Integration of functions containing parameters and the specialization problem

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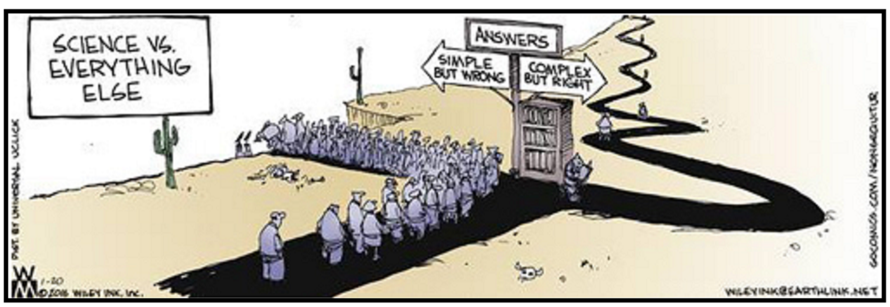
Abstract. We discuss the calculation and presentation of integrals when parameters are present. We pay special attention to how this is done, or should be done, in tables of integrals and in computer algebra systems. Specifically, we consider two issues: the need for expressions to be *comprehensive* and *continuous*. We present methods for achieving these goals both in manual calculation and in automatic symbolic computation.

Introduction



There are many reference books that publish tables of integrals, for example [1, 3, 6]. An alternative to integral tables is provided by computer algebra systems (CAS), which are already ubiquitous and available on platforms of all sizes. These software systems evaluate integrals using a mixture of integral tables and algebraic algorithms. A feature common to all sources of integrals is the fact that the formulae usually contain parameters. No one wants a table of integrals that contained separate entries for x, x^2 and x^{42}, rather than one entry for x^n, and many tables include additional parameters for user convenience; for example, there will be entries for integrals containing $\sin ax$, rather than the sufficient, but less convenient, $\sin x$.

Although parameters add greatly to the scope and convenience of integral tables, there can be difficulties and drawbacks occasioned by their use. We shall use the word *specialization* to describe the action of substituting specific values (usually numerical, but not necessarily) into a formula. The *specialization problem* is a label for a cluster of problems associated with formulae and their specialization, the problems ranging from inelegant results to invalid ones. For example, in [4] an example is given in which the evaluation of an integral by specializing a general formula misses a particular case for which a more elegant expression is possible. The focus here, however, is on situations in which specialization leads to invalid or incorrect results. To illustrate the problems, consider an example from a fine old Russian textbook [7, ch8, p346, (5)],

$$I_1 = \int \left(\alpha^{\sigma z} - \alpha^{\lambda z}\right)^2 \, dz = \frac{1}{2\ln\alpha}\left(\frac{\alpha^{2\lambda z}}{\lambda} + \frac{\alpha^{2\sigma z}}{\sigma} - \frac{4\alpha^{(\lambda+\sigma)z}}{\lambda+\sigma}\right) . \tag{1}$$

Expressions equivalent to this are returned by Maple, Mathematica and many other systems, such as the Matlab symbolic toolbox. It is easy to see that the specialization $\sigma = 0$ leaves the integrand in (1) well defined, but the expression for its integral on the right-hand side is no longer defined. If we pursue this further, we see that there are multiple specializations for which (1) fails, *viz.* $\alpha = 0$, $\alpha = 1$, $\lambda = 0$, $\sigma = 0$, $\lambda = -\sigma$, and combinations of these. The question of how or whether to inform computer users of these special cases has been discussed in the CAS literature many times [2]. A list of every special case for (1) is as follows.

$$I_1 = \begin{cases} \dfrac{1}{2\lambda\ln\alpha}\left(\alpha^{2\lambda z} - \alpha^{-2\lambda z} - 4z\lambda\ln\alpha\right) \;, & \left[\begin{array}{l} \lambda+\sigma = 0 \;, \\ \alpha \neq 0 \;, \; \alpha \neq 1 \;, \; \sigma \neq 0 \;; \end{array}\right. \\ z + \dfrac{1}{2\lambda\ln\alpha}\left(\alpha^{\lambda z}(\alpha^{\lambda z} - 4)\right) \;, & \left[\begin{array}{l} \sigma = 0 \;, \\ \alpha \neq 0 \;, \; \alpha \neq 1 \;, \; \lambda \neq 0 \;; \end{array}\right. \\ z + \dfrac{1}{2\sigma\ln\alpha}\left(\alpha^{\sigma z}(\alpha^{\sigma z} - 4)\right) \;, & \left[\begin{array}{l} \lambda = 0 \;, \\ \alpha \neq 0 \;, \; \alpha \neq 1 \;, \; \sigma \neq 0 \;; \end{array}\right. \\ \text{ComplexInfinity} \;, & \left[\begin{array}{l} \alpha = 0 \;, \\ \Re(\lambda z)\,\Re(\sigma z) < 0 \;; \end{array}\right. \\ \text{Indeterminate} \;, & \left[\begin{array}{l} \alpha = 0 \;, \\ \Re(\sigma z)\,\Re(\lambda z) \geq 0 \;; \end{array}\right. \\ \dfrac{1}{2\ln\alpha}\left(\dfrac{\alpha^{2\lambda z}}{\lambda} + \dfrac{\alpha^{2\sigma z}}{\sigma} - \dfrac{4\alpha^{(\lambda+\sigma)z}}{\lambda+\sigma}\right) \;, & \text{otherwise, (generic case)} \;. \end{cases} \tag{2}$$

Conditions are here shown as in printed tables; otherwise they could be presented using the logical $\vee$ and $\wedge$ operators.

To generalize this, we can denote a function depending on parameters by $f(z;\mathbf{p})$, with z being thought of as the main argument, the integration variable, and $\mathbf{p}$ representing the set of parameters. Then (2) is called a comprehensive antiderivative.

Definition 0.1. A *comprehensive antiderivative* of a parametric function $f(z;\mathbf{p})$ is a piecewise function $F(z;\mathbf{p})$ containing explicit consequents[1] for each special case of the parameters.

Computer algebra systems are reluctant to return comprehensive expressions because they can quickly lead to unmanageable computations, and as well many users might regard them as *too much information*. Instead, tables and CAS commonly adopt the approach of identifying a *generic* case, which is then the only expression given; in the case of CAS, the generic case is returned without explicitly showing the conditions on the parameters. In the case of tables, any special case values would be used to simplify the integrand and then the resulting integrand and its antiderivative would be displayed as a separate entry at an appropriate place in the table.

Definition 0.2. A *generic antiderivative* is one expression chosen from a comprehensive antiderivative that is valid for the widest class of constraints.

We have written a Mathematica package that automatically generates comprehensive anti-derivatives for integrands containing parameters.

1. Continuity in parameters

The example (2) dramatically illustrates the potential size of comprehensive antiderivatives, but is too cumbersome for explaining ideas. We turn to simpler examples. We begin with the comprehensive antiderivative known to all students of calculus:

$$\int z^{\alpha}\,\mathrm{d}z = \begin{cases} \ln z\ , & \text{if } \alpha = -1\ , \\ \dfrac{z^{\alpha+1}}{\alpha+1}\ , & \text{otherwise (generic case).} \end{cases} \tag{3}$$

Substituting $\alpha = -1$ into the generic case gives $1/0$ and not $\ln z$. Often when a substitution fails, a limit will succeed, so we try the limit as $\alpha \to -1$. This also fails, but we can examine *how* the limit fails by expanding the generic case as a series about $\alpha = -1$, that is treating $\alpha - 1 = \varepsilon$ as a small quantity.

$$\frac{z^{\alpha+1}}{\alpha+1} = \frac{e^{\varepsilon \ln z}}{\varepsilon} = \frac{1 + \varepsilon \ln z + O\left(\varepsilon^2\right)}{\varepsilon}\ . \tag{4}$$

If we can remove the leading term of the series, namely $1/\varepsilon$, then the next term gives us $\ln z$ as desired. But an integral is determined only up to a constant! So,

[1] The expression that is the consequence of specialization.

an equally correct integral is

$$\int z^\alpha \, \mathrm{d}z = \frac{z^{\alpha+1}}{\alpha+1} - \frac{1}{\alpha+1} \ ,$$

and now the limit as $\alpha \to -1$ is exactly $\ln z$. Thus the comprehensive antiderivative [5]

$$\int z^\alpha \, \mathrm{d}z = \begin{cases} \ln z \ , & \text{if } \alpha = -1 \ , \\ \dfrac{z^{\alpha+1} - 1}{\alpha+1} \ , & \text{otherwise.} \end{cases} \tag{5}$$

is continuous with respect to α, and the generic antiderivative now contains the exceptional case as a removable discontinuity.

Definition 1.1. Given a function $f(z;\mathbf{p})$ and an expression $F(z;\mathbf{p})$ for the indefinite integral of $f(z;\mathbf{p})$, that is,

$$F(z;\mathbf{p}) = \int f(z;\mathbf{p}) \, \mathrm{d}z \ ,$$

and given a point in parameter space $\mathbf{p}_c$ at which $F(z;\mathbf{p})$ is discontinuous with respect to one or more members of $\mathbf{p}$, a function $C(\mathbf{p})$, which serves as a constant of integration with respect to z, and which has the property that $F(z;\mathbf{p})+C(\mathbf{p})$ is continuous with respect to $\mathbf{p}$ at $\mathbf{p}_c$ is called a Kahanian constant of integration[2].

Definition 1.2. A comprehensive antiderivative in which each consequent contains an appropriate Kahanian constant of integration is a Kahanian antiderivative.

We have written a Mathematica package that computes Kahanian antiderivatives.

References

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[2]Since it is a function of $\mathbf{p}$, one can question whether it should be called a constant. It is constant with respect to z, and seems a useful extension of calculus terminology.

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