Notes on Gaussian process regression

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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

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.

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

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!

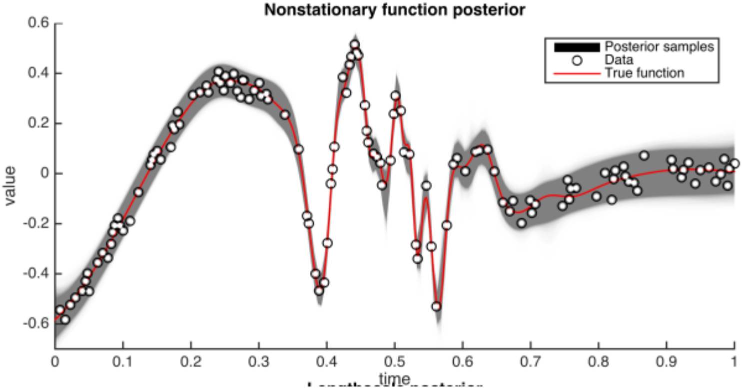
Warping GPs

- 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

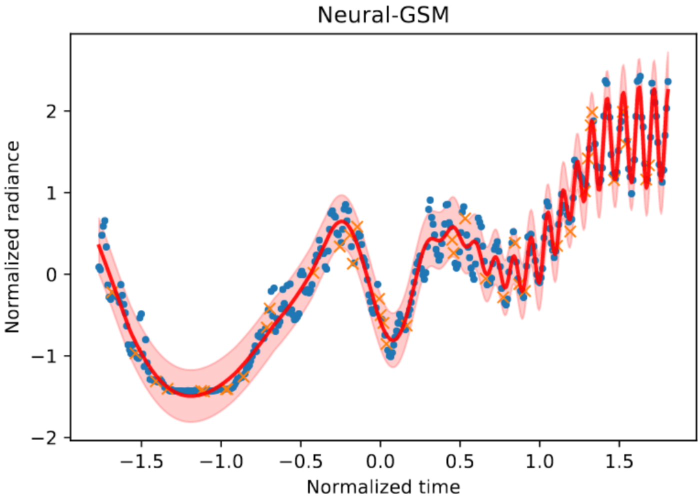
- Gaussian processes train in $\mathcal{O}(n^3)$; this is too slow for $n > \mathcal{O}(10^3)$ datapoints
- When faced with big data, we could train a GP by selecting a subset of data to work with
  - This throws away useful information
- Alternative: learn a set of representative latent variables, and 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).


Neural-GSM
Normalized radiance
Normalized time
2
1
0
−1
−2
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

Next steps

Coursework marking, then...

- 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