

## STATISTICAL ANALYSIS AND DATA MINING

Research Article

**Predicting simulation parameters of biological systems using a Gaussian process model**Xiangxin Zhu , Max Welling, Fang Jin, John Lowengrub

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## Abstract

Finding optimal parameters for simulating biological systems is usually a very difficult and expensive task in systems biology. Brute force searching is infeasible in practice because of the huge (often infinite) search space. In this article, we propose predicting the parameters efficiently by learning the relationship between system outputs and parameters using regression. However, the conventional parametric regression models suffer from two issues, thus are not applicable to this problem. First, restricting the regression function as a certain fixed type (e.g. linear, polynomial, etc.) introduces too strong assumptions that reduce the model flexibility. Second, conventional regression models fail to take into account the fact that a fixed parameter value may correspond to multiple different outputs due to the stochastic nature of most biological simulations, and the existence of a potentially large number of other factors that affect the simulation outputs. We propose a novel approach based on a Gaussian process model that addresses the two issues jointly. We apply our approach to a tumor vessel growth model and the feedback Wright–Fisher model. The experimental results show that our method can predict the parameter values of both of the two models with high accuracy. © 2012 Wiley Periodicals, Inc. *Statistical Analysis and Data Mining*, 2012

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