Gillespie Algorithm: Key Formulas and Concepts

1. Purpose of the Gillespie Algorithm

The Gillespie algorithm simulates the stochastic time evolution of chemical reactions, especially in systems where molecule counts are low and fluctuations are significant. It avoids deterministic differential equations and instead models reaction events as probabilistic, discrete events.

2. Key Definitions

- Propensity (a_i): Probability per unit time that a given reaction i will occur.
- Total Propensity (a_0): Sum of all individual propensities.

   a_0 = sum of all a_i

3. Role of Random Numbers

Two uniform random numbers r1 and r2 in (0, 1) are used per step:
- r1 determines the time until the next reaction (tau).
- r2 determines which reaction occurs.

4. Formula for Time to Next Reaction

The time tau until the next reaction is drawn from an exponential distribution:

   $tau = (1 / a_0) * \ln(1 / r1)$

This is derived using inverse transform sampling on the exponential distribution.

5. Reaction Selection Rule

The reaction index j is chosen such that:

   sum of a_i (up to j-1) < r2 * a_0 <= sum of a_i (up to j)

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This ensures a reaction is chosen according to its relative probability.

6. Summary of Gillespie Steps

1. Compute all propensities a_i and total a_0.

2. Generate r1 and r2 in (0,1).

3. Compute time to next reaction:

    tau = (1 / a_0) * ln(1 / r1)

4. Select reaction j such that:

    sum of a_i < r2 * a_0 <= sum of a_i

5. Update system state and advance time by tau.