Stochastic Modeling and Computations
Skolkovo Institute of Science and Technology — April 15, 2016
M. Chertkov, S. Belan, and V. Parfenyev

Problem Set II

This problem set is due by **Wed May 18**, 11:59 pm Moscow time.
Solutions should be turned in through the course web-site in an electronic format. Remember, your goal is to communicate. Full credit will be given only to the correct solution which is described clearly.

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1. **(25 points)** *Spanning Trees.*

   Problem 4. *Spanning Trees.* Let G be an undirected complete graph. A simple MCMC algorithm to sample uniformly from the set of spanning trees of G is as follows: Start with some spanning tree; add uniformly-at-random some edge from G (so that a cycle forms); remove uniformly-at-random some link from this cycle; repeat. Suppose now that the graph G is positively weighted, i.e., each edge e has some cost $c_e > 0$. Suggest an MCMC algorithm that samples from the set of spanning trees of G, with the probability proportional to the overall weight of the spanning for the following cases: (i) the weight of any sub-graph of G is the sum of costs of its edges; (ii) the weight of any sub-graph of G is the product of costs of its edges. In addition, (iii) estimate the average weight of a spanning tree using the algorithm of uniform sampling. Finally, (iv) implement all the algorithms on some small (but non-trivial) weighted graph of your choice. Verify that the algorithm converges to the right value.

2. **(10 points)** *Tree Learning.*

   The spanning-tree-structured graphical model consists of five nodes: x_1, x_2, x_3, x_4 and x_5. Mutual information for all pairs of nodes estimated empirically is

$$
\begin{aligned}
I(x_1, x_2) &= 0.55,\\
I(x_1, x_3) &= 0.34,\\
I(x_1, x_4) &= 0.11,\\
I(x_1, x_5) &= 0.59,\\
I(x_2, x_3) &= 0.68,\\
I(x_2, x_4) &= 0.03,\\
I(x_2, x_5) &= 0.25,\\
I(x_3, x_4) &= 0.01,\\
I(x_3, x_5) &= 0.22,\\
I(x_4, x_5) &= 0.10.
\end{aligned}
$$

   Reconstruct most probable tree spanning the nodes.

3. **(25 points)** *Elementary Diffusion.*

   Consider a particle jumping over nodes of the one-dimensional chain, where the states are labeled $n = 0, \pm 1, \pm 2, \ldots$. Left and right jumps are performed with the rates μ and λ respectively. Assume that at the moment of time $t = 0$ the particle was located at the node $n = 0$.

   (i) Using any programming language perform and illustrate a sample of a particle path/trajectory.

   (ii) Find $P(n, t)$ numerically, where $P(n, t)$ is the probability to observe a particle at the position n at the moment of time t. In order to simulate the particle motion split the time axis into discrete intervals and for any time step implement decision (on where to move next) according to the rates.

   (iii) Solve (ii) analytically by solving the master equation, which is stated in continuous time as follows (this is a discrete time analog of the Fokker-Planck equation),

$$\partial_t P(n,t) = -(\lambda + \mu) P(n,t) + \mu P(n+1,t) + \lambda P(n-1,t). \tag{1}$$

   (iv) Replace a discrete variable n in this equation by a continuous variable x. Under what assumptions can you do it? Solve the resulting (continuous time, continuous space) equation analytically and compare the result with the simulations performed in (ii). (*Hint:* if $\lambda = \mu$ then the right-hand side is just $\lambda \partial_x^2 P(x,t)$.)

   (v) For the original case of discrete space and setting $\lambda = 0$, solve the problem exactly. Compare the solution with (proper version of) the simulations performed in (ii).

4. **(30 points)** *Mortal Brownian Particle.*

   Unstable Brownian particle moves within the interval $0 < x < L$ between two absorbing walls starting from the initial position x_0. The decay (mortality) rate of the particle is α and the diffusion coefficient is D.

   (i) Calculate the survival probability $p(t)$ of the particle analytically.

   (ii) Find the expected lifetime of the particle analytically and by direct numerical simulations for $L = 1$, $x_0 = 0.5$, $D = 1$ and $\alpha = 1$.

   (iii) Assume that $x_0 = L/2$. What is the probability that the particle will be absorbed before it decays? Answer this question analytically or numerically.

   (iv) Find analytically the probability that the particle will be absorbed at the left wall.

   (*Hint:* The probability distribution of an unstable Brownian particle is described by the equation, $\partial_t n = D\partial_x^2 n - \alpha n$.)