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Efficient Method of Estimating Second-Order Sensitivities for Stochastic Discrete Biochemical Systems

Biochemical systems involving some small molecular populations may exhibit stochastic fluctuations that can influence cellular dynamics, thus discrete stochastic models are essential to accurately represent them. Additionally, their models are often stiff due to reactions occurring on widely separated time-scales. Sensitivity analysis is crucial for understanding how parameter changes affect system dynamics and second-order sensitivities provide concavity information and capture interactions between parameters. We propose a finite-difference technique for estimating second-order parametric sensitivities in moderately stiff to stiff stochastic discrete models of biochemical systems. This method uses an adaptive tau-leaping scheme combined with a coupling strategy for nominal and perturbed processes, to achieve both accuracy and computational efficiency. Moreover, this approach may be extended to models of reaction-diffusion systems. This is joint work with Silvana Ilie.