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Exercise sheet #4

Numerics of stochastic differential equations

Wintersemester 2015/16

'A mathematician is a blind man in a dark room looking for a black cat which isn't there.'
Charles R. Darwin

Hand in until: Tuesday, 12th January, 10:15am

Exercise 1 [2 points]. (Continuous Semigroups I)
Consider a continuous-time Markov process $(X_t)_{t\geq 0}$ with semigroup $S_t : K \to K$ on a Banach space $(K, \|\cdot\|)$. Let L be its the infinitesimal that is defined by

$$Lf = \lim_{t\to 0} \frac{S_t f - f}{t}\,, \quad f \in K$$

assuming that the limit exists in $(K, \|\cdot\|)$.

Show that $LS_t = S_t L$.

Exercise 2 [2 points]. (Continuous Semigroups II)
Let $(X_t)_{t\geq 0}$ be a time-homogeneous, one-dimensional diffusion process with generator

$$L = \frac{a(x)}{2}\frac{\partial^2}{\partial x^2} + b(x)\frac{\partial}{\partial x}\,,$$

with the shorthand $a(x) = (\sigma(x))^2$.

Prove that

$$a(x) = \lim_{t\to 0} \frac{\mathbb{E}_x((X_t - x)^2)}{t}\,, \quad b(x) = \lim_{t\to 0} \frac{\mathbb{E}_x(X_t - x)}{t}\,,$$

where $\mathbb{E}_x(\cdot) = \mathbb{E}(\cdot|X_0 = x)$ denotes the expectation over all realizations of X_t starting at $X_0 = x$.

Exercise 3 [6 points]. (Committor probabilities)
Let $X_t = W_t + x$ be a one-dimensional Brownian motion starting at $X_0 = x$. Let $A = [a_1, a_2] \subset \mathbb{R}$ and $B = [b_1, b_2] \subset R$ with $b_1 > a_2$; further let $C = [a_2, b_1]$. Let τ_A and τ_B be the first hitting times of A and B, and define for any $x \in C$ the committor function as

$$q(x) = \mathbb{P}(\tau_A > \tau_B | X_0 = x).$$

(a) Show that the committor function solves the linear elliptic boundary value problem

$$\frac{1}{2}\Delta q = 0 \;\; \forall x \in C, \quad q|_A = 1, \quad q|_B = 0.$$

(b) Consider now a symmetric random walk $(Z_n)_{n\in\mathbb{N}_0}$ on a lattice with spacing Δz and transition probabilities $\mathbb{P}(Z_{n+1} = z \pm \Delta z | Z_n = z) = \frac{1}{2}$. Use the Markov property of Z_n to show that the committor probability q satisfies the discrete boundary value problem

$$\frac{1}{2}\Delta_d q = 0 \;\; \forall x \in C, \quad q|_A = 1, \quad q|_B = 0\,,$$

with suitable definitions of the sets A, B and C, and Δ_d being the finite-difference discretization of the Laplacian on the lattice with spacing Δz.

(c) Compare the results from (a) and (b), noting that $L_d = P - I$ is the generator of Z_n, with P denoting the transition matrix of the Markov chain. (*Hint:* finite difference approximation.)

Exercise 4 [6 points]. (Markov chain Monte Carlo)
Let $(X_t)_{t\geq 0}$ be an Itô process given by the SDE

$$dX_t = -\nabla V(X_t)dt + \sqrt{2\epsilon}dB_t \tag{1}$$

with $\epsilon > 0$ a real parameter, and the potential function $V(x) = (x^2 - 1)^2$.

(a) Compute the invariant density ρ_∞ up to the normalization constant.

(b) One way to sample ρ_∞ numerically is by using a long trajectory. The hope is that the system converges to ρ_∞ fast enough such that one eventually ends up sampling ρ_∞. We want to try this out. Numerically integrate (1) with $X_0 = -1$ using forward Euler for $\epsilon = 0.15$ with $\Delta t = 0.05$. Use $N = 10^4, 10^5$ and 10^6 steps. Create a histogram of all the positions visited and compare with (a), using a suitable norm or statistical distance such as the Kullback-Leibler divergence. What are the problems you observe? What happens if you change Δt?

(c) The Metropolis-Hastings algorithm can be used to sample distributions which are known up to their normalization constant. The algorithm creates a Markov chain $(X_n)_n$ which has the chosen distribution (here ρ_∞) as invariant distribution. It consists of two steps:

(i) Proposal step: Starting from X_n, create a new state $\tilde{X}_{n+1}$ drawn from some proposition density $T(X_n, \tilde{X}_{n+1})$.

(ii) Acceptance step: Compute the Metropolis-Hastings ratio

$$r(X_n, \tilde{X}_{n+1}) = \frac{T(\tilde{X}_{n+1}, X_n)\rho_\infty(\tilde{X}_{n+1})}{T(X_n, \tilde{X}_{n+1})\rho_\infty(X_n)}$$

and accept the proposition with probability $\min\Big(1, r(X_n, \tilde{X}_{n+1})\Big)$. In this case set $X_{n+1} = \tilde{X}_{n+1}$, otherwise $X_{n+1} = X_n$.

Implement the Metropolis-Hastings algorithm using the Euler discretization of (1) as the proposal step. Convince yourself that

$$\tilde{X}_{n+1} \sim \mathcal{N}\left(X_n - \Delta t \nabla V(X_n), 2\epsilon\Delta t\right)$$

and calculate $T(X_n, \tilde{X}_{n+1})$. Use the result of (a) for the computation of $r(X_n, \tilde{X}_{n+1})$. Use the same parameters as in (b) for the implementation. Create a histogram of the positions X_n and compare your results with (a) and (b). What do you observe? Use your algorithm to try out different values for Δt and try to find the optimal choice. What happens if Δt becomes either much larger or much smaller?

(d) Repeat (c), but this time use $\tilde{X}_{n+1} \sim \mathcal{N}(0, 0.5^2)$ for the proposal step.