

## ISE-INFORMS Research Seminar

### Practical Heteroskedastic Gaussian Process Modeling for Large Simulation Experiments

#### SPEAKER INFORMATION

**Dr. Robert B. Gramacy**  
Professor  
Department of Statistics

#### SEMINAR SESSION INFORMATION

**DATE:** Wednesday, March 22

**TIME:** 12:15pm

**LOCATION:** Durham 260

**PROVIDED:** Pizza and Soda

**Abstract:** We present a unified view of likelihood based Gaussian process regression for simulation experiments exhibiting input-dependent noise. Replication plays an important role in that context, however previous methods leveraging replicates have either ignored the computational savings that come from such design, or have short-cut full likelihood-based inference to remain tractable. Starting with homoskedastic processes, we show how multiple applications of a well-known Woodbury identity facilitate inference for all parameters under the likelihood (without approximation), bypassing the typical full-data sized calculations. We then borrow a latent-variable idea from machine learning to address heteroskedasticity, adapting it to work within the same thrifty inferential framework, thereby simultaneously leveraging the computational and statistical efficiency of designs with replication. The result is an inferential scheme that can be characterized as single objective function, complete with closed form derivatives, for rapid library-based optimization. Illustrations are provided, including real-world simulation experiments from manufacturing and the management of epidemics.

**Biography:** Dr. Gramacy is a Professor of Statistics in the College of Science at Virginia Tech. Previously He was an Associate Professor of Econometrics and Statistics at the Booth School of Business, and a fellow of the Computation Institute at The University of Chicago. He specializes in areas of real-data analysis in the physical, engineering and biological sciences. His research interests include Bayesian modeling methodology, statistical computing, Monte Carlo inference, nonparametric regression, sequential design, and optimization under uncertainty. His work resulted in several software packages for general use in areas such as big data regression, and computer model emulation.

**Faculty and Students are invited**