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The Integration of a Class of Special Functions with the Risch Algorithm

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We indicate how to extend the Risch algorithm to handle a class of special functions defined in terms of integrals. Most of the integration machinery for this class of functions is similar to the machinery in the algorithm which handles logarithms. A program embodying much of the extended integration algorithm has been written. It was used to check a table of integrals and it succeeded in finding some misprints in it.

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by

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The purpose of this memorandum is to point out the similarity for the purposes of integration of the logarithm function and a class of special functions defined in terms of integrals. Note that

$$\log(h(x)) = \int_a^{h(x)} \frac{1}{t}\, dt,$$

that is, the logarithm can be defined as an integral. Note also that we do not restrict ourselves to a single function log(x), but consider the family of functions log(h(x)). Here we shall consider the class of special functions F defined by

$$F(h(x)) = \int_a^{h(x)} g(t)dt,$$

where a is a constant, and g(t) can be obtained by rational operations upon the variable t and by exponential and logarithmic terms involving t. The function g may also contain special function terms not involving F, but it must not be integrable in terms of the allowed functions. This class of special functions includes

the error function $\quad \mathrm{erf}(h(x)) = \frac{2}{\sqrt{\pi}} \int_0^{h(x)} e^{-t^2}\, dt,$

the exponential integral $\quad E_i(h(x)) = \int_{-\infty}^{h(x)} \frac{e^t}{t}\, dt,$

and the Spence function $\quad Sp(u(x)) = -\int_1^{u(x)} \frac{\log t}{t - 1}\, dt.$

We claim that much of the machinery for integrating expressions involving such special functions is contained in the logarithm case of the Risch algorithm [1]. An extension to the Risch algorithm is to be preferred to traditional integration methods (e.g., integration by parts, substitution of variables) because it is a decision procedure. This means that the procedure should be able to obtain the integral if it is expressible in closed form or to show that the integral cannot be so expressed. Traditional methods cannot make such a decision and are particularly weak if the integrand involves division in a nontrivial way. On the other hand the Risch algorithm we shall employ is weak in that it does not handle algebraic expressions (e.g., $\sqrt{x}$). However, such a restriction has been removed by Risch in extensions to the algorithm described in [3,4].

Our description of the steps necessary to extend the Risch algorithm will concentrate on the particular case of the error function. We have extended the current state of our implementation of the Risch algorithm to handle the error function. At the present time our implementation of the Risch algorithm contains a nearly complete implementation of the logarithm case and a partial implementation of the exponential case. Details about the approach taken in our implementation are to be found in [2].

The first thing one notices in attempting an extension is that the introduction of special functions will cause a modification to be made to the Liouville theorem which is basic to the Risch algorithm. The Liouville theorem says, roughly speaking, that the integral of an expression E is the sum of an expression which is rational in the logarithmic and exponential terms already in E and constant multiples of new logarithmic terms. The argument for the validity of such a theorem is based on the realization that differentiation does not introduce new exponential or logarithmic terms. Moreover, differentiation will not get rid of existing exponentials and logs except for constant multiples of logs occurring in a sum.

The generalized version of the Liouville theorem says that constant multiples of special functions can be included in the integral as well as constant multiples of logs. In any particular situation one would be looking for integrals involving a given set of special functions only; say, error functions and exponential integrals. In such a case the generalized version of the Liouville theorem particularizes to give the form of the integral as

$$w + \sum_{i=1}^{q} c_i \log(v_i) + \sum_{j=1}^{r} d_j \operatorname{erf}(u_j) + \sum_{k=1}^{s} e_k E_i(t_k) \quad ,$$

where w, v_i, u_j, and t_k are rational expressions in the exponential, logarithmic and special function terms already in the integrand, and the c_i, d_j, and e_k are constants.

It is important to note how constant multiples of special functions arise in the integral. The situation in the log case is quite simple -- the integrand must be of the form

$$c \frac{v'}{v} \qquad \left(\int c \frac{v'}{v} = c \log v\right).$$

Let us recall from [2] that the integrand can be expressed in the partial fraction decomposition

$$P + \frac{R_1}{S_1} + \frac{R_2}{S_2^2} + \dots + \frac{R_k}{S_k^k} \quad ,$$

where P, R_i, and S_i are polynomials in the main variable in the integrand with coefficients involving the rational, logarithmic, and other special function terms in the integrand. It is clear that new log terms involving the main variable (if any) must arise from the rational terms

$$\frac{R_i}{S_i^{\,i}} \quad .$$

The other new log terms (i.e., not involving the main variable) arise through the recursive use of the integration process in the polynomial part. Such terms must also be obtained from rational terms at some point in the recursion.

The form of the integrand leading to the error function term is

$$ce^{-u^2} u' \qquad \left(\int ce^{-u^2} u' = c\frac{\sqrt{\pi}}{2} \operatorname{erf}(u) \right).$$

Based on this form it is clear that the main variable at the point in the integration process when the error function arose was an exponential. Furthermore, the term arose when integrating the polynomial part of the expression or rational terms of the form

$$\frac{A}{(e^f)^k} \quad .$$

(The latter terms are treated like polynomial terms in the algorithm, when e^f is the main variable).

We shall now indicate how the algorithm can be extended to handle the error function. Let us suppose the erf(u(x)) is the main variable in the integrand, and the integrand has the form

$$P + \sum_{i=1}^{k} \frac{R_i}{S_i^{\,i}} ,$$

where P, R_i, and S_i are polynomials in erf(u(x)).

For rational terms a reduction in the degree of the numerator can be made. Thus for $i > 1$,

$$\int \frac{R}{S^i}\, dx \to \frac{A}{S^{i-1}} + \int \frac{B}{S^{i-1}}\, dx ,$$

where A and B are polynomials in erf(u(x)) obtained by a simple computation based on the gcd of S and S'. For i=1, the denominator is completely factored and we proceed as in [2] to find logarithmic terms.

For example, consider the integral

$$\int e^{-x^2}\left(\frac{\operatorname{erf}(x) - 1}{\operatorname{erf}^2(x)}\right) dx$$

The reduction procedure should yield

$$\int e^{-x^2}\left(\frac{\operatorname{erf}(x) - 1}{\operatorname{erf}^2(x)}\right) dx = \frac{\sqrt{\pi}}{2}\ \frac{1}{\operatorname{erf}(x)} + \int \frac{e^{-x^2}}{\operatorname{erf}(x)}\ dx.$$

The latter term need not be factored since the denominator is linear in erf(x). This term yields

$$\frac{\sqrt{\pi}}{2} \log \operatorname{erf}(x).$$

So the integral is

$$\frac{\sqrt{\pi}}{2} \frac{1}{\text{erf}(x)} + \frac{\sqrt{\pi}}{2} \log \text{erf}(x).$$

Now let us consider the polynomial part. Suppose the expression to be integrated is

$$A_n(x)\ \text{erf}^n(u) + A_{n-1}(x)\ \text{erf}^{n-1}(u) + \ldots + A_0(x),$$

where the A_i do not involve erf(u). Then the integral, if it exists, must be of the form

$$B_{n+1}\ \text{erf}^{n+1}(u) + B_n\ \text{erf}^n(u) + \ldots + B_0\ ,$$

where the B_i do not involve erf(u), and only B_0 may contain new logarithmic or error-function terms.

We can obtain values for the B_i (or decide the nonintegrability of the expression in logarithmic, exponential, or error-function terms) by a process similar to the one described in [2]. An example which uses this method is given below. Consider

$$\int \text{erf}^2(x)\ dx$$

integral: $B_3\ \text{erf}^3(x) + B_2\ \text{erf}^2(x) + B_1\ \text{erf}(x) + B_0$

integrand: $A_2\ \text{erf}^2(x) + A_1\ \text{erf}(x) + A_0$; $A_2 = 1$, $A_1 = 0$, $A_0 = 0$.

Differentiating the general form of the integral, we obtain

$$B_3' \operatorname{erf}^3(x) + \left(\frac{6}{\sqrt{\pi}} B_3 e^{-x^2} + B_2'\right) \operatorname{erf}^2(x) + \left(\frac{4}{\sqrt{\pi}} B_2 e^{-x^2} + B_1'\right) \operatorname{erf}(x)$$

$$+ \left(\frac{2}{\sqrt{\pi}} B_1 e^{-x^2} + B_0'\right) = \operatorname{erf}^2(x).$$

By matching coefficients, starting with B_3, we obtain $B_3' = 0$. Therefore, B_3 is a constant, say b_3.

$$\frac{6}{\sqrt{\pi}} b_3 e^{-x^2} + B_2' = 1$$

By integrating (trivially on the left-side, by a recursive call to the integration procedure on the right), we obtain

$$3b_3 \operatorname{erf}(x) + B_2 = x + \text{constant}.$$

So $b_3 = 0$, $B_2 = x + b_2$

$$\frac{4}{\sqrt{\pi}} (x + b_2) e^{-x^2} + B_1' = 0$$

$$\frac{4}{\sqrt{\pi}} b_2 e^{-x^2} + B_1' = - \frac{4x}{\sqrt{\pi}} e^{-x^2}$$

Integration yields

$$2b_2 \operatorname{erf}(x) + B_1 = \frac{2}{\sqrt{\pi}} e^{-x^2} + \text{constant}$$

So $b_2 = 0$, $B_1 = \frac{2}{\sqrt{\pi}} e^{-x^2} + b_1$

$$\frac{2}{\sqrt{\pi}} \left(\frac{2}{\sqrt{\pi}} e^{-x^2} + b_1 \right) e^{-x^2} + B_0' = 0$$

$$\frac{2}{\sqrt{\pi}} b_1 e^{-x^2} + B_0' = \frac{-4}{\pi} e^{-2x^2}$$

Integrating

$$b_1 \operatorname{erf}(x) + B_0 = - \sqrt{\frac{2}{\pi}} \operatorname{erf}(x\sqrt{2}) + \text{constant}$$

(See below for a discussion of such an integration step).

So $b_1 = 0$, $B_0 = -\sqrt{\frac{2}{\pi}} \operatorname{erf}(x\sqrt{2}) + b_0$

Substituting these results into the general form of the integral, we obtain

$$x \operatorname{erf}^2(x) + \frac{2}{\sqrt{\pi}} e^{-x^2} \operatorname{erf}(x) - \sqrt{\frac{2}{\pi}} \operatorname{erf}(x\sqrt{2}) + b_0$$

It thus appears that when the main variable is erf(u(x)) the algorithm is quite similar to the log case as we have claimed. The algorithm must also be modified in the exponential case. We have to permit constant multiples of error-function terms to be included in the solution. This follows from our previous discussion. That is, if the main variable is $e^{u(x)}$, then

$$\int A(x) e^{ku(x)}\, dx = B e^{ku(x)} + c \operatorname{erf}(p(x)),$$

where c is a constant, k is a nonzero integer, and p(x) is so defined that

$e^{-p^2} = e^{ku}$. By differentiation we obtain

$$Ae^{ku} = (B' + kBu')\, e^{ku} + c \frac{2}{\sqrt{\pi}} e^{-p^2} p'$$

$$= (B' + kBu' + \frac{2c}{\sqrt{\pi}} p')\, e^{ku}$$

Hence

$$A = B' + kBu' + \frac{2c}{\sqrt{\pi}} p' \ .$$

We are given A, u, and k. Our object is to find B and c, when these exist, where $-p^2 = ku$. B is restricted to being rational in the logarithmic, exponential, and error-function terms which A contains. Moreover, since we do not allow algebraic expressions except for algebraic constants, we shall restrict p accordingly. Note that -ku can be expressed as a rational expression in the variable of integration and any additional defined variables representing logs, exponentials and error-functions. We want to know if -ku is a perfect square. This can be decided by factoring. If -ku is a perfect square, let p be a square root of it. Otherwise ignore the error function terms and proceed as usual.

Rearranging the equation above, we obtain

$$B' + kBu' = A - \frac{2c}{\sqrt{\pi}} p' \ .$$

We can now use the machinery of the Risch algorithm to solve for B and c, if they exist. A solution for B and c must be unique for if it were not it would imply that an error-function term is algebraically dependent on an exponential and terms of lower complexity. We shall assume that except for purely constant expressions such functions do not exist.

As an example, let us consider

$$\int \frac{e^{-2x^2}}{x^2}\, dx = Be^{-2x^2} + c \operatorname{erf}(p).$$

Here $-p^2 = -2x^2$, so let $p = \sqrt{2}\, x$

Differentiating

$$\frac{1}{x^2} e^{-2x^2} = (B' - 4Bx)\, e^{-2x^2} + \frac{2\sqrt{2}}{\sqrt{\pi}} e^{-2x^2}$$

$$B' - 4Bx = \frac{1}{x^2} - \frac{2\sqrt{2}}{\sqrt{\pi}} c$$

B must be rational in x. Its denominator is x. The numerator is linear at most. So $B = \frac{a + bx}{x}$.

Substituting

$$\frac{-a}{x^2} - 4a - 4bx = -\frac{2\sqrt{2}}{\sqrt{\pi}} c$$

$$a = -1, \quad 4 = \frac{-2\sqrt{2}}{\sqrt{\pi}} c, \text{ so } c = -\sqrt{2}\sqrt{\pi}\,, \quad -4bx = 0, \quad \text{so } b = 0\ .$$

The integral therefore is

$$\frac{-e^{-2x^2}}{x} - \sqrt{2}\sqrt{\pi}\, \operatorname{erf}(x\sqrt{2}).$$

We shall now discuss the problems encountered in generalizing our analysis of the error function extension to the Risch algorithm. A very important factor to be considered in the following is that the number of useful special functions in most fields of application is relatively stable and not very large.

For each special function one must perform an analysis of the ways in which constant multiples of an instance of it can enter into the integral. This involves some pattern recognition, and it seems difficult to obtain a simple algorithm to perform the task in general. However, for each special function definable by an integral that we have encountered, the analysis is quite simple [see 5].

We must also know in what ways the special function interacts with previous functions. The algorithm assumes the algebraic independence of all the terms. Hence, we must not let algebraically dependent expressions appear in the integrand. An example of such a dependence is given below.

$$A_i(h(x)) = \int_0^{h(x)} \frac{1}{\log t} \, dt = E_i\left(\log(h(x))\right)$$

There may also be algebraic relationships between different instances of the same function (e.g., $\log(ab) = \log a + \log b + 2k\pi i$). In these cases we presently have to rely on previous analyses of the simplification rules associated with the special functions under consideration. Divining the simplification rules applicable to any given special function relative to a given set of functions seems very difficult at present.

It should also be clear that the fact that an expression is not integrable in terms of existing functions does not necessarily make its integral a suitable candidate for a special function. For example, note that

$$\int \frac{\log x - \frac{1}{x}}{\log^2 x}\, dx = \frac{1}{\log x} + \int \frac{1}{\log x}\, dx .$$

Because of this relationship the integral on the left is a bad candidate for a special function. A little consideration will reveal several restrictions on what one might call "primitive" integrals. Restricting special functions to those defined by such primitive integrals will make the extension a good deal easier.

In order to debug the program, we used our version of the Risch algorithm extended to handle the error function to check a fine table of integrals of the error function compiled by W. D. Maurer in 1958 [6]. (A more recent table, emphasizing definite integrals is [7]). The program unfortunately cannot check the correctness of the entire set of integrals because some entries involve algebraic expressions such as $\sqrt{x}$ and others involve definite integrals. The program has so far uncovered a misprint in

$$\int x \,\mathrm{erf}^2 x \, dx = \left(\frac{x^2}{2} - \frac{1}{4}\right) \mathrm{erf}^2 x + \frac{x}{\sqrt{\pi}}\, e^{-x^2}\, \mathrm{erf}\, x + \underline{\frac{1}{2\pi}}\, e^{-2x^2},$$

where the underlined expression was $2\sqrt{\pi}$.

A potentially controversial disagreement between the program and the table occurred in

$$\int x^2\, \mathrm{erf}(ax + b)\, e^{px}\, dx = \frac{1}{p^3}\, \mathrm{erf}(ax + b)\, e^{px}\, (2 - 2px + p^2x^2)$$

$$+ \frac{pax - pb + \frac{p^2}{2a} - 2a}{a^2p^2\sqrt{\pi}}\, e^{-(ax+b)^2 + px}$$

$$- \frac{\frac{p^4}{a} - 4p^3b + 4ab^2p^2 - \underline{2ap^2} + 8a^2bp + 8a^3}{4a^5p^3}\, e^{\frac{p}{a}\left(\frac{p}{4a} - b\right)}\, \mathrm{erf}\left(ax + b - \frac{p}{2a}\right).$$

The underlined term in the table was $-3xp^2$. However, Maurer specifically indicated that he did not check the third term in the integral. We have decided not to check the integral either. Readers are therefore welcome to enter the arena with a certification of either of the proposed solutions, or with another solution of their choosing.

Maurer recently informed us that he spent at least forty hours checking by hand the solution to the above problem before he gave up on it. The PDP-6 at MIT spent eight minutes on the problem. We believe that the machine's time can be reduced to a few seconds by making changes to the simplifier used in the program. Currently the simplifier rerepresents expressions quite frequently due to a fear that new logarithmic or error function terms were obtained in the lower levels of the recursion. The algebraic manipulations in the program are mostly performed using a rational function representation, but this representation does not allow one to introduce new variables. When a new variable appears, the old expressions must be rerepresented to account for its existence. Fortunately the simplifier's fears are usually groundless, and appropriate modifications to it should yield considerable savings in execution time.

Risch has pointed out to us that Ostrowski [8] gives an algorithm which is, in the case where no algebraic expressions appear, an extension of the Risch algorithm for the log case. Ostrowski deals with integrals of rational expressions involving a function defined in terms of an integral. However, he considers only a single function (e.g., log(x) or erf(x + 1)) rather than a family of functions. Hence he deals with the case when a log or special function is the main variable of integration, but does not handle cases where constant multiples of special functions can appear in the integral. As we have seen, the problems that remain unsolved in such cases are essentially simplification problems.

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