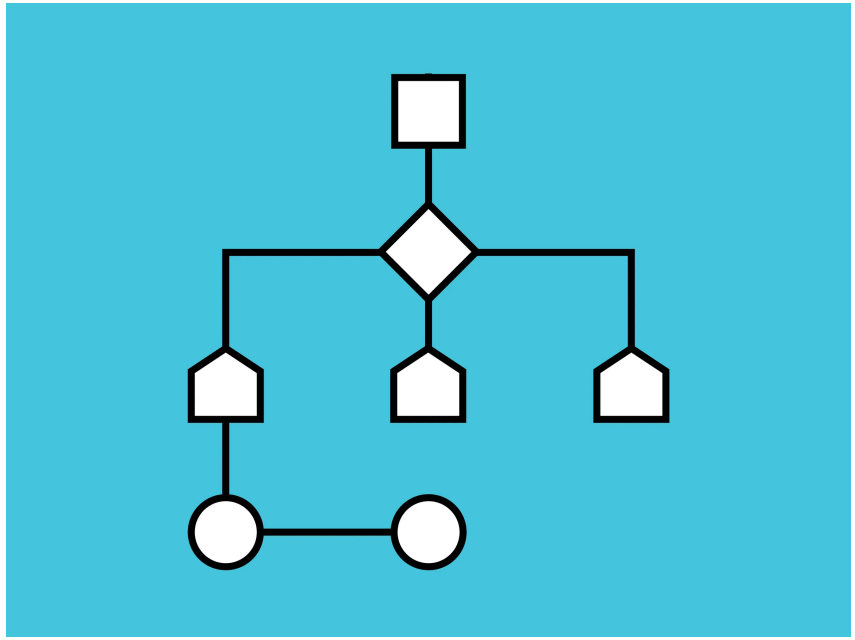
How to derive the Gillespie algorithm



How are stochastic algorithms constructed?

From the master equation / Kolmogorov forward equation ?

- $p_{ij}(t) = P(X(t) = j \mid X(0) = i)$ transition probabilities.
- $P(t) = \left(p_{ij}(t)\right)$

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$a_i\, dt$ = the probability that the reaction i will occur in the infinitesimal time interval $(t, t + dt)$

where $a_i(\boldsymbol{x})$ is the total rate (or the propensity) of the reaction i

Rejection sampling algorithm

Most straightforward method.

1. Discretize the time-axis in small enough time-steps Δt.
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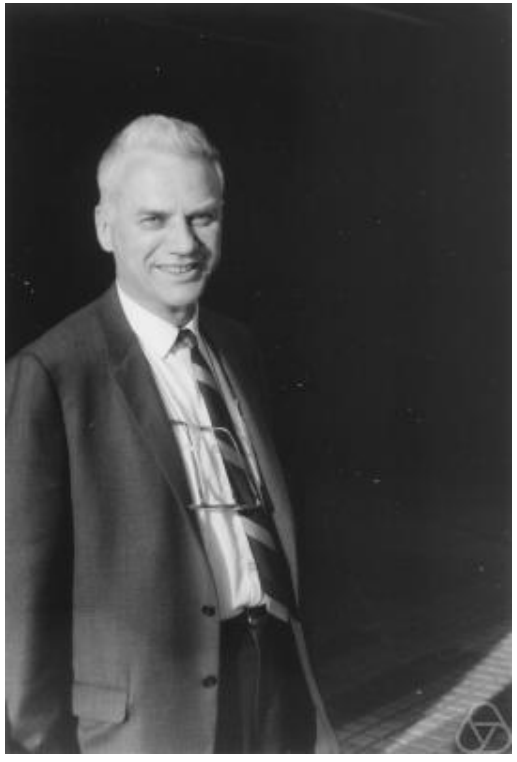
1. **When does the next reaction occur?**
2. **Which reaction occurs next?**

The Doob-Gillespie algorithm

Joseph L. Doob (1942 and 1945)



First implementation

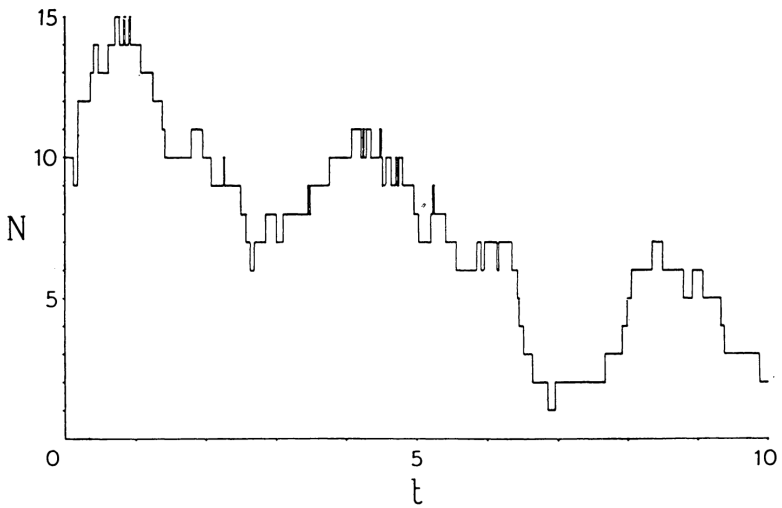
An Artificial Realization of a Simple "Birth-and-Death" Process

By David G. Kendall

Magdalen College, Oxford

[Received November 1st, 1949]

Manchester Mark 1



The graph shows the variation with time (t) in the number of individuals (N) in an artificial population developing in accordance with the simple birth-and-death process ($\lambda = \mu = \frac{1}{2}$).

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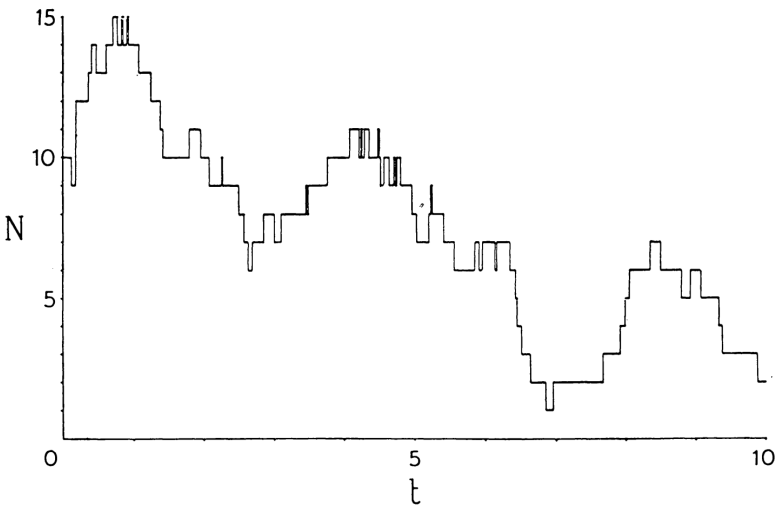

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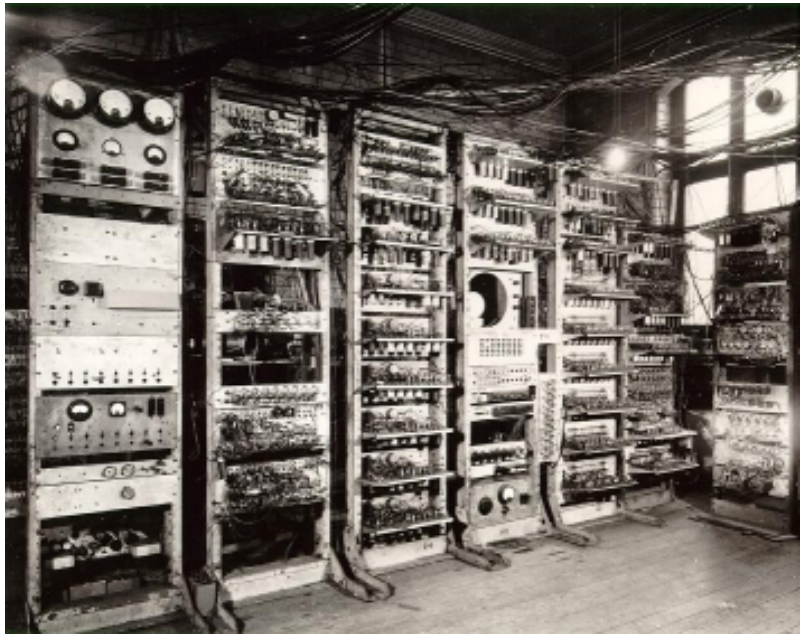

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A General Method for Numerically Simulating the Stochastic Time Evolution of Coupled Chemical Reactions

DANIEL T. GILLESPIE

Research Department, Naval Weapons Center, China Lake, California 93555

Received January 27, 1976; revised April 21, 1976

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$$p(\tau, i) = a_0 e^{-a_0\tau} \times \frac{a_i}{a_0}$$

$$p(\tau, i) = p(\tau) \times p(i \mid \tau)$$

Sampling τ and i

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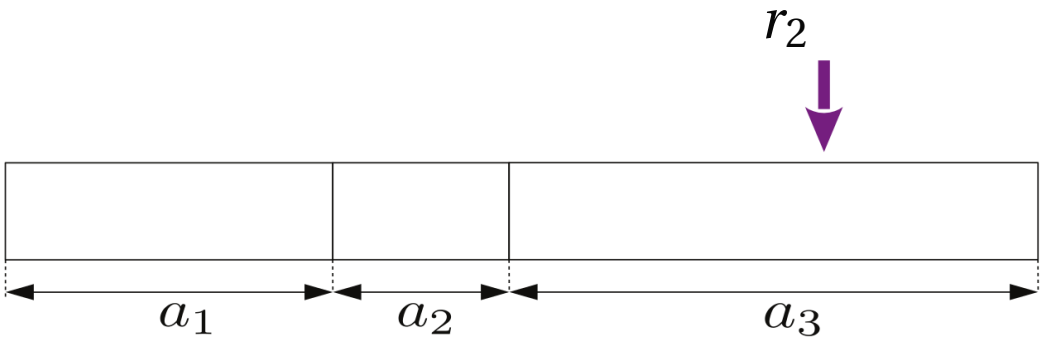
- draw a reaction i in a discrete distribution for which $P(X = i) = \frac{a_i}{a_0}$.



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6. Save $(\boldsymbol{x}, t)$ as desired and return to Step 1, or else end the simulation

An alternative: the First-Reaction Method

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One can prove that the joint probability $p(\tau, i)$ which is generated by this method is the one we want:

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⚠The first reaction might change the propensities a_i of other reactions making previous calculations obsolete.