# Towards Better Simplification of Elementary Functions

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## ABSTRACT

We present an algorithm for simplifying a large class of elementary functions in the presence of branch cuts. This algorithm works by:

**(a)** verifying that the proposed simplification is correct as a simplification of multi-valued functions;

**(b)** decomposing **C** (or $\mathbf{C}^n$ in the case of multivariate simplifications) according to the branch cuts of the relevant functions;

**(c)** checking that the proposed identity is valid on each component of that decomposition.

This process can be interfaced to an `assume` facility, and, if required, can verify that simplifications are valid "almost everywhere".

## 1. INTRODUCTION

Simplification of elementary functions is a vexed question in computer algebra. One reason for this is that simplification itself is vexed — what do we mean by "simpler"? Is $1 + x + x^2 + \cdots + x^{1000}$ "simpler" than $\frac{x^{1001}-1}{x-1}$? A related question is the following: does simplification mean expression in terms of the most compact formula, or expression in terms of the fewest primitives — is $\arctan(z)$ simpler or less simple than $\frac{1}{2i}(\log(1+iz) - \log(1-iz))$? However, even if one is not concerned by this, there is always the fact that many of the elementary functions are, in principle, multi-valued, and how does one know that the simplifier is respecting the standard choice of branch cuts [1, 8]? Much of the work on simplifying (denesting) radicals (e.g. [4]) concentrates on radicals of numbers because of the difficulty of deciding branch cuts for radicals of functions.

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In Maple[1] one has the choice between the `simplify` command, which is, in principle, completely correct, but often does not simplify when it should,[2] and the `simplify(..., symbolic)` command, which often simplifies to things that are not equal. Indeed, it has been commented that the command should be called "oversimplify". More information about the various approaches to the treatment of inverse elementary functions can be found in [5, 7].

In this paper we propose an approach that:

- is always correct;
- should do significantly better than the current approaches to the problem;
- will inter-operate with the `assume` facility — see step 3 in section 4;
- is capable of producing "simplification with health warnings" — see the last paragraph of section 5.2.

**Notation:** Terms like log, arctan (as well as $\sqrt{\ }$) denote single-valued functions from **C** to **C**, with the branch cuts as in [1, 8]. Capitalised variants, such as Log, Arctan and Sqrt denote multi-valued functions, regarded as mapping **C** into sets of values, and defined via their inverses, so that $\mathrm{Log}(z) = \{w : \exp(w) = z\} = \{\log z + 2n\pi i \mid n \in \mathbf{Z}\}$ and $\mathrm{Sqrt}(z) = \{w : w^2 = z\} = \{\pm\sqrt{z}\}$. The same notation is used for arbitrary expressions denoting elementary functions, so that $G$ is the multi-valued version of $g$.

The arithmetic operations are assumed to act on these sets element-wise, so that $A + B = \{a + b \mid a \in A, b \in B\}$. The same is true for unary functions, so that $\tan(\mathrm{Arctan}(x)) = \{\tan w \mid w \in \mathrm{Arctan}(x)\}$.

**Elem** denotes the set of elementary formulae (referred to as functions in [14]), whereas $\mathbf{Elem}_{\mathbf{C}\to\mathbf{C}}$ denotes the set of single-valued elementary functions from **C** to **C**, i.e. **Elem** regarded as single-valued functions and with the branch cuts interpreted in the sense of [1, 8]. These functions may not

[1]This is not a particular criticism of Maple, whose simplification features are probably the equal of any other systems, and, with the `assume` facility [15], probably better.

[2]For example, it will not simplify $\sqrt{1-z}\sqrt{1+z} - \sqrt{1-z^2}$ to 0, even though this simplification is valid — see section 5.1.

be total (e.g. $\log(0)$ is not defined), but are defined almost everywhere. When we write $f(z) = g(z)$ this is assumed to be true if *both* are undefined at $z$.

## 2. OVERALL APPROACH

The overall approach of this algorithm is in three steps. We will describe it for the case of univariable expressions, and treat the generalisation in section 6.

1. Find a possible simplification $g$ of the candidate $f$, e.g. by using `simplify(...,symbolic)`.
2. Check algebraically that the simplification is correct in the multi-valued sense, i.e. that $\forall z : f(z) \in G(z)$.
3. Check semi-numerically that the simplification is correct in the single-valued, branch-cut respecting, sense, i.e. that $f = g$ rather than $f = \hat{g}$ for any other $\hat{g} \in G$. At this stage, we can take into account any assumptions on the values of variables.

Step 1 will not be discussed further in this paper, except to note that it would be possible to combine steps 1 and 2 in practice.

Other approaches are possible, such as making a single simplification, and then checking that this is correct in the single-valued, branch-cut respecting sense. The problem with this is that a chain of simplifications, some of which are not valid in that sense, may still be valid as a simplification since the branch cuts may effectively cancel out.

One challenge is what to do if the ultimate simplification as proposed in step 1 is not deemed to be correct by the later stages. One possible solution is for step 1 to maintain a list of intermediates, and to work backwards through this list. Probably only experimentation can suggest the correct strategy here.

## 3. CHECKING MULTIVALUED CORRECTNESS

This can be done roughly as in a standard simplifier such as `simplify(...,symbolic)`. Most standard simplification "rules", which are in fact not true in the single-valued case, *are* true in the multi-valued sense. A partial list of such rules in given in Table 1, generally with a counter-example for the single-valued case. At this stage of the research, we do not have a complete list of these rules, which seems to be an under-researched area of mathematics.

This area is not trivial: for example, while $\mathrm{Arctan}(x) = \{\arctan(x) + n\pi \mid n \in \mathbf{Z}\}$, $\mathrm{Arcsin}(x) = \{\arcsin(x) + 2n\pi \mid n \in \mathbf{Z}\} \cup \{\pi - \arcsin(x) + 2n\pi \mid n \in \mathbf{Z}\}$. This problem combines with another one, that of the lack of a cancellation law, so that, if $A = \mathrm{Arcsin}(x)$,

$$\begin{aligned} A - A &= \{2n\pi \mid n \in \mathbf{Z}\} \cup \{2\arcsin(x) - \pi + 2n\pi \mid n \in \mathbf{Z}\} \\ &\quad \cup \{\pi - 2\arcsin(x) + 2n\pi \mid n \in \mathbf{Z}\} \\ &= \{2n\pi \mid n \in \mathbf{Z}\} + \\ &\quad \{0, 2\arcsin(x) - \pi, \pi - 2\arcsin(x)\}. \end{aligned}$$

**Table 1: Correct multi-valued simplification rules**

| Rule | Single-valued counter-example |
|---|---|
| $\mathrm{Log}(x) + \mathrm{Log}(y) = \mathrm{Log}(xy)$ | $x = y = -1$ |
| $\mathrm{Log}(x) - \mathrm{Log}(y) = \mathrm{Log}(\frac{x}{y})$ | $x = 1,\ y = -1$ |
| $-\mathrm{Log}(x) = \mathrm{Log}(\frac{1}{x})$ | $x = -1$ |
| $\overline{\mathrm{Log}(x)} = \mathrm{Log}(\overline{x})$ | $x = -1$ |
| $\mathrm{Sqrt}(x)\,\mathrm{Sqrt}(y) = \mathrm{Sqrt}(xy)$ | $x = y = -1$ |
| $\mathrm{Sqrt}(x)^2 = \{x\}$ | no counter-example |
| $\mathrm{Sqrt}(x^2) = \{\pm x\}$ | not single-valued |
| $\mathrm{Arctan}(x) + \mathrm{Arctan}(y) = \mathrm{Arctan}\left(\frac{x+y}{1-xy}\right)$ | $x = y = 1$ |
| $\tan(\mathrm{Arctan}(x)) = \{x\}$ | no counter-example |
| $\mathrm{Arctan}(\tan(x)) = \{x + n\pi \mid n \in \mathbf{Z}\}$ | $x = \pi$ |
| $\sin(\mathrm{Arcsin}(x)) = \{x\}$ | no counter-example |
| $\mathrm{Arcsin}(\sin(x)) = \{x + 2n\pi \mid n \in \mathbf{Z}\} \cup \{-x + (2n+1)\pi \mid n \in \mathbf{Z}\}$ | $x = \pi$ |

Note that $A - A$ still depends on $x$, unlike the case of $\mathrm{Arctan}(x) - \mathrm{Arctan}(x) = \{n\pi \mid n \in Z\}$.

The process of simplifying under the scenario of trying to find a $g \in \mathbf{Elem}$ such that $f \in G$ goes as follows: use the standard (but only the correct) single-valued simplification rules as long as possible, then, when it is necessary to do so, replace the single-valued function by the corresponding multi-valued function, and then use the multi-valued simplification rules as in Table 1.

## 4. CHECKING SINGLE-VALUED CORRECTNESS

This is the nub of the problem. To state the problem formally for functions $\mathbf{C} \to \mathbf{C}$:

SIMPLIFICATION PROBLEM 1. *Given $f, g \in \mathbf{Elem}_{\mathbf{C}\to\mathbf{C}}$ and the fact that $f \in G$, is $f = g$? That is, $\forall z \in \mathbf{C} : f(z) = g(z)$.*

In its full generality, of course, this problem is undecidable — see [13]. We could also ask the questions that computer algebra systems never ask (deliberately!):

SIMPLIFICATION PROBLEM 2. *Given $f, g \in \mathbf{Elem}_{\mathbf{C}\to\mathbf{C}}$ and the fact that $f \in G$, is $f = g$ almost everywhere? That is, $\exists M \subset \mathbf{C} : \mu(M) = 0 \wedge \forall z \in \mathbf{C} \setminus M : f(z) = g(z)$.*

In the special case of $f$ and $g$ both analytic (no branch cuts at all) it suffices that they agree on any infinite set of points in a bounded domain for them to be equal everywhere.

There are analogues to these problems from $\mathbf{R} \to \mathbf{C}$ and even for $\mathbf{R} \to \mathbf{R}$ — see section 6. We do not have a complete answer to any of these problems, but we do have answers in the case[3] when the only nesting of elementary functions in

[3]The reasons for these restrictions are explored in section 7.1, and they are enough to make the problem decidable.

the formula for $f$ and $g$ is of square roots inside other functions, and where inverse functions only occur in the numerators. In this case, for most[4] values of $x$, we can distinguish $g$ from the other values of $G$.

In this case, we can proceed as follows.

1. Determine all the branch cut loci of $f$ and $g$. In view of the restriction on the nesting of $f$, these will all be defined by algebraic (more accurately semi-algebraic) equations in $\Re(z)$ and $\Im(z)$.

2. Determine a decomposition of $\mathbf{C}$ (viewed as $\mathbf{R}^2$) determined by these branch cuts. This could be done by cylindrical algebraic decomposition [6], though, as we will see in the examples, the current technology for this is often overkill. On each component, $f$ is equal to some fixed $\hat{g} \in G$.

3. For each component $C$ of the decomposition, choose an $x \in C$ such that $g(x)$ is defined and distinguishable from $\hat{g}(x)$ for all other $\hat{g} \in G$, and check numerically that $f(x) = g(x)$ to within this distinguishing accuracy, which can be taken to be $\frac{|g(x)-\hat{g}(x)|}{4}$. Note that our restrictions rule out functions like $1/\operatorname{Arctan}(x)$, where the branches have accumulation points.

In the presence of an "assume" facility, we can replace step 3 by the following, where $\widehat{\mathbf{C}}$ is that portion of $\mathbf{C}$ that is allowed by the assumptions.

3' For each component $C$ of the decomposition with $C \cap \widehat{\mathbf{C}} \neq \emptyset$, choose[5] an $x \in C$ such that $g(x)$ is defined and distinguishable from $\hat{g}(x)$ for all other $\hat{g} \in G$, and check numerically that $f(x) = g(x)$ to within this distinguishing accuracy, which can be taken to be $\frac{|g(x)-\hat{g}(x)|}{4}$.

# 5. EXAMPLES

## 5.1 Square roots: $\sqrt{1-z}\sqrt{1+z} \stackrel{?}{=} \sqrt{1-z^2}$

It is clearly true, from the fifth rule in Table 1, that $\operatorname{Sqrt}(1-z)\operatorname{Sqrt}(1+z) = \operatorname{Sqrt}(1-z^2)$, so that $\sqrt{1-z}\sqrt{1+z} \in \operatorname{Sqrt}(1-z^2)$. Hence all that remains to do is check the single-valued correctness. Following the algorithm above, this goes as follows.

1. The branch cut for $\sqrt{z}$ is the negative real axis, i.e. $\{z \mid \Re(z) < 0 \wedge \Im(z) = 0\}$. Hence the branch cut for $\sqrt{1-z}$ is along

$$\{z \mid \Re(z) > 1 \wedge \Im(z) = 0\}. \tag{1}$$

Similarly, the branch cut for $\sqrt{1+z}$ is along

$$\{z \mid \Re(z) < -1 \wedge \Im(z) = 0\}. \tag{2}$$

[4] A typical example of why this is only true for "most" values is $x\operatorname{Arctan}(x)$ where all the different values of $\operatorname{Arctan}(x)$ give the same value of $x\operatorname{Arctan}(x)$ at $x = 0$.

[5] Note that it is not necessary to choose an $x \in C \cap \widehat{\mathbf{C}}$, since generic truth/falsity is invariant on components.

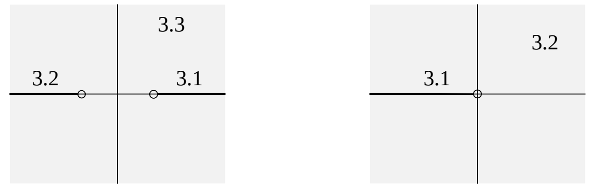


**Figure 1: Decompositions for $\sqrt{1-z}\sqrt{1+z}$ and $\log z$**

Also the branch cut for $\sqrt{1-z^2}$ is along

$$\{z^2 \mid \Re(z) > 1 \wedge \Im(z) = 0\}, \tag{3}$$

which is just the union of the sets in (1) and (2).

2. Hence we have to determine a decomposition of $\mathbf{C}$ by the equations in (1) and (2). By hand it is obvious that there are three connected components: (1), (2) and their complement (which is connected). See Figure 1, where the components are labelled by their step number in this algorithm.

3. We now need to make a check for each component. In the notation of the algorithm in section 4, $g = \sqrt{1-z^2}$ and $G = \{\pm\sqrt{1-z^2}\} = \{g, -g\}$.

3.1 **component (1).** If we take[6] $z = 2$, then $g(z) = \sqrt{-3} = 0 + \sqrt{3}i$ while $-g(z) = -\sqrt{-3} = 0 - \sqrt{3}i$, so the two are distinguishable. $f(2) = \sqrt{-1}\sqrt{3} = \sqrt{3}i = g(z)$, so on this component $f = g$.

3.2 **component (2).** If we take $z = -2$, then $g(z) = \sqrt{-3} = 0 + \sqrt{3}i$ while $-g(z) = -\sqrt{-3} = 0 - \sqrt{3}i$, so the two are distinguishable. $f(-2) = \sqrt{3}\sqrt{-1} = \sqrt{3}i = g(z)$, so on this component $f = g$.

3.3 **the complement** If we take $z = 0$, then $g(z) = \sqrt{1} = 1$ while $-g(z) = -\sqrt{1} = -1$, so the two are distinguishable. $f(0) = \sqrt{1}\sqrt{1} = 1 = g(z)$, so on this component $f = g$.

- Hence, throughout $\mathbf{C}$, $\sqrt{1-z}\sqrt{1+z} = \sqrt{1-z^2}$, as required.

We should note, though, that the sets defined in equations (1) and (2) are not directly acceptable to cylindrical algebraic decomposition algorithms. Instead (1) has to become the pair of equations $\Re(z) = 1$; $\Im(z) = 0$ and (2) becomes the pair of equations $\Re(z) = -1$; $\Im(z) = 0$. These decompose $\mathbf{C} = \mathbf{R}^2$ into six two-dimensional regions, seven one-dimensional regions and two zero-dimensional regions ($\pm 1$). The same analysis can be carried out, but we will not bore the reader with 15 cases similar to those above. A clustering algorithm [2, 3] would not help directly, but one that knew about the original formulation might. This is an important area for future research.

[6] There is no algorithmic requirement to take a point like this where there is good simplification. As long as we choose a value of $z$ such that $g(z) \neq -g(z)$, and can evaluate $f(z)$ and $g(z)$ with error bounded by $\frac{1}{4}|g(z) - (-g(z))|$, we can determine whether $f(z) = g(z)$ or $f(z) = -g(z)$.

## 5.2 Logarithms: $\log\left(\frac{1}{z}\right) \stackrel{?}{=} -\log x$

The multivalued form of this is already the third rule of Table 1, so we know that $\log\left(\frac{1}{z}\right) \in -\operatorname{Log}(z) = \{-\log(z) + 2n\pi i \mid n \in \mathbf{Z}\}$, and all that remains is to check the single-valued correctness. We proceed as follows.

1. The branch cut of $-\log z$ is the same as that of $\log z$, viz.
$$\{z \mid \Re(z) < 0 \wedge \Im(z) = 0\}. \qquad (4)$$
The branch cut of $\log\left(\frac{1}{z}\right)$ is $\{z \mid \Re\left(\frac{1}{z}\right) < 0 \wedge \Im\left(\frac{1}{z}\right) = 0\}$, which in fact is the same set as given in equation (4).

2. Hence we have to determine a decomposition of $\mathbf{C}$ determined by equation (4). This leads to two sets: (4) and its complement. See Figure 1.

3. We now have to examine the issue of single-valued correctness on each component.

3.1 **component (4).** A suitable point would be $z = -1$. $-\operatorname{Log}(-1) = \{(2n+1)\pi i \mid n \in \mathbf{Z}\}$, of which $-\log(-1) = -\pi i$. But $\log\left(\frac{1}{-1}\right) = \log(-1) = \pi i$, so on this component $\log\left(\frac{1}{z}\right) \neq -\log(z)$.

3.2 **complement of (4).** A suitable point would be $z = 1$. $-\operatorname{Log}(1) = \{2n\pi i \mid n \in \mathbf{Z}\}$, of which $-\log(1) = 0$. $\log\left(\frac{1}{1}\right) = \log(1) = 0$, so on this component $\log\left(\frac{1}{z}\right) = -\log(z)$.

The conclusion is that the simplification proposed is false (Simplification Problem 1), but is true except on a set of measure zero (Simplification Problem 2). If there had been an assumption of the form $\Re(z) \geq 0$, then the component (4) would not have been legal, step 3.1 would not have run, and the simplification would have been declared to be valid throughout the region of assumption.

It would also be possible, in the absence of any assumptions, for a system to return that the simplification was valid, either because it had been told to ignore sets of measure zero (e.g. `simplify(...,measurezero)`) or by printing out a warning to the user and continuing.

# 6. MULTIVARIATE SIMPLIFICATION

The case of multivariate simplifications is in principle the same: we merely have to decompose $\mathbf{C}^n$ (viewed as $\mathbf{R}^{2n}$) rather than $\mathbf{C}$, where $n$ is the number of variables. If a variable is `assume`d to be real, then we can replace $\mathbf{C}$ by $\mathbf{R}$ for that variable, and thus reduce the dimensionality of the real space we have to decompose — important since the complexity is doubly exponential in the dimension [10]. We will consider one example, first over $\mathbf{R}^2$ then over $\mathbf{C}^2 = \mathbf{R}^4$.

Table 1 states
$$\operatorname{Arctan}(x) + \operatorname{Arctan}(y) = \operatorname{Arctan}\left(\frac{x+y}{1-xy}\right). \qquad (5)$$

To what extent is this valid as a single-valued equation, i.e.
$$\arctan(x) + \arctan(y) \stackrel{?}{=} \arctan\left(\frac{x+y}{1-xy}\right). \qquad (6)$$

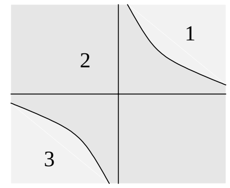


**Figure 2: Decomposition for** $\arctan(x) + \arctan(y)$

## 6.1 $\mathbf{R} \to \mathbf{R}$

We are assuming in this subsection that $x$ and $y$ are known to be real. It is not obvious why there is a problem here, since arctan is a continuous, bijective, differentiable function $(-\infty,\infty) \to (-\pi/2, \pi/2)$. Indeed, we can define $\arctan(-\infty) = -\pi/2$, $\arctan(\infty) = \pi/2$ to get a bijection $[-\infty,\infty] \to [-\pi/2, \pi/2]$.

Unfortunately, $[-\infty,\infty]$ is not the right domain for this sort of analysis. One way of seeing this is to observe that, although $(-\infty,\infty) = \mathbf{R} \subset \mathbf{C}$, the analytic completion of $\mathbf{C}$ is the one-point completion $\mathbf{C} \cup \{\infty\}$, and $[-\infty,\infty] \not\subset \mathbf{C} \cup \{\infty\}$.

In fact, arctan has a branch cut[7] at infinity. When $x = \infty$ (or $y = \infty$), this might seem to cause a problem, since $\frac{x+y}{1-xy}$ tends to $\frac{-1}{y}$. However, the problem this causes is masked by the another, more serious, problem.

It is possible for $\frac{x+y}{1-xy}$ to pass through $\infty$ even when both $x$ and $y$ are finite, namely when $xy = 1$. If $\frac{x+y}{1-xy}$ goes from "large and positive" to "large and negative", then $\pi$ is subtracted from the value of its arctan, and *vice versa*. We need to add a correction term, which can be done in various ways, e.g.[8]

$$\arctan(x) + \arctan(y) = \arctan\left(\frac{x+y}{1-xy}\right) + \begin{cases} \pi & x > 0, xy > 1 \\ 0 & x \geq 0, xy \leq 1 \\ -\pi & x < 0, xy \geq 1 \end{cases} \qquad (7)$$

See Figure 2.

This can be restated more compactly in terms of the "unwinding number" [7, 9] as

$$\arctan(x) + \arctan(y) = \arctan\left(\frac{x+y}{1-xy}\right) + \pi\mathcal{K}\left(2i(\arctan(x) + \arctan(y)\right). \qquad (8)$$

which is coupled more clearly to the problem of "overflow" across regions in adding the two arctan terms, and the boundary cases are dealt with consistently.

Equation (7) divides the $(x,y)$-plane into three regions (the

[7]Some people refer to this a jump discontinuity, which of course it is, but it is better to think of it as a branch cut, since it could be moved elsewhere by another choice of branch cut: indeed, as pointed out in [8], there is no agreement on where the branch cut for the closely related function arccot should go.

[8]For the cases when $xy = 1$, we are assuming a single $\infty$, with $\arctan(\infty) = \frac{\pi}{2}$.

two entries with zero correction term define one region, open on the lower-left boundary and closed on the top-right boundary. If we proceed algorithmically, by cylindrical algebraic decomposition [6], we in fact decompose the place into seven regions, as given in Table 2. The technique of clustering [3]

**Table 2: Cylindrical Decomposition of $(x, y)$-plane for equation (6)**

| $x$ | $xy$ | dimension | correction |
|---|---|---|---|
| $>0$ | $>1$ | 2 | $\pi$ |
| $>0$ | $=1$ | 1 | 0 |
| $>0$ | $<1$ | 2 | 0 |
| $=0$ | — | 1 | 0 |
| $<0$ | $>1$ | 2 | $-\pi$ |
| $<0$ | $=1$ | 1 | $-\pi$ |
| $<0$ | $<1$ | 2 | 0 |

would reduce this, ideally to three regions as in equation (7), but certainly to five regions, which are described in Table 3.

**Table 3: 5 Regions of the $(x, y)$-plane for equation (6)**

| | $R_1$ | $R_2$ | $R_3$ | $R_4$ | $R_5$ |
|---|---|---|---|---|---|
| $xy$ | $<1$ | $=1$ | $=1$ | $>1$ | $>1$ |
| $x$ | — | $>0$ | $<0$ | $>0$ | $<0$ |
| Fig. 2 region | 2 | 2 | 3 | 1 | 3 |

Evaluation at $x = y = 0$ shows that equation (5) is true there, and therefore throughout $R_1$. Similarly, evaluation at $x = y = 1$ shows that it is true there, and so throughout $R_2$. Evaluation at $x = y = -1$ shows that equation (5) is false, and needs a correction factor of $-\pi$ at that point, and therefore throughout $R_3$. By hand or in floating-point, evaluation at $x = y = 2$ shows that equation (5) is false, and needs a correction factor of $\pi$ at that point, and therefore throughout $R_4$. However, it seems impossible to persuade Maple (release V.5) to simplify[9] $2\arctan 2+\arctan\frac{4}{3}$ to $\pi$ (to be fair, though, Maple V7 does manage to do this). *Mutatis mutandis*, the same remarks apply to $x = y = -2$ and $R_5$. Hence the proposed simplification is not valid. Note that the assumption[10] $xy < 1$ would mean that only $R_1$ would be considered, and the simplification would then be declared valid.

Of course, we have chosen values of $x$ and $y$ at which the arctan function has a simple expression, but the algorithm does not need to do that, since it knows that the indeterminacy in $\operatorname{Arctan}\left(\frac{x+y}{1-xy}\right)$ is a multiple of $\pi$. Any point at which it can evaluate $\arctan(x) + \arctan(y)$ and $\arctan\left(\frac{x+y}{1-xy}\right)$ to an accuracy better than $\pi/4$, and therefore test whether the two are equal to an accuracy better than $\pi/2$, will do.

[9]Of course, direct simplification of this would use equation (5), which would spoil the point, but it ought to be doable via complex logarithms.

[10]Unfortunately, this assumption cannot be declared in Maple. One could declare $y > 0 \wedge x < \frac{1}{y}$, but this would only cover part of the desired region.

If we were considering the very similar proposed simplification $x\arctan(x) + x\arctan(y) \stackrel{?}{=} x\arctan\left(\frac{x+y}{1-xy}\right)$, and we knew that

$$x\arctan(x) + x\arctan(y) \in x\operatorname{Arctan}\left(\frac{x+y}{1-xy}\right) \quad (9)$$

from the rules in Table 1, the procedure above for $R_1$ would not quite have worked. The indeterminacy in the right-hand side of equation (9) is $\{xn\pi \mid n \in \mathbf{Z}\}$, which is zero at the sample point $x = y = 0$. Hence we would need to take a different sample point, say $x = y = \frac{1}{2}$ and evaluate to an accuracy better than $\pi/8$. Indeed $2\arctan\left(\frac{1}{2}\right) = \arctan\left(\frac{4}{3}\right)$, either symbolically, if we can persuade a system to do it, or numerically, if we trust the guarantees of accuracy, so the simplification is valid in $R_1$.

## 6.2 $\mathbf{C} \to \mathbf{C}$

The definition of $\arctan x$ is [1, 8]

$$\frac{1}{2i}\left(\log(1 + ix) - \log(1 - ix)\right).$$

Hence its branch cuts in the complex plane are along $1+ix \in (-\infty, 0]$, i.e. $x \in [i, i\infty)$, and along $1 - ix \in (-\infty, 0]$, i.e. $x \in (-i\infty, -i]$. These do not disconnect the complex plane, so the only special cases are along them. The same is true of $\arctan y$ and $\arctan\left(\frac{x+y}{1-xy}\right)$. There is still the critical locus $xy = 1$, as in the real case.

We now have to determine how these interact. Write $x = x_R + ix_I$ etc. Then we have to consider various intersections.

- The intersection of the two branch cuts for $\arctan x$ and $\arctan y$, This is clearly possible, since the two constraints are independent.
- The intersection of the branch cuts for $\arctan\left(\frac{x+y}{1-xy}\right)$ with the branch cuts for $\arctan x$. If one solves for the two (real) equations resulting from $\Re\left(\frac{x+y}{1-xy}\right) = 0$ and $x_R = 0$, one is left with, *inter alia*, the resultant

$$-3y_Ry_I^2 - y_I^6y_R - 3y_I^2y_R^5 - 3y_I^4y_R^3 - y_R^7 + y_R + y_R^3 + 2y_R^3y_I^2 - y_R^5 + 3y_I^4y_R. \quad (10)$$

  The only solutions of this have $|y_R| \leq 1$ and $|y_I| \leq 1$, and therefore are not on the branch cut for $\arctan y$, except that when $y_R = 0$, $y_I$ is unconstrained. Hence it is in fact possible to be on all the branch cuts of arctan simultaneously, say with $x = y = 2i$, and $\frac{x+y}{1-xy} = \frac{4}{5}i$.
- The intersection of the branch cuts for $\frac{x+y}{1-xy}$ with the branch cuts for $\arctan x$. This is identical to the previous case.
- The intersection of the branch cut for $\arctan x$ with the critical locus $xy - 1$. It then follows that $y_R$ has to be zero (since $x_Iy_R = 0$), so the point is also on the branch cut of $\arctan y$, and possibly on the branch cut for $\arctan\left(\frac{x+y}{1-xy}\right)$.

- The intersection of the branch cut for arctan $\left(\frac{x+y}{1-xy}\right)$ with the critical locus $xy-1$ cannot happen.

In sum, the situation here is very complicated, but can be reduced to a finite number of regions which need to be tested. It turns out that the move to the complex plane does not, in fact, add any further complication.

# 7. CONCLUSIONS

We have presented an outline of an algorithm for simplifying elementary functions correctly, possibly in the presence of an `assume` facility, and possibly, but only *when required* to ignore exceptional cases of measure zero. The algorithm works for cases where the only nesting allowed is that of square roots inside other elementary functions, and inverse (potentially multivalued) functions may only occur in the numerator.

## 7.1 Why this restriction?

One reason for the restriction on nesting is that the branch cuts are then given by algebraic equations, so that cylindrical algebraic decomposition [6] is then feasible. Extensions of this technique do exist [11], though implementations are rarer.

Another reason for the restriction on nesting is that, without it, the branch cut structure might no longer be finite. For example, $\log\sin x$ has infinitely many branch cuts, of the form $((2n-1)\pi, 2n\pi)$ for all $n \in \mathbf{Z}$.

The main reason for this restriction, however, is that it is otherwise hard, possibly impossible, to determine the distance between branches. In some cases this can be done, though we are currently unable to make this algorithmic. We give a few examples of functions that violate our restriction.

- $\operatorname{Arctan}\left(x \operatorname{Arctan}\left(\frac{1}{x}\right)\right)$. Let us suppose that we wish to evaluate this at $x=2$. Assuming the outer Arctan always takes the principal branch, the value for various branches of the inner Arctan is given in Table 4.

**Table 4: Values of** $\operatorname{Arctan}(2\operatorname{Arctan}(1/2))$

| branch | Value |
|---|---|
| arctan $-\pi$ | -1.38621133788 |
| arctan | 0.74769230366 |
| arctan $+\pi$ | 1.43298836482 |
| arctan $+2\pi$ | 1.49682270728 |
| arctan $+3\pi$ | 1.52027518705 |
| arctan $+4\pi$ | 1.53244221290 |
| arctan $+5\pi$ | 1.53288779388 |

As we can see (or by consideration of the formula) the values tend to $\pi/2$, and the separation tends to zero. However, the values are monotone, and hence we can assert that, provided we can evaluate to a precision of

$$\frac{1.43298836482 - 0.74769230366}{4} = 0.17133976529,$$

we can tell whether or not we are on the principal branch.

- We are not so fortunate when we apply many–one functions to multi-valued functions. Consider

$$\sin\left(\operatorname{Arctan}(x)^2\right)$$

at $x=1$. Values of this for various branches of the Arctan expression are given in Table 5. From this we can see that the values most certainly are not monotone, and indeed the branch closest (in the table) to the principal one is the arctan $-3\pi$ branch. It seems very likely that the values for the different branches are scattered throughout $(-1,1)$, and in fact it can be shown[11] that

$$\liminf_{|n|\to\infty} \left|\sin\left(\arctan(1)^2\right) - \sin\left((\arctan(1)+n\pi)^2\right)\right| = 0.$$

**Table 5: Values of** $\sin\left(\operatorname{Arctan}(1)^2\right)$

| branch | Value |
|---|---|
| arctan $-3\pi$ | 0.53223226469052394255108411324973 |
| arctan $-3\pi$ | -0.68844319556276953646396461406407 |
| arctan $-2\pi$ | -0.92846670306661207702727154343231 |
| arctan $-\pi$ | -0.66801107797394745302320860026876 |
| arctan | 0.57846878935455793874901827368615 |
| arctan $+\pi$ | -0.21379811148627617791348823769380 |
| arctan $+2\pi$ | -0.29610307588996806435608381265315 |
| arctan $+3\pi$ | -0.54395136438824375909319106070388 |
| arctan $+4\pi$ | 0.71808846220316247330302549263127 |
| arctan $+5\pi$ | 0.96016428952194522990132251781603 |

- We can see the reason for restricting inverse functions to the numerator: consider the function $\operatorname{Arctan}(x)/\operatorname{Arctan}(2x)$ evaluated at $x=1$. Depending on the choices of branch in the numerator and denominator, we can (by the theory of continued fractions) approximate the principal value $\arctan(1)/\arctan(2)$ arbitrarily closely, as shown in Table 6.

**Table 6: Values of** $\operatorname{Arctan}(1)/\operatorname{Arctan}(2)$

| numerator branch | denominator branch | Value |
|---|---|---|
| arctan | arctan | 0.70938813438026133678959 |
| arctan $+2\pi$ | arctan $+3\pi$ | 0.67115767953116559118826 |
| arctan $+7\pi$ | arctan $+10\pi$ | 0.70031959034809923217896 |

Of course, provided we are not worried about sets of measure zero, we can always clear denominators before checking whether $f=g$.

## 7.2 Future Algorithmic Development

The algorithm we have presented uses the following subalgorithms, all of which could benefit from improvement.

[11] We can make the absolute value as small as we like by choosing $n$ such that $n\pi$ is sufficiently close to an integer multiple of 4.

- Simplification of multi-valued elementary functions, using rules as in Table 1. This table could do with being completed, and it has to be recognised that these multi-valued functions do not form a ring — see the example of $\mathrm{Arcsin}(x) - \mathrm{Arcsin}(x)$ after Table 1 — and hence standard computer algebra systems may need substantial modification to handle this multi-valued simplification.
- Cylindrical algebraic decomposition [6]. Here the difficulty is that the semi-algebraic sets we are using to partition the complex plane, as in equation (1), cannot be given directly to cylindrical algebraic decomposition, and the transformation of them may lead to far larger decompositions than are desirable. A clustering algorithm [2, 3] would help (e.g. reducing the seven regions in Table 6.1 to the five in Table 6.1), but in general it would need to be aware of the *original* set of semi-algebraic sets, rather than the transformed set of constraints — see the last paragraph of section 5.1.
- Recognition of the nearest elements to $g(z)$ in $G(x)$. The difficulties with extending this are brought out in the previous subsection.
- Numerical evaluation of elementary functions with guaranteed error bounds. Much work has been done on this [12], but such algorithms are not normally available in computer algebra systems.

It is clear that we have only scratched the surface of what could be done by following this approach to simplification. There is also work to be done on lifting some of the restrictions on the forms allowed in $f$ and $g$.

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