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Simulating stochastic quantum systems with polynomial chaos expansions

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Abstract

We present an approach to the simulation of quantum systems driven by classical stochastic processes that is based on the polynomial chaos expansion, a well-known technique in the field of uncertainty quantification. The polynomial chaos expansion represents the system density matrix as a series of orthogonal polynomials in the principle components of the stochastic process and yields a sparsely coupled hierarchy of linear differential equations. We provide practical heuristics for truncating this expansion based on results from time-dependent perturbation theory and demonstrate, via an experimentally relevant one-qubit numerical example, that our technique can be significantly more computationally efficient than Monte Carlo simulation.

Problem statement

Hamiltonian describing the system dynamics includes driving by a classical, stationary, Gaussian stochastic process

$$H(t;\Omega(t)) = H_0(t) + \Omega(t)V$$

We're interested in finding the state of the system, averaged over the stochastic process.

$$\rho(\tau) = \langle U(\tau;\{\Omega(t)\})\rho(0)U(\tau;\{\Omega(t)\})\rangle_\Omega$$

General approach

A simple approach would be **Monte Carlo**: generate a set of realizations of the stochastic process which are consistent with the known statistics, unitarily evolve the state of the time-dependent, deterministic, system in accordance with the Schrodinger-von Neumann equation, and average the results over the realizations.

Monte Carlo converges slowly, so we apply a classical technique, the **Polynomial Chaos Expansion** (**PCE**). The PCE begins by performing a **Karhunen-Loeve** (**KL**) decomposition of the noise, also know as principle component analysis, representing the continuous time stochastic process as a sum over deterministic functions with random coefficients. Depending on the details of the process, many of the principle components can be discarded, so the stochastic part of the evolution can be described in terms of only a few random variables. The density matrix can then be written as a polynomial in these random variables, and the evolution of the coefficients of this polynomial is described by a sparsely coupled hierarchy of differential equations.

Karhunen Loeve Decomposition

The KL decomposition expresses the stochastic process as a sum over deterministic functions weighted by normally distributed random variables, $\xi_n \in \mathcal{N}(0,1)$

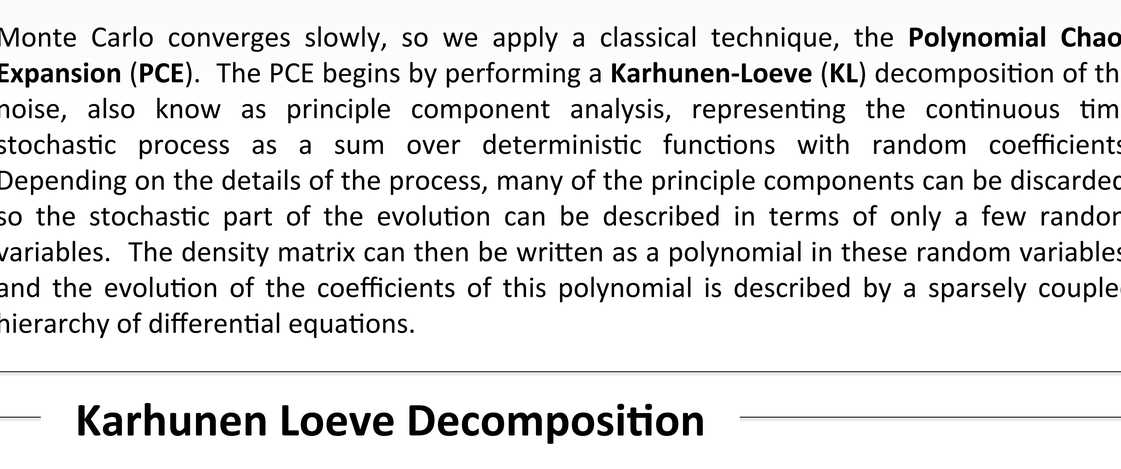
$$\Omega(t) = \sum_{n=1}^{\infty} \sqrt{\lambda_n} g_n(t)\xi_n$$

The functions are given as the eigenvalues and eigenvectors of the Fredholm equation, an integral equation over the correlation function of the stochastic process,

$$\int_0^\tau C(t_1,t_2)g_n(t_2)dt_2 = \lambda_n g_n(t_1)$$

We keep only those terms which cause the highest transition rates,

$$\Gamma_n^{jk} = \frac{1}{\tau}\left|\langle j\,|V|\,k\rangle \int_0^\tau e^{i(E_j-E_k)t}\sqrt{\lambda_n}g_n(t)dt\right|^2$$



Polynomial Chaos Expansion

We begin by working in a rotating frame with respect to the known Hamiltonian,

$$\tilde{H}(t;\Omega(t)) = \Omega(t)U_0(t)^\dagger V U_0(t) \equiv \Omega(t)\tilde{V}(t)$$

So the evolution equation for the system is

$$i\frac{d\rho(t;\{\Omega(t)\})}{dt} = \Omega(t)V(t)^\times\rho(t;\{\Omega(t)\}) \qquad A^\times B = [A,B]$$

Replace the stochastic process by the truncated KL expansion,

$$i\frac{d\rho(t;\vec{\xi})}{dt} = \sum_{n=1}^{S}\sqrt{\lambda_n}g_n(t)\xi_n V(t)^\times\rho(t;\vec{\xi})$$

And expand the state in Hermite polynomials over the random variables,

$$\rho(t;\vec{\xi}) = \sum_{n=0}^{\infty}\phi_n(t)\Phi_n(\vec{\xi}) \qquad \Phi_{\mathbf{n}}(\vec{\xi}) = \prod_{j=1}^{S}\mathrm{He}_{n_j}(\xi_j)$$

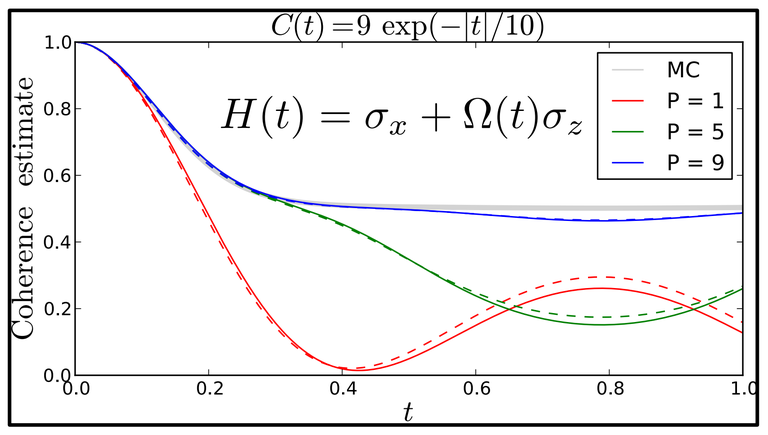
Evolution of the coefficients is described by the coupled differential equations,

$$i\frac{d\phi_{\mathbf{m}}(t)}{dt} = \sum_{n=1}^{S}\sum_{||\mathbf{l}||_1=0}^{P}\sqrt{\lambda_n}g_n(t)V(t)^\times\phi_{\mathbf{l}}(t)G_{\mathbf{m}n\mathbf{l}}$$

The hierarchy is sparse, as indicated by the form of the **Galerkin projection**

$$G_{\mathbf{m}n\mathbf{l}} = ((\mathbf{m}_n+1)\delta_{\mathbf{m}_n+1,\mathbf{l}_n} + \delta_{\mathbf{m}_n-1,\mathbf{l}_n})\prod_{j\neq n}\delta_{\mathbf{m}_j\mathbf{l}_j}$$

Numerical Results



Our PCE method is capable of reproducing the results of MC simulations with high accuracy, significantly faster than MC. For the example chosen, Monte Carlo required approximately 4000 iterations for convergence, while the most accurate PCE results report here (P = 9 and S = 3) required the solution of only 220 coupled equations and ran approximately 20 times faster than the MC simulation. Note that because $\tau_c/\tau = 10$ in our simulation, only one eigenvalue of the KLE is dominant. In this regime, it is more efficient to keep the stochastic dimension small ($S \leq 3$) and increase the PCE order for improved accuracy. As the order increases from P = 1 to P = 9, the accuracy of the PCE coherence increases as a function of time, compared to the converged MC result.

For more details, please see

Young, K. and Grace, M, *Simulation of stochastic quantum systems using polynomial chaos expansions*, arXiv:1209:3289, in press at Physical Review Letters

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