Comment on Article by Chkrebtii, Campbell, Calderhead, and Girolami[*]

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Discussion

The article presented by the authors addresses the issue of discretization uncertainty when differential equation systems are solved numerically, and particularly, its effect on the inference of unknown system parameters. I wish, firstly, to congratulate the authors for a very nice piece of work which, to my knowledge, is one of the first papers to highlight the issue and provide a Bayesian solution for it. Nevertheless, I do have several concerns with the article which I hope that the authors can help clarify and discuss.

On Discretization Uncertainty

What represents discretization uncertainty? The authors take the solution, u, of the differential equation system and its derivative, u_t, to be distributed according to a Gaussian process a priori. On discretizing over the ordered partition $\mathbf{s} = \{s_1, s_2, \cdots, s_N\}$, the discretization uncertainty is propagated as $f_n = f(s_n, u^{n-1}(s_n), \theta)$ where $u^{n-1}(s_n)$ is sampled from the marginal predictive prior $[u(s_n)|f_{n-1}, f_{n-2}, \cdots, f_1]$. This current f_n then is used to update the mean and covariance functions of the Gaussian process as in Algorithm 1 for the next step from $n \rightarrow n+1$. At step $n+1$, $u^n(s_{n+1})$ is sampled from $[u^n(s_{n+1})|f_n, f_{n-1}, \cdots, f_1]$, f_{n+1} is evaluated as $f_{n+1} = f(s_{n+1}, u^n(s_{n+1}), \theta)$, and the mean and covariance functions are again updated as in Algorithm 1. This process is repeated until $n = N$, the size of the discretization grid chosen. The posterior $[u(\mathbf{s}), u_t(\mathbf{s})|f_N, f_{N-1}, \cdots, f_1]$ is the discretization uncertainty, according to the authors, as shown in Figure 1.

But why should Algorithm 1 terminated at $n = N$ be interpreted as the final discretization uncertainty? That is, why should it be interpreted as the discretization uncertainty *associated with the grid* $\mathbf{s}$? One could potentially repeat the iterative process again for a second time, obtain a new sequence of f_ns, say $f_n^{(2)}$, $n = 1, 2, \cdots, N$, and update the mean and covariance functions as in Algorithm 1. To elaborate, I am assuming that $u^*(0)$ is fixed so $f_1^{(2)} = f(s_1, u^*(0), \theta)$ will not change, but based on this f_1, the mean and covariance functions can be updated again from the final posterior $[u(\mathbf{s}), u_t(\mathbf{s})|f_N, f_{N-1}, \cdots, f_1]$ from the first cycle. Then, obtain $u^{1,(2)}(s_2) \sim$