Statistical physics

lecture 14

Szymon Stoma

01-02-2010

$$G(s,t) = \left(1 - (1-s)e^{-kt}\right)^{n_0}$$

$$G(s,t) = \left((1 - e^{-kt}) + se^{-kt}\right)^{n_0}$$

$$G(s,t) = (q + s(1-q))^{n_0}$$

$$G(s,t) = \sum_{n=0}^{n_0} \binom{n_0}{n} q^{n_0-n} \left[s(1-q)\right]^n$$

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$$\textbf{\textit{A Simple Example}}:\quad S_1 \xrightarrow{c_1} 0\,.$$

$$a_1(x_1) = c_1 x_1,\quad \nu_1 = -1.\ \text{Take } X_1(0) = x_1^0\,.$$

RRE: $\dfrac{dX_1(t)}{dt} = -c_1 X_1(t)$. Solution is $X_1(t) = x_1^0\, \mathrm{e}^{-c_1 t}$.

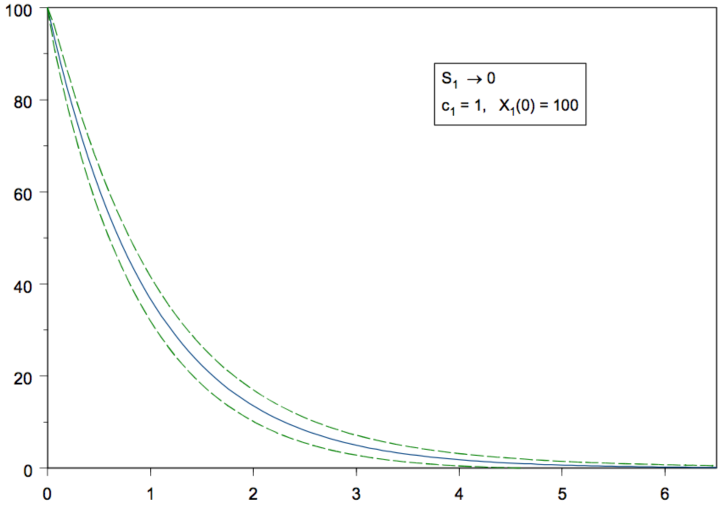
CME: $\dfrac{\partial P(x_1,t\,|\,x_1^0,0)}{\partial t} = c_1\Big[(x_1+1)P(x_1+1,t\,|\,x_1^0,0) - x_1 P(x_1,t\,|\,x_1^0,0)\Big]$.

Solution: $P(x_1,t\,|\,x_1^0,0) = \dfrac{x_1^0\,!}{x_1!\,(x_1^0 - x_1)!}\, \mathrm{e}^{-c_1 x_1 t}\left(1-\mathrm{e}^{-c_1 t}\right)^{x_1^0 - x_1}\quad (x_1 = 0,1,\ldots,x_1^0)$

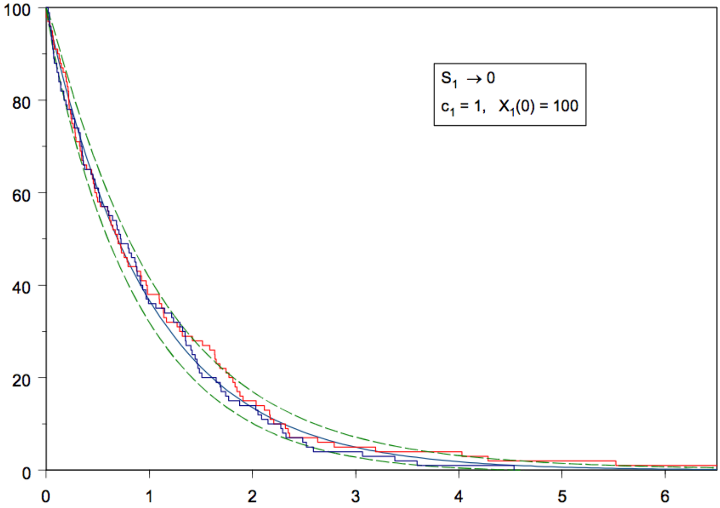
which implies $\langle X_1(t)\rangle = x_1^0\,\mathrm{e}^{-c_1 t}$, $\mathrm{sdev}\{X_1(t)\} = \sqrt{x_1^0\,\mathrm{e}^{-c_1 t}\left(1-\mathrm{e}^{-c_1 t}\right)}$.

SSA: Given $X_1(t) = x_1$, generate $\tau = \dfrac{1}{c_1 x_1}\ln\left(\dfrac{1}{r}\right)$, then update:

$$t \leftarrow t + \tau,\quad x_1 \leftarrow x_1 - 1\,.$$



$S_1 \to 0$
$c_1 = 1, \quad X_1(0) = 100$
100
80
60
40
20
0
0
1
2
3
4
5
6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Problem - dimerization kinetics in a bacteria cell:

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\begin{aligned}
R_1, k_1 : 2P &\rightarrow P_2 \\
R_2, k_2 : P_2 &\rightarrow 2P
\end{aligned}
$$

Solution:

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\begin{aligned}
\frac{dP}{dt} &= 2k_2 P_2 - k_1 PP \\
\frac{dP_2}{dt} &= k1PP - 2k_2 P_2
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We can use this system to build a conversation equation:

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\frac{dP}{dt} + 2\frac{d2P}{dt} &= 0 \\
\Longrightarrow \frac{d(P + 2P_2)}{dt} &= 0 \\
\Longrightarrow P + 2P_2 &= c
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,where c will be initial concentration.

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$$\frac{dP}{dt} = 2k_2P_2 - k_1PP$$
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So we can convert this system into one equation by assuming $P_2 = (c - P)/2$:

$$\frac{dP}{dt} = k_2(c - P) - k_1PP$$

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Size of the E.coli:

- rod shaped, $l = 2\mu m$ long, $r = 0.5\mu m$ of diameter
- $V = \pi r^2 l = \pi \left(0.5 \times 10^{-6}\right)^2 2 \times 10^{-6} m^3$
- $V = \pi/2 \times 10^{-18} m^3$
- $V = \pi/2 \times 10^{-15} dm^3$

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We need to assume something about the dimensions:

- Initial concentration of P is $0.5 \mu mol\ dm^{-3} = 5 \times 10^{-7} mol\ dm^{-3}$
- Volume of a bacteria $V = 10^{-15} dm^3$
- $k_1 = 5 \times 10^5$
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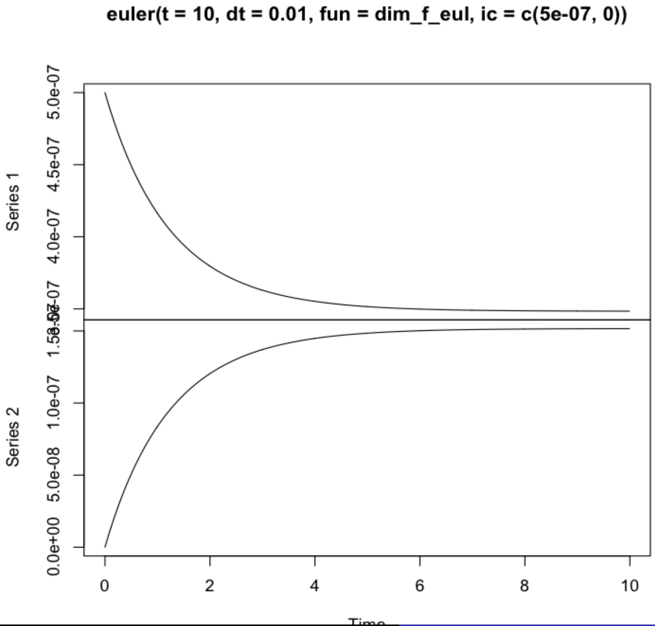
euler(t = 10, dt = 0.01, fun = dim_f_eul, ic = c(5e-07, 0))
Series 1
Series 2
5.0e-07
4.5e-07
4.0e-07
1.0e-07
5.0e-08
0.0e+00
0
2
4
6
8
10
Time

How about stochastical simulations?

$$\emptyset \longrightarrow S$$

- deterministic rate law: k
- for a volume V, $kn_A V$ molecules/second
- stochastic rate law: c
- $c = kn_A V$

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$$S \rightarrow ?$$

- deterministic rate law: $k[S]$
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$$S + R \rightarrow ?$$

- deterministic rate law: $k[S][R]$
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To perform a stochastical simulation we need to switch from concentrations:

- $\bar{P} = PVn_A = 5 \times 10^{-7} mol\, dm^{-3} \times 10^{-15} dm^3 = 5 \times 10^{-22} \times 6.0221367 \times 10^{23} = 301$
- $c_1 = 2k_1/(n_A V) = 2 \times (5 \times 10^5)/(6.0221367 \times 10^{-7}) = 1.66 \times 10^{-3}$
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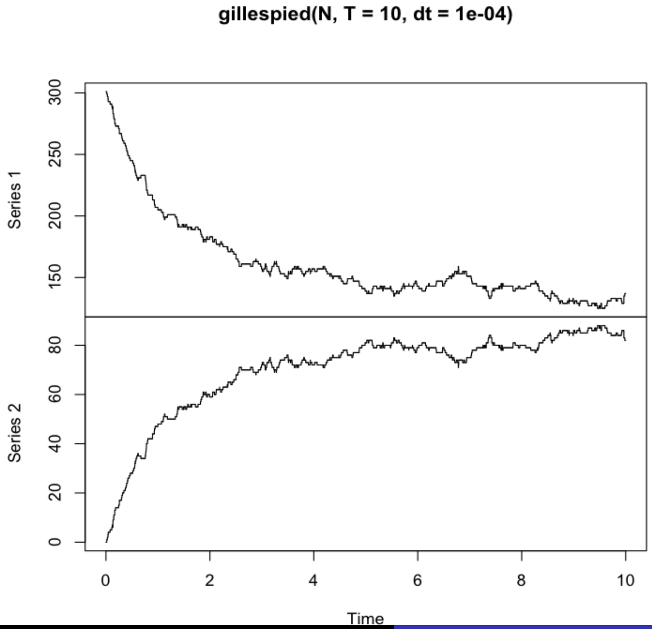
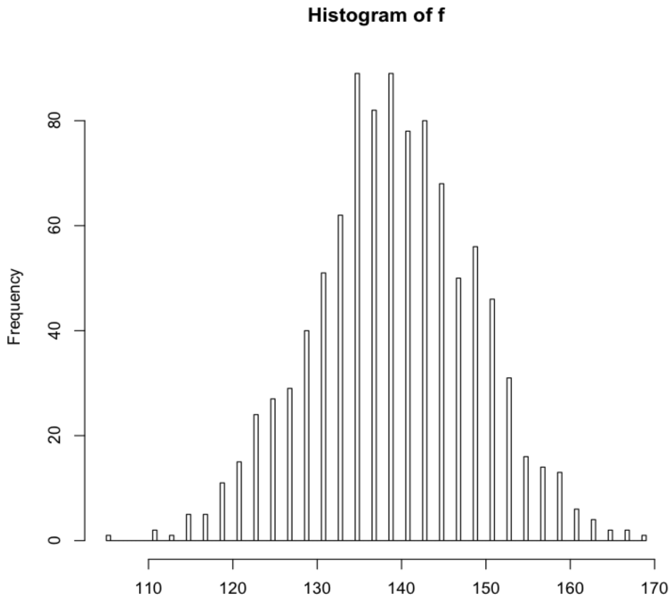
Gillespie algorithm

1. Initialize the system at $t = 0$ with rates $c_1, \ldots, c_m$ and initial numbers of molecules $x_1, \ldots, x_n$
2. For each $i = 1, \ldots, m$ calculate $h_i(x, c_i)$
3. Calculate $h_0(x, c) = \sum_{i=1}^{m} h_i(x, c_i)$, a combined reaction hazard
4. Sample a time for the next event dt from $Exp(h_0(x, c))$
5. $t = t + dt$
6. Sample the reaction index i from the discrete random variable with prob. $h_i(x, c_i)/h_0(x, c), i = 1, \ldots, m$
7. Update x according to the reaction R_i
8. If $t < t_{max}$ goto 2

Example

$$N = (Pr, T, Pre, Post, M, R),\ Pr = (P, P_2)',$$
$$T = (Dimer, UnDimer), Pre = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, Post = \begin{pmatrix} 0 & 1 \\ 2 & 0 \end{pmatrix}, R =$$
$$(c_1 y_1 (y_1 - 1)/2, c_2 y_2)', M = (301, 0)', c = (1, 0.2)'$$


gillespied(N, T = 10, dt = 1e-04)
Series 1
300
250
200
150
Series 2
80
60
40
20
0
0
2
4
6
8
10
Time


Histogram of f
Frequency
0
20
40
60
80
110
120
130
140
150
160
170

A word about parameter estimation