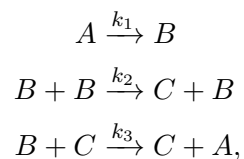


Stan/Torsten tutorial example: autocatalysis kinetics

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We consider the kinetics of an autocatalytic reaction [1]. The structure of the reactions is



where k_1 , k_2 , k_3 are the rate constants and A , B and C are the chemical species involved. The corresponding ODEs are

$$\begin{aligned}x_1' &= -k_1x_1 + k_3x_2x_3 \\ x_2' &= k_1x_1 - k_2y_2^2 - k_3x_2x_3 \\ x_3' &= k_2y_2^2\end{aligned}$$

Given $k_1 = 0.04$, $k_2 = 1.0e4$, $k_3 = 3.0e7$, we seek the initial condition for $x_1(t = 0)$, combined with initial condition $x_2(t = 0) = 0.0$ and $x_3(t = 0) = 0.0$.

References

- [1] H. H. Robertson. *Numerical analysis, an introduction, chapitre The solution of a set of reaction rate equations*. Academic Press, 1966.