examples of growth of perturbations in chemical organizations

Canonical name	ExamplesOfGrowthOfPerturbationsInChemicalOrganizations
Date of creation	2014-05-31 15:55:20
Last modified on	2014-05-31 15:55:20
Owner	rspuzio (6075)
Last modified by	rspuzio (6075)
Numerical id	33
Author	rspuzio (6075)
Entry type	Example

We will examine several simple examples of chemical systems where we start with one species of molecules (or a closed subset of species) then intoruduce a small perturbation and evolve the system using mass action dynamics. We want to know whether this perturbation will grow and, if so, at what rate. Ultimately, we would like to link the behavor to some feature of the reaction system, perhaps related to Rosen's theory of M-R systems.

To get started, consider a trivial case, $A + B \to B + B$. The system of equations which describes this system is:

$$\frac{dx}{dt} = -kxy$$
$$\frac{dy}{dt} = kxy$$

It is easy enough to solve this system. We begin by noting that $\frac{d}{dt}(x+y) = 0$, hence $x + y = x_0 + y_0$. Substituting this back in to the second equation, we conclude that

$$\frac{dy}{dt} = k(x_0 + y_0 - y)(y).$$

This equation can readily be solved to yield the implicit solution

$$kt = \frac{1}{x_0 + y_0} \log \frac{y}{x_0 + y_0 - y} \cdot \frac{x_0}{y_0}$$

which can be solved to produce the explicit solution

$$y = x_0 + y_0 - \frac{x_0 + y_0}{1 + \frac{y_0}{x_0} \exp(k(x_0 + y_0)t)}.$$

Looking at the solution, we see that it starts out at $y = y_0$ and grows towards $y = x_0 + y_0$ as $t \to \infty$. This is as we expect — as time goes on, whatever A's there are left react with B's to turn into B's until we are left with nothing but B's.

If we suppose that, at the initial time $t = 0$, there is only a tiny proportion of B's, i.e. $y_0 \ll x_0$, then we may make an expansion of the fraction and conclude that y grows exponentially for small values of t:

$$\frac{1}{1 + \frac{y_0}{x_0} \exp(k(x_0 + y_0)t)} \approx 1 - \frac{y_0}{x_0} \exp(k(x_0 + y_0)t)$$

$$y \approx \frac{y_0}{x_0} \exp(k(x_0 + y_0)t)$$

We can also come to this conclusion by bounding y without solving the equation first. For a simple equation like this which is readily solved, this is hardly needed but, for larger, more complicated equations, it becomes important and this simple example can serve as a illustration of the general technique.

Theorem 1. *Let C be a real number such that $0 < C < 1$ and let x_0 and y_0 be strictly positive real numbers such that $0 < y_0 < C(x_0 + y_0)$. Set $t_1 = \frac{1}{k(x_0+y_0)} \log C \frac{x_0+y_0}{y_0}$. Then there exists a function $f\colon [0, t_1) \to [0, C(x_0 + y_0))$ such that f satisfies the differential equation*

$$\frac{df(t)}{dt} = k(x_0 + y_0 - f(t))f(t).$$

and, for all $t \in [0, t_1)$,

$$y_0 \exp((1 - C)k(x_0 + y_0)t) \leq f(t) \leq y_0 \exp(k(x_0 + y_0)t).$$

Proof. By the existence theorem, there exists a positive real number t_0 and a function $f\colon [0, t_0) \to \mathbb{R}$ such that $f(0) = y_0$ and f satifies the differential equation. Since $f(0) = y_0 < C(x_0 + y_0)$, by continuity there exists a positive real number t_2 and a function $f\colon [0, t_0) \to [0, C(x_0 + y_0))$ which satisfies the same differential equation with the same initial condition. Furthermore, we assume that t_2 is maximal.

Starting with this condition $f(t) < C(x_0 + y_0)$ and doing some algebra, we conclude that

$$(1 - C)k(x_0 + y_0) \leq \frac{1}{y}\frac{dy}{dt} \leq k(x_0 + y_0)$$

Now, $\frac{1}{y}\frac{dy}{dt} = \frac{d}{dt}(\log y)$ so, by the mean value theorem, we conclude that

$$(1 - C)k(x_0 + y_0)t \leq \log \frac{y}{y_0} \leq k(x_0 + y_0)t.$$

Exponentiating,

$$y_0 \exp((1 - C)k(x_0 + y_0)t) \leq y \leq y_0 \exp(k(x_0 + y_0)t).$$

We can ensure that the bound on y is satisfied if the condition $C(x_0+y_0) \geq y_0 \exp(k(x_0+y_0)t)$ is met, which amounts to demanding that $0 \leq t \leq t_1$ where $t_1 = \frac{1}{k(x_0+y_0)} \log C \frac{x_0+y_0}{y_0}$.

□