Symbolic-numeric approach for the investigation of kinetic models

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Chemical kinetics equations

Chemical kinetics equations

$$N_a^A X^a \underset{k_A^-}{\overset{k_A^+}{\rightleftarrows}} M_a^A X^a$$

$A = \overline{1,m}$, $a = \overline{1,n}$, M_a^A, N_a^A – the number of components of type X^a in the left and right sides, respectively.

$$s_A^+ = k^+ \prod_a x^{a\,N_a}$$

$$s_A^- = k^- \prod_a x^{a\,M_a}$$

x^a – the substance concentration X^a

Master equation

$$\partial_t p(\mathsf{x}, t) = \sum_A [(s_A^-(\mathsf{x} + r^A) P(\mathsf{x} + r^A, t) - s_A^+(\mathsf{x}) P(\mathsf{x}, t)) +$$

$$+ (s_A^+(\mathsf{x} - r^A) P(\mathsf{x} - r^A, t) - s_A^-(\mathsf{x}) P(x, t))],$$

$$\mathsf{r}^A = \mathsf{M}^A - \mathsf{N}^A$$

$$\mathsf{x} = (x_1, x_2, \dots, x^n)^T$$

$$\partial_t p(\mathsf{x},t) = \sum_A [\sum_j (\frac{(r^A \nabla)^j}{j!} s_A^-(\mathsf{x}) P(\mathsf{x},t)) +$$

$$+ \sum_j (\frac{(-r^A \nabla)^j}{j!} s_A^+(\mathsf{x}) P(\mathsf{x},t))].$$

$$\partial_t p(\mathsf{x}, t) = -\partial_a [A^a(\mathsf{x}) p(\mathsf{x}, t)] + \frac{1}{2} \partial_a \partial_b [B^{ab}(\mathsf{x}) p(X, t)], a = \overline{1, n}, b = \overline{1, n},$$

where

$$A^a(\mathsf{x}) = r_a^A [s_A^+(\mathsf{x}) - s_A^-(\mathsf{x})],$$

$$B^{ab}(\mathsf{x}) = r_a^A r_b^A [s_A^+(\mathsf{x}) - s_A^-(\mathsf{x})].$$

$$\mathrm{d}\mathsf{x} = \mathsf{a}(\mathsf{x})\mathrm{d}t + \mathsf{b}(\mathsf{x})\mathrm{d}\mathsf{W},$$

where W – n-dimensional Wiener process, the coefficient a corresponds to the coefficient A, $\mathsf{B} = \mathsf{b}\mathsf{b}^T$

Differential equation system:

$$\frac{\mathrm{d}\mathsf{x}}{\mathrm{d}t} = r_a^A[s_A^+(x) - s_A^-(x)].$$

$$X \xrightarrow{k_1} 2X$$
$$X \xrightarrow{k_2} 0$$

$$r^1 = 1, \quad r^2 = -1.$$

$$s_1^+ = k_1^+ x,$$
$$s_2^+ = k_2^+ x.$$

$$A(x) = r^1 s_1^+ + r^2 s_2^+ = k_1^+ x - k_2^+ x = (k_1 - k_2)x$$

$$B(x) = r^1(r^1)s_1^+ + r^2(r^2)s_2^+ = (k_1 + k_2)x$$

$$\mathrm{d}x = (k_1 - k_2)x\mathrm{d}t + \sqrt{(k_1 + k_2)x}\mathrm{d}W$$

Malthusian growth model (simple exponential growth mode)

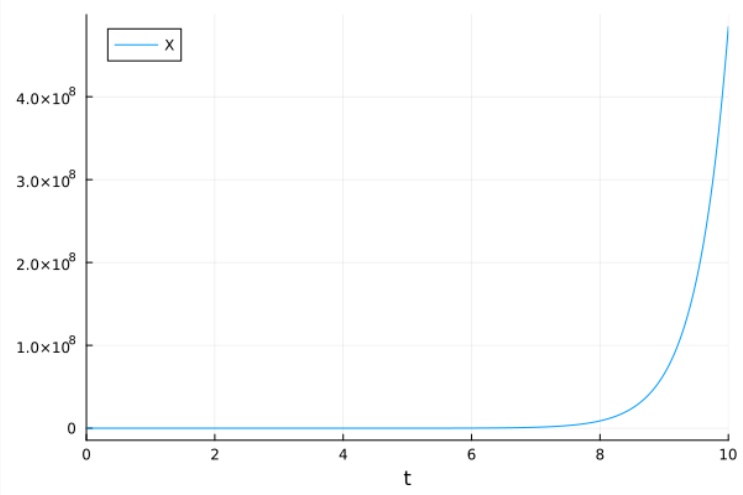

Рис. 1: Malthusian growth model, where $k_1 = 5.0, k_2 = 3.0$

$$X \overset{k_1^+}{\to} 2X$$

$$X + X \overset{k_2^+}{\to} X$$

$$r^1 = 1, \quad r^2 = -1$$

$$s_1^+ = k_1^+ x^1,$$

$$s_2^+ = k_2^+ x^2,$$

$$A(x) = r^1 s_1^+ + r^2 s_2^+ = k_1^+ x - k_2^+ x^2$$

$$B(x) = r^1 (r^1)^T s_1^+ + r^2 (r^2)^T s_2^+ = k_1^+ x + k_2^+ x^2$$

$$\mathrm{d}x = (k_1^+ x - k_2^+ x^2)\mathrm{d}t + \sqrt{(k_1^+ x - k_2^+ x^2)}\mathrm{d}W$$

Verhulst's logistic curve

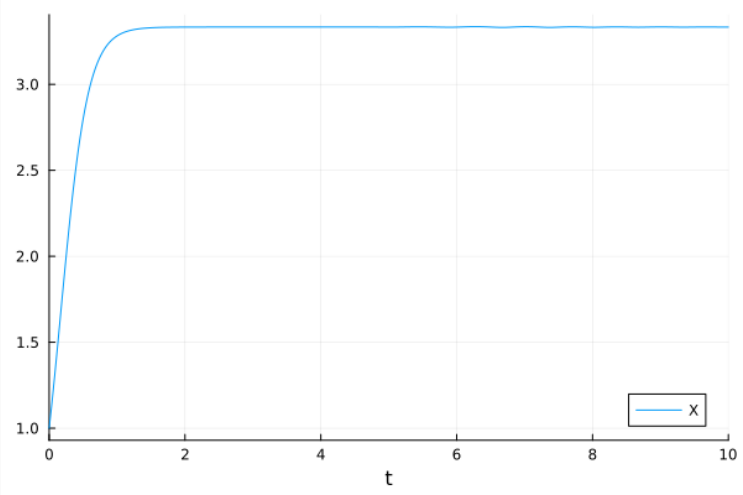

Рис. 2: Verhulst's logistic curve, where $k_1 = 5.0, k_2 = 3.0$

$$X \xrightarrow{k_1^+} 2X$$
$$X + Y \xrightarrow{k_2^+} 2Y$$
$$Y \xrightarrow{k_3^+} 0$$

$$r^1 = (1, 0)^T, \quad r^2 = (-1, 1)^T, \quad r^3 = (0, -1)^T$$

$$s_1^+ = k_1^+ x,$$
$$s_2^+ = k_2^+ xy,$$
$$s_3^+ = k_3^+ y,$$

$$A(x,y) = r^1 s_1^+ + r^2 s_2^+ + r^3 s_3^+ = \begin{pmatrix} k_1^+ x - k_2^+ xy \\ k_2^+ xy - k_3^+ y \end{pmatrix}$$

$$B(x,y) = r^1 (r^1)^T s_1^+ + r^2 (r^2)^T s_2^+ + r^3 (r^3)^T s_3^+ = \begin{pmatrix} k_1^+ x + k_2^+ xy & -k_2^+ xy \\ -k_2^+ xy & k_2^+ xy + k_3^+ y \end{pmatrix}$$

$$\mathrm{d}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} k_1^+ x - k_2^+ xy \\ k_2^+ xy - k_3^+ y \end{pmatrix} \mathrm{d}t + b(x,y)\mathrm{d}\begin{pmatrix} W_1 \\ W_2 \end{pmatrix}$$

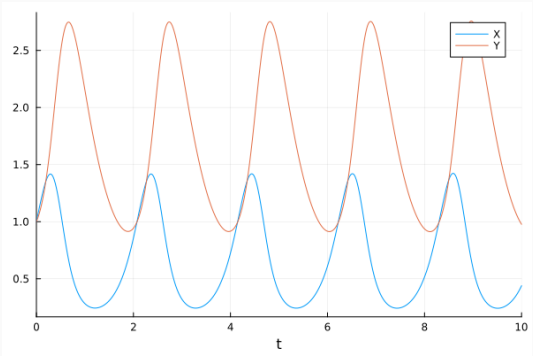

Рис. 3: Lotka–Volterra model, where $k_1 = 5.0, k_2 = 3.0, k_3 = 2.0$

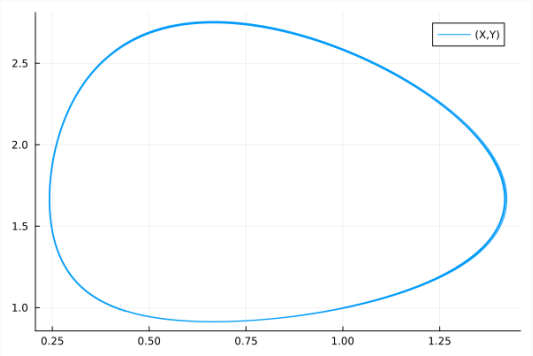

Рис. 4: Lotka–Volterra model, where $k_1 = 5.0, k_2 = 3.0, k_3 = 2.0$

Advantages of the Catalyst.jl library

- Catalyst.jl excels BioNetGen, COPASI, GillesPy2, Matlab and SimBiology in terms of performance.
- Simple and straightforward reaction notation.
- Models can be converted to symbolic models of ODE, CDE and stochastic chemical kinetics (jump processes).
- Non-integer reaction intensity coefficients are supported.