Symbolic Solution of Polynomial Differential Equations Via Cauchy–Riemann Equations.

Applications to Kinetic Differential Equations.

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- No symbolic solution, except
  - in kinetics: Z. Szabó, Rodiguin, and Rodiguina, G. Lente
  - in differential equations: Kamke
- Another subclass will be solved.
- Cauchy–Riemann equations.
- Applications outside kinetics.
- Applications in kinetics.

Cauchy–Riemann–Erugin Equations

- Consider:

$$\dot{x} = u \circ (x, y), \quad \dot{y} = v \circ (x, y), \tag{1}$$

- Assume:

$$\partial_1 u = \partial_2 v, \quad \partial_2 u = -\partial_1 v. \tag{2}$$

- We then write (1) satisfying (2) in the form:

$$\dot{z} = u \circ (x, y) + iv \circ (x, y) = f \circ z \tag{3}$$

- Solve the equation (3) for $z := x + iy$.
- Determine the real and imaginary parts of the solution.
- Find simple realization (few complexes and reaction steps).

Linear Systems

Trivial introductory example

In case of

$$\dot{x} = a + bx + cy, \quad \dot{y} = A + Bx + Cy, \quad (a, b, c, A, B, C \in \mathbb{R})$$

the Cauchy–Riemann conditions imply $C = b, B = -c$. Thus

$$\dot{x} = a + bx + cy, \quad \dot{y} = A - cx + by.$$

If it is to be kinetic as well, then $a, A \geq 0$ and $c = 0$, or

$$\dot{x} = a + bx \quad \dot{y} = A + by.$$

Linear Systems

For $z := x + iy$ one has

$$\dot{z} = a + iA + (b - ic)z, \quad z(0) = x_0 + iy_0 \tag{4}$$

if $x(0) = x_0, y(0) = y_0$. The solution of (4) is

$$z(t) = e^{(b-ic)t}\left(z(0) + \frac{a+iA}{b-ic}\right) - \frac{a+iA}{b-ic},$$

and by applying Euler's formula we obtain

$$x(t) = e^{bt}\left(\cos(bt)(x_0 + \frac{ab-Ac}{b^2+c^2}) + \sin(bt)(y_0 + \frac{ac+Ab}{b^2+c^2})\right) - \frac{ab-Ac}{b^2+c^2},$$
$$y(t) = e^{bt}\left(\sin(bt)(x_0 + \frac{ab-Ac}{b^2+c^2}) + \cos(bt)(y_0 + \frac{ac+Ab}{b^2+c^2})\right) - \frac{ac+Ab}{b^2+c^2}.$$

FHJ Graphs

$\dot{x} = a + bx, \quad \dot{y} = A + by$

The FHJ graphs of one realization for different values of b can be seen in the figures.

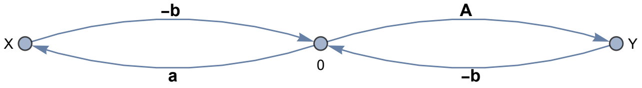


Figure: A reaction with a minimal number of complexes and reaction steps with $b < 0$.

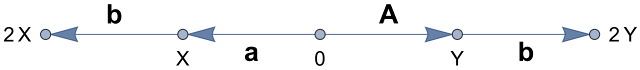


Figure: A reaction with a minimal number of complexes and reaction steps with $b > 0$.

Solution of the kinetic case

$c = 0$

$$x(t) = (x_0 + \frac{a}{b})e^{bt} - \frac{a}{b},$$
$$y(t) = (y_0 + \frac{A}{b})e^{bt} - \frac{A}{b} \quad (t \in \mathbb{R}).$$

Even the general case can be solved with the classical methods.
This is not the case for the systems below, although the computation difficulties may be cumbersome even using the proposed new method.

Second-degree systems

Start from

$$\dot{x} = a \quad +bx + cy \quad +dx^2 + exy \quad +fy^2, \quad \dot{y} = A \quad +Bx + Cy \quad +Dx^2 + Exy$$

It is of Cauchy–Riemann–Erugin form if:

$$\dot{x} = a + bx + cy + dx^2 + exy - dy^2,$$
$$\dot{y} = A - cx + by - \frac{e}{2}x^2 + 2dxy + \frac{e}{2}y^2.$$

For z we have

$$\dot{z} = a + iA + (b - ic)z + (d - i\frac{e}{2})z^2, \quad z(0) = x_0 + iy_0.$$

with the solution:

$$z(t) = z_1 + \frac{z_2 - z_1}{1 - \frac{z(0)-z_2}{z(0)-z_1}e^{(d-i\frac{e}{2})(z_2-z_1)t}} = z_2 + \frac{z_1 - z_2}{1 - \frac{z(0)-z_1}{z(0)-z_2}e^{(d-i\frac{e}{2})(z_1-z_2)t}}$$

z_1, z_2 are roots of $f(z) := a + iA + (b - ic)z + (d - i\frac{e}{2})z^2$.

Kinetic case

$a, A \geq 0$; $d, e \leq 0$, and either $b < 0$, or $b = 0$, or $b > 0$.

$$\dot{x} = a + bx + dx^2 + exy - dy^2, \quad \dot{y} = A + by - \frac{e}{2}x^2 + 2dxy + \frac{e}{2}y^2 + dy.$$

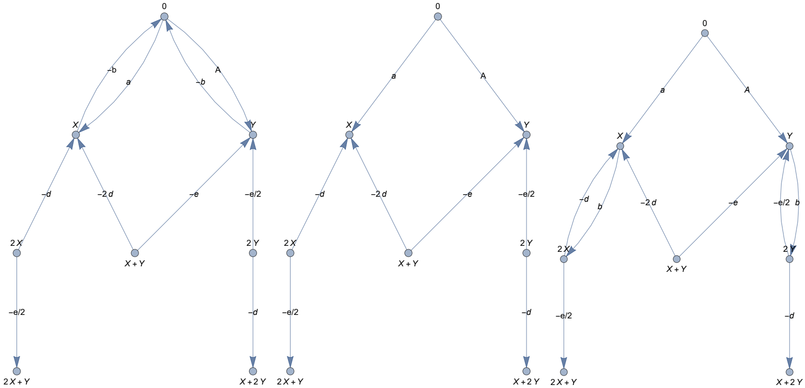


Figure: The canonic realization for $b < 0, b = 0, b > 0$ respectively. Can you find "better" realizations?

A second-degree example

Example

The reaction

$$2\mathrm{X} \xrightarrow{1} \mathrm{X} + \mathrm{Y} \underset{1}{\overset{2}{\longleftrightarrow}} 0, \quad 2\mathrm{Y} \xrightarrow{1} \mathrm{X} + \mathrm{Y}$$

induces the kinetic differential equation

$$\dot{x} = 1 - x^2 - 2xy + y^2, \quad \dot{y} = 1 + x^2 - 2xy - y^2$$

that also satisfies Cauchy–Riemann's conditions. Adjoining the initial conditions $x(0) = 2$, $y(0) = 1$ leads to the (complex) initial value problem:

$$\dot{z} = 1 + i + (-1 + i)z^2, \quad z(0) = 2 + i.$$

A second degree/example, cont.

Complex solution and real and imaginary parts

Example

$$z(t) = \frac{(1+i)(-2ie^{2\sqrt{2}t} + 3(1+\sqrt{2})e^{4\sqrt{2}t} + 3 - 3\sqrt{2})}{-8e^{2\sqrt{2}t} + 3(2+\sqrt{2})e^{4\sqrt{2}t} + 6 - 3\sqrt{2}} \quad (t \in \mathbb{R}).$$

Therefore,

$$x(t) = \frac{2e^{2\sqrt{2}t} + 3(1+\sqrt{2})e^{4\sqrt{2}t} + 3 - 3\sqrt{2}}{-8e^{2\sqrt{2}t} + 3(2+\sqrt{2})e^{4\sqrt{2}t} + 6 - 3\sqrt{2}} \quad (t \in \mathbb{R}),$$

$$y(t) = \frac{-2e^{2\sqrt{2}t} + 3(1+\sqrt{2})e^{4\sqrt{2}t} + 3 - 3\sqrt{2}}{-8e^{2\sqrt{2}t} + 3(2+\sqrt{2})e^{4\sqrt{2}t} + 6 - 3\sqrt{2}} \quad (t \in \mathbb{R}).$$

Proposition

The denominator of the above expressions is never zero.

Third-degree systems

with complete solution

Start from:

$$\dot{x} = a + bx + cy + dx^2 + exy + fy^2 + gx^3 + hx^2y + jxy^2 + ky^3,$$
$$\dot{y} = A + Bx + Cy + Dx^2 + Exy + Fy^2 + Gx^3 + Hx^2y + Jxy^2 + Ky^3.$$

It is of Cauchy–Riemann–Erugin form if:

$$\dot{z} = a + iA + (b - ic)z + (d - i\frac{e}{2})z^2 + (h - i\frac{g}{3})z^3, \quad z(0) = x_0 + iy_0.$$

The solution is:

$$(z(t) - z_1)(z(t) - z_2)(z(t) - z_3) =$$

$$(z(0) - z_1)(z(0) - z_2)(z(0) - z_3)\exp{(z_1 - z_2)(z_1 - z_3)(z_2 - z_3)(a - i\frac{b}{3})t},$$

where z_1, z_2 and z_3 are the roots of the polynomial
$f(z) := a + iA + (b - ic)z + (d - i\frac{e}{2})z^2 + (h - i\frac{g}{3})z^3$

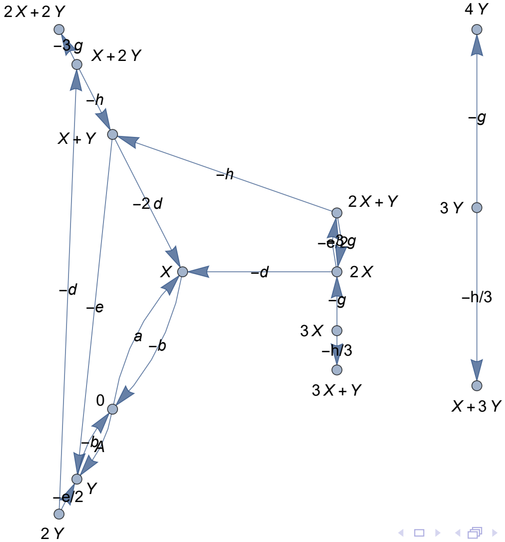
Kinetic case

$$\dot{x} = a + bx + dx^2 + exy - dy^2 + gx^3 + hx^2y - 3gxy^2 - \frac{h}{3}y^3,$$
$$\dot{y} = A + by - \frac{e}{2}x^2 + 2dxy + \frac{e}{2}y^2 - \frac{h}{3}x^3 + 3gx^2y + hxy^2 - gy^3.$$

Note that terms of the same degree only depend on **two parameters** even in the general case.

FHJ Graph

realizations for $b < 0$ and $g < 0$



A third-degree example

Example

The initial value problem:

$$\dot{x} = -3x + 6xy + x^3 - 3xy^2, \quad \dot{y} = 1 - 3y - 3x^2 + 3y^2 + 3x^2y - y^3,$$
$$x(0) = 1, \quad y(0) = 2.$$

can be rewritten as: $\dot{z} = (z - i)^3, \quad z(0) = 1 + 2i$ with the solution

$$z(t) = i + \frac{2}{\sqrt{1-8t}}, \quad (t \in]-\infty, \frac{1}{8}[),$$

thus $x(t) = \frac{2}{\sqrt{1-8t}}, \quad (t \in]-\infty, \frac{1}{8}[), y(t) = 1, \quad (t \in \mathbb{R}).$

Can we have such a simple cubic equation in kinetics?

Unfortunately, not.

Proposition

The right-hand side $(az + bi)^3$, $\quad (a, b \in \mathbb{R})$ *can never come from a kinetic differential equation.*

R^{th}-Degree Systems

Seemingly no kinetic relevance, but nice.

Theorem

Let $R \in \mathbb{N}_0$, and suppose that the polynomials u, v defined as

$$u(x,y) := \sum_{r=0}^{R}\sum_{s=0}^{r} a_r^s x^{r-s} y^s, \quad v(x,y) := \sum_{r=0}^{R}\sum_{s=0}^{r} A_r^s x^{r-s} y^s$$
$$(a_r^s, A_r^s \in \mathbb{R}, s = 0,1,2,\dots,r; r = 0,1,2,\dots,R)$$

satisfy the Cauchy–Riemann equations. Then, for the complex-valued function $z := x + iy$ one has

$$\dot{z} = a_0^0 + iA_0^0 + \sum_{r=1}^{R}(a_r^0 - i\frac{a_r^1}{r})z^r.$$

(Two parameters are left!—Kinetic: $a_0^0, A_0^0 \geq 0, a_1^1 = 0$.)

Proof

A direct comparison of the coefficients in the Cauchy–Riemann equations gives

$$A_r^s = \frac{r-s+1}{s} a_r^{s-1} \qquad (s = 1, 2, 3, \dots, r; r = 1, 2, 3, \dots, R), \tag{5}$$

$$A_r^s = -\frac{s+1}{r-s} a_r^{s+1} \qquad (s = 0, 1, 2, \dots, r-1; r = 1, 2, 3, \dots, R). \tag{6}$$

Eqs.(5) and (6) imply

$$a_r^s = -\frac{(r-s+2)(r-s+1)}{s(s-1)} a_r^{s-2} \quad (s = 2, 3, \dots, r; r = 2, 3, \dots, R). \tag{7}$$

The recursive application of (5) and (7) proves the theorem.

Generalized Cauchy–Riemann equations

Suppose, u and v are the real and imaginary parts of the multivariate complex function f. Then:

$$\frac{\partial u}{\partial x_j} = \frac{\partial v}{\partial y_j}, \quad \frac{\partial u}{\partial y_j} = -\frac{\partial v}{\partial x_j}.$$

If we consider differential equations in four variables then we obtain: $\dot{z}_1 = f_1 \circ (z_1, z_2)$, $\dot{z}_2 = f_2 \circ (z_1, z_2)$.where, $f_1 = u_1 + iv_1$ and $f_2 = u_2 + iv_2$. Let us start from:

$$\begin{aligned}
\dot{x}_1 &= j_1 x_1^2 + j_2 x_2^2 + j_3 y_1^2 + j_4 y_2^2 \\
&+ j_5 x_1 x_2 + j_6 y_1 y_2 + j_7 x_1 y_1 + j_8 x_1 y_2 + j_9 x_2 y_1 + j_{10} x_2 y_2 \\
&+ j_{11} x_1 + j_{12} x_2 + j_{13} y_1 + j_{14} y_2 + j_{15}, \qquad (8) \\
\dot{y}_1 &= k_1 x_1^2 + k_2 x_2^2 + k_3 y_1^2 + k_4 y_2^2 \\
&+ k_5 x_1 x_2 + k_6 y_1 y_2 + k_7 x_1 y_1 + k_8 x_1 y_2 + k_9 x_2 y_1 + k_{10} x_2 y_2 \\
&+ k_{11} x_1 + k_{12} x_2 + k_{13} y_1 + k_{14} y_2 + k_{15}, \qquad (9)
\end{aligned}$$

Multivariate case, contd.

$$
\begin{aligned}
\dot{x}_2 &= J_1 x_1^2 + J_2 x_2^2 + J_3 y_1^2 + J_4 y_2^2 \\
&\quad + J_5 x_1 x_2 + J_6 y_1 y_2 + J_7 x_1 y_1 + J_8 x_1 y_2 + J_9 x_2 y_1 + J_{10} x_2 y_2 \\
&\quad + J_{11} x_1 + J_{12} x_2 + J_{13} y_1 + J_{14} y_2 + J_{15}, \qquad (10) \\
\dot{y}_2 &= K_1 x_1^2 + K_2 x_2^2 + K_3 y_1^2 + K_4 y_2^2 \\
&\quad + K_5 x_1 x_2 + K_6 y_1 y_2 + K_7 x_1 y_1 + K_8 x_1 y_2 + K_9 x_2 y_1 + K_{10} x_2 y_2 \\
&\quad\quad + K_{11} x_1 + K_{12} x_2 + K_{13} y_1 + K_{14} y_2 + K_{15}. \qquad (11)
\end{aligned}
$$

We arrive at:

$$
\dot{z}_1 = (j_1 - i\frac{j_7}{2}) z_1^2 + j_{11} z_1 + j_{12} z_2 + (j_{15} + i k_{15}), \qquad (12)
$$

$$
\dot{z}_2 = (J_1 - i\frac{J_7}{2}) z_2^2 + J_{11} z_1 + J_{12} z_2 + (J_{15} + i K_{15}). \qquad (13)
$$

Comparison with the method of Calogero

Calogero and Payandeh, 2021

Theorem

Consider

$$\dot{x}_1 = a_0^0 + a_1^0 x_1 + a_1^1 x_2 + a_2^0 x_1^2 + a_2^1 x_1 x_2 + a_2^2 x_2^2, \tag{14}$$

$$\dot{x}_2 = A_0^0 + A_1^0 x_1 + A_1^1 x_2 + A_2^0 x_1^2 + A_2^1 x_1 x_2 + A_2^2 x_2^2, \tag{15}$$

and assume that

$$4a_2^2 A_2^0 - a_2^1 A_2^1 = 0, \quad A_1^0(2a_2^0 - A_2^1) + 2A_2^0(A_1^1 - a_1^0) = 0 \tag{16}$$

$$a_2^1 A_1^0 - 2a_1^1 A_0^2 = 0, \quad 2(-a_2^1 + A_2^2)A_2^0 + (2a_2^0 - A_2^1)A_2^1 = 0 \tag{17}$$

hold. Then, the explicit symbolic solution of (14)–(15) *can be constructed by applying the steps of the algorithm given in the paper.*

Comparison with the method of Calogero

- Cauchy–Riemann–Erugin systems satisfy the Calogero–Payandeh equalities (their method implies ours) **generally...**
- Not all Cauchy–Riemann–Erugin systems can be solved by the method of Calogero and Payandeh; for example, the linear systems cannot, because they do not satisfy the above-mentioned technical conditions.
- There is a significant overlap in the scopes of the two methods concerning two-variable second-degree systems.
- Computational difficulties. We have seen that in the linear case, our method requires lengthier calculations than the traditional approach. However, in the second-degree case, our method and Colagero's are effective as opposed to the traditional methods.

Summary, further possibilities, acknowledgement

We have shown how to solve

- some further kinetic differential equations, and
- some further polynomial differential equations

Further possible extensions

- Reaction-diffusion equations
- Approximation of "almost" CRE type equations
- Use of quaternions?

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References

F. Calogero and F. Payandeh.
Solution of the system of two coupled first-order ODEs with second-degree polynomial right-hand sides.
Mathematical Physics, Analysis and Geometry, 24(3):29, 2021.

J. Giné and V. G. Romanovski.
Integrability conditions for Lotka–Volterra planar complex quintic systems.
Nonlinear Analysis: Real World Applications, 11(3):2100–2105, 2010.

E. Kamke.
Differentialgleichungen: Lösungsmethoden und Lösungen.
Springer-Verlag, 2013.

G. Lente.
Deterministic Kinetics in Chemistry and Systems Biology: The Dynamics of Complex Reaction Networks.
Springer, 2015.

N. M. Rodiguin and E. N. Rodiguina.
Consecutive Chemical Reactions: Mathematical Analysis and Development (English edn.).
D. Van Nostrand Co., New York, 1964.

Z. G. Szabó.
Kinetic characterization of complex reaction systems.
In Ch. Bamford and C. F. H. Tipper, editors, *Comprehensive Chemical Kinetics*, volume 2, chapter 1, pages 1–80.
Elsevier, Amsterdam, Oxford, New York, 1969.