Combined Error Estimates for Numerical Continuation of Stochastic Systems

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Summary. Numerical continuation methods for dynamical systems have been successfully applied to a wide variety of applications. In particular, parametric studies of ordinary, partial and delay differential equations can be carried out very efficiently using various existing software tools. Applications range from engineering and applied mathematics to virtually all fields in the natural sciences. However, studying stochastic dynamical systems numerically has turned out to be challenging. In this contribution, I am going to outline one possible broad framework how to incorporate noise-driven effects into the classical deterministic continuation framework. In particular, I shall show how one can efficiently continue the local fluctuations of stochastic partial differential equations (SPDEs), also with a view towards large-scale applications for the stochastic Navier-Stokes equation. Since the numerical approximation of a large scale problem involves several sources of error, I shall also explain, how to prove combined error estimates (CERES). This approach to provide a CERES can be extended to a wide variety of problems. Large-scale stochastic and multiscale systems seem to be key classes of examples. In these contexts, it is often extremely difficult to determine just based on numerical experiments, which part of a CERES dominates so better theory is called for.

Introduction

As a starting point, fix a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and consider a general stochastic differential equation (SDE) given by

$$\frac{dx}{dt} = \dot{x} = f(x;\mu) + \sigma F(x;\mu)\dot{W} \tag{1}$$

where $W = (W_1, W_2, \ldots, W_k)^T$ is k-dimensional Brownian motion, $\sigma > 0$ controls the noise level, $\mu \in \mathbb{R}^p$ are parameters and $f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ and $F : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^{n\times k}$ are sufficiently smooth maps; the SDE (1) is interpreted in the Itô sense with white noise $\dot{W}$ as the usual generalized derivative. Currently, most studies that investigate the dynamics of (1) numerically are centered around Monte-Carlo algorithms and their variations. The strategy is to use forward integration of the SDE and a strategy which requires, at least, three different components:

(S1) Sample over a sufficiently large number of initial conditions $x(0) \in \mathbb{R}^n$ and determine which initial conditions lead to similar dynamics.

(S2) Sample over a sufficiently large number of noise realizations $\omega \in \Omega$ and compute the required averaged quantities of interest over s sample paths.

(S3) Sample over the parameters $\mu \in \mathbb{R}^p$ and plot the bifurcation diagram at each point by repeating steps (S1)-(S2).

There are some strategies that slightly alleviate the computational requirements for carrying out (S1)-(S3), such as quasi-Monte-Carlo methods based on discrepancy theory or multilevel-Monte-Carlo based upon a coarse-/fine-sampling hierarchy. Nevertheless, any slightly larger problem suffers strongly from the curse of dimensionality. Indeed, just elementary count yields $n \times p \times s$ as the "total dimension of the problem" where usually $s, n \gg 1$ and even p is often very large. Of course, trying to solve the Fokker-Planck partial differential equation (PDE) associated to (1) numerically for $n \gg 1$ is also computationally prohibitive. A key perspective to see the difficulty is that one would usually not even attempt (S1)-(S3) in the ODE case with $\sigma = 0$ where (S2) can be skipped entirely nor would one try to solve the Liouville equation for the density numerically. Indeed, consider the deterministic part of (1) given by

$$\dot{x} = f(x;\mu). \tag{2}$$

For (2) there are well-known tools how to study the dynamical behaviour depending upon the parameters $\mu \in \mathbb{R}^p$ based upon numerical continuation. The key insights of this framework are to focus on dynamical objects (equilibria, periodic orbits, invariant manifolds, etc.), instead of individual paths or densities, and to employ Newton's method for parametrized algebraic nonlinear equations. The methods also extend naturally to PDEs and delay equations. Although stochastic systems are of high current interest, no natural numerical continuation approach has been available. In this contribution, I shall outline one possibility and its extensions currently under development for SPDEs.

Basic Idea for SDE Numerical Continuation

We take the viewpoint that the noise level $\sigma > 0$ is "not too large" which is quite natural as extremely large noise indicates that the model might have not been derived to suitable physical modelling accuracy in the first place. Suppose that (2) has hyperbolic stable equilibrium point $x^* = x^*(\mu)$ for a given range of parameter values, say $\mu \in \mathbb{R}$ for simplicity. Assuming that $F(x^*;\mu) \neq 0$ and Taylor expanding the approximation of (1) to lowest order yields

$$\dot{X}_t = A(x^*;\mu)X_t + \sigma F(x^*;\mu)\dot{W} \tag{3}$$

where $A = A(x;\mu) = (D_x f)(x;\mu) \in \mathbb{R}^{n\times n}$ is the usual Jacobian matrix. Equation (3) is an n-dimensional Ornstein-Uhlenbeck process with covariance matrix

$$C(t) := \mathrm{Cov}(X(t)) = \sigma^2 \int_0^t U(t,s)F(x^*;\mu)F(x^*;\mu)^T U(t,s)^T ds$$

where $U(t,s)$ is the fundamental solution of $\dot{U} = A(x^*;\mu)U$. Differentiation shows that $C(t)$ satisfies the ODE $\dot{C} = A(x^*;\mu)C + CA(x^*;\mu)^T + \sigma^2 F(x^*;\mu)F(x^*;\mu)^T$. Since x^* is a hyperbolic stable equilibrium point, it follows that the eigenvalues of the linear operator $L(C) := A(x^*;\mu)C + CA(x^*;\mu)^T$ are $\{2\lambda_j\}_{j=1}^n$ where λ_j are the eigenvalues of $A(x^*;\mu)$. Therefore, the covariance ODE has a stable equilibrium solution which is obtained by solving

$$0 = A(x^*;\mu)C + CA(x^*;\mu)^T + \sigma^2 F(x^*;\mu)F(x^*;\mu)^T. \tag{4}$$

Note that (4) is a Lyapunov equation. We denote the solution of (4) simply as C or $C(x^*(\mu);\mu)$. It is standard to define a covariance neighbourhood

$$\mathcal{B}(h) := \left\{x \in \mathbb{R}^n : (x-x^*)^T C^{-1}(x-x^*) \le h^2\right\} \tag{5}$$

where h is a parameter that can be interpreted as a probabilistic confidence level. Essentially, $\mathcal{B}(h)$ yields the information about local fluctuations and important noise directions near x^*. Hence, we would like to solve for $\mathcal{B}(h)$ for $x^*(\mu)$ along the entire branch of equilibrium points obtained via continuation $\gamma := \{(x^*(\mu),\mu)\} \subset \mathbb{R}^n \times \mathbb{R}$. The algebraic equation is a uniquely solvable Lyapunov matrix equation of the form

$$AC + CA^T + B = 0 \tag{6}$$

where $A = A(x^*;\mu)$ and $B := \sigma^2 F(x^*;\mu)F(x^*;\mu)^T$. Although direct numerical methods for (6) exist, for our case new aspects arise since we want to solve (6) along an entire equilibrium branch. Indeed, most numerical continuation algorithms require an approximation of the $n \times (n+1)$ Jacobian matrix $(D_{(x,\mu)}f)(x^*(\mu_1),\mu_1)$ to compute a point $(x^*(\mu_2),\mu_2) \in \gamma$ starting from $(x^*(\mu_1),\mu_1) \in \gamma$. Therefore, the matrix $A = (D_x f)(x^*(\mu_1);\mu_1)$ is available at each continuation step. Furthermore, computing the matrix B requires at most one matrix multiplication at a given point $(x^*(\mu_1),\mu_1)$; for purely additive noise B can even be precomputed for all equilibrium points. Solving (6) at $(x^*(\mu_1),\mu_1)$ gives a matrix $C(x^*(\mu_1);\mu_1)$. If $|\mu_1 - \mu_2|$ is small then $C(x^*(\mu_1);\mu_1)$ is already an excellent initial guess to find $C(x^*(\mu_2);\mu_2)$! In fact, one may compute even better initial guesses by a predictor step. Hence, except for the first point on the equilibrium curve, we always have an initial guess available for an iterative method of solving the Lyapunov equation. Efficient methods for iterative solution of matrix Lyapunov equations are available and are still under active development (e.g. ADI or rational-Krylov methods). The SDE example (1) can naturally be extended to SPDEs by using a spatial discretization. In this contribution, I shall outline the cubic-quintic Allen-Cahn SPDE

$$\partial_t u = \Delta u + \mu u + u^3 - u^5 + \xi, \qquad u = u(x,t), \tag{7}$$

as one standard test problem, where $\xi = \xi(x,t)$ is a trace-class space-time white noise. Furthermore, I shall sketch, how to prove error estimates in this context combining the errors from discretization, linearization, reduction and low-rank approximation of the covariance matrix into one estimate. Furthermore, I shall outline, how to apply the methods to an SPDE arising in climate science describing the periodic Atlantic meridional overturning circulation (AMOC). The contribution is a summary of results obtained recently in the following works:

- Numerical continuation for SDEs [Kue12]
- Software development and gluing [Kue15a]
- Extension to SPDEs and cubic-quintic Allen-Cahn [Kue15b]
- Application to climate science [BVM$^+$16]
- CERES for local fluctuations of SPDEs [KK16]

References

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