

Gaussian Process Probabilistic Programming

Will Tebbutt, Wessel Bruinsma, and Richard E. Turner {wct23,wpb23,ret26}@cam.ac.uk



- Write programmes specifying the relationship between a collection of Gaussian processes (GPs)
- Both Julia and Python implementations available: Stheno.jl and Stheno

• GP perspective: adopt a **process-centric** as opposed to **kernel-centric** approach to model specification

• PP perspective: useful corner-case where **exact** inference is **tractable**

Implementing GPPPs: Maths Code

$$\begin{split} s &\sim \mathcal{GP}(0, k_{\mathsf{quadratic}} + k_{\mathsf{EQ}}), & \mathsf{s} &= \mathsf{GP}(\mathsf{Quadratic}() + \mathsf{EQ}()) \\ a &| s &= \mathsf{d}^2 s / \mathsf{d} t^2, & \mathsf{a} &= \nabla(\nabla(\mathsf{s})) \\ &\varepsilon_s &\sim \mathcal{GP}(0, k_{\mathsf{noise}}), & \varepsilon_- \mathsf{s} &= \mathsf{GP}(0, \, \mathsf{Noise}()) \\ &\varepsilon_a &\sim \mathcal{GP}(0, k_{\mathsf{noise}}), & \varepsilon_- \mathsf{a} &= \mathsf{GP}(0, \, \mathsf{Noise}()) \\ &y_s \,|\, s, \varepsilon_s &= s + \varepsilon_s, & y_- \mathsf{s} &= s + \varepsilon_- \mathsf{s} \\ &y_a \,|\, a, \varepsilon_v &= a + \varepsilon_a, & y_- \mathsf{a} &= a + \varepsilon_- \mathsf{a} \\ &p(s \,|\, y_s(t) = \mathsf{obs_s}, y_a(t) = \mathsf{obs_a})? & \mathsf{s_posterior} &= \mathsf{s} \mid & (y_- \mathsf{s}(t) \leftarrow \mathsf{obs_s}, \, y_- \mathsf{a}(t) \leftarrow \mathsf{obs_a}) \end{split}$$

Kernel and mean function of the posterior: $kernel(s_posterior)$ and $mean(s_posterior)$

Background

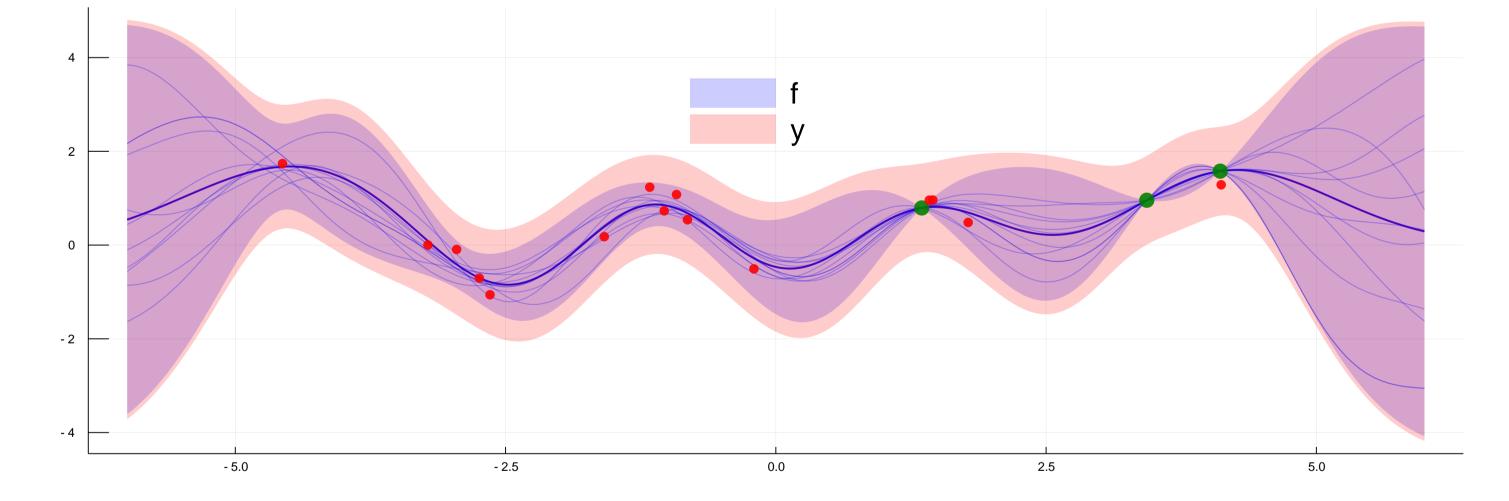
A Gaussian Process Probabilistic Program (GPPP) is a GP.

- GP: useful prior for real-valued functions, closed under affine transformation [1]
- A programme comprises a collection of primitive GPs and affine transforms thereof
- This collection defines a GP on an augmented domain
- Mean function and kernel on augmented domain deduced automatically from programme structure
- Strictly more general than traditional GP packages (e.g. [2]), enables inspection of distribution of any component of the model
- Usable as a primitive distribution in a general PPL

[1] C. E. Rasmussen and C. K. I. Williams, Gaussian Processes for Machine Learning. MIT Press, 2006.

[2] D. G. Matthews, G. Alexander, M. Van Der Wilk, T. Nickson, K. Fujii, A. Boukouvalas, P. León-Villagrá, Z. Ghahramani, and J. Hensman, "Gpflow: A gaussian process library using tensorflow", *The Journal of Machine Learning Research*, vol. 18, no. 1, pp. 1299–1304, 2017.

Partially-Noisy Nonlinear Regression



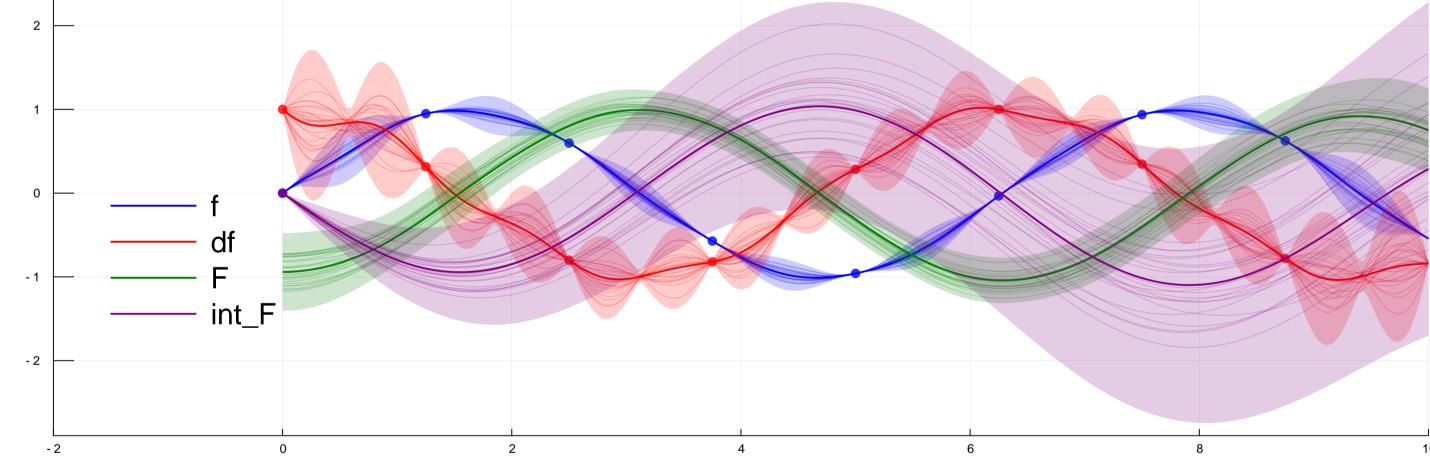
Omodel function $gp(\sigma^2)$ f = 1.5 * GP(EQ()) $\varepsilon = GP(Noise(\sigma^2))$ $y = f + \varepsilon$ return f, yend f, y = gp()# Sample from the prior.

Xf = rand(Uniform(-5, 5), 3)
Xy = rand(Uniform(-5, 5), 15) $f_-, y_- = rand([f(Xf), y(Xy)])$ # Compute posterior processes. $f', y' = (f, y) \mid$ $(f(Xf) \leftarrow f_-, y(Xy) \leftarrow y_-)$

Specify generative model.

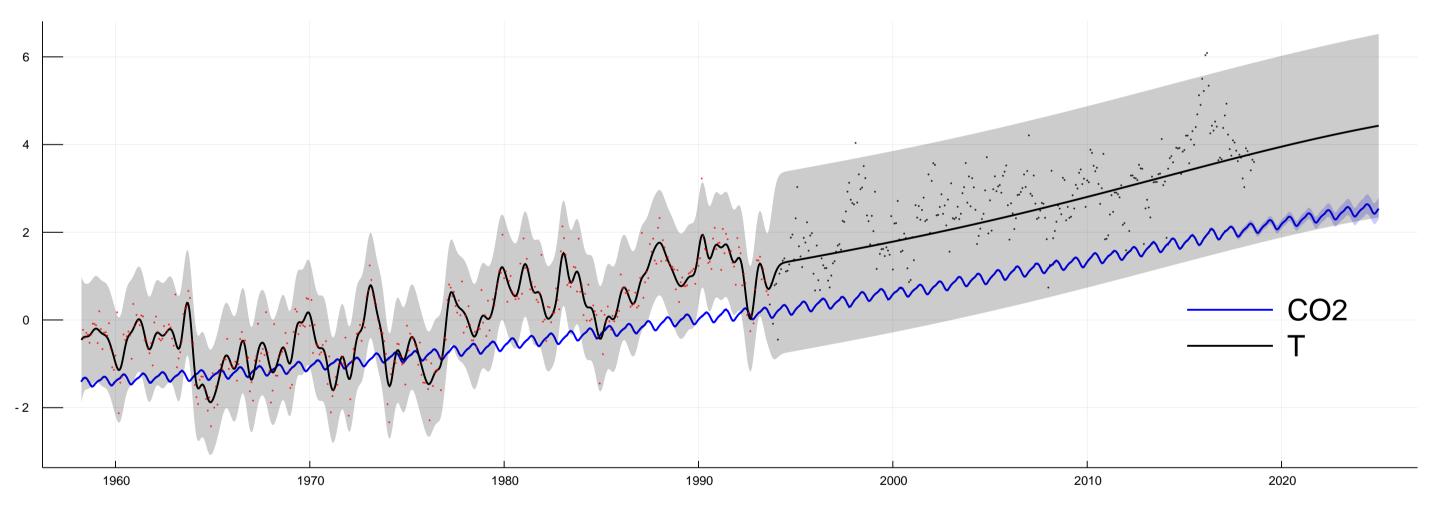
- Small number of observations f_ of latent process f
- Larger number of observations y_ of noisy process y
- Condition on both to infer posterior over f and y

Probabilistic Integration



- Infer the double integral of f
- Make observations of f and its gradient, df
- Nestable AD enables multiple integration
- Take care to fix the integration constants

Toy Climate Problem



@model function climate(θ)

Joint latent trend.

- trend = GP(...)

 # Specify model for CO2.
 co2_trend = trend * θ[1]
 co2_wiggle = GP(...)
 co2_period = GP(...)
 co2_period + GP(Noise(...))

 # Specify model for T.
 Thrend = for trend * θ[2]
- # Specify model for T.
 T_trend = f_trend * θ[2]
 T_wiggle = GP(...)
 T = T_trend + T_wiggle +
 GP(Noise(...))

return co2, T end

- Goal: predict T (temperature) given co_2 (CO₂ concentration)
- Idea: jointly model co_2 and T
- Infer long term trend in both co_2and T
- Account for short-term fluctuations separately
- Trend recovered; irreducible variation in T accounted for