Numerical Scheme for Bilevel Langevin

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Numerical methods

We have two numerical schemes: one to simulate the system of SDE's that corresponds to the stocBio algorithm (without Neumann series) and one to simulate the Brownian dynamics system above. We set up the timesteps as follows: t_i for $i \in 1, \ldots, N$, with $t_1 = t_{start}, t_N = t_{end}$. Let $t_{i+1} = t_i + \delta t$, where $\delta t = \frac{t_{end} - t_{start}}{N}$. Additionally, set $\sigma = \sqrt{2/\beta}$. For the stocBio system, we have the updates

$$\begin{aligned} X_{t_{i+1}} &= X_{t_i} - \nabla_x F(X_{t_i}, \lambda_{t_i})\delta t/\epsilon + \sigma \mathcal{N}(0, dt) \\ \lambda_{t_{i+1}} &= \lambda_{t_i} - \left(\nabla_\lambda C((X_{t_i}, \lambda_{t_i})) + \nabla_{\lambda x} F(X_{t_i}, \lambda_{t_i})\, (\nabla_{xx} F(X_{t_i}, \lambda_{t_i}))^{-1} \nabla_x C((X_{t_i}, \lambda_{t_i}))\right) \delta t + \sigma \mathcal{N}(0, dt). \end{aligned}$$

We simulate the Brownian dynamics setup using the following scheme:

$$\begin{aligned} X_{t_{i+1}} &= X_{t_i} - \nabla_x F(X_{t_i}, \lambda_{t_i})\delta t/\epsilon + \sigma \mathcal{N}(0, dt) \\ X^j_{t_{i+1}} &= X^j_{t_i} - \nabla_x F(X^j_{t_i}, \lambda_{t_i})\delta t/\epsilon + \sigma \mathcal{N}(0, dt) \qquad j = 1, \ldots, M \\ \lambda_{t_{i+1}} &= \lambda_{t_i} + \left(-\frac{1}{\epsilon} \nabla_\lambda F(X_{t_i}, \lambda_{t_i}) + \frac{1}{\epsilon} approx\_int((X_{t_i}, \lambda_{t_i}))\right) \delta t \\ &\quad - \left(\nabla_\lambda C((X_{t_i}, \lambda_{t_i})) + \nabla_{\lambda x} F(X_{t_i}, \lambda_{t_i})\, (\nabla_{xx} F(X_{t_i}, \lambda_{t_i}))^{-1} \nabla_x C((X_{t_i}, \lambda_{t_i}))\right) \delta t + \sigma \mathcal{N}(0, dt). \end{aligned}$$

In the above scheme we define $approx\_int((X_{t_i}, \lambda_{t_i})) = \frac{1}{M} \sum_{j=1}^M \nabla_\lambda F(X^j_{t_i}, \lambda_{t_i}) \approx \int \nabla_\lambda F(x, \lambda_{t_i})\, \mu_t(dx \mid \lambda_{t_i})$.