What Might “Understand a Function” Mean?

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Abstract. Many functions in classical mathematics are largely defined in terms of their derivatives, so Bessel’s function is “the” solution of Bessel’s equation, etc. For definiteness, we need to add other properties, such as initial values, branch cuts, etc. What actually makes up “the definition” of a function in computer algebra? The answer turns out to be a combination of arithmetic and analytic properties.

1 Introduction

The claim is often made (these days generally informally) that a given computer algebra system “understands” tan, or some other function, generally a function defined through some analytic process. Here we ask three questions.

1. What does this mean?
2. What might it mean?
3. How should a system “understand” such a new function?

More generally, to what extent does such an analytic process, or a built-in function, define a function, and what properties does such a function have?

Notation: throughout this paper, the term ‘function’ means a total[1] function from $\mathbf{R}$ to $\mathbf{R}$ or $\mathbf{C}$ to $\mathbf{C}$. The principles apply to functions $\mathbf{R}^n$ to $\mathbf{R}$ or $\mathbf{C}^n$ to $\mathbf{C}$, but we shall not consider such functions here. C will denote an arbitrary field of constants (of characteristic zero). From the point of view of differential algebra, x will be the variable of differentiation/integration, i.e. $x' = 1$. From the point of view of functions, x is the variable being evaluated. Functions such as log have the meaning given in [1], as refined by [9].

We remind the reader of a couple of definitions from differential algebra.

Definition 1. *θ is said to be* elementary *over a differential field K if one of the following is true:*

(a) *θ is algebraic over K;*
(b) *$\theta' = \eta'/\eta$ for some $\eta \in K$ (we write $\theta = \log \eta$);*
(c) *$\theta' = \eta'\theta$ for some $\eta \in K$ (we write $\theta = \exp \eta$).*

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[1] Or at least “total with singularities”. We then define equality $f = g$ to mean that, at all x where f and g are both defined, $f(x) = g(x)$ [12]. A full exposition of removable singularities would be a paper in itself.

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The object f is said to be elementary over K if it can be expressed in some $K(\theta_1, \ldots \theta_n)$ with each θ_i elementary over $K(\theta_i \ldots \theta_{i-1})$. If K is omitted, $C(x)$ is assumed.

Much of the theory of integration [5] is cast in terms of elementary functions. We can generalise the concept as follows.

Definition 2. *θ is said to be* Liouvillian *over a differential field K if one of the following is true:*

(a) *θ is algebraic over K;*
(b) *$\theta' = \eta$ for some $\eta \in K$ (we write $\theta = \int \eta$);*
(c) *$\theta' = \eta'\theta$ for some $\eta \in K$ (we write $\theta = \exp \eta$).*

The object f is said to be Liouvillian over K if it can be expressed in some $K(\theta_1, \ldots \theta_n)$ with each θ_i Liouvillian over $K(\theta_i \ldots \theta_{i-1})$. If K is omitted, $C(x)$ is assumed.

Note that, even if K is a field of functions embedded in $\mathbf{R} \to \mathbf{R}$ (or $\mathbf{C} \to \mathbf{C}$), there is no requirement that f should be such a function: we have merely stated a property of the *abstract* derivative of f. In practice, we also want each θ_i to be an elementary (resp. Liouvillian) *function* as well, i.e. that its numerical values, as well as its differential properties, be specified.

Definition 3. *Let K be a field of functions in $\mathbf{R} \to \mathbf{R}$ (or $\mathbf{C} \to \mathbf{C}$). $f(x)$, a function from $\mathbf{R} \to \mathbf{R}$ (or $\mathbf{C} \to \mathbf{C}$) is said to be an* elementary *(resp.* Liouvillian*) function if it lies in some elementary (resp. Liouvillian) extension $K(\theta_1, \ldots \theta_n)$ of K.*

However, even this is not enough.

Definition 4. *Let K be a field of functions in $\mathbf{R} \to \mathbf{R}$ (or $\mathbf{C} \to \mathbf{C}$). $f(x)$, a function from $\mathbf{R} \to \mathbf{R}$ (or $\mathbf{C} \to \mathbf{C}$) is said to be a* proper elementary *(resp.* Liouvillian*) function if it lies in some elementary (resp. Liouvillian) extension $K(\theta_1, \ldots \theta_n)$ of K, where each is θ_i proper elementary (resp. Liouvillian) over $K(\theta_i \ldots \theta_{i-1})$, and, for each x where both are defined,*

$$(f')(x) = \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon}. \tag{1}$$

Furthermore, we require that the right-hand side of (1) be defined almost everywhere.

As examples of the various pathologies that can occur, we give the following examples, where K is the field $\mathbf{Q}(x)$ of rational functions $\mathbf{C} \to \mathbf{C}$ equipped with the derivation induced by $x' = 1$.

1. $K(\theta)$ where $\theta' = \frac{1}{x}$. Here θ is merely an abstract symbol, not a function at all.
2. $K(\theta)$ where $\theta' = \frac{1}{x}$ and $\theta : x \mapsto 0$. Here θ is elementary, and a function, but not a proper elementary function since equation (1) is violated.

3. $K(\theta)$ where $\theta' = \frac{1}{x}$ and $\theta : x \mapsto \begin{cases} 1 & x \in \mathbf{Q} \\ 0 & x \notin \mathbf{Q} \end{cases}$. Here equation (1) is satisfied, but only because the right-hand side is nowhere defined, and therefore this falls foul of the last clause in definition 4.
4. $K(\theta = \log(x)+42)$ where $\theta' = \frac{1}{x}$. This is indeed a proper elementary function in the sense of definition 4, even though it is not "what we all mean by" $\log x$.
5. $K(\theta)$ where $\theta' = \frac{1}{x}$ and $\theta : x \mapsto \log x + \begin{cases} 0 & x > 0 \\ -i\pi & x < 0 \end{cases}$. As a function $\mathbf{R} \to \mathbf{R}$ this is $\log |x|$, and is a proper elementary function in our sense. Whether it is "what we all mean by" $\log x$ has been debated elsewhere [31].

2 What Does It Mean?

1. Numerical evaluation. Generally speaking, if the input is real, this means real evaluation where possible. To do numerical evaluation, one has to choose the branch cuts (if there are any) of the relevant function — see [9].
2. Plotting — generally a consequence of the above, though more can in fact be done [2] if the function is better "understood".
3. Differentiation. This property is generally hard-coded for some functions, with an extension mechanism for others, e.g. defining `diff/f` for a function `f` in Maple, or giving a symbol a `!*DF` property in REDUCE.
4. Integration. This is the difficult one, and is discussed during much of the rest of this paper.
5. Special values. This is not the same as numerical evaluation (though the two can easily be confused): $\sin(\pi)$ is precisely 0, whereas

$$\sin(3.14159265358979323846264 33) = 8.32795 \times 10^{-26}$$

(with an appropriate setting of `Digits` or the equivalent). This is a case where the precise nature, and the adherence [4], of the branch cuts is critical: $\log(-1.0 + \epsilon i)$ might be near either of πi or $-\pi i$, but $\log(-1)$ has (with the standard definitions) to be πi.
6. Simplification. Some of this is built in, e.g. for even/odd functions, as in $\sin(-x)$ and $\cos(-x)$: other simplifications can be invoked via commands such as `expand` or `collect`, or by giving functions properties (REDUCE).

3 Defining Functions

There are various ways by which new functions can be defined.

3.1 By Explicit Formulae, Normally Composition

"Let $h(x) = f(g(x))$". Provided that f and g are "understood", and that the system knows the chain rule, this more or less means that the system "understands" h, at least as well as it understands $f(g(x))$. This may be "not at all", as in the case of the real-valued function $\log \log \sin x$, which is nowhere defined.

Numerical and symbolic evaluation and plotting are, at least conceptually, simple. Difficulties can arise, though, if we expect the algebra system to remove removable singularities, i.e.

$$h(x) = \begin{cases} f(g(x)) & g(x) \text{ well-defined} \\ \lim_{y\to x} f(g(y)) & \text{otherwise.} \end{cases} \tag{2}$$

Expecting a system to perform (2) automatically is, in the author's opinion, expecting too much, though possibly systems might provide some help in this direction. Problems ought, where possible, to be signalled at definition time rather than at use time, so an explicit, tool-supported, definition mechanism is probably what should be provided. An example of what can go wrong is provided by $\arctan\left(\frac{1}{1-x}\right)$, where there is a jump discontinuity at $x = 1$ corresponding to the "discontinuity at infinity" of arctan.

3.2 By Indefinite Integration

One might define erf to be the integral[2] of $\exp(-x^2)$, or, more formally,

$$\operatorname{erf}(x) = \int_0^x \exp -t^2 \, \mathrm{d}t,$$

in order to fix the constant of integration.

Such a definition tells us explicitly how to evaluate the function numerically[3], and implicitly how to differentiate the new function. Risch's algorithm [27,5] will tell us whether this is a 'new' function or can be defined in terms of previously known ones (though current systems are not always good at getting the constant of integration right).

Indefinite integration is much harder. All integration algorithms for elementary functions rely on Liouville's principle: that the only new elementary functions which can be introduced are logarithms, and that only with constant coefficients. This theorem remains true even if the integrand is not elementary. However, this is not what one actually wants. Just as we added a new logarithm to compute $\int \frac{1}{x \log x} = \log\log x$, we would like to add new error functions, or whatever is in the domain of discourse, and this is not always obvious. The first term in the following integral (taken from [7]) is pretty obvious, but it is far from clear where the last term comes from.

$$\int \operatorname{erf}(ax)\operatorname{erf}(bx) = x\operatorname{erf}(ax)\operatorname{erf}(bx) +$$

$$\frac{e^{-a^2x^2}\operatorname{erf}(bx)}{\sqrt{\pi}a} + \frac{e^{-b^2x^2}\operatorname{erf}(ax)}{\sqrt{\pi}b} - \operatorname{erf}\left(\sqrt{a^2+b^2}x\right)\left(\frac{a}{b}+\frac{b}{a}\right)\frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{a^2+b^2}}$$

[2] In practice, one introduces a multiplicative factor of $2/\sqrt{\pi}$ to keep the statisticians happy, but the principle is the same.

[3] And hence how to plot it. However, there are much better, and more stable, ways of plotting an integral than via a sequence of *de novo* numerical evaluations.

Similarly [8]

$$\int \frac{x}{\log^2 x} = 2\,\mathrm{li}(x^2) - \frac{x^2}{\log x}, \tag{3}$$

where $\mathrm{li}(x) = \int \frac{1}{\log x}$, and one could wonder where the $\mathrm{li}(x^2)$ comes from.

In general, one needs a fresh generalisation of Liouville's Principle for each new function generator introduced. Some such have been proved [3,7,8,19,20], but even the most general [30] is far from complete: it deals with EL-elementary extensions subject to the restriction that, for each H in case (e) below, the degree of the numerator of H does not exceed the degree of the denominator by more than 1.

Definition 5. *θ is said to be EL-elementary over a differential field K if one of the following is true:*

(a) *θ is algebraic over K;*
(b) *$\theta' = \eta'/\eta$ for some $\eta \in K$ (we write $\theta = \log \eta$);*
(c) *$\theta' = \eta'\theta$ for some $\eta \in K$ (we write $\theta = \exp \eta$);*
(d) *$\theta' = \zeta' R'(\zeta)\eta G(\eta))$ and $\eta' = \zeta' R'(\zeta)\eta$ for some $\zeta \in K$ (we might[4] write $\eta = \exp(R(\zeta))$ and $\theta = \int G(\exp(R(\zeta)))$);*
(e) *$\theta' = \zeta' \frac{S'(\zeta)}{S(\zeta)} H(\eta))$ and $\eta' = \zeta' \frac{S'(\zeta)}{S(z\eta)}$ for some $\zeta \in K$ (we might[4] write $\eta = \log(S(\zeta))$ and $\theta = \int H(\log(S(\zeta)))$),*

where each of G, H, R, S are prescribed[5] rational functions of one variable. The function f is said to be EL-elementary over K if it can be expressed in some $K(\theta_1, \ldots \theta_n)$ with each θ_i EL-elementary over $K(\theta_i \ldots \theta_{i-1})$. If K is omitted, $C(x)$ is assumed.

For example, error functions would be coped with by having $(G, R) = (t \mapsto t, t \mapsto -t^2)$.

Special values are essentially then problems of definite integration. Tricks such as evaluating $\mathrm{erf}(\infty)$ by writing

$$\begin{aligned}
\mathrm{erf}^2(\infty) &= \left(\int_0^\infty \frac{2}{\sqrt{\pi}} e^{-x^2}\,\mathrm{d}x\right)\left(\int_0^\infty \frac{2}{\sqrt{\pi}} e^{-y^2}\,\mathrm{d}y\right)\\
&= \int_0^\infty \int_0^\infty \frac{4}{\pi} e^{-x^2-y^2}\,\mathrm{d}x\mathrm{d}y\\
&= \int_0^\infty \int_0^{\pi/2} \frac{4}{\pi} e^{-r^2} r\mathrm{d}r\mathrm{d}\theta\\
&= 1
\end{aligned}$$

are within the scope of heuristics rather than algorithms at the current time.

[4] The use of "might" here indicates that the problem of introducing new constants by this formulation of such an extension is a delicate one.

[5] This is the original definition from [30]. In practice the (G, R) and (H, S) are prescribed pairs of rational functions, so that a given G goes with a given R, etc.

Even/odd simplifications are generally possible, but deducing further rules is again a matter for heuristics. If $F = \int_0 f$, then

$$F(a+b) = \int_0^a f + \int_a^{a+b} f = F(a) + \int_a^{a+b} f,$$

and if the last term can be transformed into $\int_0^c f$, then a simplification can be deduced.

3.3 By First Order Linear Differential Equations

In general, one would consider a y defined by

$$y' + fy = g, \tag{4}$$

with an initial condition equivalent to the constant of integration discussed above. Let $F = \int f$ and $y = z\exp(-F)$. Then (4) becomes

$$z'\exp(-F) - fz\exp(-F) + fz\exp(-F) = g, \tag{5}$$

i.e. $z' = g\exp(F)$. Hence

$$y = \exp(-F) \int \left(g\exp(F)\right), \tag{6}$$

and the problem is reduced to the previous one, i.e. the solution is Liouvillian over the field generated by f and g.

However, there are some caveats here [11]. The first is that any logarithms with rational coefficients in F have to be expressed explicitly, and the exponentiation has to perform the "simplification" $\exp\log(h)) \mapsto h$, thereby possibly adding radicals to the mix. The second is that, if F has any components other than logarithms with rational coefficients, then $\int (g\exp(F)) = G\exp(F)$, and then $\exp(-F)$ and $\exp(F)$ cancel, and the integration is in fact the solution of the original differential equation.

3.4 By Higher Order Linear Differential Equations

If we take second-order linear differential equations with coefficients in $C(x)$, there are four possibilities [22] (generalised in [29] to Liouvillian coefficients).

(1) There is a solution of the form $e^{\int f}$, where f is a rational function. In this case, the differential operator factorises, and we get a first order equation, the solutions of which are always Liouvillian.

(2) The first case is not satisfied, but there is a solution of the form $e^{\int f}$, where f satisfies a quadratic equation with rational functions as coefficients. In this case, the differential operator factorises and we get a first order equation, the solutions of which are always Liouvillian.

(3) The first two cases are not satisfied, but there is a non-zero Liouvillian solution. In this case, every solution is an algebraic function.
(4) The non-zero solutions are not Liouvillian.

We could extend the definition of "Liouvillian" to allow solutions of second-order differential equations (normally called "Eulerian"), and ask whether differential equations can be solved in terms of Eulerian functions [28], and so on, but the underlying differential Galois theory becomes intractable.

Is this function "new"?. A more fundamental question might be: "can special function g, defined as a solution of equation *(g)*, be expressed in terms of special function f, defined as a solution of equation *(f)*?" Assuming that *(f)* and *(g)* have order greater than one, this would be more precisely defined as "can special function g, defined as a solution of equation *(g)* with given initial conditions, be defined in terms of a basis $f_1, \ldots, f_n$ of solutions of *(f)*?"

An example is given by the Bessel functions. [1, chap. 9] defines J_ν as solutions of

$$x^2y'' + xy' + (x^2 - \nu^2)y = 0, \tag{7}$$

whereas in [1, chap. 10], j_n is defined as solutions of

$$x^2y'' + 2xy' + (x^2 - n(n+1))y = 0. \tag{8}$$

These are connected by $j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+\frac{1}{2}}(x)$. Can such a relationship be deduced automatically? *If* we know that $j_n(x)$ should be of the form[6] $J_{n+\frac{1}{2}}(x)/f(x)$, the fact that $f(x)$ is of the form $c\sqrt{x}$ can be deduced relatively easily. If we assume merely that $j_n(x)$ is of the form $J_k(x)/f(x)$, the correct solution can still be deduced. Similarly, if we are faced with

$$x^2y'' + 2xy' + 4(x^4 - n(n+1))y = 0, \tag{9}$$

and if we suspect that the solution is of the form $J_n(f(x))$, deducing $f(x) = x^2$ is not too hard. However, given

$$4\,(y''(x))\,x^2 + \left(16\,x^4 - 16\,n^2 + 1\right) y\,(x) \tag{10}$$

and the suspicion that y is of the form $J_n(f(x))g(x)$, the author knows of no way of recovering the true answer — $J_n(x^2)\sqrt{x}$. It is possible that the results of [21] might help us to know which equation was related to which other equation, but, despite the call in [24], little seems to have been done in this direction.

Properties of the Function. The differential equation and suitable initial conditions will, in general, allow numerical evaluation, and thence plotting[3]. Formal integration of the differential equation will lead to a corresponding equation for the integral, so the question of integration reduces to the "is it related" question.

Even/odd simplification rules can be deduced from the differential equation, where appropriate. More general rules, and special values, are even more intractable than they are for integrals.

[6] The author is not sure whom the factor $\sqrt{\frac{\pi}{2}}$ is meant to please.

3.5 By Functional Equations

The simplest functional equation is the polynomial one: y such that $P(x, y) = 0$. If this is soluble by radicals, then we can import the branch cut for logarithm (though the result may be messy, and we need to worry about false solutions, as in Cardan's formula for the cubic [25]).. If it is not soluble by radicals, then there appears to be no "natural" placement for the branch cuts.

About the simplest non-algebraic functional equation is $ye^y = x$, whose solution is the Lambert W function [10]. This is not elementary or Liouvillian [6], but can also be defined by a non-linear differential equation: $W'(x) = \frac{W(x)}{(1+W(x))x}$. Just as log has infinitely many variants, separated by $2k\pi i$, which can be chosen to have a common branch cut, conventionally[7] the negative real axis, with the cut itself adhering [4] to the upper half-plane, so W has infinitely many branches, but the description is somewhat more complex [10,17].

The analysis of W was very much *ad hoc*, and the author knows of no systematic approach to such equations, unless they can be reduced to differential equations, as in the next section.

3.6 By Non-linear Differential Equations

The Lambert W function (see above) is one such. The question posed above "is this function definable in terms of that one", becomes even more relevant in this setting, and there are some surprising results: [14] gives the solution[8] to

$$(4y + 2x + 3)y' - 2y - x - 1 = 0 \tag{11}$$

as

$$4096 \exp\left(-W\left(32768 \exp(8x + c)\right) + 8x + c\right) - \frac{x}{2} - \frac{5}{8}. \tag{12}$$

The author knows of no way of deducing this in any sensible manner. The constant 5/8 is easy enough to determine, as is the 1/2, but the overall structure of the integral, necessary for any 'method of undetermined coefficients' to succeed, is not obvious.

3.7 By Definite Integration

The classic example of this is the Γ function, defined by

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} \mathrm{d}t. \tag{13}$$

This is continuous over the whole of the complex plane, except for $z{=}0,-1,-2\ldots$. It cannot be defined by a differential equation [16]. As far as the author was[9]

[7] There is nothing special about this choice: see [9].

[8] A reviewer pointed out that the solution can also be found by Maple as $W(c\exp(8x)) - \frac{x}{2} - \frac{5}{8}$, but this does not fully answer the question: does equation (11) have a solution in the form of (12) with fully undetermined coefficients?

[9] The reviewer pointed out [15], which has some techniques for negative results.

aware, there have been no attempts to systematise this analysis. There are heuristics in some packages (e.g. Maple), which sometimes produce differential equations. Hence it seems that, at the current time, there is nothing that a system can do *in general* except say "OK: you seem to have defined a function, which I can (generally) evaluate numerically".

3.8 Interrelations Between Methods

As we have seen, W can be defined either by a functional equation or by a (nonlinear) differential equation. In this case, going from the functional equation to the differential equation is fairly straight-forward, and mechanised in Maple's `PDEtools`, but the author knows no general way of reversing the process, or of knowing whether it is reversible.

4 Branch Cuts

These are inevitable for certain functions defined by integration or other analytic processes. Just to remind ourselves, let us look again at the branch cut for log. $\oint_C \frac{1}{x}\mathrm{d}x = 2\pi i$, where C is the unit circle (traversed counter-clockwise). Hence any *continuous* definition of $\log z = \int_1^z \frac{1}{x}\mathrm{d}x$ is bound to be multi-valued by multiples of $2\pi i$. Hence the minimum[10] branch cut necessary is a cut from 0 to (complex) infinity, with the value of log decreasing by $2\pi i$ as one crosses the branch cut in the direction of C (and increasing if one crosses it the other way). This poses two questions.

- What shape and where should the cut be?
- What happens *on* the cut?

In answer to the first, Occam's razor suggests that the cut might as well be a straight line from the origin to complex infinity. Note that this is not *mathematically necessary*, merely philosophically desirable[11]. Occam's razor again suggests that the cut might as well be along one of the axes. The current favourite [1] seems to be along the negative real axis, though the positive real axis has also been used.

In answer to the second question, clearly any behaviour is possible. Adherence to one side or the other (i.e. the value on the cut is the limit as you approach the cut from a given direction) seems a reasonable stipulation, as does the fact that the decision be taken consistently on the cut (if t parameterises the cut, we could insist on upper continuity for rational t, and lower continuity for irrational t, but this seems perverse) where possible. We stipulate "where possible" because

[10] We could always add "unnecessary" and cancelling branch cuts by arbitrary (but cancelling) amounts, but we will assume that this is not done.

[11] We note that the International Date Line, which can be viewed as a branch cut of $\sqrt[7]{\quad}$ is, for geopolitical reasons, not a straight line, but is piecewise straight, at least in its current incarnation [13, `international_date.html`].

branch cuts may bifurcate or merge: see [17, Figure 2] Beyond this, logic and Occam's razor make no suggestions. There are two common schools of thought, both of which can lay claim to being "consistent" in their own ways.

Independent. consistency. Here we have a rule for all branch cuts. The common one is "counter-clockwise consistency", advocated in [18], see also [26]. Here one defines continuity on the branch cut as continuity with the region from which one approaches the cut when circling the origin counter-clockwise.

Dependent. consistency. Here one stipulates that, if h can be derived from g, i.e. $h(x) = f_1(g(f_2(x)))$ where f_1 and f_2 have no, or "simpler" cuts, then the branch cuts and adherence of h are derived from those of g. This is largely the approach taken in [1]: one defines the branch cuts for log and the rest follow. Difficulties occur when there are alternative definitions for h, say $h = \hat{f}_1(g(\hat{f}_2(x)))$, which might induce different branch cuts or adherence. Hence this approach only makes sense when a *particular* definition of h in terms of g is fixed. [26].

5 Conclusion

There has been comparatively little systematic work in this area: an early attempt was [24], which urged the consideration of [21], but little has been done in this direction. Perhaps the most interesting is [23].

To define functions completely, one has to know the branch cuts and their behaviour, and nothing has been done about automating this — largely because there is no consistent philosophy here. Indeed, it would be a significant step forward to have a system capable of checking that a definition of, say, a proper Liouvillian function and its branch cuts *was* consistent.

Hence the answer to the question "how should a system understand a new function" at the moment seems to be "we don't know, in general".

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