

Summary of the Gillespie algorithm

The Gillespie algorithm [1] provides a way of mimicking the dynamics of a system of reactants by, in a recursive manner, defining all currently possible processes in it as so-called reactions, and then executing a single reaction selected from the set of reactions. Each reaction corresponds not to a type of process but indeed to a unique process. For example, in a system containing identical molecules which may each spontaneously undergo a certain type of chemical reaction, each individual molecule has its own reaction associated to it within the scope of the Gillespie algorithm. The selection of the executed reaction is random, and the probability of being selected varies for each reaction. After a reaction has been executed, others may become impossible or new ones may need to be considered, and hence both the set of reactions and their probabilities need to be updated after each reaction step. The picking likelihood, so-called propensity, of each reaction is the main influence on the behavior of the system and is a property that depends on kinetic parameters as well as underlying system mechanisms. It can be thought of as an average frequency at which the reaction happens per unit time. The propensities of the reactions within the system are also key to determine the duration of the simulated reactions. More precisely, for each step this time value is picked randomly from an exponential distribution between 0 and infinity, the average of which corresponds to the inverse of the sum of all reaction propensities currently in the system (see Figure 1). As a result, on average the time picked, i.e. the duration of the reaction, decreases as the propensity sum increases and vice versa. By formulating the dynamics in this fashion, we may mimic the situation in a real system, where a large number of reactions corresponds to a high concentration of reactants, and the resulting time between reactions turns out to be small due to the high frequency of reactant encounters. Conversely, a small number of reactions corresponds to a small number of reactants and long times between individual reactant encounters. The algorithm proceeds recursively in reaction picking and time calculation until there are no reactions left to pick from, at which point the propensity sum is 0, and the average time for a next reaction to take place approaches infinity. This mimics the situation in a system in which everything that can happen has happened, and the system state remains constant for an infinite amount of time. This procedure, common to any simulation using a Gillespie algorithm, is summarized below:

- 1) Calculate the propensity sum a from the individual propensities of all N reactions currently in the system:

$$a = \sum_{i=1}^N a_i. \quad (1)$$

- 2) Generate a random number r_1 from a uniform distribution between 0 and a .
- 3) Pick the reaction to be executed in the current step by finding the number j for which the following equation holds:

$$\sum_{i=1}^j a_i \leq r_1 < \sum_{i=1}^{j+1} a_i. \quad (2)$$

- 4) Generate a random number r_2 from a uniform distribution between 0 and 1.
- 5) Transform r_2 such that it represents a number drawn from an exponential distribution between 0 and infinity whose average is $\frac{1}{a}$. To do so, calculate the duration of the step τ via

$$\tau = \frac{1}{a} \ln\left(\frac{1}{r_2}\right). \quad (3)$$

- 6) Execute the reaction and update the table of reactions.

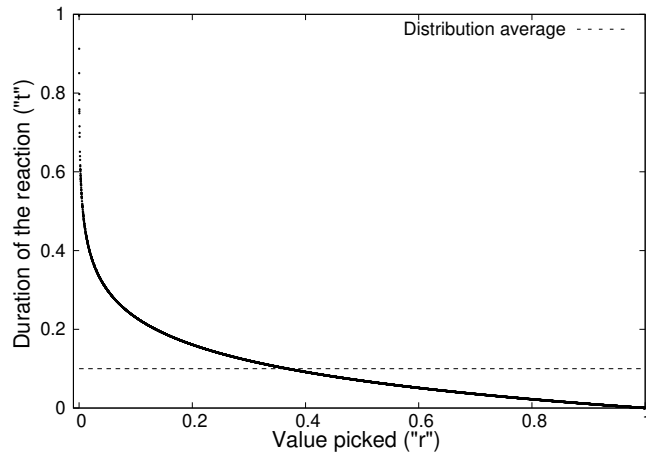


Figure 1: Visualization of a transformation applied to random numbers ("r") picked from a uniform distribution between 0 and 1. The transformation $t(r) = \frac{1}{a} \ln(\frac{1}{r})$ was applied to each "r" picked, with $\frac{1}{a} = 0.1$, leading to the "t" values following an exponential distribution between 0 and $+\infty$ whose average value is equal to $\frac{1}{a}$. 10 000 values are represented.

- 7) Repeat from 1) until the propensity sum a reaches 0 or the simulation time reaches a specified limit.

References

- [1] D. T. Gillespie, "A general method for numerically simulating the stochastic time evolution of coupled chemical reactions," *Journal of Computational Physics*, vol. 22, no. 4, pp. 403 – 434, 1976.