A short note on the Lyapunov function for complex-balanced chemical reaction networks

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January 23, 2014

Abstract

A very short proof is presented that the usual Lyapunov function of chemical reaction network theory is, in fact, a strict Lyapunov function. The proof is essentially the same as that presented in a series of lectures by Marty Feinberg at the University of Wisconsin in 1979, though the reliance on "complex-space" has been removed, making this particular argument slightly more intuitive.

This note largely follows a small portion of Marty Feinberg's lectures [1]. The major difference between the argument presented here and those presented in [1] is that here we will not utilize "complex-space." How complex-balancing implies the usual Lyapunov function is, in fact, a strict Lyapunov function then becomes quite clear. We stress, however, that the main argument is essentially that of [1].

We follow the notation of [1]. Let $\{\mathcal{S}, \mathcal{C}, \mathcal{R}\}$ be a deterministically modeled chemical reaction system with mass-action kinetics. Suppose that there are precisely N species. We denote the kth reaction by $y_k \to y_k'$, and denote the span of the reaction vectors by $S = \text{span}\{y_k' - y_k\}$. The ODE governing the dynamics of the system is

$$\dot{x}(t) = \sum_k \kappa_k x(t)^{y_k}(y_k' - y_k). \tag{1}$$

Assume that the system is complex-balanced with complex-balanced equilibrium $\overline{c} \in \mathbb{R}^N_{>0}$. This means that for each $\eta \in \mathcal{C}$,

$$\sum_{k:\eta = y_k} \kappa_k(\overline{c})^{y_k} = \sum_{k:\eta = y_k'} \kappa_k(\overline{c})^{y_k}, \tag{2}$$

where the sum on the left is over all reactions for which η is the source complex, and the sum on the right is over all reactions for which η is the product complex.

Now define the function V by

$$V(x) = \sum_{i=1}^N x_i(\ln(x_i) - \ln \overline{c}_i - 1) + \overline{c}_i.$$

The fact that V is a Lyapunov function for the system is captured in the following result.

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Theorem 0.1. Suppose that $x \in \mathbb{R}^N_{>0}$ with $x - \overline{c} \in S$. Then

$$\nabla V(x) \cdot \sum_k \kappa_k x^{y_k}(y_k' - y_k) = \sum_k \kappa_k x^{y_k}(y_k' - y_k) \cdot (\ln(x) - \ln(\overline{c})) \leq 0,$$

with equality if and only if $x = \overline{c}$.

Proof. Note that

$$\sum_k \kappa_k x^{y_k}(y_k' - y_k) \cdot (\ln x - \ln \overline{c}) = \sum_k \kappa_k (\overline{c})^{y_k} \left(\frac{x}{\overline{c}}\right)^{y_k} \left(\ln\left\{\left(\frac{x}{\overline{c}}\right)^{y_k'}\right\} - \ln\left\{\left(\frac{x}{\overline{c}}\right)^{y_k}\right\}\right).$$

Using that for any real numbers $a, b \in \mathbb{R}$ we have $e^a(b-a) \leq e^b - e^a$ with equality if and only if $a = b$ (consider secant lines of e^x), we have

$$\begin{aligned}
\sum_k \kappa_k (\overline{c})^{y_k} \left(\frac{x}{\overline{c}}\right)^{y_k} \left(\ln\left\{\left(\frac{x}{\overline{c}}\right)^{y_k'}\right\} - \ln\left\{\left(\frac{x}{\overline{c}}\right)^{y_k}\right\}\right) &\leq \sum_k \kappa_k (\overline{c})^{y_k} \left(\left(\frac{x}{\overline{c}}\right)^{y_k'} - \left(\frac{x}{\overline{c}}\right)^{y_k}\right) \\
&= \sum_{\eta \in \mathcal{C}} \left[\sum_{k:\eta = y_k'} \kappa_k (\overline{c})^{y_k} \left(\frac{x}{\overline{c}}\right)^{y_k'} - \sum_{k:\eta = y_k} \kappa_k (\overline{c})^{y_k} \left(\frac{x}{\overline{c}}\right)^{y_k}\right] \\
&= \sum_{\eta \in \mathcal{C}} \left(\frac{x}{\overline{c}}\right)^{\eta} \left[\sum_{k:\eta = y_k'} \kappa_k (\overline{c})^{y_k} - \sum_{k:\eta = y_k} \kappa_k (\overline{c})^{y_k}\right] \\
&= 0,
\end{aligned}$$

where the final equality holds by (2), i.e. by complex-balancing at $\overline{c}$.

Thus, we have a strict inequality unless

$$(y_k' - y_k) \cdot (\ln(x) - \ln(\overline{c})) = 0,$$

for all k. That is, we have a strict inequality unless

$$\ln(x) - \ln(\overline{c}) \in S^{\perp}. \tag{3}$$

Following precisely the argument on page $4 - 33$ of [1], we now note that if both $x - \overline{c} \in S$ and (3) hold, then

$$0 = (x - \overline{c}) \cdot (\ln(x) - \ln(\overline{c})) = \sum_{i=1}^{N} (x_i - \overline{c}_i)(\ln(x_i) - \ln(\overline{c}_i)),$$

which, by the monotonicity of log function, can only happen if $x_i = \overline{c}_i$ for all i. □

References

[1] M. Feinberg, *Lectures on chemical reaction networks*, Delivered at the Mathematics Research Center,Univ. Wisc.-Madison. Available for download at `http://crnt.engineering.osu.edu/LecturesOnReactionNetworks`, 1979.