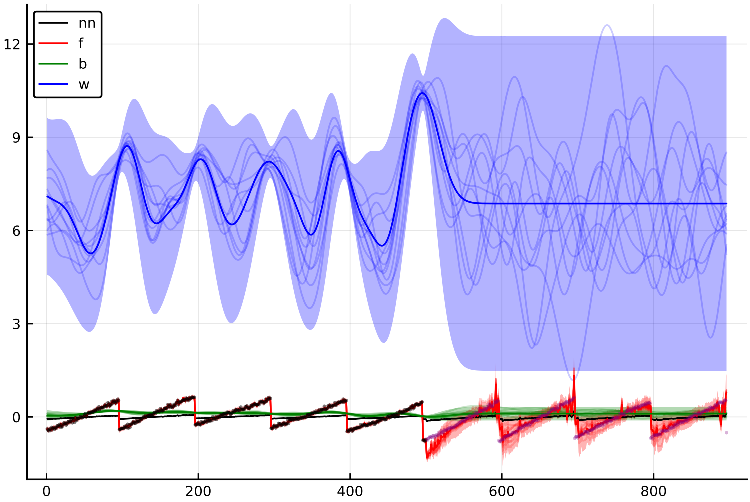
Flux + Stheno: Modulated Noisy Sawtooth

GP-modulated NN



Flux + Stheno: Modulated Noisy Sawtooth

GP-modulated NN



Flux + Stheno: Non-toy problems

Body of literature on GPs + Deep Learning / Neural Networks, including:

- [Calandra et al., 2016]
- [Wilson et al., 2016]
- [Snelson et al., 2004]
- [Al-Shedivat et al., 2016]

Turing + Stheno

- Embed a GPPP within a non-Gaussian probabilistic programme
- Use HMC to perform inference

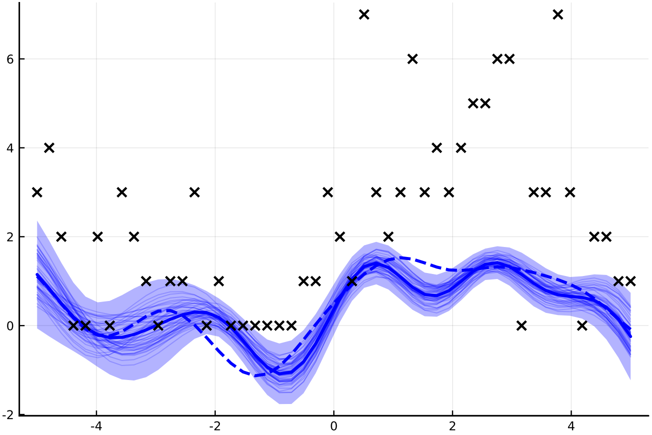
Turing + Stheno

Poisson Regression

```
@model poisson_regression(y) = begin
    f = GP(eq(), TuringGPC())
    fx ~ f(x, 1e-9)
    y ~ Product(Poisson.(exp.(fx)))
    return fx, y
end
```

Turing + Stheno

Poisson Regression



Turing + Stheno

The State of Integration

- Very much a WIP
- Pain points well understood
- Not there yet

To Conclude

The Gaussian Process Probabilistic Programme

- Gaussian processes are interpretable, tractable, and flexible probabilistic models for functions
- The GPPP lets you manipulate GPs in a flexible way that was previously tricky
- Can (in principle) be used as a component distribution in more general non-Gaussian PPLs (e.g. Turing, Gen, Soss, etc)
- Stheno.jl is a concrete implementation of these ideas in Julia

To Conclude

Stheno: Smaller Todos

- Better documentation / write up
- GPU support
- Better integration with Turing.jl
- Plotting
- Stochastic Variational Inference (e.g. for mini-batching)
- Some form of MLJ integration

To Conclude

Stheno: Larger Todos

- Improve bus factor
- State-space methods for low-dimensional (e.g. spatio-temporal) problems
- Optimisations for vector-valued / matrix-valued GPs

To Conclude

Thanks

- Wessel Bruinsma, Rich Turner, various members of the Cambridge MLG
- Hong Ge and the Turing team
- Invenia Labs

To Conclude
Links

- Julia: `https://www.github.com/willtebbutt/Stheno.jl`
- Python: `https://www.github.com/wesselb/stheno`
- These slides: `https://willtebbutt.github.io`

Bibliography I

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Pseudo Points

- the GPPP makes inter-domain pseudo-points [Lázaro-Gredilla and Figueiras-Vidal, 2009] trivial
- Yields improved statistical / representational efficiency in certain cases e.g. [Van der Wilk et al., 2017]
- Can provide computational advantages in others
- Open research area
- Stheno has excellent support for a vanilla form of the SOTA variational pseudo-point approximation
- Straightforward to extend to slightly different scenarios