106d Parameter Estimation for Stochastic Differential Models: Application to a Model of Polymer Rheology

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Stochastic differential equations (SDEs) can be used to model a wide variety of systems, from materials, such as polymers and their rheological behaviour, to the stock market. Reliable methods for the integration of SDE models, such as Itô integration, have been developed. A key issue in using SDEs for practical applications is the estimation of model parameters. This is made difficult by the stochastic nature of the model, which makes the computation of derivatives unreliable, and by the high computational cost of the model evaluations.

The objective of this work is to propose a parameter estimation method for SDE systems which overcomes these issues, providing values of the optimal parameters estimates and their confidence intervals. The parameter estimation problem is formulated using a maximum likelihood objective function and a modified Levenberg-Marquardt algorithm is proposed for its solution.

We address the issue of gradient calculation by deriving the sensitivity equations for the SDE model. The integration of the augmented SDE systems shows that the analytical gradients are more reliable, less noisy and faster to compute than numerical gradients which are obtained by a finite difference method. The noise in the resulting gradients is comparable to the noise in the state variables. The issue of computational efficiency is addressed by varying the SDE simulation size from iteration to iteration. The key idea is that, when the parameter values are some distance away from the optimal solution, the search direction can be obtained reliably from relatively small and noisy simulations. As a result, we adjust the size of simulation according to the proximity of the parameter iterate to the optimal solution, as indicated by the magnitude of the sensitivities. Finally, we address the impact of noise on the convergence criterion.

Uncertainty in the parameters estimated arises from experimental error and from the stochastic nature of the model. To obtain confidence intervals, we use a global uncertainty analysis. We sample normally distributed experimental trajectories, and, for a set of trajectories, we estimate the cumulative probability that a given set parameters is optimal, based on knowledge of the simulation noise. We repeat this for a set of uniformly distributed parameters. The results of this analysis give an estimate of expected ‘true' values of the parameters and their confidence intervals.

The parameter estimation algorithm has been applied to a model of polymer melt rheology, (H. C. Öttinger, 1999, J. Rheol., 43, 1461; J. Fang, M. Kröger and H. C. Öttinger, 2000, J. Rheol., 44, 1293). This model is based on theories of non-equilibrium thermodynamics, and it incorporates advanced phenomena of polymer dynamics such as double reptation, convective constraint release, chain stretching, and avoiding independent alignment. The model parameters are related to the dynamic properties as well as the architecture of polymer chains. The model is used to predict transient viscosity under different flow conditions as a function of time. The algorithm is applied to two polymers: a model polymer, with known parameter values and pseudo experimental data generated from simulations, and a polyacrylate. Results of these case studies show that the algorithm provides good estimates of the parameters and their confidence intervals.