Elementary modeling of a Markov process

The goal of this project is to model so-called Markov jump processes, widely used in population dynamics, chemical kinetics, theory of radioactive decay, etc. These processes describe systems with discrete states (e.g. given by a number of particles of a given type), with stochastic transitions between these states (see https://en.wikipedia.org/wiki/Markov_chain). The transitions do not depend on the past, but just on the present configuration, and are described through rates. The simplest Markov process is the Poisson process, where at a given rate r particles of type A are added to the system. This means that during small time interval Δt , the probability that a particle will be added is $r\Delta t$. From the theory of Markov processes it follows that the time intervals between the events of adding a particle $\tau = t_{i+1} - t_i$ are distributed according to the exponential distribution with density

$$w(\tau) = re^{-r\tau}$$

If the number of particle is N, then at the transition $N \to N+1$. If one neglects fluctuations, the mean number of particles grows deterministically via mean-field equations

$$\frac{dN}{dt} = r .$$

More complex processes are the birth and death processes, where each existing particle can produce a new one with rate r_b , or disappear with rate r_d . Because the particles are independent, the transition can happen with any of them, and the rates of transitions $N \to N+1$ and $N \to N-1$ are $r_b N$ and $r_d N$, respectively. The mean-field equations are

$$\frac{dN}{dt} = r_b N, \qquad \frac{dN}{dt} = -r_d N$$

To describe a saturation of the population growth, one uses a logistic (Verhulst) nonlinear mean-field equation

$$\frac{dN}{dt} = r_b N - r_{nl} N^2$$

which can be considered as a superposition of a linear birth process and of a nonlinear death process.

To model a superposition of elementary Markov processes, one uses **the Gllespie algorithm** https://en.wikipedia.org/wiki/Gillespie_algorithm. This algorithm is based on the fact, that for a superposition of several processes with rates r_1, r_2, \ldots, r_n the time between the events is a random variable distributed exponentially with rate $r = \sum_{k=1}^{n} r_k$. Which of n events happens, can be modeled by choosing a discrete random number p out of n possibilities having probabilities $\frac{r_1}{r}, \frac{r_2}{r}, \ldots, \frac{r_n}{r}$.

Below you have to model several Markov processes with Gillespie algorithm, and compare the results to mean-field equations.

Task 1: Model a death process $A \xrightarrow{r} \emptyset$ with initial number of particles N(0) = 20 and rate r = 0.1. Present several sample realization of the Markov process; calculate the average $\langle N(t) \rangle$ and the standard deviation.

Task 2: Model the gene expression for a single cell. The mean field equations read [M. Scott, Tutorial: Genetic circuits and noise, http://www.math.uwaterloo.ca/~mscott/NoiseTutorial.pdf.]

$$\frac{dM}{dt} = \lambda_m - d_m M$$
$$\frac{dP}{dt} = \lambda_p M - d_p P$$

for $\lambda_m = 1$, $\lambda_p = 1$, $d_m = 0.2$, $d_p = 0.02$.

Find the equilibrium distribution density of P and compare with to theoretical approximate prediction

$$w(P) \approx \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(P - \langle P \rangle)^2}{2\sigma^2}\right]$$

where $\langle P \rangle = \frac{\lambda_m \lambda_p}{d_m d_p}$ and $\sigma^2 = \langle P \rangle (1 + \frac{\lambda_p}{d_m + d_p})$. Plot the density in normal and logarithmic scales. Calculate the skewness and the kurtosis of the distribution.

Task 3: Model of extinction in the logistic (Verhulst) process.

$$\frac{dN}{dt} = \lambda N - dN^2$$

for $\lambda = 1, d = 0.1$.

Here the mean level of the population is $N_0 = \frac{\lambda}{d}$, but there are stochastic deviations. If at some time N = 0, the population extincts, but for large \hat{N} this is rather unprobable.

Find a dependence of the mean extinction time starting from $N(0) = N_0 = \lambda/d$ on the values of N_0 (vary these in the interval $10 \le N_0 \le 20$).

Task 4: SIR model of epidemic spreading. Here there are 3 types of individuals: S - susceptible, I - infected, R - recovered. The rate of infection is proportional to the probability of S and I to meet, i.e. to SI. The rate of recovering is constant. One neglects all other processes like death rate etc. The mean-field equations are

$$\frac{dS}{dt} = -bSI$$

$$\frac{dI}{dt} = bSI - cI$$

$$\frac{dR}{dt} = cI$$

Elementary events here is infection, at which $S \to S - 1$, $I \to I + 1$; and recovery at which $I \to I - 1$, $R \to R + 1$. The epidemic ends when I = 0.

4.1: Solve mean-field equations for b = 0.02 and c = 0.3, starting from S = 30, I = 1, R = 0. Find the state at $t \to \infty$, which gives an average number of totally infected persons.

4.2 Apply the Gillespie method, simulate epidemic spreading as a stochastic process, and find a distribution of overall infected persons during the epidemic for S = 30, I = 1, R = 0.