

# Papers, splines, and other ideas

Mark Blyth



### Presentation overview

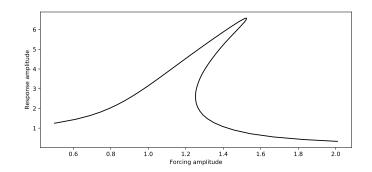
₭ Splines discretisation progress

- Some ideas: projects that will enhance CBC, and make it more powerful for studying neurons
  - Lots of exciting ideas; these ones are limited to the project-relevant ones



# CBC code progress

- Rewritten for a new solver
- Works for Fourier

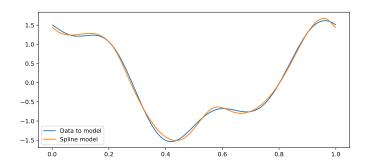




 ✓ Newton iterations fail to converge with splines discretisation

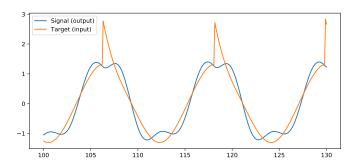
- Working hypothesis: splines models are structurally unstable; small perturbations cause big changes
  - Finite differences evaluates gradients by using small perturbations
  - Finite differences perturbations lead to discontinuous changes in the model





#### Spline model describes data fairly accurately





Control-target input is discontinuous during Jacobian estimation



- Newton iterations fail to converge with splines discretisation
- Working hypothesis: splines models are structurally unstable; small perturbations cause big changes
  - Finite differences evaluates gradients by using small perturbations
  - Finite differences perturbations lead to discontinuous changes in the model
- Currently a best-guess conjecture
  - Need to play about more to see if this is actually the case
  - ► Need to test different finite-differences stepsizes



# Novel discretisors

Ideal: journal paper comparing...

- **K** Splines
  - Knot selection methods?
- Wavelets
- Collocation
- **K** Fourier

Compare for noise-robustness, dimensionality, computational speed

Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - ▶ Produce Bayesian inference method for Fourier harmonics

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - ▶ Replace 'simple' splines / wavelets / collocation with Bayesian alternative

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - Replace 'simple' splines / wavelets / collocation with Bayesian alternative
  - 'Intelligently' select the best discretisor

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - Replace 'simple' splines / wavelets / collocation with Bayesian alternative
  - 'Intelligently' select the best discretisor
- Extension 2: reversible-jump MCMC for Fourier model identification

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - Replace 'simple' splines / wavelets / collocation with Bayesian alternative
  - 'Intelligently' select the best discretisor
- Extension 2: reversible-jump MCMC for Fourier model identification
  - Automatically determine best number of Fourier harmonics for any given signal

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - Replace 'simple' splines / wavelets / collocation with Bayesian alternative
  - 'Intelligently' select the best discretisor
- Extension 2: reversible-jump MCMC for Fourier model identification
  - Automatically determine best number of Fourier harmonics for any given signal
  - Similar to how BARS auto-chooses knot numbers and locations, but instead Fourier harmonics

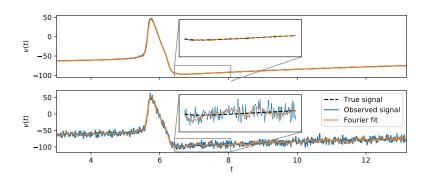
- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - Replace 'simple' splines / wavelets / collocation with Bayesian alternative
  - 'Intelligently' select the best discretisor
- Extension 2: reversible-jump MCMC for Fourier model identification
  - Automatically determine best number of Fourier harmonics for any given signal
  - Similar to how BARS auto-chooses knot numbers and locations, but instead Fourier harmonics

Why Bayesian?

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - Replace 'simple' splines / wavelets / collocation with Bayesian alternative
  - 'Intelligently' select the best discretisor
- Extension 2: reversible-jump MCMC for Fourier model identification
  - Automatically determine best number of Fourier harmonics for any given signal
  - Similar to how BARS auto-chooses knot numbers and locations, but instead Fourier harmonics
- Why Bayesian?
  - Automatic Occam's razor

- Extension 1 [discussed in meetings]: selecting discretisation method based on model evidence
  - Produce Bayesian inference method for Fourier harmonics
  - Replace 'simple' splines / wavelets / collocation with Bayesian alternative
  - 'Intelligently' select the best discretisor
- Extension 2: reversible-jump MCMC for Fourier model identification
  - Automatically determine best number of Fourier harmonics for any given signal
  - Similar to how BARS auto-chooses knot numbers and locations, but instead Fourier harmonics
- Why Bayesian?
  - Automatic Occam's razor
  - Optimally balances goodness-of-fit against model complexity; ensures simplest, most generalizable discretisations; statistically optimal

# The sweetspot problem



- Sweetspot problem: too few harmonics don't fit; too many harmonics overfit noise
- Bayesian Fourier model selection would find the sweet spot by automatically trading goodness-of-fit against model complexity

As removed from NODYCON abstract

- As removed from NODYCON abstract
  - Project surrogate of system output onto fundamental harmonic

- As removed from NODYCON abstract
  - Project surrogate of system output onto fundamental harmonic
  - Subtract out surrogate's fundamental harmonic

- As removed from NODYCON abstract
  - Project surrogate of system output onto fundamental harmonic
  - Subtract out surrogate's fundamental harmonic
  - Replace fundamental harmonic with harmonic forcing term

- As removed from NODYCON abstract
  - Project surrogate of system output onto fundamental harmonic
  - Subtract out surrogate's fundamental harmonic
  - Replace fundamental harmonic with harmonic forcing term
  - Feed the modified surrogate back into the system as the new control target

- As removed from NODYCON abstract
  - Project surrogate of system output onto fundamental harmonic
  - Subtract out surrogate's fundamental harmonic
  - Replace fundamental harmonic with harmonic forcing term
  - Feed the modified surrogate back into the system as the new control target

Should converge rapidly, implicitly represent an infinite number of harmonics, improve computational speed by avoiding DFT, improve noise-robustness by employing surrogate noise-filtering

- As removed from NODYCON abstract
  - Project surrogate of system output onto fundamental harmonic
  - Subtract out surrogate's fundamental harmonic
  - Replace fundamental harmonic with harmonic forcing term
  - Feed the modified surrogate back into the system as the new control target

Should converge rapidly, implicitly represent an infinite number of harmonics, improve computational speed by avoiding DFT, improve noise-robustness by employing surrogate noise-filtering

Further extension: something resembling a Picard iteration

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output

- CBC strategies solve for input=output
  - ► Harder to solve if output is corrupted by noise, or subject to stochastic dynamics both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics both prevalent with neurons
     'True' stochasticity measurement noise means evaluating the IO man for the
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0

- CBC strategies solve for input=output
  - ► Harder to solve if output is corrupted by noise, or subject to stochastic dynamics both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>
- These two approaches are identical in the noise-free case

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>
- These two approaches are identical in the noise-free case
  - Control target is a solution to one if and only if it's a solution to the other

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>
- These two approaches are identical in the noise-free case
  - Control target is a solution to one if and only if it's a solution to the other
- Minimizer approach is better in the noisy case

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>
- These two approaches are identical in the noise-free case
  - Control target is a solution to one if and only if it's a solution to the other
- Minimizer approach is better in the noisy case
  - If the system is subject to noise or stochastics, output will never truly equal input

- CBC strategies solve for input=output
  - ► Harder to solve if output is corrupted by noise, or subject to stochastic dynamics both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>
- These two approaches are identical in the noise-free case
  - Control target is a solution to one if and only if it's a solution to the other
- Minimizer approach is better in the noisy case
  - If the system is subject to noise or stochastics, output will never truly equal input
  - Noninvasive solution will therefore minimize control action [minimizer works], but will not result in input-output=0 [solver won't work]

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics – both prevalent with neurons
  - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>
- These two approaches are identical in the noise-free case
  - Control target is a solution to one if and only if it's a solution to the other
- Minimizer approach is better in the noisy case
  - If the system is subject to noise or stochastics, output will never truly equal input
  - Noninvasive solution will therefore minimize control action [minimizer works], but will not result in input-output=0 [solver won't work]
  - Bonus: lots of research on stochastic gradient descent (stochastic optimization) to help with this

- CBC strategies solve for input=output
  - Harder to solve if output is corrupted by noise, or subject to stochastic dynamics both prevalent with neurons
    - 'True' stochasticity measurement noise means evaluating the IO map for the same input won't necessarily give the same output
    - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Solver approach: input output = 0
- Minimizer approach: find input that minimizes (input output)<sup>2</sup>
- ★ These two approaches are identical in the noise-free case
- Control target is a solution to one if and only if it's a solution to the other
- Minimizer approach is better in the noisy case
   If the system is subject to noise or stochastics, output will never truly equal input
  - Noninvasive solution will therefore minimize control action [minimizer works], but will not result in input-output=0 [solver won't work]
  - Bonus: *lots* of research on stochastic gradient descent (stochastic optimization) to help with this
     Research output: comparison of convergence time, noise-robustness for

Covers same issues as before, but in a different way

- Covers same issues as before, but in a different way
  - How do we decide when we've found a solution to a system, if the system is stochastic?

- Covers same issues as before, but in a different way
  - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?

- Covers same issues as before, but in a different way
  - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Mewton iterations are slow, even with Jacobian updates

- Covers same issues as before, but in a different way
  - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Mewton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)

- Covers same issues as before, but in a different way
  - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Newton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)
- IDEA: surrogates-based approach

- Covers same issues as before, but in a different way
  - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Newton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)
- IDEA: surrogates-based approach
  - ▶ Build a surrogate of the input→output map

- Covers same issues as before, but in a different way
  - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Newton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)
- IDEA: surrogates-based approach
  - ▶ Build a surrogate of the input→output map
  - Choose next function evaluation based on knowledge-gradient or expected improvement

- Covers same issues as before, but in a different way
  - ► How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Newton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)
- IDEA: surrogates-based approach
  - ▶ Build a surrogate of the input→output map
  - Choose next function evaluation based on knowledge-gradient or expected improvement
  - With a probabilistic approach, this should converge much faster than Newton, and in a noise-robust way

- Covers same issues as before, but in a different way
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Mewton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)
- **№** IDEA: surrogates-based approach
  - ▶ Build a surrogate of the input→output map
  - Choose next function evaluation based on knowledge-gradient or expected improvement
  - With a probabilistic approach, this should converge much faster than Newton, and in a noise-robust way
  - Use a splines model for the input-output map, as GPR doesn't handle MIMO well

- Covers same issues as before, but in a different way
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- Newton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)
- **№** IDEA: surrogates-based approach
  - ▶ Build a surrogate of the input→output map
  - Choose next function evaluation based on knowledge-gradient or expected improvement
  - With a probabilistic approach, this should converge much faster than Newton, and in a noise-robust way
  - Use a splines model for the input-output map, as GPR doesn't handle MIMO well
  - Extension of Barton-Renson conference paper: uses explicit MIMO models, knowledge gradients, explicit noise modelling

- Covers same issues as before, but in a different way
  - How do we decide when we've found a solution to a system, if the system is stochastic?
  - ► How do we decide if input≠ output because we haven't converged, or just because of noise?
- We Newton iterations are slow, even with Jacobian updates
  - Especially big issue for larger-dimensional discretisations (as with neurons!)
- **★** IDEA: surrogates-based approach
  - ▶ Build a surrogate of the input→output map
  - Choose next function evaluation based on knowledge-gradient or expected improvement
  - With a probabilistic approach, this should converge much faster than Newton, and in a noise-robust way
  - Use a splines model for the input-output map, as GPR doesn't handle MIMO well
    - Extension of Barton-Renson conference paper: uses explicit MIMO models, knowledge gradients, explicit noise modelling
- Aim main paper at a numerical methods audience; possibly additional journal paper comparing CBC speeds, noise-robustnesses for various numerical solvers

# Results Efficier

Efficient discretisation methods

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)
  - Allows the discretisation of spiking, neuron-like signals

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)
  - Allows the discretisation of spiking, neuron-like signals
- Intelligent discretisation methods

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)
  - Allows the discretisation of spiking, neuron-like signals
- Intelligent discretisation methods
  - Bayesian'ly determine the best discretisor class [eg. Fourier vs. splines], best discretisation approach within that class [eg. number of knots / harmonics]

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)
  - Allows the discretisation of spiking, neuron-like signals
- Intelligent discretisation methods
  - Bayesian'ly determine the best discretisor class [eg. Fourier vs. splines], best discretisation approach within that class [eg. number of knots / harmonics]
  - Allows the optimal discretisation of spiking, neuron-like signals, without needing a human in the loop

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)
  - Allows the discretisation of spiking, neuron-like signals
- Intelligent discretisation methods
  - Bayesian'ly determine the best discretisor class [eg. Fourier vs. splines], best discretisation approach within that class [eg. number of knots / harmonics]
  - Allows the optimal discretisation of spiking, neuron-like signals, without needing a human in the loop
  - Ensures CBC is accurate, by guaranteeing discretisation actually describes the target signal

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)
  - Allows the discretisation of spiking, neuron-like signals
- Intelligent discretisation methods
  - Bayesian'ly determine the best discretisor class [eg. Fourier vs. splines], best discretisation approach within that class [eg. number of knots / harmonics]
  - Allows the optimal discretisation of spiking, neuron-like signals, without needing a human in the loop
  - Ensures CBC is accurate, by guaranteeing discretisation actually describes the target signal
- Noise-robust solvers for accurate CBC calculations

- Efficient discretisation methods
  - Alternative approaches to Fourier (splines, collocation, wavelets)
  - Allows the discretisation of spiking, neuron-like signals
- Intelligent discretisation methods
  - ▶ Bayesian'ly determine the best discretisor class [eg. Fourier vs. splines], best discretisation approach within that class [eg. number of knots / harmonics]
  - Allows the optimal discretisation of spiking, neuron-like signals, without needing a human in the loop
  - Ensures CBC is accurate, by guaranteeing discretisation actually describes the target signal
- Noise-robust solvers for accurate CBC calculations
  - Solve the CBC equations accurately, even faced with measurement noise [and stochasticity?]



# Testing the new methods

Any CBC rigs I could demonstrate these methods on?



# Next steps

- Edit NODYCON paper
- Edit continuation paper
- Keep working on splines discretisation code
- Test other discretisor methods