APS Scientific Computation Seminar Series

Speaker:
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Title:
Widely Applied Kriging: From Mechanics to MRI

Date:
February 19, 2024

Time:
1:00 PM (Central Daylight Savings Time)

Location:
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Abstract:
The process of iteratively selecting experiments based on prior results is common to essentially all forms of research. While this practice is deeply intwined with scientific intuition and hypothesis-driven research more generally, there are many components of experimental design where the behavior of an unknown system can be effectively learned by algorithmically building an approximation of the system and sequentially choosing experimental conditions most likely to progress toward the user-driven goal. Kriging is an especially general example of such an algorithm based upon Gaussian process regressions (GPRs) and we have used this approach extensively to guide experimental research. In this talk, I will some discuss examples of how we have used Kriging and what we have learned about how to understand, interpret, and guide long-term research campaigns. I will begin by discussing our use of GPRs as a method to sub-sample magnetic resonance images. This will allow us to discuss concepts of stationary vs. non-stationary kernels in GPRs. We find this approach to be more effective and data-efficient than comparable methods based upon deep learning. Next, I will discuss our integration of Kriging with an autonomous experimentation system designed to study the mechanical properties of 3D-printed polymer structures. The resulting self-driving lab allowed us to experimentally evaluate the acceleration inherent to Kriging, which we found to require ~30x fewer experiments than grid-based searching. We also explore methods of using transfer learning to incorporate further information into GPRs by integrating simulation. Finally, we discuss a two-year experimental campaign in which we identified the most mechanical efficient structure realized to date. In carrying out this campaign, we had key learnings about how to monitor and interact with a SDL using Kriging to select experiments and we will conclude the talk discussing these general lessons.