Exercise 3

If you have questions or need suggestions: donati[at]zib.de

Master equation of a pure birth process

Consider a population of n individuals that can increase by one individual at a rate of μ:

$$n \xrightarrow{\mu} n+1\,. \tag{1}$$

The *transition rate* μ (units [time^{-1}]) represents the probability that an event occurs in an infinitesimal timestep, then the *transition probability* (unit less) in a timestep Δt is defined as

$$P(n+1,\, t+\Delta t|\, n,\, t) = \mu\Delta t\,. \tag{2}$$

The probability $P(n, t+\Delta t)$ to have n individuals at time $t+\Delta t$ is given by the sum of

- the probability there were $n-1$ individuals at time t, times the probability to increase the population by one in Δt (eq. 2):
$$P(n-1,t)\cdot \mu\Delta t\,,$$
- the probability there were n individuals at time t, times the transition probability that no increase will occur:
$$P(n,t)\cdot (1-\mu\Delta t)\,.$$

Then

$$P(n,t+\Delta t) = P(n-1,t)\cdot \mu\Delta t + P(n,t)\cdot(1-\mu\Delta t)\,. \tag{3}$$

Rearranging eq. 3 and taking the limit $\Delta t \to 0$ yields the *master equation*

$$\boxed{\frac{\partial P(n,t)}{\partial t} = \mu P(n-1,t) - \mu P(n,t)} \tag{4}$$

The solution of eq. 4 is the Poisson distribution

$$P(n,t) = \frac{1}{n!}(\mu t)^n e^{-\mu t} \tag{5}$$

Pen-and-paper exercise

- Derive the solution defined in eq. 5 of the master equation eq. 4.

  Hint: Use the probability generating function

  $$G(z,t) = \sum_{n=0}^{\infty} z^n \cdot P(n,t)\,, \tag{6}$$

  where z is a complex number.

Computational exercise Simulate the pure birth process using the following algorithms.

- *Time-driven simulation.* In a time-driven simulation, the timeline is discretized in equal timesteps Δt, then at each time step, we calculate the probability that an event occurs.
  1. Define a timestep such that $\mu\Delta t < 1$ and set a certain number of timesteps N_{steps}.
  2. Define an array n with N_{steps} entries to save the time evolution of the population.
  3. Initialize a for-loop over time t.

4. At each timestep draw a random number u from a uniform distribution $\mathcal{U}(0,1)$, then upate the population array:

$$n[t+1] = \begin{cases} n[t]+1 & \text{if } u < \mu\Delta t \\ n[t] & \text{else} \end{cases} . \tag{7}$$

Set $\mu = 0.5$ and generate an ensemble of 5000 trajectories of length 50000 timesteps. Build the distribution at specific timesteps (i.e. build the histogram) and compare with the exact solution defined in eq. 5.

- *Event-driven event simulation.* In an event-driven simulation, the simulation runs from event to event, and then the timeline is not uniformly discretized. In other words, instead of calculating the probability of an event occurring within a given timestep, we calculate how much time elapses between one event and the next. For this purpose, we implement the Gillespie algorithm.

  1. Define a certain number of timesteps N_{steps}.
  2. Define an array t with N_{steps} entries to save the evolution of the timeline.
  3. Define an array n with N_{steps} entries to save the time evolution of the population.
  4. Assume the system starts at time $t[0] = 0$.
  5. Initialize a for-loop over the index k.
  6. Draw a random number τ from the distribution $P(\tau) = \mu \exp(-\mu\tau)\tau$. For this purpose, draw a random number u from the uniform distribution $\mathcal{U}(0,1)$, then calculate

  $$\tau = -\frac{\log(u)}{\mu} .$$

  7. Update the array $t[k+1] = t[k] + \tau$.
  8. Update the array $n[k+1] = n[k] + 1$

  Set $\mu = 0.5$ and generate an ensemble of 5000 trajectories of length 50 timesteps. Build the distribution at specific timesteps (i.e. build the histogram) and compare with the exact solution defined in eq. 5.