

# CS-E5795 Computational Methods in Stochastics

## Exam 11.12.2023

Basic function calculator is allowed.

1. The probability density function (PDF) for bacteria to die at time  $t$  is that of the exponential distribution  $f_T(t) = \lambda e^{-\lambda t}$ , where  $t \geq 0$  and  $\lambda > 0$ .

a) (3 p) If  $T$  is the expected lifetime of a unit (some constant number) of bacteria, then the probability that a unit has survived up to time  $t$  is  $\Pr\{T > t\} = 1 - F_T(t)$ , where  $F_T(t)$  is the cumulative distribution function (CDF). Derive the conditional distribution of the remaining lifetime  $\Pr\{T - t > x | T > t\}$  of units, that is, the probability of a unit to survive a further time  $x > 0$ . Based on the result, does this process have memory?

b) (3 p) Derive and describe how you would simulate event times of bacterial deaths having the above PDF  $f_T(t) = \lambda e^{-\lambda t}$  by using the inverse transformation/distribution method. In what order does this method give event times?

2.

a) (3 p) Derive/describe the very short procedure of sampling from a bivariate density  $\pi(x, y)$  that is the basis for Gibbs sampling. Justify the steps.

b) (3 p) The probability density function  $\pi(\cdot)$  for states  $x$  and  $y \in S$  is stationary. Write down the detailed balance condition between  $x$  and  $y$ .

If the potential energy of state  $x$  is greater than the potential energy of state  $y$ ,  $E(x) > E(y)$ , what can you say about  $\pi(x)$  and  $\pi(y)$ ? Can reversibility and/or detailed balance hold in this case?

3.

a) (1 p) You know the transition matrix  $P(t)$  for a Markov chain in discrete space and continuous time  $t$ . How do you compute  $P(t + t')$ ?

b) (1 p) What is the initial condition (at  $t = 0$ ) for this transition matrix?

c) (2 p) The defining equation for the Markov chain in discrete space and continuous time  $t$  is given by  $\frac{dP(t)}{dt}$ , in which the transition matrix for hazards  $Q = \frac{d}{dt} P(t)|_{t=0} = \frac{P(t+dt) - P(t)}{dt}|_{t=0}$  is used. Either derive this  $\frac{dP(t)}{dt}$  or write it down with a statement on why, given the definition of  $Q$ , it has to be of this form - one of the two suffices.

d) (2 p) A Markov chain  $X_0, X_1, X_2, X_3, \dots, X_n, \dots$  has the transition probability matrix

$$P = \begin{bmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{bmatrix}.$$

The states are labelled as  $S = \{0, 1, 2\}$ .

What is the probability distribution of the values of  $X_2$  under the condition that  $X_0 = 1$ ?

4.

a) (3 p) Describe with equations and diagrams in phase space coordinates the two steps comprising Hamiltonian Monte Carlo (HMC) method. When appropriate, explain reasons for the details in the procedure? What is the motivation for using HMC? (Do not include implementation of boundary conditions in your explanation.)

b) (3 p) What is the potential function  $U(q)$  to be used in the Hamiltonian Monte Carlo (HMC) method for simulating the Weibull distribution, whose probability density function is

$$f(q) = \begin{cases} \alpha \beta^{-\alpha} q^{\alpha-1} e^{-\left(\frac{q}{\beta}\right)^\alpha} & \text{if } q > 0 \\ 0 & \text{otherwise} \end{cases}$$

Here,  $\alpha > 0$  and  $\beta > 0$ . Give the potential also in the minimal form for using in HMC. Justify this minimal form.