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Qualitative Analysis of a Biological-Chemical Reaction Model of Multi-Molecule Systems

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Abstract

This article discuss the limit cycle of the

$$\begin{cases} \dot{x} = 1 - x^p y^{p+1} \\ \dot{y} = \theta y(x^p y^p - 1) \end{cases} \quad p \ge 1, p \in Z, x \ge 0, y \ge 0, \theta \ge 0$$

and branching problem of Hopf, whose parameter is Theta，giving the direction and stability Of Hopf branch and its approximate expression based on of small amplitude cycle.

*Keywords:*stability ,limit cycle ,Hopfbranch

1. One Introduction

Multi-molecular reaction model among Biochemical reactions is

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$$[A_0]\xrightarrow{K_1} A_1, A_1 \xrightarrow{K_2} 0 \quad \text{(Output)}$$
$$pA_1 + qA_2 \xrightarrow{K_3} (p+q)A_2 \quad \text{(Adduct reaction)} \tag{1}$$
$$A_2 \xrightarrow{K_4} \text{(Output)}$$

The corresponding mathematical model is：

$$\frac{dx_1}{dt} = k_1x_0 - k_2x_1 - pk_3x_1^p x_2^q$$
$$\frac{dx_2}{dt} = pk_3x_1^p x_2^q - k_4x_2$$

This article discusses the situation as follow $q = p+1, p \ge 1, p \in Z, k_2 = 0$
In the model (1)

$$\alpha = \frac{1}{k_1x_0}[\frac{k_1x_0}{r^q k_3 p}]^{\frac{1}{p}}\ ,\ \ \beta = (\frac{k_1x_0}{r^q k_3 p})^{\frac{1}{p}}\ ,\quad \gamma = \frac{k_1x_0}{k_4}$$

Transfore to

$$\tau = \alpha t, x_1 = \beta x, x_2 = \gamma y\ ,\ \text{to}\ \theta = \frac{k_4}{k_1x_0}(\frac{k_1x_0}{r^q k_3 p})^{\frac{1}{p}}$$

So Model (1) becomes into a systerm as follow

$$\begin{cases} \dfrac{dx}{dt} = 1 - x^p y^{p+1} = P(x,y) \\ \dfrac{dx}{dt} = \theta(x^p y^p - 1) = Q(x,y) \end{cases} \quad x \ge 0, y \ge 0, p \ge 1, p \in Z, \theta > 0$$

In the first quadrant $(1)_\theta$ only get a unique equilibrium,that is point（1,1）， and the corresponding characteristic equation of the variational equations is

$$\lambda^2 + p(1-\theta)\lambda + \theta p = 0 \tag{2}$$

（2）The characteristic roots the second equation is

$$\lambda_{1,2} = \frac{1}{2}(-p(1-\theta) \pm \sqrt{p^2(1-\theta)^2 - 4\theta p}$$

It is obvious that the equilibrium of the system is unstable when $\theta > 1$,while the system is stable when $\theta < 1$, Next we focuse on the qualitative form of the $(1)_\theta$ system.

2. Second, nonexistence of the periodic orbit

Theorem 1 the $(1)_\theta$ system does not have a limit cycle.when $\theta \ge 2^{\frac{1}{p}}$

Proof: First , if $(1)_\theta$ systerm has limit cycle, then the limit cycle will intersect with the hyperbolic, notes that

The tangent of the system is $x=0$,the solution is y=0, so the limit cycle of the system will not intersect with two straight lines, so we use Dulac function

$$B(x,y)=x^{-p}y^{-(p+1)}e^{-p(\theta x+y)}$$

$$\frac{\partial[B(x,y)P(x,y)]}{\partial x}=x^{-(p+1)}y^{-(p+2)}e^{-p(\theta x+y)}(x^p y^p p\theta xy^2-py-p\theta xy)$$

$$\frac{\partial[B(x,y)Q(x,y)]}{\partial x}=x^{-(p+1)}y^{-(p+2)}e^{-p(\theta x+y)}(-x^p y^p p\theta xy^2+p\theta xy+p\theta xy^2)$$

$$\frac{\partial(BP)}{\partial x}+\frac{\partial(BQ)}{\partial y}=x^{-(p+1)}y^{-(p+1)}e^{-p(\theta x+y)}p(\theta xy-1)$$

According to Dulac determine theorem, if the $(1)_\theta$ system has a limit cycle it certainly intersect with the hyperbola $\theta xy-1=0$.

Next,when $\theta\geq 2^{\frac{1}{p}}$, limit cycle of $(1)_\theta$ system and the hyperboa $L=y-\frac{1}{2^{\frac{1}{p}}x}=0$ are tangent and this limit cycle will not intersect with $(1)_\theta$ system .Follow the trajectories of the $(1)_\theta$ system,

$$\frac{dL}{dt}\Big|_{L=0}=\frac{dy}{dt}-2^{\frac{1}{p}}\frac{1}{x^2}\frac{dx}{dt}=\frac{1}{x^3}(-\frac{1}{2^{1+\frac{1}{p}}}\theta x^2+\frac{1}{2^{\frac{1}{p}}}x-\frac{1}{2^{1-\frac{2}{}}})$$

Here the following discriminant of quadratic algebraic equation,

$$-\frac{1}{2^{1+\frac{1}{p}}}\theta x^2+\frac{1}{2^{\frac{1}{p}}}x-\frac{1}{2^{1-\frac{2}{p}}})=0$$

when $\theta\geq 2^{\frac{1}{p}}$,

$$\Delta=\frac{1}{2^{\frac{2}{p}}}(1-\frac{\theta}{2^{\frac{1}{p}}})\leq 0$$

Due to the hyperbola $\theta xy-1=0$, when $\theta\geq 2^{\frac{1}{p}}$,the hyperbola coincides with it in the bottom ,so when $\theta\geq 2^{\frac{1}{p}}$, the limit cycle of $(1)_\theta$ can not intersect the hyperbola $\theta xy-1=0$, so there is no limit cycle.

3. Hopf bifurcation

In order to discuss the Hopf bifurcation of the $(1)_\theta$ system,we transform the system into

$$\frac{d}{dt}\begin{pmatrix}u\\v\end{pmatrix}=A\begin{pmatrix}u\\v\end{pmatrix}+\begin{pmatrix}-f(u,v)\\\theta f(u,v)\end{pmatrix},\text{其中 } A=\begin{pmatrix}-p & -(p+1)\\\theta p & \theta p\end{pmatrix} \quad (1)_\mu$$

$$f(u,v)=\frac{p(p-1)}{2}u^2+\frac{p(p+1)}{2}v^2+p(p+1)uv+\frac{p^2(p+1)}{2}uv^2+\frac{p(p^2-1)}{2}u^2v$$
$$+\frac{1}{6}p(p-1)(p-2)u^3+\frac{1}{6}p(p^2-1)v^3+G(u,v)$$

thereinto $G(u,v)$ is a more than three times polynomial about u, v .we take

$$\theta=\theta(\mu)=1+\mu,\mu=\mu^{\mathrm{H}}(\varepsilon)=\sum_{i=2}^{\infty}\mu_i^H\varepsilon^i$$

$(0<\varepsilon<\varepsilon_H)$ as a bifurcation parameter, then a pair of conjugate eigenvalues of (2) are

$$\lambda=\lambda(\mu)=\alpha(\mu)+\omega(\mu)\ i\ ,\ \ \overline{\lambda}=\overline{\lambda}(\mu)=\alpha(\mu)\ -\omega(\mu)\ i$$

$$\alpha(\mu)=\frac{1}{2}p\mu,\omega(\mu)=\frac{1}{2}\sqrt{4(1+\mu)p-p^2\mu^2}$$

$$\alpha(0)=\alpha_0=0,\ \ \alpha'(0)=\frac{1}{2}p>0,\omega(0)=\omega_0=\sqrt{p},\omega'(0)=\frac{1}{2}\sqrt{p}$$

Accordingly.we know that:

\Theorem 3 there is $\varepsilon_H>0,$ when $0<\varepsilon<\varepsilon_H$, systerm $(1)_\mu$ at least has one limit cycle near the equilibrium point (1,1) (small amplitude periodic solution)

Next we discuss the stability of systerm $(1)_\mu$ when $\mu=0$,the direction and the stability of Hopf branch，at this time, the feature vector $(\zeta_1,\ \zeta_2)$ of matrix A which eigenvalue is $\lambda(0)=\omega_0 i=\sqrt{pi}$ must fulfill

$$\begin{cases}-(p+\sqrt{pi}\zeta_1-(p+1)\zeta_2=0\\ p\zeta_1+(p-\sqrt{pi}\zeta_2=0\end{cases}$$

Then Select

$\zeta_1=1,\ \ \zeta_2=-\frac{1}{p+1}(p+\sqrt{pi})$, And make $B=\begin{pmatrix}1 & 0\\ -\frac{p}{p+1} & \frac{\sqrt{p}}{p+1}\end{pmatrix}$

Then transform,we

Get

$$\begin{pmatrix}u\\ v\end{pmatrix}=B\begin{pmatrix}y_1\\ y_2\end{pmatrix}$$

$$\begin{pmatrix}\frac{dy_1}{dt}\\ \frac{dy_2}{dt}\end{pmatrix}=\begin{pmatrix}0 & -\sqrt{p}\\ \sqrt{p} & 0\end{pmatrix}\begin{pmatrix}y_1\\ y_2\end{pmatrix}+\begin{pmatrix}F^1(y_1,y_2)\\ F^2(y_1,y_2)\end{pmatrix}\qquad(3)$$

Here we know

$$F^1(y_1,y_2)=\frac{p(2p+1)}{2(p+1)}y_1^2-\frac{p\sqrt{p}}{p+1}y_1y_2-\frac{p^2}{2(p+1)}y_2^2-$$

$$\frac{p^5+p^4-p^3+p^2+p}{3(p+1)^2}y_1^3-\frac{\sqrt{p}}{(p+1)^2}(\frac{1}{6}p^5-\frac{1}{2}p^4-\frac{2}{3}p^3-\frac{1}{2}p^2-\frac{1}{2}p)y_1^2y_2$$

$$-\frac{p^3}{(p+1)^2}y_1y_2^2-\frac{p^2(p-1)\sqrt{p}}{6(p+1)^2}y_2^3+G(y_1,y_2)$$

$$F^2(y_1,y_2)=-\frac{1}{\sqrt{p}}F^1(y_1,y_2)$$

Therein, $G(u,v)$ is a more than three times polynomial about u, v

$$g_{11}=\frac{1}{4}[\frac{\partial^2F^1}{\partial y_1^2}+\frac{\partial^2F^1}{\partial y_2^2}+i(\frac{\partial^2F^2}{\partial y_1^2}+\frac{\partial^2F^2}{\partial y_2^2})]=\frac{1}{4}(p-i\sqrt{p})$$

$$g_{11}=\frac{1}{4}[\frac{\partial^2F^1}{\partial y_1^2}-\frac{\partial^2F^1}{\partial y_2^2}-2\frac{\partial^2F^2}{\partial y_1\partial y_2}+i(\frac{\partial^2F^2}{\partial y_1^2}-\frac{\partial^2F^2}{\partial y_2^2}+2\frac{\partial^2F^1}{\partial y_1\partial y_2})]=\frac{1}{4}(\frac{3p^2-p}{p+1}-i\frac{\sqrt{p}(5p+1)}{p+1})$$

$$g_{20}=\frac{1}{4}[\frac{\partial^2F^1}{\partial y_1^2}-\frac{\partial^2F^1}{\partial y_2^2}+\frac{\partial^2F^2}{\partial y_1\partial y_2}+i(\frac{\partial^2F^2}{\partial y_1^2}-\frac{\partial^2F^2}{\partial y_2^2}-2\frac{\partial^2F^1}{\partial y_1\partial y_2})]=\frac{1}{4}(3p-i\sqrt{p})$$

$$C_1(0)=\frac{i}{2\sqrt{p}}(g_{20}g_{11}-2|g_{11}|^2-\frac{1}{3}|g_{02}|^2)+\frac{1}{2}g_{21}$$

$$=\frac{p}{16(p+1)^2}[2(p+1)^2-(\frac{5}{3}p^4-3p^3+\frac{4}{3}p^2+2p+4)$$

$$+\frac{\sqrt{p}}{16}[\frac{1}{2}p-\frac{3}{2}+\frac{1}{(1+p)^2}(\frac{1}{3}p^5+p^4-\frac{3}{2}p^3-\frac{15}{6}p^2-\frac{11}{6}p+\frac{1}{6})]i$$

$$\mu_2^H=-\operatorname{Re}C_1(0)/\alpha'(0)=\frac{1}{8(P+1)^2}\left[\frac{5}{3}p^4+3p^3+\frac{4}{3}p^2+2p+4-2(p+1)^2\right]=\frac{f(p)}{8(p+1)^2}$$

Among which

$$f(p)=\frac{5}{3}p^4+3p^3+\frac{4}{3}p^2+2p+4-2(p+1)^2$$

As for

when $p\in N$ there is $f(p)>0$,

Therefore, for any $p\in N$ there is $\mu_2^H>0$ $\beta_2=2\operatorname{Re}C_1(0)<0$

$$\operatorname{Im}C_1(0)=\frac{\sqrt{p}}{16}\left[\frac{1}{2}p-\frac{3}{2}+\frac{1}{(1+p)^2}\left(\frac{1}{3}p^5+p^4-\frac{3}{2}p^3-\frac{5}{2}p^2-\frac{11}{6}p+\frac{1}{6}\right)\right]$$

$$\tau_2 = -\left(\mathrm{Im}\, C_1(0) + \mu_2^H \omega'(0)/\omega_0\right)$$

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} + B\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} 1+\varepsilon\cos\sqrt{pt}/T + O(\varepsilon^2) \\ 1+\dfrac{\varepsilon}{p+1}\left(-p\cos\sqrt{pt}/T + \sqrt{p}\sin\sqrt{pt}/T + O(\varepsilon^2)\right) \end{pmatrix} \qquad (4)$$

from $\mu_2^H > 0, \beta_2 < 0,$ see $[4]$ we know that.

Theorem 4 system There is $\theta = \overline{\theta},$ when $1 < \theta < \overline{\theta} \le 2^{\frac{1}{p}}$, $(1)_\theta$ systerm has a stable limit cycle, and its approximate expression is given by (4) equation.

The above exposition shows that the model $(1)_\theta$ of multi-cellular biochemical reactions, when $0 < \theta < \theta^* < 1$, the equilibrium $(1,1)$ is globally asymptotically stable in the first quadrant, when $1 < \theta < \overline{\theta} < 2^{\frac{1}{p}}$ there is a stable oscillations, when $\theta > 2^{\frac{1}{p}}$,the oscillations disappear.

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