

1 Introduction

1.1 Define the problem

1. complex models in physics/natural science
2. research and large-scale commercial usage
3. expensive: to address the cost, use of prior knowledge and iterative/sequential learning is key
4. computer experiments - Sacks et al. (1989)
 - (a) prediction
 - (b) calibration (inverse problem) - Kennedy & O'Hagan (2001)
 - (c) surrogates Draws from predictive equations derived from a fitted model can act as a surrogate for the data-generating mechanism. If the fit is good – model flexible yet well-regularized, data rich enough and fitting scheme reliable then such a surrogate can be quite valuable. Gathering data is expensive, and sometimes getting exactly the data you want is impossible or unethical. A surrogate could represent a much cheaper way to explore relationships, and entertain “what ifs?”. How do surrogates differ from ordinary statistical modeling? One superficial difference may be that surrogates favor faithful yet pragmatic reproduction of dynamics over other things statistical models are used for: interpretation, establishing causality, or identification. As you might imagine, that characterization oversimplifies.
 - (d) Gaussian Process/kriging
 - (e) framework consistent with both classical MLE: Santner et al. (2003) and Bayesian methods: Higdon et al. (2004)
 - (f) functional outcome (discretized, basically multivariate) outcome
5. DoE:
 - (a) why simple space filling design is not sufficient in most applications, particularly in high-dimensional space
 - (b) criterion based, use criterion to find areas with more uncertainty

- (c) exploit-explore: Challenge: *trade off exploration by gathering data for estimating the expected payoff function over the ..context-action?.. space, and to exploit by choosing an action deemed optimal based on the gathered data. The objective function is designed as a sample from a Gaussian process defined over the joint ..context-action?.. space – Krause & Ong (2011)*
- (d) sequential and real-time updates

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1.2 Motivating example

1.3 Computer Experiments Using Gaussian Processes

1.4 Citations Tests

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References

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