



Bayesian local surrogate models for the control-based continuation of multiple-timescale systems

Mark Blyth (speaker), Lucia Marucci and Ludovic Renson

University of Bristol
BrisSynBio
Imperial College London

ONLINE, FEBRUARY 16 - 19, 2021



- Numerical continuation is the standard tool for computational bifurcation analysis
- Continuation traces out implicitly defined manifolds, and as such, requires a model to define these manifolds
- Usable models are not always available
- Can we apply the same methods in cases where a usable model is unavailable?



- Control-based continuation is a reformulation of the traditional continuation paradigm

$$\dot{x} = f(x) + u(x, x^*)$$

$u \equiv 0 \Rightarrow$ system operates under natural dynamics

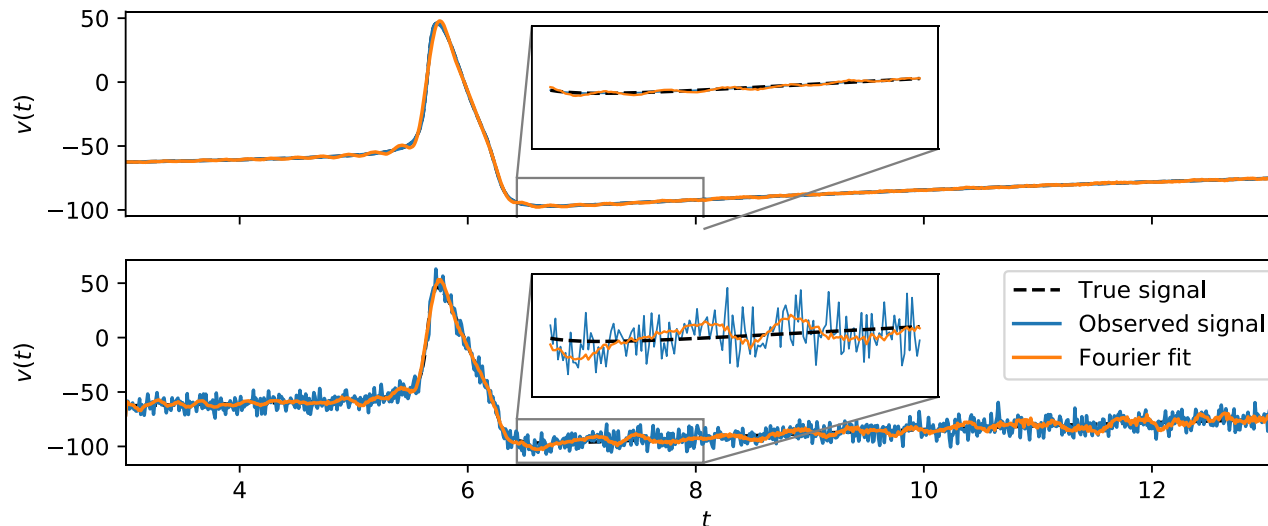
$$u = k_p (x^* - x)$$

Zero-problem: $x^* - x = 0$

- Nonlinear oscillations require discretising before they can be studied



- All continuation methods use nonlinear solvers for prediction-correction steps
- Functions cannot be used as solver inputs and outputs; instead, they must be discretised
- CBC applications use Fourier discretisation
- Multiple-timescale systems typically require many Fourier harmonics
- Larger numbers of Fourier harmonics cause less noise-robustness
- We can't filter the noise off using simple filters





- Noise reduces the discretisation accuracy, and it can't be filtered off easily; instead we propose a surrogates approach
- Surrogates are a statistical regression model

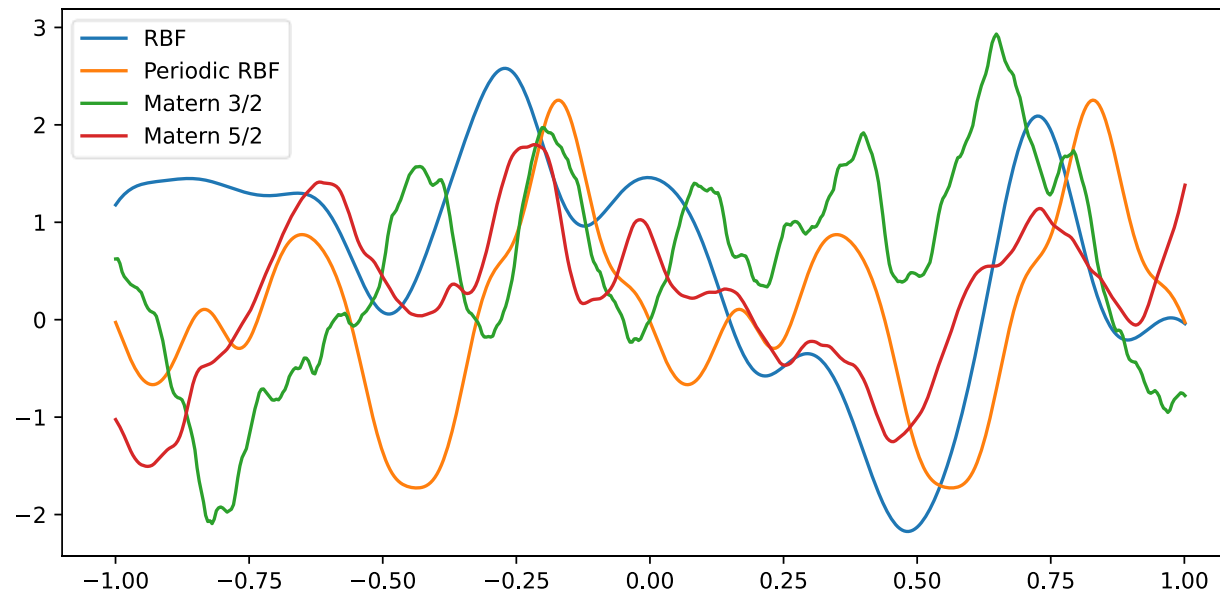
$$\text{Assume } x_i = f(t_i) + \varepsilon_i,$$

$$\varepsilon_i \sim N(0, \sigma^2).$$

- A well-fitted model allows us to separate samples into signal and noise
- Challenge: find some function $f(t)$ that is sufficiently general to describe the signals of interest

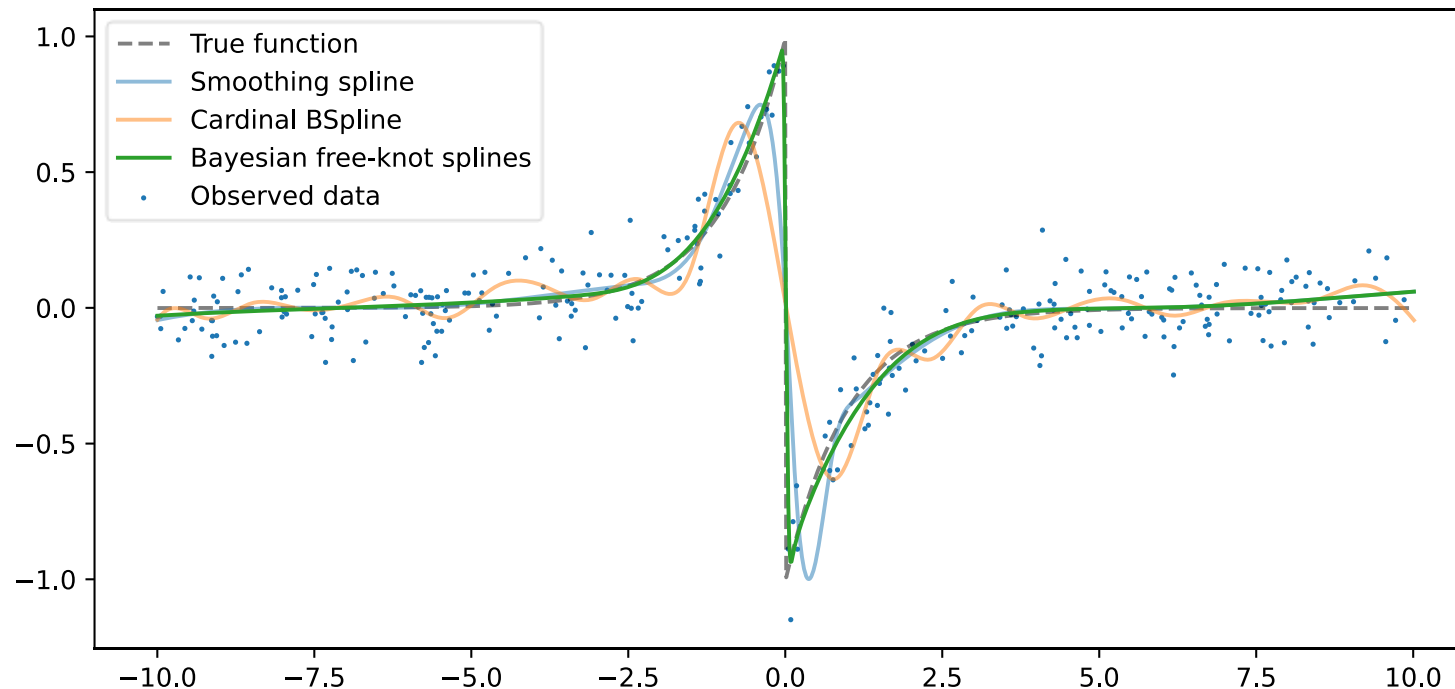


- Gaussian processes generalise the normal distribution to infinite dimensions
- Gaussian process regression is a nonparametric function-space regression method
- Bayesian methods require priors; GP priors are covariance functions
- We use periodic and non-periodic RBF and Matern 3/2, and Matern 5/2 kernels





- Spline regressors are maximally smooth piecewise-polynomial curves
- BSplines are a set of basis functions over an associated set of spline curves
- Choosing good BSpline knots can be hard
- Bayesian inference can be used to maintain a distribution over spline curves





- Surrogates are tested on noise-corrupted outputs from simulations of two multiple-timescale models
- Goodness-of-fit is quantified by fitting the models to noisy data, then comparing the actual and predicted values at unseen datapoints

SNR (dB)	$\sigma = 0$ -	$\sigma = 0.05$ 30.0	$\sigma = 0.1$ 24.0
Bayesian splines	2.11×10^{-4}	1.20×10^{-3}	3.00×10^{-3}
GPR: Periodic Matern 3/2	6.40×10^{-6}	5.63×10^{-4}	1.48×10^{-3}
GPR: Periodic RBF	3.60×10^{-7}	8.43×10^{-4}	2.92×10^{-3}
GPR: Matern 3/2	5.75×10^{-5}	2.40×10^{-3}	5.46×10^{-3}
GPR: Matern 5/2	3.59×10^{-5}	2.08×10^{-3}	5.27×10^{-3}
GPR: RBF	3.53×10^{-5}	2.09×10^{-3}	6.96×10^{-3}

van der Pol MSPE

SNR (dB)	$\sigma = 0$ -	$\sigma = 1$ 37.4	$\sigma = 2$ 31.4
Bayesian splines	8.00×10^{-2}	0.185	0.597
GPR: Periodic Matern 3/2	1.80×10^{-4}	0.213	0.641
GPR: Periodic RBF	3.36×10^{-2}	0.406	0.806
GPR: Matern 3/2	3.24×10^{-2}	0.759	1.82
GPR: Matern 5/2	1.72×10^{-2}	0.915	1.91
GPR: RBF	5.61×10^{-1}	1.78	2.60

Hodgkin-Huxley MSPE



- CBC is a method for analysing the bifurcation structure of black-box and physical systems
- Oscillatory dynamics require discretising to be tracked
- It is difficult to accurately Fourier-discretise noisy multiple-timescale signals
- Bayesian regression models can be used instead to average out the noise
- Future work includes alternatives to Fourier discretisation, however these are often even less noise-robust