Uncertainty Quantification for Generalized Langevin Dynamics

Eric Hall,* Markos Katsoulakis, Luc Rey-Bellet
(*hall@math.umass.edu)

Problem
The generalized Langevin equation (GLE) is given by
\[ dX_t = V_d dt, \quad X_0 = x_0, \]
\[ mdV_t = \nabla U(X_t) dt - \int_0^t K(t-s)V_{t-s} dW_s + F(t) dt, \quad V_0 = v_0. \]

When \( A \) can be represented by a positive Prony series, \( A(t) = \sum_{i=1}^{\infty} e^{-\alpha_i t} \langle c_i \rangle \), the non-Markovian GLE can be mapped into a higher dimensional Markovian problem in \( N_f \) extended variables [1]. The extended variable GLE,
\[ mdV_t = \nabla U(X_t) dt + \sum_{i=1}^{N_f} S_i dt, \]
\[ dX_t = V_t dt, \]
\[ dS_i = -\frac{1}{\tau_i} S_i dt - \frac{C_i}{\tau_i} V_t dt + \frac{1}{\tau_i} \sqrt{2 \lambda_i} f_i dW_i, \]

contains many parameters that must be tuned and is therefore an ideal candidate for sensitivity analysis (SA) and uncertainty quantification (UQ). Thus for a given observable \( S(t; \alpha; f) = \frac{1}{2} \mathbb{E}[\hat{f}(X_t^\alpha)] \), for dynamics depending on a parameter \( \alpha \). However, well known SA techniques such as linear response, likelihood ratio, pathwise methods, and information theoretic bounds are not applicable to all parameters of interest in \( \mathbb{R} \). Finite difference (FD) estimators are applicable to all parameters of interest, but introduce a bias and have large variance.

Results
In [2] we give reduced variance FD estimators for goal oriented sensitivity indices via a coupling method. Consider the FD estimator \( S_{\text{FD}}(t; \alpha; f) = \frac{1}{2} \mathbb{E}[\hat{f}(X_t^\alpha)] \), given by \( S_{\text{FD}}(t; \alpha; f) = \frac{1}{2} \mathbb{E}[\hat{f}(X_t^\alpha)] \). The variance of the estimator is controlled by
\[ \frac{\text{Var}[\hat{f}(X_t^\alpha) - f(X_t^\alpha)]}{\text{Var}[\hat{f}(X_t^\alpha) - 2 \text{Cov}[\hat{f}(X_t^\alpha), f(X_t^\alpha)]]. \]

The variance can be reduced, relative to independent sampling of \( f(X_t^\alpha) \) and \( f(X_t^\alpha) \), by coupling the processes: \( \hat{Z}_t = (X_t^\alpha; \hat{X}_t^\alpha) \). Then for \( d\hat{Z}_t = \hat{B}(\hat{Z}_t) dt + \hat{L}(\hat{Z}_t) dW_t \), an optimization problem, where the constraints are derived by requiring that the statistics of the marginals of the coupled process match the nominal and perturbed processes, suggests an optimal coupling locally in time (how to choose \( \hat{B} \) and \( \hat{L} \)). For convex potentials the optimal coupling is to simulate \( X^\alpha \) and \( \hat{X}^\alpha \) with a common random path.

\[ M = 10^3, \epsilon = 0.01 \]
\[ S_{\text{FD}}(t; \epsilon; \text{VACF}) \sim 1 \text{sd} \]

Above, a smaller sample size \( M \) is required to obtain meaningful estimates for sensitivities for the common random path coupled FD estimators for the convex potential \( U(X) = \omega X^2/2 \). Below, the relative sensitivity of the VACF to perturbations in the parameters \( c_1, c_2, \) and \( \omega \) is not known a priori.

\[ M = 10^4, \epsilon = 0.01 \]
\[ S_{\text{FD}}(t; \epsilon; \text{VACF}) \sim 1 \text{sd} \]

Summary
In [2] we give efficient and easily implemented FD estimators for goal oriented sensitivity indices that apply to all parameters of interest in \( \mathbb{R} \) by coupling the nominal and perturbed dynamics appearing in the FD through a common random path. For convex potentials this coupling is optimal relative to independent sampling and, for many sensitivity indices, the reduction to the variance of the estimator is in the order of the bias squared—mitigating the effect of the bias error on the computational cost.

References