The Persistence of Irrationals in Some Integrals

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Abstract: Computer algebra systems are expected to simplify formulas they obtain for symbolic integrals whenever they can, and often they succeed. However, the formulas so obtained may then produce incorrect results for symbolic definite integrals.

Introduction: Suppose that $f(z)$ is a rational function with integer coefficients. Its indefinite integral $F(z) := \int f(z)\,dz$ consists of a sum of rational functions and logarithms and arctans of rational functions; usually their coefficients cannot all be integers too but must be derived from certain algebraic numbers, the poles of $f(z)$. However, when the integral $F(z)$ can have an unusually simple form, say with integers for all coefficients of all the rational functions that appear in it, then such a form might well seem preferable to every other. In other words, taken from p. 170 of the book by J.H. Davenport *et al.* (1988),

> " The real problem is to find the integral without using any algebraic numbers other than those needed in the expression of the result. The problem has been solved by ... "

The book cites solutions published independently in 1976 by B. M. Trager and by M. Rothstein; D. Lazard and R. Rioboo (1990) present an improved solution. They all perform predictably many exclusively rational operations to find a simple form $F(z)$ for the integral when it exists. But it may be too simple.

The example $f(z)$ presented here has the following properties:

* $f(z)$ is rational with integer coefficients, ...
* ... and so is $\tan(F(z)) = \tan(\int f(z)\,dz)$, but ...
* $\int_X^Y f(z)\,dz = F(Y) - F(X) + L\pi$ for some small integer L which is best determined with the aid of irrational algebraic numbers none of which appears in the expression of the result F obtained by Trager *et al.* F is wrong without $L\pi$.
* $\int_X^Y f(z)\,dz$ has a closed form with all coefficients integers.

The example is

$$f(z) := (z^4 - 3z^2 + 6)/(z^6 - 5z^4 + 5z^2 + 4) \ , \quad \text{and}$$

$$\int f(z)\,dz = F(z) := \arctan(\ (z^3 - 3z)/(z^2 - 2)\ ) \ ; \quad \text{but}$$

$$\int_X^Y f(z)\,dz \neq F(Y) - F(X) \quad \text{in general. However,}$$

$$\Phi(z) := \arctan((2z^2+1)(z^2-3)z/(z^6-3z^4+2z^2+2)) + 3\arctan z$$

satisfies $\int_X^Y f(z)\,dz = \Phi(Y) - \Phi(X)$ always.

The Conventional Approach: To integrate $f(z)$ symbolically, we first derive its partial fraction expansion from its poles. Our example $f(z)$ has six of them: $\pm\iota\alpha$, $\beta \pm \iota\gamma$ and $-\beta \pm \iota\gamma$ where

$$\iota = \sqrt{(-1)} \ ,$$

$$\alpha = \sqrt{(\ \sqrt[3]{((83 + 3\sqrt{321})/54)} + \sqrt[3]{((83 - 3\sqrt{321})/54)} - 5/3\ )}$$

$$= 0.71522\,52384\ \ldots \ ,$$

$$\beta = \ldots = 1.66614\,75736\ \ldots \ ,$$

$$\gamma = \ldots = 0.14238\,73808\ \ldots \ .$$

Exact expressions for β and γ involving the surds that appear in α are available but not worth the space needed to display them.

After the partial fraction expansion of $f(z)$ has been simplified (not a trivial task), its indefinite integral $\Phi(z) := \int f(z)\,dz$ turns out to be a sum of logarithms which simplifies to

$$\Phi(z) := \arctan(z/\alpha) + \arctan((z-\beta)/\gamma) + \arctan((z+\beta)/\gamma)$$

after complex conjugates have been paired. Now for any real X and Y the definite integral $\int_X^Y f(z)\,dz = \Phi(Y) - \Phi(X)$ can be computed unexceptionably except for its complexity. Simplifying it produces something as simple as $F(Y) - F(X) + L\pi$ with a small integer L, and removes all traces of the irrational algebraic numbers α, β and γ, but at horrendous computational cost. Later a cheap way to compute L will be explained.

The Methods of Trager *et al.*: These methods, presented in works cited above, use only rational arithmetic (with complex integers) to produce a sum of complex conjugate logarithms that simplify to $\int f(z)\,dz = F(z)$ presented above. But this $F(z)$ jumps down by π as z increases past $-\sqrt{2}$, and does the same again as z increases past $\sqrt{2}$. That is why $\int_X^Y f(z)\,dz = F(Y) - F(X) + L\pi$ where L is the number of these jump-points ($-\sqrt{2}$ and $+\sqrt{2}$) that lie strictly between X and Y. Thus, two irrational algebraic numbers are *needed* in the expression of the result even though they do not *appear* in it. Omitting L is a common mistake.

Apparently the *constant* of integration in $F(z)$ is only piecewise constant, with jumps at $z = \pm\sqrt{2}$. Are these jumps, or their irrationality, mere artifacts of Trager's method? They may be.

Persistent Irrationality: Choose any two integers m and n free from nontrivial common factors and not both zero, and redefine

$$F(z) := \arctan(\,(m\,A(z) - n\,B(z))/(m\,B(z) + n\,A(z))\,) \quad \text{with}$$
$$A(z) := z^3 - 3z, \qquad B(z) := z^2 - 2.$$

As m and n vary, this $F(z)$ runs through *all* integrals of $f(z)$ that can be produced directly by the methods of Trager *et al.*; $F(z)$ has integer coefficients and $dF(z)/dz$ simplifies to

$$F'(z) = (\,A'(z)B(z) - A(z)B'(z)\,)/(\,A^2(z) + B^2(z)\,) = f(z)$$

except at arguments z where $F(z)$ jumps. These jumps are poles z of $(mA - nB)/(mB + nA)$. How many and where are these poles?

Regardless of m and n, there are three poles. By expanding the equation $B/A + n/m = 0$ in partial fractions it may be confirmed that each interval $-\sqrt{3} \le z < 0$ and $0 < z \le \sqrt{3}$ contains a pole; and the third lies at $z = 0$ if $m = 0$, at $z = \infty$ if $n = 0$, and otherwise between $-\mathrm{sign}(n/m)\,\infty$ and $-\mathrm{sign}(n/m)\sqrt{3}$. As z increases past a pole, $F(z)$ jumps down by $-\pi\,\mathrm{sign}(f(z)) = -\pi$. (More elaborate examples can jump up here and down there.) That is why $\int_X^Y f(z)\,dz = F(Y) - F(X) + L\pi$ wherein L counts poles strictly between X and Y. How many of the poles are irrational?

At least two poles are irrational. To see why, suppose one of them is at $z = r$, a rational number. Then $n/m = -B(r)/A(r)$, so the other two poles must be zeros z of

$$(B(r)A(z) - A(r)B(z))/(z-r) = (r^2 - 2)z^2 + rz + 6 - 2r^2 .$$

This quadratic must have irrational zeros because its discriminant $8r^4 - 39r^2 + 48$ is not a rational square, as can be confirmed by a little computation modulo 3.

The Cauchy Index of a Rational Function: The integer L in formulas like

$$\int_X^Y f(z)\,dz = F(Y) - F(X) + L\pi$$

above can be computed using solely rational operations via *Sturm Sequences*; in fact, $L := V(Y) - V(X)$ where the *Cauchy Index* $V(\ldots)$ is determined as follows:

Take any $F(z) := \arctan(\,A(z)/B(z)\,)$ where now $A(z)$ and $B(z)$ are polynomials with real rational coefficients and no commom zero z ; this means that $A(z)/B(z)$ is a rational function in lowest terms. Set $B_0 := B$, $B_1 := A$, and by repeated long division compute the remainders $B_{k+1} := Q_k B_k - B_{k-1}$ and quotients Q_k with $\deg(B_1) > \deg(B_2) > \ldots > \deg(B_K) = 0$. Each $B_k(z)$ is a polynomial with real rational coefficients; and the last of them, B_K , is a nonzero constant. (If it were zero then B_{K-1} would be a nonconstant divisor of both A and B .) The sequence

$$B_0(z),\ B_1(z),\ B_2(z),\ \ldots,\ B_K$$

has the properties of a Sturm sequence; no two adjacent terms in it can vanish simultaneously because otherwise induction would imply $B_K = 0$ too. And if any term but the first vanishes then the two terms on either side of it must have opposite signs.

Let $V(z)$ count the number of times adjacent terms $B_k(z)$ have opposite signs. For this purpose assign either a $+$ sign or a $-$ sign to a term that vanishes. Then $V(z)$ is a piecewise constant function with jumps only at poles z of $B_1(z)/B_0(z)$ where this reverses sign. In fact, the jump in $V(z)$ turns out to be the same as the jump in $-F(z)/\pi$, so $F(z) + V(z)\pi$ is continuous and its derivative is $f(z)$, as required.

For example, we find the Sturm sequence for $A(z) = z^3 - 3z$ and $B(z) = z^2 - 2$ to be

$$z^2 - 2\ ,\quad z^3 - 3z\ ,\quad 2 - z^2\ ,\quad z\ ,\quad -2$$

whence

$$V(z) = \begin{cases} 1 & \text{for } -\infty \le z < -\sqrt{2}\ , \\ 2 & \text{for } -\sqrt{2} < z < \sqrt{2}\ , \\ 3 & \text{for } \sqrt{2} < z \le +\infty\ , \end{cases}$$

and so $\arctan(\,A(z)/B(z)\,) + V(z)\pi$ is continuous. Note that this continuity persists even at the zeros of $B(z)$ provided the signs of $A/(\pm 0)$ and of $\pm\infty$ are properly correlated to ensure that the correct sign is chosen for $\arctan(\pm\infty) = \pm\pi/2$. The rules followed by IEEE standards 754 and 854 for floating-point arithmetic automatically achieve the proper correlation here too.

For more applications of the Cauchy Index $V(\ldots)$ see the paper by T. Sakkalis (1988) and citations therein.

Closed Forms for $\int_X^Y f(z)\,dz$: Replacing L by the Cauchy Index yields a formula

$$\int_X^Y f(z)\,dz = F(Y) - F(X) + (V(Y) - V(X))\pi$$

in which $F(z) = \arctan(\,A(z)/B(z)\,)$ and $V(z)$ is the Cauchy Index of $A(z)/B(z)$, but this is no "closed form" in the usual sense unless we have a closed form for $V(\ldots)$.

When all real zeros of $B(z)$ are known, tabulating $V(z)$ there provides a kind of closed form for it. In our example, given

$$A(z) := z^3 - 3z \quad \text{and} \quad B(z) := z^2 - 2 \ ,$$
$$V(z) \ = \ (z > -\sqrt{2}) \ + \ (z \geq \sqrt{2}) \ + \ 1 \ ,$$

where the predicates in parentheses are treated as 1 if true, 0 if false, and we assert $B(\pm\sqrt{2}) = +0$ in the absence of roundoff. (If roundoff had to be taken into account, the predicates might have to be adjusted.)

Another way to represent $V(z)\pi$ exploits the identity

$$\arctan(x) + \arctan(1/x) \ = \ \mathrm{sign}(x)\,\pi/2 \ ;$$
$$\begin{aligned} V(z)\pi \ &= \ \arctan(z+\sqrt{2}) - \arctan(1/(-\sqrt{2} - z)) \\ &\quad + \arctan(z-\sqrt{2}) + \arctan(1/(z-\sqrt{2})) + 2\pi \\ &= \ \arctan(B(z)/B'(z)) \ + \arctan(B'(z)/B(z)) \\ &\quad + \arctan(B'(z)/B''(z)) + \arctan(B''(z)/B'(z)) + 2\pi \ . \end{aligned}$$

Evidently the given integral $\int f(z)\,dz$ can be expressed as a sum of several arctans simpler than the sum of three arctans $\Phi(z)$ above. How few arctans of continuous real rational functions with integer coefficients suffice to represent that integral? The best I can find has two:

$$\int f(z)\,dz = \arctan((2z^2+1)(z^2-3)z/(z^6-3z^4+2z^2+2)) + 3\arctan z \ .$$

At present, I know no general way to find such a thing whenever it exists. However, D. Lazard informed me recently in a letter that his student Renaud Rioboo may have solved that problem.

Conclusion: The simplicity of some integration formulas for rational functions may be superficial; before deducing definite integrals from them we may have to estimate irrational algebraic numbers, or count sign-changes by computing Sturm sequences, or rework the formulas somehow to remove spurious jumps.

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