

Bayesian Quantification of Uncertainty in Systems with Intrinsic Noise

Stochastic Dynamical Systems: Analysis of Dynamics and Predictability

Khachik Sargsyan, Cosmin Safta, Bert Debusschere, Habib Najm

Sandia National Laboratories

P.O. Box 969, Livermore, CA, 94551-0969

bjdebus@sandia.gov

Abstract

Uncertainty quantification (UQ) and sensitivity analysis techniques are typically challenged by the presence of intrinsic variability in stochastic systems [2, 1]. In this work, we develop UQ methods to study the dependence of output quantities of interest with respect to uncertain input parameters in such systems. Spectral polynomial chaos (PC) expansions are used to represent the relationship between input parameters and noisy output observables. Spectral projections using full tensor product quadrature suffer from the curse of dimensionality, *i.e.* in the presence of large number of input parameters. While sparse grid quadrature methods are known to alleviate this issue for a moderate number of dimensions, we have shown that they fail strongly for noisy systems, no matter how small the amplitude of the noise.

We developed a Bayesian framework to infer PC coefficients and arrive at an *uncertain* PC expansion that effectively incorporates the parametric uncertainty and the intrinsic noise of the model. The expansion is obtained using an initial sampling at a number of input configurations that are chosen to cover the high-dimensional input space sufficiently well. The intrinsic noise, as well as the uncertainty arising from the lack of sufficient sampling, are represented by the posterior probability distribution of the PC coefficients. By using conjugate priors in conjunction with gaussian likelihood functions, this high-dimensional Bayesian inference is made analytically tractable.

The approach is demonstrated on the analysis of the stochastic reaction network of gene regulation in *Bacillus subtilis*. *B. subtilis* is a key gram-positive bacterium commonly found in soil [4], with specific relevance to bioremediation and enhanced oil recovery. Competence in *B. subtilis* is a stochastically regulated state that allows cells to take up DNA from the environment, and it is characterized by sporadic fast jumps in the number of transcription factor comK molecules. We investigated the dependence of competence on the rate constants of all 16 reactions involved in the network. To properly represent the various dynamical regimes across the input parameter space, e.g. always vegetative, always competent, or intermittently competent, a piecewise polynomial representation is constructed using a nearest-neighbor classification approach, leading to a mixture-PC representation of the input-output relationship. Furthermore, a variance decomposition has been performed to arrive at sensitivity information indicating specific input parameters and combinations thereof that have the strongest effect on the competence transition[3].

- [1] K. Sargsyan, B. Debusschere, H. Najm, and O. Le Maître. Spectral representation and reduced order modeling of the dynamics of stochastic reaction networks via adaptive data partitioning. *SIAM Journal on Scientific Computing*, 31(6):4395–4421, 2010.
- [2] K. Sargsyan, B. Debusschere, H. Najm, and Y. Marzouk. Bayesian inference of spectral expansions for predictability assessment in stochastic reaction networks. *J. Comput. Theor. Nanosci.*, 6(10):2283–2297, 2009.
- [3] K. Sargsyan, C. Safta, B. Debusschere, and H. Najm. Multiparameter spectral representation of noise-induced competence in *Bacillus subtilis*. *in preparation*, 2011.
- [4] G. M. Suel, R. P. Kulkarni, J. Dworkin, J. Garcia-Ojalvo, and M. B. Elowitz. Tunability and noise dependence in differentiation dynamics. *Science*, 315(5819):1716 – 1719, 2007.