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On the Aris-Amundson model

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Abstract. The work is devoted to the study of the real roots of the system of transcendental Aris–Amundson equations. It is shown that the number of real roots is related to the number of real roots of some entire function (resultant). The number of complex roots is investigated.

Keywords: systems of transcendental equations, resultant, simple root.

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Introduction

Finding the number of real roots of polynomials is a classical algebraic problem. The Hermite method of quadratic forms, the Sturm method, the Descartes sign rule, and the Byudan–Fourier theorem are devoted to this problem (see, for example, [1]). Further development of these methods for polynomials can be found in the work [2] and the monograph [3]. For entire functions, the question of localization of real positive roots was considered in the classical works of N. G. Chebotarev [4] (pp. 28–56), as well as in the work of [5] (we refer to the collected works of N. G. Chebotarev, since his original works are hardly accessible).

For systems of equations, the number of real roots was studied in the articles [6–8]. In the article [9], the number of real roots was related to the number of real roots of the resultant.

The monographs [10,11] consider algebraic and transcendental systems of equations. Systems of transcendental equations arise, for example, in the study of equations of chemical kinetics [12]. One of the problems that arise there is the problem of the number of real positive roots of a system of equations in a reaction polyhedron. As an example, the Aris-Amundson system has been studied.

1. Multiple roots of the resultant

Let us consider one of the models of a continuous perfectly stirred reactor, the so-called Aris-Amundson model in the dimensionless form (see [12, ch. 2])

$$\frac{dx}{d\tau} = f(y)(1-x) - x = f_1(x,y), \quad \frac{dy}{d\tau} = \beta f(y)(1-x) - s(y-1) = f_2(x,y), \tag{1}$$

where $f(y) = Dae^{\gamma(1-1/y)}$. All constants are positive.

The stationary states of the system (1) are solutions of the stationarity system

$$f_1(x,y) = 0, \quad f_2(x,y) = 0, \tag{2}$$

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which can be written as

$$Dae^{\gamma(1-1/y)}(1-x)-x=0,$$

$$\beta Dae^{\gamma(1-1/y)}(1-x)-s(y-1)=0.$$

Denoting $Da=b$, $t=\gamma\,(1-1/y)$, we get the system

$$be^t(1-x)-x=0,\quad \beta be^t(1-x)-s\frac{t}{\gamma-t}=0. \tag{3}$$

Obviously, the system (3) has no roots with zero coordinates.

Earlier in the work [13], the Zeldovich–Semenov model was studied in a similar way. The main idea of the study is the application of the multidimensional theory of residues, the study of power sums of roots and residue integrals (see [10, 11]).

Then we get

$$be^t\cdot\frac{\beta(\gamma-t)-st}{\beta(1-t)}-\frac{st}{\beta(\gamma-t)}=0.$$

Thus, the entire function of the first order of growth can serve as the resultant of the system (2)

$$F(t)=be^t(\beta\gamma-t(\beta+s))-st=0.$$

Let us check it for multiple zeros. We convert it to the form

$$\varphi(t)=be^t-\frac{st}{\beta\gamma-t(\beta+s)}.$$

Calculating the derivative, we get

$$\varphi'(t)=be^t-\frac{s\beta\gamma}{(\beta\gamma-t(\beta+s))^2}.$$

Obviously, if $F(t)=0$ and $F'(t)=0$ at some point t, then $\varphi(t)=0$ and $\varphi'(t)=0$ at this point. The converse is also true.

Then from the equalities $\varphi(t)=0,\ \varphi'(t)=0$ we get

$$t_{1,2}=\frac{\beta\gamma\mp\sqrt{\beta^2\gamma^2-4\beta^2\gamma-4\beta\gamma s}}{2(\beta+s)}.$$

Substituting these values, for example, into the first equation, we get

$$b\cdot\exp\left(\frac{\beta\gamma\mp\sqrt{\beta^2\gamma^2-4\beta^2\gamma-4\beta\gamma s}}{2(\beta+s)}\right)=\frac{s}{\beta+s}\cdot\frac{\beta\gamma\mp\sqrt{\beta^2\gamma^2-4\beta^2\gamma-4\beta\gamma s}}{\beta\gamma\pm\sqrt{\beta^2\gamma^2-4\beta^2\gamma-4\beta\gamma s}}. \tag{4}$$

Thus, in equality (4), there is an exponential function on the left, and a power function on the right. Therefore, they cannot match for almost all parameter values. Then for almost all parameter values there are no multiple roots of the function $\varphi(t)$ (and therefore $F(t)$).

Proposition 1. *For almost all parameter values the function $\varphi(t)$ (and therefore $F(t)$) has no multiple roots.*

2. The number of real roots of the resultant

Next, we use the following statement (see [14]).

Theorem 1. *If the system (2) with real coefficients is such that it has no roots with zero coordinates and all zeros of the resultant $F(t)$ are simple, then the number of real roots of the system (2) coincides with the number of real roots of the function $F(t)$.*

From the system (2) we get $1-x = 1+\dfrac{s}{\beta}(1-y)$, $x = \dfrac{s}{\beta}(y-1)$. We substitute it into the first equation

$$be^{\gamma(1-1/y)}\cdot\left(1+\frac{s}{\beta}(1-y)\right)+\frac{s}{\beta}(1-y)=0.$$

The resultant looks like

$$\varphi(y)=be^{\gamma(1-1/y)}\cdot\frac{\beta-s(y-1)}{s(y-1)}-1,$$

and we find the number of roots of $\varphi(y)$.

First, we find the intervals of increase and decrease of $\varphi(y)$.

$$\varphi'(y)=\frac{be^{\gamma(1-1/y)}}{s}\cdot\frac{-(\gamma s+\beta)y^2+\gamma(\beta+2s)y-\gamma(\beta+s)}{y^2(y-1)^2}.$$

The derivative $\varphi'(y)=0$ if and only if

$$-(\gamma s+\beta)y^2+\gamma(\beta+2s)y-\gamma(\beta+s)=0.$$

Solving the resulting quadratic equation, we find the discriminant

$$D=\gamma^2\beta^2-4\gamma\beta^2-4\gamma\beta s.$$

Solutions to the quadratic equation are

$$y_{1,2}=\frac{\gamma(\beta+2s)\mp\sqrt{\gamma^2\beta^2-4\gamma\beta^2-4\gamma\beta s}}{2(s\gamma+\beta)}.$$

If $D>0$, that is, $\gamma\beta-4(\beta+s)>0$, then

$$\psi(y)=-(\gamma s+\beta)y^2+\gamma(\beta+2s)y-\gamma(\beta+s)$$

has two real roots $y_1<y_2$.

Since the graph of the function $\psi(y)$ is a parabola with branches down, then $\psi(y)<0$ on the interval $(-\infty;y_1)\cup(y_2;\infty)$ and $\psi(y)>0$ in the interval $(y_1;y_2)$.

If $D=0$, that is, $\gamma\beta-4(\beta+s)=0$, then $\psi(y)$ has one real root y_0 and $\psi(y)<0$ on the interval $(-\infty;y_0)\cup(y_0;\infty)$.

If $D<0$, that is, $\gamma\beta-4(\beta+s)<0$, then $\psi(y)$ has no real roots and $\psi(y)<0$ on the entire real line.

Let us show that if $D\geqslant 0$, then the roots of $\psi(y)$ lie to the right of 1, that is, $1<y_1\leqslant y_2$. Note beforehand that if $D\geqslant 0$, then $\gamma>4$.

Indeed, $D\geqslant 0$ is equivalent to the inequality $\gamma\geqslant 4+\dfrac{4s}{\beta}$, which implies that $\gamma>4$ $(\beta,s>0)$.

Assume that $y_1=\dfrac{\gamma(\beta+2s)-\sqrt{D}}{2(s\gamma+\beta)}>1$. This inequality is equivalent to $\beta(\gamma-2)>\sqrt{D}$. Since $\gamma>4$, the left and right sides of the last inequality are non-negative, which means it is equivalent to $\beta^2(\gamma-2)^2 > \gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s$. Simplifying it, we get the equivalent condition $4\beta(\beta+\gamma s) > 0$, which is always true, since $\beta, \gamma, s > 0$. Thus, our assumption that $y_1 > 1$ is correct. That is, for $D \geqslant 0$, the condition $1 < y_1 \leqslant y_2$ is satisfied.

It follows from the above that if $D > 0$, that is, $\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s > 0$, then $\varphi'(y)$ has two real roots $1 < y_1 < y_2$ and $\varphi'(y) < 0$ on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_1) \cup (y_2; +\infty)$, $\varphi'(y) > 0$ in the interval $(y_1; y_2)$. So $\varphi(y)$ decreases on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_1) \cup (y_2; +\infty)$ and $\varphi'(y)$ increases in the interval $(y_1; y_2)$.

It also follows from the above that if $D > 0$, that is, $\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s > 0$, then $\varphi'(y)$ has two real roots $1 < y_1 < y_2$ and $\varphi'(y) < 0$ on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_1) \cup (y_2; +\infty)$, $\varphi'(y) > 0$ in the interval $(y_1; y_2)$. So $\varphi(y)$ decreases on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_1) \cup (y_2; +\infty)$ and $\varphi'(y)$ increases in the interval $(y_1; y_2)$.

If $D = \gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s = 0$, then $\varphi'(y)$ has one real root $y_0 > 1$ and $\varphi'(y) < 0$ on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_0) \cup (y_0; +\infty)$. So $\varphi(y)$ decreases on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_0) \cup (y_0; +\infty)$.
If $D = \gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s = 0$, then $\varphi'(y)$ has one real root $y_0 > 1$ and $\varphi'(y) < 0$ on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_0) \cup (y_0; +\infty)$. So $\varphi(y)$ decreases on the set $(-\infty; 0) \cup (0; 1) \cup (1; y_0) \cup (y_0; +\infty)$.

If $D = \gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s < 0$, then $\varphi'(y)$ has no real roots and $\varphi'(y) < 0$ over the entire domain of $\varphi'(y)$, which means $\varphi(y)$ decreases over the entire domain of definition of $\varphi(y)$.

For a more accurate understanding of the behavior of the function $\varphi(y)$, we find the limits of $\varphi(y)$ at $\pm\infty$ and at the break points: $\lim\limits_{y\to-\infty} \varphi(y) = -be^{\gamma} - 1 < 0$, $\lim\limits_{y\to 0-0} \varphi(y) = -\infty$, $\lim\limits_{y\to 0+0} \varphi(y) = -1$, $\lim\limits_{y\to 1-0} \varphi(y) = -\infty$, $\lim\limits_{y\to 1+0} \varphi(y) = +\infty$, $\lim\limits_{y\to+\infty} \varphi(y) = -be^{\gamma} - 1 < 0$

Now we find the number of roots of the function $\varphi(y)$.

1. If

$$\begin{cases} D > 0, \\ \varphi(y_1) < 0, \\ \varphi(y_2) > 0, \end{cases}$$

or more precisely

$$\begin{cases} \gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s > 0, \\ be^{\frac{\gamma\beta - \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s}}{2(\beta+s)}} \cdot \dfrac{\gamma\beta + \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s} - 2(\beta+s)}{2s} - 1 < 0, \\ be^{\frac{\gamma\beta + \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s}}{2(\beta+s)}} \cdot \dfrac{\gamma\beta - \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s} - 2(\beta+s)}{2s} - 1 > 0, \end{cases}$$

then $\varphi(y)$ has three real roots $1 < Y_1 < Y_2 < Y_3$.

For example, if $b = 0.04$, $\gamma = 10$, $\beta = 1$, $s = 1$, we get the discriminant $D = 20 > 0$, $y_1 = \dfrac{15-\sqrt{5}}{11} \approx 1.16035745659093 > 1$, $y_2 = \dfrac{15+\sqrt{5}}{11} \approx 1.5669152706818 > y_1$, $\varphi(y_1) \approx -0.16584745271763 < 0$, $\varphi(y_2) \approx 0.13869366143044 > 0$ and the function $\varphi(y)$ has three real roots $Y_1 \approx 1.073488201 > 1$, $Y_2 \approx 1.356686984 > Y_1$, $Y_3 \approx 1.733497054 > Y_2$ (see Fig. 1).

Another example: for $b = 0.001$, $\gamma = 10$, $\beta = 10$, $s = 1$ we get the discriminant $D = 5600 > 0$, $y_1 = = 3 - \dfrac{\sqrt{14}}{2} \approx 1.129171306 > 1$, $y_2 = 3 + \dfrac{\sqrt{14}}{2} \approx 4.870828694 > y_1$, $\varphi(y_1) \approx -0.76011792742972 < 0$, $\varphi(y_2) \approx 3.4763004785113 > 0$ and the function $\varphi(y)$ has three real roots $Y_1 \approx 1.011153756 > 1$, $Y_2 \approx 1.812214562 > Y_1$, $Y_3 \approx 9.890609328 > Y_2$ (see Fig. 2).

2. When the following conditions are met

$$\begin{cases} \gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s > 0, \\ be^{\frac{\gamma\beta - \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s}}{2(\beta+s)}} \cdot \dfrac{\gamma\beta + \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s} - 2(\beta+s)}{2s} - 1 = 0 \end{cases}$$

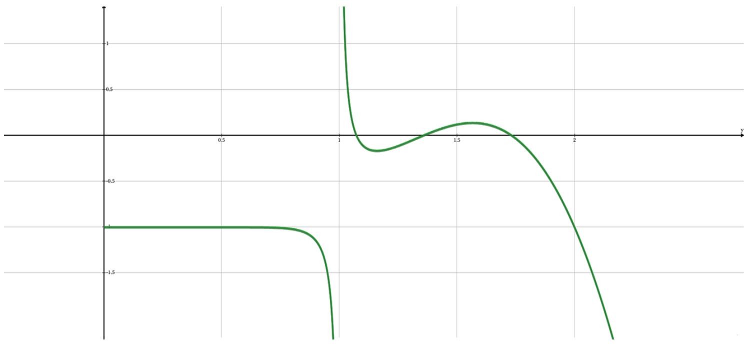

Fig. 1. $\varphi(y)$ has 3 real roots

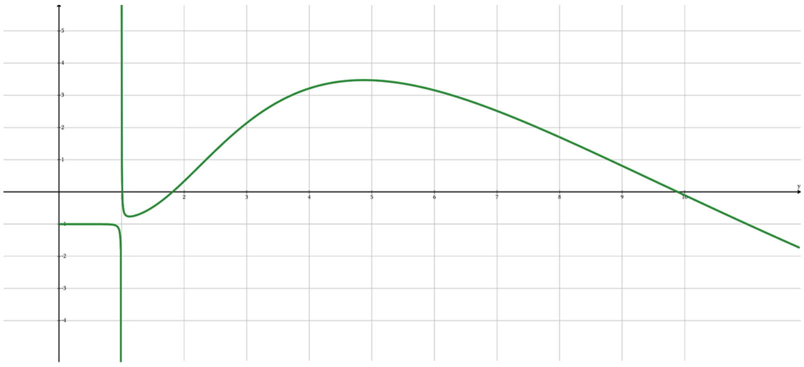

Fig. 2. $\varphi(y)$ has 3 real roots

(the case when y_1 is a multiple real root of $\varphi(y)$) or

$$\begin{cases} \gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s > 0, \\ be^{\frac{\gamma\beta + \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s}}{2(\beta+s)}} \cdot \dfrac{\gamma\beta - \sqrt{\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s} - 2(\beta+s)}{2s} - 1 = 0 \end{cases}$$

(the case when y_2 is a multiple real root of $\varphi(y)$), the function $\varphi(y)$ has two real roots $1 < Y_1 < Y_2$.

An example when Y_1 is a multiple real root ($Y_1 = y_1$) is the following: for $\gamma = 10$, $\beta = 10$, $s = 1$, $b = = \dfrac{(4-\sqrt{14}) \cdot e^{\frac{40-10\sqrt{14}}{-6+\sqrt{14}}}}{16+\sqrt{14}}$ we get the discriminant $D = 5600 > 0$, $y_1 = 3 - \dfrac{\sqrt{14}}{2} \approx 1.129171307 > 1$, $y_2 = 3 + \dfrac{\sqrt{14}}{2} \approx 4.870828694 > y_1$, $\varphi(y_1) = 0$, $\varphi(y_2) \approx 17.6604210584 > 0$ and the function $\varphi(y)$ has two real roots $Y_1 = y_1 = 3 - \dfrac{\sqrt{14}}{2} \approx 1.129171307 > 1$, $Y_2 \approx 10.73089616 > Y_1$ (see Fig. 3).

3. If

$$\gamma^2\beta^2 - 4\gamma\beta^2 - 4\gamma\beta s < 0,$$

the function $\varphi(y)$ has one real root $Y_1 > 1$.

Proposition 2. *The resultant has no more than 3 real roots, therefore, the system (2) has, according to Theorem 1, no more than 3 real roots.*

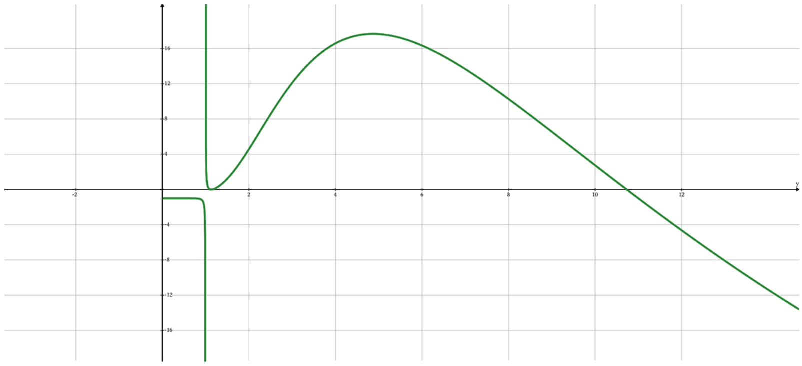

Fig. 3. $\varphi(y)$ has 2 real roots

3. Complex roots of the system

Recall Hadamard's theorem for entire functions of finite order of growth (see, for example, [15]). Expressions $E(u,0) = 1-u$, $E(u,p) = (1-u)e^{u+\frac{u^2}{2}+\cdot+\frac{u^p}{p}}$, $p = 1,2,\ldots$ are called *approximate multipliers*.

If a function $f(t)$ on the complex plane has a finite order of growth ρ and $t_1,\ldots,t_n,\ldots$ its zeros, then there exists an integer $p \leqslant \rho$ independent of n such that the product

$$\prod_{n=1}^{\infty} E\left(\frac{t}{t_n}, p\right) \tag{5}$$

converges for all t if the series converges

$$\sum \left(\frac{r}{r_n}\right)^{p+1},$$

where $r_1, r_2, \ldots$ are the absolute values of the zeros of the function $f(t)$, and this series converges for all values of r if $p+1 \geqslant \rho$.

The product (5) with the smallest of the integers p for which the series converges is called the *canonical product* constructed from zeros $f(t)$, and this smallest p is called its *genus*.

Theorem 2 (Hadamard). *If the an entire function $f(t)$ of order ρ has zeros t_1, t_2, ..., and $f(0) \neq 0$, then*

$$f(t) = e^{Q(t)}P(t),$$

where $P(t)$ is the canonical product constructed from zeros $f(t)$, and $Q(t)$ is a polynomial of degree no higher than ρ.

Consider the resultant

$$F(t) = be^t(\beta\gamma - t(\beta+s)) - st.$$

This is a entire function of the first order of growth.

If it has a finite number of zeros, then according to Hadamard's theorem it will have the form

$$F(t) = e^t \cdot P_m(t),$$

where $P_m(t)$ is a certain polynomial. From here

$$e^t = \frac{st}{b(\beta\gamma - t(\beta+s))} \cdot P_m(t),$$

which is impossible, since there is a transcendental function on the left, and a rational one on the right.

Thus, the resultant $F(t)$ has an infinite number of complex roots t_k, $|t_k| \to +\infty$ as $k \to \infty$.

From the system (3), we express x and y in terms of t and get

$$y = \frac{\gamma}{\gamma - t}, \quad x = \frac{st}{\beta(\gamma - t)}.$$

Then at the points t_k we have $x_k = \dfrac{st_k}{\beta(\gamma - t_k)}$, $y_k = \dfrac{\gamma}{\gamma - t_k}$. Therefore, $x_k \to -\dfrac{s}{\beta}$, $y_k \to 0$ as $k \to \infty$.

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О модели Ариса-Амундсона

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Аннотация. Работа посвящена исследованию вещественных корней системы трансцендентных уравнений Ариса–Амундсона. Показано, что число вещественных корней связано с числом вещественных корней некоторой целой функции (результанта). Исследовано число комплексных корней.

Ключевые слова: системы трансцендентных уравнений, результант, простой корень.