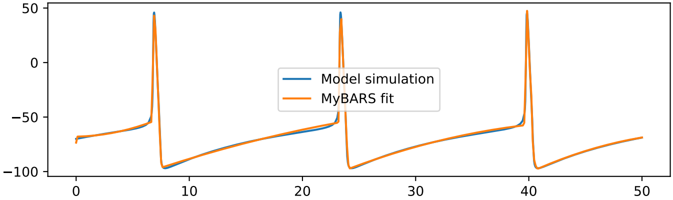
More model fitting

Mark Blyth

Presentation points

- Models for wind tunnel data
- A BARS redesign
- BARS potential pitfalls

An exciting aside



My BARS implementation works!

- Gives okay results *[some sharp corners?]*
- Allows arbitrary interpolation
- Slower than the C implementation

BARS - wind tunnel

2500 datapoints, 41s run-time

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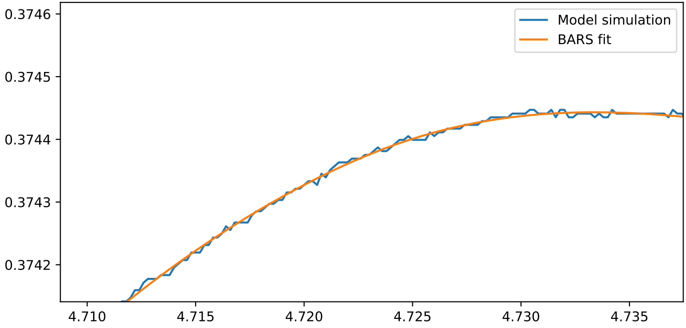
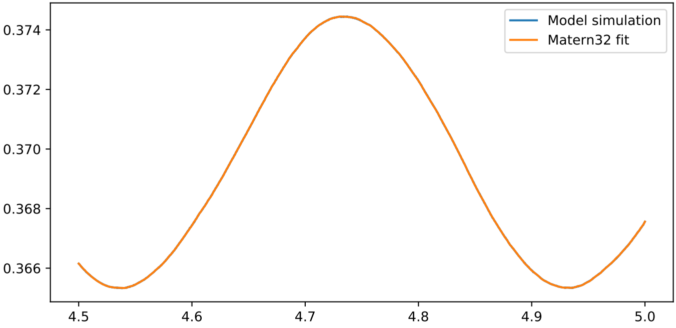


2500 datapoints, 40s run-time

Matern32 (GPR) - wind tunnel



2500 datapoints, 119s run-time

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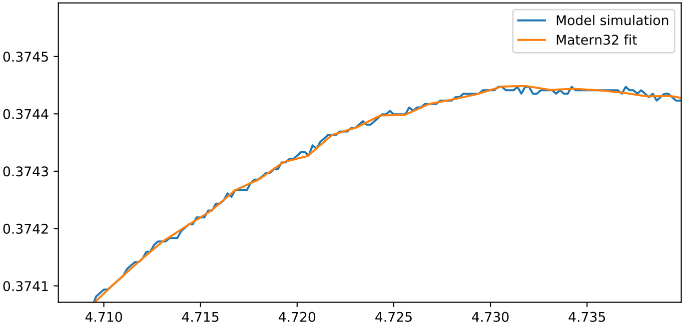

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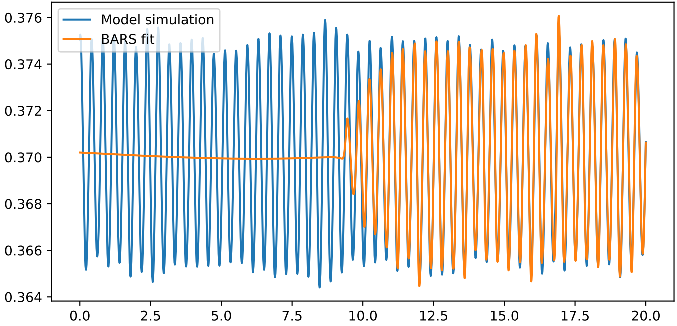
Timings

- Unoptimized C code is still faster than optimized python / matlab
  - BARS is using optimized C implementation, GPRs is using my unoptimized python implementation
  - GPFlow, GPyTorch would be much faster for GPR
  - Probabilistic programming might speed up BARS
- Both methods are $\mathcal{O}(n^3)$; require inverting $n \times n$ matrix
  - Both perform poorly on lots of datapoints!

BARS



10,000 datapoints *[crashes with full dataset]*, 142s run-time

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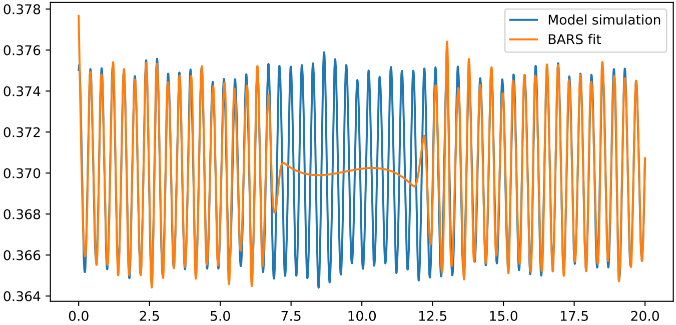

10,000 datapoints *[crashes with full dataset]*, max. number of knots *[80]*, more burn-in; 590s (9 mins 50s) run-time

BARS issues

- C implementation doesn't allow validation
  - Can't interpolate at arbitrary points
  - Python implementation does! But it's slower
- C implementation caps the max. number of knots
  - Python implementation doesn't! But it's slower
  - Doesn't work for long time series
- $\mathcal{O}(n^3)$ means data need downsampling to be used
  - Took about 10 minutes to fit a model to 10% of the data

Experimental data

- If experiments use small numbers of periods (1, 2, 3), current methods work
  - Similar to how I tested models on small numbers of neuron spikes
  - Few periods = less data = fewer knots needed, and quicker fit obtained
- More datapoints mean we need to get creative...
  - Sparse variational BARS
  - Periodic BARS
  - Semiperiodic methods

Or... speed up BARS by not using BARS

A new BARS approach

IDEA: Bayesian adaptive *evolutionary* splines; genetic algorithm

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  - Each MCMC acceptance/rejection becomes an evolutionary scoring step

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5. Can maximise posterior, instead of likelihood, by including a prior term

BARS vs evolution

- Would be interesting to compare this to the MCMC method
  - MCMC sets up a Markov chain whose stationary distribution is the posterior
  - This aims to find a Markov chain whose stationary distribution is the argmax
  - Grounds for a rigorous justification / proof of convergence
- Evolution will likely be faster
  - Could leverage existing genetic optimization packages
  - Easily parallelised for more speed-up
  - No RJ-MCMC makes it easier target for probabilistic programming

SV-BARS

Another idea: remodel BARS to work similarly to sparse GPR

- BARS typically uses 3000+ MCMC steps
  - Each MCMC step requires inverting an $n \times n$ matrix – SLOW
- Choose a *[small]* set of maximally informative surrogate datapoints (x_i^*, y_i^*)
- Run MCMC step on surrogate datapoints
  - Much faster to invert the smaller matrix
- Well-chosen surrogate points means we get the same result as running on real data
- Fewer datapoints means it runs a lot faster

SV-BARS implementation

- Find a set of m inducing points (x_i^*, y_i^*)
  - Find inducing points by minimising $D_{\mathrm{KL}}\left[p_y \| p_{y^*}\right]$
  - Use variational Bayes to approximate this
- Find posterior knots $p(k, \xi | y^*)$ *[instead of $p(k, \xi | y)$]*
  - $\mathcal{O}(m^3), m \ll n$
  - Sparse GPR is $\mathcal{O}(nm^3)$, so if my complexity is correct, we get a bigger speed-up / outperform SVGPR!

Would require learning RJ-MCMC, variational Bayes, sparse GPR in-depth

Periodic BARS

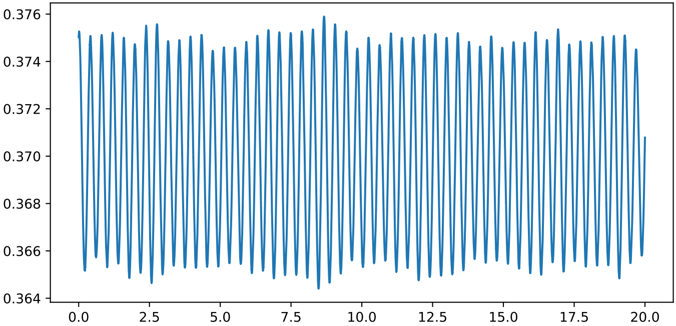
An approach for if we need to model more than a few spikes:

- Assume data are given by $y_i = f(x_i) + \varepsilon$
  - $f(t) = f(t + T)$
- Find either
  - T-periodic knot-set
  - T-periodic basis splines
    - Nicer approach

…in such a way that we…

- minimise fitting time
- balance fit against number of knots

Semiperiodic methods



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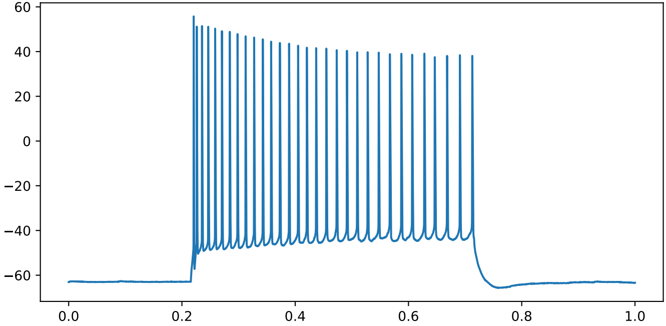

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- Would likely give similar results to sparse BARS

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- (Semi)periodic BARS would be less generally applicable, but potentially faster when applicable

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   - Periodic BARS is a less general method

My proposal

- Validate models
  - Also try simple data transformations for GPR
- Write up notes on *everything* so far

Then...

1. Adapt BARS for sparsity, evolution
   - Fast, SOTA, scalable
   - Needs variational Bayes learned
2. Demonstrate sparse BARS on other problems (NDC, comp-synth-bio, ML)
   - Not sure which problems would benefit from splines?
3. Apply the shiny new splines method to CBC