The Unifying View on Ordinary Differential Equations and Automatic Differentiation, **yet with a Gap to Fill**

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Conventions

Differentiation is understood as for holomorphic functions in the complex plane.

Automatic Differentiation is understood as the *optimized* formulas for *n*-order differentiation of composite functions (in contrast to non-optimized formulas of Faa di-Bruno).

ODEs are specifically regarded as **generators** of the *n*-order derivatives and of the Taylor expansion of the solution.

Elementary functions are defined wider than the conventional list by Liouville. Elementariness is viewed as a property to satisfy explicit rational ODEs.

What was unified?

The ideas seemingly unrelated such as…

- General elementary functions;
- The class of elementary ODEs closed with regard to their solutions;
- The transformations of all elementary ODEs to the special formats, ***enabling...***
  - Optimized computability of *n*-order derivatives, ***enabling...***
    - The modern Taylor integration method as a tool of efficient analytic continuation, ***revealing…***
    - Special points unreachable via integration of ODEs – the ***regular*** points of the solution where the ***elementariness*** is ***violated***.

…comprise the pieces of ***one big picture – the Unifying View*** [2]

The two definitions of ***elementariness***:

vector elementariness vs. ***scalar elementariness***

A vector-function $\boldsymbol{u(t)}=(u_1, \ldots, u_m)$ is elementary at and near an initial point if it satisfies (generally) a wider system of $n \geq m$ rational ODEs

$$\begin{cases} \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ u_k' = r_k(u_1, \ldots, u_n)\ ; \quad k = 1, \ldots, n \\ \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \end{cases}$$

regular at the initial point.

Since R. Moore (1960) it is the main definition. The fundamental results in the Unifying view were proved with namely this definition (except one in slide 3.1 not yet proved for this definition)

A function $u_1(t)$ is elementary at and near an initial point if it satisfies a rational m-order ODE

$$u_1^{(m)} = R(u_1, u_1', \ldots, u_1^{(m-1)})$$

regular at the initial point.

The equivalence of both definitions is not established, depending on the not yet proved **Conjecture** (slide 6). With this definition it is *not known* how to prove the fundamental results in the Unifying view (except one result in slide 3.1)

New type of special points

proven only for the *scalar elementariness* [1]

Theorem: The function $x(t) = \frac{e^t - 1}{t}$ and several others (see below) can satisfy **rational ODE** $x^{(m)} = R(x, x', \ldots, x^{(m-1)})$ **only if it is singular at t=0**, hence it can satisfy **no polynomial ODE** $x^{(m)} = P(x, x', \ldots, x^{(m-1)})$.

This Theorem means that the point $t=0$ represents a new type of a special point in the function $x(t)$: the point where its <u>*scalar elementariness*</u> is violated. However it is not known whether its <u>*vector-elementariness*</u> is violated at $t=0$ – unless both definitions are equivalent, which takes place if **the Conjecture** (slide 6) is true.

An infinite class of functions similar to $x(t)$ in that their *scalar elementariness* at $t=0$ is violated was found. Here are some examples:

$$\frac{e^t - 1}{t} \qquad \frac{\sin t}{t} \qquad \frac{\ln(t+1)}{t} \qquad \cos t^{1/2}$$

and also the solution of the IVP $tx'' - x = 0, \quad x(0) = 0, \quad x'(0) = 1.$

The gap: A not yet established equivalence between…

One n-order rational ODE (in u_1) at a *regular point*	and	System of m 1st order rational ODEs at a *regular point*
$u_1^{(n)} = f(t, u_1, u_1', \ldots, u_1^{(n-1)})$		$\begin{cases} \cdot\ \cdot\ \cdot\ \cdot\ \cdot \\ u_k' = g_k(t, u_1, \ldots, u_m)\ ; \quad k = 1, \ldots, m \\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot \end{cases}$

Here the terms ***rational*** and ***regular*** are critical. The equivalency does take place if arbitrary holomorphic right hand sides are allowed, and also for rational ODEs if we do not ask regularity of the target ODE at the initial point – see the Table:

Source	*Target*	*The target is…* Rational	*The target is…* Holomorphic
One n-order ODE →	System of m 1st order ODEs	Yes	Yes
System of m 1st order ODEs →	One *regular* n-order ODE	?	Yes
	One possibly *singular* n-order ODE	Yes	

→ means "*converts into*"

Fundamental transforms of the elementary systems

$$\begin{cases} \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ u_k{}' = g_k(t, u_1, \ldots, u_m)\ ; \quad k = 1, \ldots, m \\ \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \end{cases}$$

An explicit 1st order system of ODEs whose right-hand sides g_k comprise an **elementary** vector-function converts to. . .

A system of ODEs whose right-hand sides are **rational** functions.

At regular points it further converts to. . .

A **canonical** system: an explicit system of algebraic and differential equations for computing n-order derivatives requiring $O(n^2)$ operations.

A system, whose right-hand sides are **polynomials**. It further converts to...

Polynomial ODEs of **degree ≤ 2**. It further converts to polynomial ODEs of degree 2 with ...

...with coefficients **0, 1 only** (Kerner)

…with **squares** only (Charnyi)

The Conjecture (for rational system)

Consider an IVP for a source system of m rational ODEs

$$x' = \frac{P_1(t, x, y, z, \ldots)}{Q_1(t, x, y, z, \ldots)}$$

$$y' = \frac{P_2(t, x, y, z, \ldots)}{Q_2(t, x, y, z, \ldots)}$$

$$\cdots\cdots\cdots\cdots$$

with all the denominators $Q_i|_{t=0} \neq 0$ so that the IVP is regular and has a unique solution $(x, y, z, \ldots)$ near $t = t_0$, in particular the derivatives $x^{(n)}|_{t=t0} = a_n, \quad n = 0, 1, 2, \ldots$

Then there exists an *explicit rational* ODE of some order n

$$x^{(n)} = \frac{F(t, x, x', \ldots, x^{(n-1)})}{G(t, x, x', \ldots, x^{(n-1)})} \qquad x^{(k)}|_{t=t0} = a_k, \quad k = 0, 1, \ldots, n-1$$

with a denominator $G|_{t=t0} \neq 0$ so that this ODE is regular at $t = t_0$ and has $x(t)$ as its unique solution. Or…

Or there exists an *implicit polynomial* ODE $H(t, x, x', \ldots, x^{(n-1)}, x^{(n)}) = 0$ regular at $t = 0$, meaning

$$\left.\frac{\partial H}{\partial X_n}\right|_{t=t0} \neq 0, \qquad (\ X_n = x^{(n)} \ ).$$

The Conjecture (for polynomial system)

Consider an IVP for a source system of m polynomial ODEs

$$x' = P_1(t, x, y, z, \ldots)$$
$$y' = P_2(t, x, y, z, \ldots)$$
$$\ldots\ldots\ldots\ldots$$

so that the IVP is regular and has a unique solution $(x, y, z, \ldots)$ near $t = t_0$, in particular the derivatives $x^{(n)}|_{t=t0} = a_n$, $n = 0, 1, 2, \ldots$ Then there exists an explicit rational ODE of some order n

$$x^{(n)} = \frac{F(t, x, x', \ldots x^{(n-1)})}{G(t, x, x', \ldots x^{(n-1)})} \qquad x^{(k)}|_{t=t0} = a_k, \quad k=0, 1, \ldots, n-1$$

with a denominator $G|_{t=t0} \neq 0$ so that this ODE is regular at $t = t_0$ and has $x(t)$ as its unique solution. Or…

Or there exists an *implicit polynomial* ODE $H(t, x, x', \ldots, x^{(n-1)}, x^{(n)}) = 0$ regular at $t = t_0$.

The Conjecture (squares only system)

Consider an IVP for a source system of m polynomial ODEs

$$x' = a_1x^2 + b_1y^2 + c_1z^2 + \dots$$
$$y' = a_2x^2 + b_2y^2 + c_2z^2 + \dots$$
$$\cdots\cdots\cdots\cdot$$

so that the IVP is regular and has a unique solution $(x, y, z, \dots)$ near $t = t_0$, in particular the derivatives $x^{(n)}|_{t=t0} = a_n$, $n = 0, 1, 2, \dots$ Then there exists an explicit rational ODE of some order n

$$x^{(n)} = \frac{F(t, x, x', \dots x^{(n-1)})}{G(t, x, x', \dots x^{(n-1)})} \qquad x^{(k)}|_{t=t0} = a_k, \quad k=0, 1, \dots, n-1$$

with a denominator $G|_{t=t0} \neq 0$ so that this ODE is regular at $t = t_0$ and has $x(t)$ as its unique solution.

For this form in squares only **the Conjecture** is proved, but only for $m=2$.

*Can we ask that the target be **explicit polynomial** rather than **rational** n-order ODE?*

If the Conjecture claimed as though the source system may be converted into an *explicit* polynomial ODE $x^{(n)} = F(t, x, x', \ldots x^{(n-1)})$ rather than into an *implicit* polynomial ODE, *the Conjecture would be false*!

A counter example illustrating this is the entire function

$$x(t) = \frac{e^t - 1}{t}$$

The function $x(t)$ satisfies the polynomial *system* of ODEs

$$x' = x - xy + y \qquad x|_{t=1} = e - 1$$

$$y' = -y^2 \qquad y|_{t=1} = 1, \qquad (\, y = 1/t \,)$$

(say at $t=1$), but $x(t)$ can satisfy *no* polynomial ODE

$$x^{(n)} = F(t, x, x', \ldots x^{(n-1)})$$

(as proved in 2008 by me and Flanders). Though $x(t)$, as holomorphic function may be analytically continued from $t=1$ to 0, $x(t)$ cannot be integrated from $t=1$ to 0 as the solution of the system, because the point $t=0$ is unreachable due to singularity of $y(t)$ at this point.

Conclusion: The target ODE in the Conjecture may be either **implicit polynomial** or **explicit rational** only.

In a **rational** ODE the denominator which is nonzero at one point $(t, x, x', \ldots x^{(n-1)})$, may reach zero at *other* points of the phase space. To ask for a target ODE with a nonzero denominator presumes that *different* target ODEs may be required for *different* initial points of the system.

The general setting

Conversion from a source system
$$\boxed{\begin{aligned} x' &= F(t, x, y, z) \\ y' &= G(t, x, y, z) \\ z' &= H(t, x, y, z) \end{aligned}}$$
of polynomial ODEs -

- to an **infinite system of ODEs** for $x^{(n)}$, $n=1, 2, \dots$:

$$x' = F_1(t, x, y, z) = F(t, x, y, z)$$

. . . .

$$x^{(n)} = F_n(t, x, y, z)$$

$$x^{(n+1)} = F_{n+1}(t, x, y, z) = \frac{\partial F_n}{\partial t} + \frac{\partial F_n}{\partial x} x' + \frac{\partial F_n}{\partial y} y' + \frac{\partial F_n}{\partial z} z' = \frac{\partial F_n}{\partial t} + \frac{\partial F_n}{\partial x} F + \frac{\partial F_n}{\partial y} G + \frac{\partial F_n}{\partial z} H$$

. . . .

This infinite system is consistent because it has the unique solution $x(t)$

If F, G, H are …	… then $F_1, F_2, F_3, \dots$ are …
Polynomials	Polynomials F_n of growing degrees
Forms of degree 2	Forms; degree of F_n is $n+1$
Forms in squares only	Forms F_n of a special structure

The general setting for forms in squares only

Conversion from a source system of ODEs in squares only

$$\begin{aligned} x' &= F_1(x, y, z) = a_{11}x^2 + a_{12}y^2 + a_{13}z^2 \\ y' &= G_1(x, y, z) = a_{21}x^2 + a_{22}y^2 + a_{23}z^2 \\ z' &= H_1(x, y, z) = a_{31}x^2 + a_{32}y^2 + a_{33}z^2 \end{aligned}$$

- to an infinite sequence of ODEs for $x^{(n)}$, $n=1,2,\ldots$

$$x' = F_1(x, y, z) = a_{11}x^2 + a_{12}y^2 + a_{13}z^2$$

. . . .

$$x^{(n+1)} = F_{n+1}(x, y, z) = \sum_{i=0}^{n} C_n^i(a_{11}F_iF_{n-i} + a_{12}G_iG_{n-i} + a_{13}H_iH_{n-i})$$

. . . .

where $F_0 = x, G_0 = y, H_0 = z,$

$$G_{n+1}(x, y, z) = \sum_{i=0}^{n} C_n^i(a_{21}F_iF_{n-i} + a_{22}G_iG_{n-i} + a_{23}H_iH_{n-i})$$

$$H_{n+1}(x, y, z) = \sum_{i=0}^{n} C_n^i(a_{31}F_iF_{n-i} + a_{32}G_iG_{n-i} + a_{33}H_iH_{n-i})$$

Questions about elimination of $y, z, \dots$ from the infinite system

$$x' = F_2(t, x, y, z, \dots)$$

$$\dots\dots\dots\dots\dots\dots$$

$$x^{(n-1)} = F_n(t, x, y, z, \dots) \qquad \text{(forms of degree } n)$$

$$x^{(n)} = F_{n+1}(t, x, y, z, \dots)$$

$$\dots\dots\dots\dots\dots\dots$$

in order to obtain an implicit polynomial ODE $P(t, x, x', \dots, x^{(n)})=0$:

The **ultimate goal** is to *eliminate* the undesired variables $y, z, \dots$ picking some m-1 equations of the infinite system, and to ensure that the obtained implicit n-order polynomial ODE $P(t, x, x', \dots, x^{(n)})=0$ is **not singular** at the initial point.

Do there exist m equations which are at least invertible in $y, z, \dots$ at the initial point (the Jacobian $J|_{t=0} \neq 0$) ?

- Not necessarily. Say, all $x^{(n)} = x = e^t$. Therefore…

We can not pick *any* m-1 equations of the infinite system for the elimination process and be sure that the process succeeds (does not end up with a zero polynomial)? However…

For big enough n there always exists an implicit polynomial ODE

$$P(t, x, x', x'', \dots, x^{(n)})=0$$

such that $P(t, x, F_2, F_3, \dots, F_{n+1})$

is a zero polynomial (see next slide).

How that implicit polynomial ODE $P(t, x, x', \ldots, x^{(n)})=0$ emerges[1]…

Consider the forms $F_n(t, x, y, z, \ldots)$ of degrees n and their weighted products $F_1^{\alpha} F_2^{\beta} \ldots F_n^{\omega}$ such that $1\alpha+2\beta+\ldots+n\omega = n$ (here $F_1 = bx+ct$).

The number of such products is the number of *partitions* of n, and it grows exponentially like $2^{\sqrt{n}}$.

Yet every monomial $F_1^{\alpha} F_2^{\beta} \ldots F_n^{\omega}$ is a form in $(t, x, y, z, \ldots)$ of degree n. The number of monomials in $t, x, y, z, \ldots$ in *n*-order forms in r variables grows as C^{r-1}_{n+r-1}: slower than the number of partitions. Beginning from a big enough n therefore some subset of monomials $F_1^{\alpha} F_2^{\beta} \ldots F_n^{\omega}$ must be *linearly dependent* satisfying the relation

$$\sum a_{\alpha\beta\ldots\omega} F_1^{\alpha} F_2^{\beta} \ldots F_n^{\omega} = 0$$

(all $a_{\alpha\beta\ldots\omega}$ being nonzero), which corresponds to a polynomial ODE $P(t, x, x', \ldots, x^{(n-1)})=0$. However we do not know which of $F_1^{\alpha} F_2^{\beta} \ldots F_n^{\omega}$ comprise the basis, and which are dependent.

May we ask that for a big enough n, $F_n \in \mathbf{Span}\{F_1^{\alpha} F_2^{\beta} \ldots F_{n-1}^{\tau}\}$? (No. That would generate an explicit polynomial ODE $x^{(n-1)} = F(t, x, x', \ldots x^{(n-2)})$ and we know that it is not always possible).

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[1]) The idea of the proof belongs to the late Harley Flanders

Say, an obtained polynomial ODE $P(t, x, x', ..., x^{(n)})=0$ happened to be singular so that

$$\left.\frac{\partial P}{\partial X_n}\right|_{t=0} = 0.$$

Is it possible to modify $P = 0$ in some way, or to obtain another polynomial ODE $Q = 0$ (having the same solution $x(t)$) so that $Q = 0$ is regular? - Not via differentiation d^k/dt^k …

If differentiation d^k/dt^k applies to a singular ODE $P = 0$, all the higher order ODEs $(d/dt)^k P = 0$ will be singular with the same critical factor as above.

Otherwise, we can seek another ODE $Q = 0$ of a higher order and of a higher degree with (unknown) indefinite coefficients asking that the ODE $Q = 0$ be regular. Then the unknown coefficients of Q are solutions of a certain linear algebraic system (which include the solution for $P = 0$). So far, no progress was achieved in this direction either.

Some conclusions

- The reported open case about equivalency of a system of ODEs to one n-order ODE could well be posed (or solved?) already in the 19th century. The question is so natural that it begs for the answer.
- This open case also presents a gap in the otherwise coherent theory – the unifying view on ODEs and AD.

Let's unite our efforts and find a proof of the Conjecture!

Thank you for the attention

References

1. A. Gofen, Unremovable "removable" singularities. Complex Variables and Elliptic Equations, Vol. 53, No. 7, July 2008, pp. 633-642. (Also here).
2. A. Gofen, The ordinary differential equations and automatic differentiation unified. Complex Variables and Elliptic Equations, Vol. 54, No. 9, September 2009, pp. 825-854. (Also here).
3. The Conjecture: the surrounding and what is known (2019)