# Notes on Gaussian process regression

Mark Blyth

# Week's goal

Last week...

- Kernel choice is critical to getting usable results from a GP (moreso than hyperparameters?)
- Stationary covariance functions aren't able to fully capture neuron dynamics
- Periodic kernels are harder to fit, but better represent our data

This week...

- Decide on a suitable kernel (something non-stationary, non-monotonic)
- Learn how it works
- Implement it

# Week's activities

- Read about modelling non-stationarity in GPs
  - Appropriate kernel choice allows us to model non-stationarity
  - There's also more general GPs that allow us to do that
  - These generalised GPs also have other nice features such as heteroscedasticity, and non-Gaussian noise
- Considered experimental issues with GPs
  - Fitting time
  - Noise type
- Wrote up notes about everything I've done with GPs so far
  - Covers some of the key developments in relevant areas of the literature

# Presentation points

1. Highlight what the requirements are for *in silico* experiments
   - Goal: identify what we want from a GP
2. Consider how experimental requirements may differ from *in silico*
   - Goal: identify what we want from a GP
3. Suggest some possible approaches
   - Goal: find some possible modelling strategies that fit our requirements
4. Compare approaches to help decide which approach is best
   - Goal: choose the strategy to work with

# Why GPs?

Always useful to remember why we're doing things!

- All existing CBC methods require us to discretise the system behaviours (outputs, control signals)
  - Neurons spike fast, so this is hard
- Discretisations are necessary in the continuation procedure either to...
  - predict and correct the control target,
  - or to iteratively zero the control action
- I'm hoping we can avoid discretisation by using simple transformations of continuous functions, rather than discretised vectors

This usage case defines our requirements of the Gaussian processes

# The best GP

The best Gaussian process model satisfies the following:

- Easy to use and understand
  - No need to re-invent the wheel
  - Simplicity is a virtue!
- Gives a *sufficiently* good model
  - Doesn't necessarily have to be perfect, depending on how we use the corrector step
- Easy to train
  - Hyperparameters are either quick and easy to tune, or the model works well even with bad hyperparameters

How simple we can go depends on the data we expect to see

# Data characteristics for *in silico* CBC

With computer experiments, we have. . .

- Reliable results with only small amounts of data
  - GP training speed doesn't matter
- Negligable noise
  - Only noise is numerical errors
- 'Nice' artificial noise
  - We know exactly what the noise distribution is
  - Noise can be exactly Gaussian
  - Noise can have constant variance

# Choice of GPs for *in silico* CBC

- Small amounts of data mean we don’t need any clever speedup methods
- Constant-variance noise means we don’t need to try modelling heteroscedastic behaviours
- Gaussian noise means we don’t have warp data into a Gaussian process
- Multiple-timescale dynamics mean we can’t rely on stationarity

The only non-standard requirement is that the covariance function must be non-stationary.

# Data characteristics for *in vitro* CBC

With real experiments, we have…

- Potentially lots of data, if we assume *KHz* sample rates
  - GPs must train quickly
- Unavoidable noise
  - Noise might not be Gaussian, especially for measurement-precision errors
  - Noise variance might change with signal amplitude (eg. multiplicative noise)

# Issues with GPs for *in vitro* CBC

- Lots of data
  - GPs are $\mathcal{O}(n^3)$ to train, so they become impractical with more than a few thousand datapoints
- Non-Gaussian noise
  - GPs are a collection of random variables, whose finite joint distribution is Gaussian
  - This mean GPs only let us model Gaussian noise
- Non-constant signal noise
  - GPs are heteroscedastic – the noise is assumed to be constant across the signal
  - This might not be true for our experiments

Luckily there's a range of solutions to all these problems!

# Nice GPs

A *'nice'* Gaussian process is stationary:

- Strong stationarity: moments (hyperparameters) remain constant across the signal
- Weak stationarity: mean, variance remain constant across the signal
- Standard kernels assume stationarity
- Stationary GP models are analytically tractable, with simple closed-form solutions

# Practical GPs

Realistic data aren't stationary; there's two main approaches to handle this:

- Learn a transformation of the data, so that the transformed data are stationary
- Learn a kernel that can handle the non-stationarity observed in the signal

Non-stationary models are not always analytically tractable, and require more advanced solution methods.

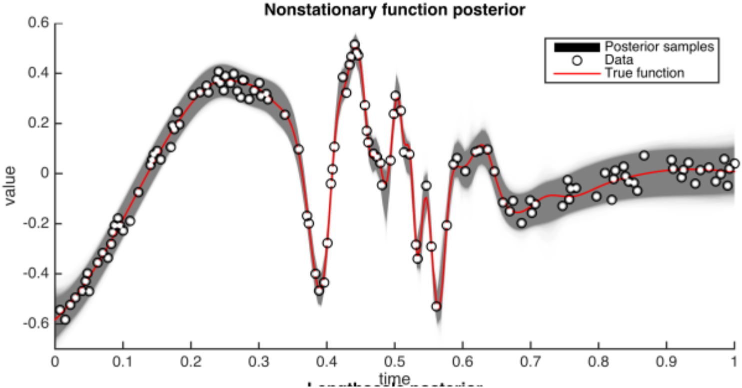
# Warping GPs

- Gaussian proesses assume observations are distributed Gaussian'ly about a true function value
- When this isn't true, we can try to learn a transformation from the original data to some latent variables, such that the latent variables *are* Gaussian
- A 'nice' GP can then be fitted to the latent variables
- This allows us to model non-Gaussian noise
- Only works when it's possible to transform the signal into a stationary GP

# Nonstationary Gaussian processes

- Take the standard square-exponential kernel
- Replace the hyperparameters with latent functions (while retaining PD)
- Model the latent functions as GPs
- Design the kernel by fitting those GPs
- There's clever optimisation techniques, but they're not necessarily fast, and they require good hyperpriors
    - Since all neuron data will look similar (in some respects), it's probably possible to train a kernel on a representative dataset; using it on novel data will then only require small optimisations

# Nonstationary GPs work well on biological data




Source: Heinonen, Markus, et al. "Non-stationary gaussian process regression with hamiltonian monte carlo." Artificial Intelligence and Statistics. 2016.

*This also shows how important kernel choice is – couldn't do that with an SE kernel!*

# Spectral kernels

- Bochner's theorem relates the power spectrum of a signal to its covariance
- A custom kernel can be designed by fitting a GP to the signal power spectrum, and inverse-Fourier-transforming the result
  - This means we only have to fit one latent GP
  - Derives the kernel directly from the data, so presumably these methods will give the most reasonable kernel for the given problem
- The resulting kernel can model non-monotonic covariance (long-term trends, eg. periodicity), and can be designed to be non-stationary
- They seem to be exactly the same as the previus non-stationary method, but designed in a perhaps easier-to-compute way
- Spectral kernels have also been developed with sparse methods in mind...

# Sparse Gaussian processes

- Gaussian processes train in $\mathcal{O}(n^3)$; this is too slow for $n > \mathcal{O}(10^3)$ datapoints
- When faced with big data, we could train a GP by selecting a subset of data to work with
  - This throws away useful information
- Alternative: learn a set of representative latent variables, and train on those
  - For $m$ latent vars, we get $\mathcal{O}(nm^2)$ complexity
- Sparse GPs let us train on a smaller number of variables, while minimising loss of information
  - KL divergence gives a measure of the difference between PDFs
  - Variational Bayesian methods give an upper bound on the KL divergence between true posterior, and sparse posterior
  - Gradient descent can then be used to minimise this upper bound

# Choice of GPs

- Spectral kernels and the pictured nonstationary GP method will both work well for neuron data
- The spectral method
  - allows sparsity, so is fast to train
  - provides efficient, easy methods for fitting latent function hyperparameters
  - provides state-of-the-art results
  - has efficient open-source code available, so is easier to use

That's therefore the method of choice

Remes, Sami, Markus Heinonen, and Samuel Kaski. "Neural Non-Stationary Spectral Kernel." arXiv preprint arXiv:1811.10978 (2018).

# Next steps

- Days / immediate: Go back and make changes to the continuation paper
- Week / medium-term: (Once the paper is finished), find code for, implement, and test the chosen GP scheme
- Weeks / longer-term: code the predictor-corrector methods, giving a completed CBC code