

A heuristic for exact calculation of n -dimensional $n+1$ -parametric integrals of some elementary and special functions

Vladimir V. Bondarenko

Department of Applied Mathematics, University of Simferopol, Simferopol, Ukraine

vvb@ccssu.crimea.ua

(05534) 2-30-60 fax: (0652) 27-23-32

Abstract

At present, an algorithm for computation of n -dimensional integrals is unknown. A heuristic for calculation of a class of n -dimensional integrals over some subspaces of Euclidean space is described. Application of the heuristic to definite integrals over n -cube and n -simplex is presented. None of the computed integrals can be converted into an entry from the most extensive integral tables [15], [16], [17] as well as from [1], [8]–[14].

1 Introduction

Multiple integrals often appear in computations because they are either a final or intermediate solution to numerous subproblems of science and engineering. For example, in physics, double and triple integrals constantly arise in mechanics, quadruple integrals (Feynman diagrams) are an essential part of relativistic quantum mechanics, 6-dimensional integrals appear in celestial mechanics and so on. Thus, a fast multiple integration facility is desirable.

The goal of the paper is to turn attention to the long-standing problem of evaluation of multiple integrals. We have to admit that the *multiple* integration is not yet developed in any computer algebra systems: an algorithm for it is unknown. Currently all multiple integrals are calculated by transforming them to repeat integrals. Moreover, even such simple procedure is quite time consuming. How to speed computation of multiple integrals up?

It is well known that a standard 1-dimensional integration strategy is as follows. A computer algebra system starts from heuristic methods (lookup process, elementary calculus methods). When these methods fail, the integral is submitted to an integration algorithm. Such a strategy is efficient because 1) the heuristics are (much) faster than the algorithm; 2) the input stream might contain integrals which can be successfully processed by the heuristics.

As a heuristic step in the multiple integration problem the author proposes to use a table lookup technique using a large enough table containing explicit formulae for n -dimensional $ln+k$ -parametric *indefinite* integrals where l is small positive integers, say 1, 2, 3. Strategy is as follows: if the search in the table is successful, then an operator depending on the integration region should be applied to the corresponding entry of the table at a given value of n ; otherwise a straightforward integration should be performed. This idea poses the following questions:

- how to decrease lookup process overheads so that the lookup would be advantageous at average?
- how to enlarge the existing set of the explicit formulae for n -dimensional integrals?
- how to describe the region and the variables of the integration?
- how to check if a given integral is a convergent one? etc.

Probably it is beyond a single article size to make a *complete* analysis of very difficult problem of multiple integration; we presents an answer to the second question. Let us recall that the theory of residues provides a very efficient method for evaluation of definite integrals involving the elementary algebraic and transcendental functions in one variable. So one might expect that it is possible to generalize the theory of residues to a multivariate case. Indeed, there is a method based on a local residues technique; the method allows us to evaluate definite multidimensional integrals of rational functions over Euclidean space \mathbb{R}^n . Unfortunately, some fundamental difficulties of topological nature impose a serious restriction to structure of the integrand which can be calculated *even for rational* functions. To give an impression of degree of the restriction, we write out one class of ‘computable’ integrals:

$$\iint_{\mathbb{R}^2} \frac{h(x_1, x_2)}{\prod_{k=1}^p ((a_k x_1 + b_k x_2 + c_k)^2 + d_k^2)^{m_k}} dx_1 dx_2, \quad a_k, b_k, c_k, d_k \in \mathbb{R}, \quad d_k \neq 0, \quad m_k \in \mathbb{N}, \quad p \in \mathbb{N}$$

where $h(x_1, x_2)$ is a polynomial in x_1, x_2 such that the integral converges absolutely [21].

Note that few n -dimensional integrals were calculated so far in view of the extreme difficulty of the problem. The integrands of a considerable part of the known integrals have a similar algebraic structure; in fact, they are

some generalizations of Euler's beta function $B(\mu, \nu) = \int_0^1 x^{\mu-1} (1-x)^{\nu-1} dx$ to multivariate case. There are 11 tabular integrals taken over n -dimensional cube and 22 integrals taken over n -dimensional simplex. At present an algorithm for computation of n -dimensional integral is unknown; so none computer algebra system can compute such integrals. Nevertheless, it is possible to compute a wide enough class of n -dimensional integrals *exactly* with the aid of the heuristic described in Section 2; application of it requires a sizable amount of symbolic computations. The key idea of the method is computation of the correct answer in a systematic way, and then constructing, via a regular approach, a *rigorous* proof of the computed explicit formula within the framework of computer algebra system or a proof development environment. The heuristic presented here is a further development of those proposed in [3] and [4]. We summarize its scope in the following table:

Table: Comparison of two methods of n -dimensional integration

	The theory of residues	The heuristic
Integral type	Definite	Indefinite and definite
Integration region	Euclidean space	(A set of subspaces of) Euclidean space
Integrand class	A subset of rational functions	A subset of elementary and special functions
Complexity	Polynomial	Polynomial or exponential

We also presents 20 integrals and a proof that none of them can be converted into the integrals in [1], [5]–[17].

2 The Heuristic

Definitions It is sufficient for our purposes to define elementary functions as functions generated by applying algebraic operation, exponentiation and logarithms to polynomials finitely many times. Let us introduce two sets of univariate functions as follows: \mathcal{E}_0 is the set consisting of the elementary functions and the error function; \mathcal{E} is the set consisting of the finite compositions of elements of the set \mathcal{E}_0 . Further, let the EGFUN (Extended GFUN) procedure returns either an explicit expression for generating function of some finite sequence, or the empty set \emptyset . Let the integrand of n -dimensional integral has the fixed form $f(\beta + \vec{a} \cdot \vec{x})$, where \vec{a} and \vec{x} are vectors in Euclidean space \mathbb{R}^n , \cdot denotes a scalar product, \setminus denotes difference of two set, $a_m \neq 0$, $\frac{\partial a_m}{\partial x_k} = 0$, $m = \overline{1, n}$, $k = \overline{1, n}$; elementary n -dimensional volume $d\Omega_n = \prod_{i=1}^n dx_i$. Let us also fix once and for all for the given structure of integrand two universal sets U_n and Y_n of $2^n + 1$ and $n + 1$ elements respectively. These sets depend only on the components of vector \vec{a} and are *independent* of function f itself: $U_n = \{0, \sum_{i \in \Sigma} a_i \mid \Sigma \in \mathcal{C}\}$, where \mathcal{C} is the set of all combinations of elements of the set $\mathcal{M} = \{1, 2, \dots, n\}$, and $Y_n = \{0, a_i \mid i = \overline{1, n}\}$. Let also define a unit n -cube $C_n = \{x_i \geq 0, x_i \leq 1 \mid i = \overline{1, n}\}$, a unit n -simplex $S_n = \{x_i \geq 0, \sum_{i=1}^n x_i \leq 1 \mid i = \overline{1, n}\}$. Let domain of function $\text{rank}(x)$ is zero or a linear polynomial in symbolic variables (i.e. ones which have no numeric value initially), $\text{rank}(0)=0$ and $\text{rank}(x) = \text{number of items in } x$, if $x \neq 0$. At last, GCD is the greatest common divisor.

Heuristic. Given a function $f(z) \in \mathcal{E}$, it tries to find, using an Integration Algorithm \mathcal{A} , explicit formula for n -dimensional $n + 1$ -parametric integral $f \cdots f f(\beta + \vec{a} \cdot \vec{x}) d\Omega_n$ taken over n -cube C_n or n -simplex S_n .

Step 1 : [Initialize]

$M \leftarrow 15$, $\mathcal{A} \leftarrow$ Algorithm [7]. *Comment:* The choice of the minimal value of M is a rather hard problem. The author's experience shows that this choice of M not leads to excessive computations; on the other hand, it was sufficient to accept it for successful calculation of all integrals computed by us.

Step 2 : [Compute indefinite integrals using algorithm \mathcal{A}]

$\mathcal{I} \leftarrow \{m! f \cdots f f(z) d^m z \mid m = \overline{1, M}\}$.

Step 3 : [Continue?]

If there is at most one unevaluated integral in the set \mathcal{I} , then return 'There is no elementary n -dimensional integral' and terminate the heuristic.

Step 4 : [Eliminate fractional powers?]

For each term z^q in the set \mathcal{I} such that q is a number if all the q_i 's $\in \mathbb{N}$, then go to step 5. Otherwise flag $\leftarrow 1$; $d \leftarrow \text{GCD}(q_1, \dots, q_m)$, $q_i \in \mathbb{Q}$ $z \leftarrow z^{1/d}$.

Step 5 : [Trivial factorization]

Represent each element \mathcal{I}_j of the set \mathcal{I} in the form $\mathcal{I}_j = \mathcal{L}_{j0}(z) + \sum_{i=1}^{i0} \mathcal{L}_{ji}(z)\mathcal{B}_{ji}(z)$, where each $\mathcal{L}_{ji}(z)$ is a polynomial and each $\mathcal{B}_{ji}(z)$ is not a polynomial.

Step 6 : [Is there a pure polynomial part only?]

If for each $\mathcal{I}_j \in \mathcal{I}$ each $\mathcal{B}_{ji}(z) \equiv 0$, then $F(z) \leftarrow \mathcal{L}_{j0}(z)$ and go to step 11.

Step 7 : [Compute the supposed generating functions at once]

For each $\mathcal{L}_i(z) \in \mathcal{L}$ do begin $Z_i(z, t) \leftarrow \text{EGFUN}(\mathcal{L}_i(z))$; if $Z_i(z, t) = \emptyset$, then $\mathcal{L} \leftarrow \mathcal{L} \setminus \mathcal{L}_i(z)$ end.

Step 8 : [Compute the remaining supposed generating functions step by step]

For each $\mathcal{L}_j(z) \in \mathcal{L}$ do begin $Z_j(z, t) \leftarrow \text{EGFUN}(\{\text{coefficient at } z^k \text{ of } \mathcal{L}_{ji}(z) \mid k = \overline{0, M}\})$; if $Z_j(z, t) = \emptyset$, then $\mathcal{L} \leftarrow \mathcal{L} \setminus \mathcal{L}_j(z)$ end.

Step 9 : [Restore the remaining supposed generating functions using a mathematical data base]

For each $\mathcal{L}_j(z) \in \mathcal{L}$ do begin scan a data base containing sequences to find a proper GF; $Z_j(z, t) \leftarrow \text{EGFUN}(\mathcal{L}_j(z))$; if $Z_j(z, t) = \emptyset$, then $\mathcal{L} \leftarrow \mathcal{L} \setminus \mathcal{L}_j(z)$ end. If $\mathcal{L} \neq \emptyset$, then output 'Failure: No matching sequence' and terminate the heuristic. *Comment:* A reference book [20] can be considered as such a 'data base'.

Step 10 : [Construct a sum?]

If for each $m = \overline{1, M}$ degree $(\mathcal{L}_{0m}(z)) < m$, then go to step 11. If integration region $R = C_n$, then $D \leftarrow \{f \cdots \int_{C_n} f(\beta + \sum_{i=1}^m a_i x_i) d\Omega_m \mid m = \overline{1, M}\}$; otherwise $D \leftarrow \{f \cdots \int_{S_n} f(\beta + \sum_{i=1}^m a_i x_i) d\Omega_m \mid m = \overline{1, M}\}$. Represent each element $D_j \in D$ in the form $D_{ji}(z) = \mathcal{P}_{j0}(z) + \sum_{i=1}^{k0} \mathcal{P}_{ji}(z)\mathcal{B}_{ji}(z)$, where each $\mathcal{P}_{ji}(z)$ is a polynomial and each $\mathcal{B}_{ji}(z)$ is not a polynomial. $\mathcal{L} \leftarrow \{\mathcal{P}_{j0}(z)\}$ and go to step 7.

Step 11 : [Construct a set for checking]

$F(z) \leftarrow \sum_i \mathcal{L}_i^*(z)\mathcal{B}_i(z)$, where the $\mathcal{L}_i^*(z)$'s are polynomials generated by the corresponding generating functions. $\mathcal{H} \leftarrow \{f(z) - (\frac{d}{dz})^m F(z) \mid m = \overline{1, 2M}\}$. *Comment:* Computation of extra M terms increases plausibility of conjecture that the computed generating functions are correct.

Step 12 : [Reject the computed generating function?]

If there is at most one element $\mathcal{H}_i \neq 0$ in the set \mathcal{H} , then output 'Failure: incorrect generating function(s)' and terminate the heuristic.

Step 13 : [Accept the computed generating function?]

Observing intermediate expressions of $\mathcal{D}^j F(\beta + \vec{a} \cdot \vec{x})$, $j = \overline{k, 1}$ and finding some useful relations, try to prove by induction that $\{f(\beta + \vec{a} \cdot \vec{x}) - \mathcal{D}^k F(\beta + \vec{a} \cdot \vec{x}) \equiv 0 \mid k \in \mathbb{N}\}$. If a proof is found, then go to step 14.

Step 14 : [Construct the explicit formula for n -dimensional integral]

If flag = 1, then $z \leftarrow (\beta + \vec{a} \cdot \vec{x})^d$; otherwise, $z \leftarrow \beta + \vec{a} \cdot \vec{x}$. If region = C_n , then return $n!^{-1} \sum_{\tau \in U_n} (-1)^{(n+\text{rank}(\tau))} \prod_{i=1}^n a_i^{-1} F(\beta + \vec{a} \cdot \vec{x})$, otherwise return $n!^{-1} \sum_{\tau \in V_n} \prod_{i=1}^n (\tau - (1 - \delta_{\tau a_i})a_i)^{-1} F(\beta + \vec{a} \cdot \vec{x})$.

Step 15 : [Give a formal proof]

Using ideas like those in the proof of the Theorem 2 (Section 4), construct a proof that the symbolic sum is formally equal to n -dimensional integral of f taken over the corresponding integration region.

Step 16 : [Compute the minimal conditions of existence of the integral]

Transform the inverse trigonometric and inverse hyperbolic functions in F into a logarithmic form. Find a solution S of linear inequalities: $\{\varphi_i > 0 \mid \varphi_i \in \mathcal{Q}\}$, where set \mathcal{Q} consists of arguments of each (nested) algebraic and logarithmic functions to ensure the minimal conditions of reality of the integral. Return S and terminate the heuristic.

Remark 1. It is possible to modify the heuristic so that it could calculate indefinite n -dimensional integrals of $f(\beta + \vec{a} \cdot \vec{x})$, $f(z) \in \mathcal{E}$. We have computed all indefinite integrals corresponding to the integrals (1)–(20) in [6].

Remark 2. The heuristic can also be extended to processing n -dimensional integrals taken over 'more complex' integration regions $\mathcal{O} \subseteq \mathbb{R}^n$ as compared to cube C_n and simplex S_n . For example, let us define the following n -dimensional regions: a unit n -sphere $P_n = \{\sum_{i=1}^n x_i^2 \leq 1\}$, a unit n -ellipsoid $E_n = \{\sum_{i=1}^n (x_i/c_i)^2 \leq 1\}$, a unit generalized n -ellipsoid $G_n = \{x_i \geq 0, \sum_{k=1}^n (x_k/c_k)^{\beta_k} \leq 1 \mid i = \overline{1, n}\}$, a positive n -half-space $H_n^+ = \{x_i \geq 0, x_i \leq \infty \mid i = \overline{1, n}\}$, a negative n -half-space $H_n^- = \{x_i \geq -\infty, x_i \leq 0, \mid i = \overline{1, n}\}$, a unit n -cone $N_n =$

$\{\sum_{i=1}^{n-1} x_i/c_i - x_n/c_n \leq 0\}$. Further, let us define the set of regions $\mathcal{D} = \{C_n, S_n, H_n^+, H_n^-, P_n, G_n, E_n, N_n\}$ and let \times denotes direct product. Then the presented heuristic can be applied to the region $\mathcal{O} = \mathcal{D}_1 \times \mathcal{D}_2 \times \cdots \times \mathcal{D}_m$ [6].

Remark 3. In reality, for recognition of the structure of sequences the author uses the GFUN package [19] which approximates the EGFUN procedure good enough. Given the first terms of the sequence, the package tries to compute either differential or algebraic equation satisfied by the generating function (GF); if possible, the package returns an explicit expression for GF. The generating function for $P_n(z)$ of Section 3 was really computed by GFUN after a little help. Unfortunately, the generating function for $Q_n(z)$ was not calculated by it. However, the package was able to compute some subexpressions of GFs in the explicit formulae for several n -dimensional integrals involving the (complementary) error function or the square of it as a factor of the integrands [6]. It seems to be valuable to expand the package facilities towards handling the quantities like $S_r(n) \equiv \sum_{j_r=1}^n \sum_{j_{r-1}=1}^{j_r} \cdots \sum_{j_2=1}^{j_3} \sum_{j_1=1}^{j_2} \prod_{m=1}^r \frac{1}{j_m}$ which have often arisen during our computations. It might be possible to use a (specialized) proof development environment for construction of the proof; but it seems to be a point of interest that in this work the author actually used a *CAS itself* in order to find an idea for a proper proof as well as to construct this proof.

Remark 4. It should be emphasized that the author could not find correct representations for the integrals of Section 3 without the essential aid of a computer algebra system *in view of an exorbitant amount of computations*. In order to obtain the correct answer for some n -dimensional integrals we needed in evaluation of 15-dimensional ones; thus, 'the paper-and-pencil' method is not applicable. Actually the integrator of Derive [18] was used intensely at steps 2 and 10, differential and recurrence equations solvers and solver for finding integer solutions to algebraic equations at steps 7, 8; at last, algebraic inequalities solver was used at step 16.

Figure: Structure of computational environment for n -dimensional integration

Derive \iff Pascal language code \iff Maple \iff GFUN procedure

Remark 5. Only a part of the computed formulae for n -dimensional integrals over n -cube C_n and n -simplex S_n is presented in the work. The explicit expressions for integrals involving $\lambda^k \arcsin^i(\lambda)$, $\lambda^k \operatorname{arcsinh}^i(\lambda)$, $i = \overline{1, 3}$, $k = \overline{1, 3}$, $\operatorname{erf}^2(\lambda)$, $\operatorname{erf}^2(\lambda) \exp(-\lambda)$, where $\lambda = \beta + \vec{a} \cdot \vec{x}$ are described in [6].

3 Integrals which cannot be derived from the integral tables

Notations Let $\beta \in \mathbb{R}$, $a_i \neq a_j$, $\lambda = \beta + \tau$. Further, $\delta_{ij} = \begin{cases} 1 & (i=j) \\ 0 & (i \neq j) \end{cases}$ is the Kronecker delta function, $\Gamma(x)$ is Euler's gamma function, $D_\nu(x)$ is the parabolic cylinder function fixed by $\frac{\partial^2}{\partial x^2} D_\nu(x) + (\nu + \frac{1}{2} - \frac{1}{2}x^2)D_\nu(x) = 0$, $D_\nu(0) = \sqrt{\pi} 2^{\nu/2} / \Gamma(\frac{1}{2} - \frac{1}{2}\nu)$, $\frac{\partial}{\partial x} D_\nu(x)|_{x=0} = -\sqrt{\pi} 2^{(\nu+1)/2} / \Gamma(-\frac{1}{2}\nu)$, $[x]$ is the integer part of number, $S_0(l) = 1$, $S_k(l) = \sum_{r=1}^l S_{k-1}(r)/r$ ($k \geq 2$), P_m^k is the number of permutations of k things taken m at a time, and polynomials $P_n(z)$, $Q_n(z)$ are defined as follows:

$$(*) \quad P_n(z) = \frac{1}{2^n} \sum_{k=0}^{[n/2]} \frac{n!}{k! (n-2k)!} (2z)^{n-2k}, \quad Q_n(z) = \sqrt{\pi} \left(\frac{d}{dt}\right)^n \exp\left((z + \frac{t}{2})^2\right) \left(\operatorname{erf}\left(z + \frac{t}{2}\right) - \operatorname{erf}(z)\right) \Big|_{t=0}.$$

At last, let us define the operators C_n^+ and S_n^+

$$C_n^+ = \sum_{\tau \in U_n} (-1)^{(n + \operatorname{rank}(\tau))} \prod_{i=1}^n a_i^{-1}, \quad S_n^+ = \sum_{\tau \in \mathcal{V}_n} \prod_{i=1}^n (\tau - (1 - \delta_{\tau a_i}) a_i)^{-1},$$

and introduce a compact notation to emphasize interconnection of the integrals:

$$\left\{ \begin{matrix} C_n \\ S_n \end{matrix} \right\} \int \cdots \int f d\Omega_n = \left\{ \begin{matrix} C_n^+ \\ S_n^+ \end{matrix} \right\} \left\{ \begin{matrix} A \\ B \end{matrix} \right\} F \text{ is equivalent to } \int \cdots \int f d\Omega_n = C_n^+ (AF), \quad \int \cdots \int f d\Omega_n = S_n^+ (BF).$$

Then the equalities for $n+1$ - and $n+2$ -parametric integrals (1)–(20) hold; they are generated by our heuristic.

We assume $\nu \in \mathbb{R}$, $\nu > 0$, $k \in \mathcal{M}$, $\{\beta > 0, \sum_{i \in \Sigma} a_i > -\beta \mid \Sigma \in \mathcal{C}\}$ for integrals 1, 3, 5, 7, 9, 19 and $\{\beta > 0, \sum_{i=1}^k a_i > -\beta \mid k = \overline{1, n}\}$ for integrals 2, 4, 6, 8, 10, 20; further, $\{|\beta| < 1, \sum_{i \in \Sigma} a_i > -\beta - 1 \mid \Sigma \in \mathcal{C}\}$ for integrals 11, 13, and $\{|\beta| < 1, \sum_{i=1}^k a_i > -\beta - 1 \mid k = \overline{1, n}\}$ for 12, 14. At last, $\{\beta \in \mathbb{C}, a_i \in \mathbb{C} \mid i = \overline{1, n}\}$ for 15–18.

$$(5)-(6) \quad \left\{ \begin{matrix} C_n \\ S_n \end{matrix} \right\} \int \cdots \int \ln(\beta + \vec{a} \cdot \vec{x}) d\Omega_n = \left\{ \begin{matrix} C_n^+ \\ S_n^+ \end{matrix} \right\} \frac{1}{n!} \left(\lambda^n \ln(\lambda) - \left\{ \begin{matrix} n! \\ 1 \end{matrix} \right\} \sum_{i=1}^n \frac{1}{i} \right),$$

$$(7)-(8) \quad \left\{ \begin{matrix} C_n \\ S_n \end{matrix} \right\} \int \cdots \int \ln^k(\beta + \vec{a} \cdot \vec{x}) d\Omega_n = \left\{ \begin{matrix} C_n^+ \\ S_n^+ \end{matrix} \right\} \frac{1}{n!} \left(\sum_{m=0}^{k-1} (-1)^m P_m^k S_m(n) \lambda^n \ln^{k-m}(\lambda) - \{n\}_1^k S_k(n) \right),$$

Remark. It is possible to use these 'basic' n -dimensional integrals for generating a number of quasi-new integrals which can be of value for different areas, by various transformations (specifically, by nonlinear substitutions).

The n -dimensional integrals (1)–(20) which were calculated with the aid of CAS are absent in the most extensive tables [15], [16], [17] as well as in [1], [8], [9], [10], [11], [12], [13], [14]. There exist algorithms which can determine whether one integral can be converted into the other one [22], [23], but these algorithms can only handle integrals with *fixed* number of variables. Nevertheless, it is possible to prove

THEOREM 1 *None of the integrals (1)–(20) can be converted, by any transformations, to the entries corresponding to n -dimensional integrals of the tables [1], [8]–[17].*

Sketch of the proof. Let us divide all 33 tabular n -dimensional integrals (including the reduction formulae) taken over unit n -cube C_n or (unit) n -simplex (S_n) S_n into 2 classes by the following attributes: 1) the total number of parametres in the integrand; 2) form of the integrand argument *and* the total number of parametres in the integrand. A (considerable) part of the tabular n -dimensional integrals cannot be transformed into the presented ones because the former integrals have *less* than $n+1$ parametres. The other part of tabular integrals and all reduction formulae have the expressions $f(\sum_{i=1}^n x_i)$, $\prod_{i=1}^n x_i^{\alpha_i} (1-x_i)^{\beta_i} f(c \prod_{i=1}^n x_i)$, $\prod_{i=1}^n x_i^{\alpha_i} f_1(\sum_{i=1}^n x_i) f_2(c \prod_{i=1}^n x_i^{\beta_i})$ and $f(1 \pm \sum_{i=1}^n x_i)$ as factors of the integrand. Therefore, the substitutions a) $x_1 \mapsto \beta + a_1 x_1$, $x_i \mapsto a_i x_i$, $i = \overline{2, n}$ and b) $x_1 \mapsto \beta \mp 1 + a_1 x_1$, $x_i \mapsto a_i x_i$, $i = \overline{2, n}$ lead to integration regions which not coincide either with C_n or with S_n . \square

Thus, new n -dimensional integrals are calculated due to the crucial aid of CAS.

4 Proof of the equalities (1)–(20)

LEMMA 1 *Let the polynomials $P_n(z)$ and $Q_n(z)$ are defined by the expressions (*). Then*

$$\frac{\partial}{\partial z} P_n(z) = n P_{n-1}(z), \quad 2P_n(z) + \frac{\partial}{\partial z} Q_n(z) - 2z Q_n(z) = n Q_{n-1}(z).$$

Proof. It is easy to check that both the sum $P_n(z)$ and the expression $P_n^*(z) = \frac{1}{2^n} e^{-z^2} \left(\frac{d}{dz}\right)^n e^{z^2}$ satisfy the equation $\frac{\partial^2 X_n(z)}{\partial z^2} + 2z \frac{\partial X_n(z)}{\partial z} - 2n X_n(z) = 0$ with the same initial conditions. Therefore $P_n(z) \equiv P_n^*(z)$. Differentiating the explicit expression for $P_n^*(z)$ and using Leibniz's formula yields

$$\frac{d}{dz} P_n(z) = \frac{1}{2^n} \left(-2ze^{-z^2} \left(\frac{d}{dz}\right)^n e^{z^2} + e^{-z^2} \left(\frac{d}{dz}\right)^n 2ze^{z^2} \right) = \frac{1}{2^n} e^{-z^2} 2n \left(\frac{d}{dz}\right)^{n-1} e^{z^2} = n P_{n-1}(z).$$

Proof of the second relation is longer, but requires no new idea. \square

LEMMA 2 *Let β be a scalar, \vec{a} be a constant vector in \mathbb{R}^n with n non-zero components a_1, a_2, \dots, a_n , \vec{x} be a vector in \mathbb{R}^n and $\lambda = \beta + \vec{a} \cdot \vec{x}$, $\mathcal{D}^n \equiv \partial^n / \partial x_1 \dots \partial x_{n-1} \partial x_n$, $\Pi = \prod_{i=1}^n a_i$. Then the following relations of the type $\mathcal{D}^n F(\lambda) = f(\lambda)$ hold:*

THEOREM 2 *The statements (1)–(20) hold.*

Proof. All formulae (1)–(20) can be proved from the unified viewpoint. Let us order the variables x_j and the components a_j of vector \vec{a} in direct lexicographic order. Without loss of generality we can assume that any $a_j \neq 0$. Otherwise, we eliminate corresponding variables from the integrand, renumber the remaining ones; trivial integration over such variables yields factor 1. First of all we will prove that the formal sums at the r.h.s. of the odd entries of (1)–(20) are equal to the corresponding integrals over cube C_n . Successive integration over the x_j 's produces the following expression with n potential substitutions \int_0^1 :

$$\int_{C_n} \cdots \int f(\beta + \vec{a} \cdot \vec{x}) \Omega_n = \prod_{j=1}^n \frac{1}{a_j} \left(\cdots \left((F(\beta + \vec{a} \cdot \vec{x})|_0^1) \Big|_0^1 \cdots \right) \Big|_0^1, \text{ where } \left(\frac{d}{dz}\right)^n F(z) = f(z).$$

At each substitution \int_0^1 over variable x_i we both ‘switch on’ component a_i in the argument of F and multiply F by 1 at the upper limit. Similarly, we ‘switch off’ (zeroize) this component a_i and multiply F by -1 at the lower limit. As none of symbolic components can be cancelled, and each substitution doubles the number of terms of the sort $F(\beta + \dots)$, therefore the total number of the terms is precisely equal to 2^n when all substitutions are performed. Further, to ‘switch on’, for example, components a_1, a_2, \dots, a_k (that is to obtain a term with these components only) after indefinite integration in \mathbb{R}^n , one must perform exactly $n - k$ substitutions at the lower limit which lead to factor $(-1)^{(n-k)}$. Therefore, to generate the above-mentioned term one must multiply expression $F(a_1, a_2, \dots, a_k)$ by factor $(-1)^{(n-k)} = (-1)^{(n+k)} = (-1)^{(n+\text{rank}(k))}$, where function $\text{rank}(k)$ is defined only on symbolic expressions and zero; the function returns number of items in x and $\text{rank}(0) = 0$. After all one needs only to sum all terms of the sort $(-1)^{(n+\text{rank}(k))}F$ (the set of all a_j ’s) over all elements of the set U_n . Therefore, the symbolic sum represents the proper n -dimensional integral over n -cube C_n .

As for unit n -simplex S_n integration region, it is sufficient to rewrite formula for integral over n -simplex via product of 1-dimensional integral over x_n by $n - 1$ -dimensional one over unit simplex S_{n-1} and integrate, with actual substitution, over variable x_n . Repeating the process $n - 1$ times produce the explicit form of the operator S_n^+ . This calculation is cumbersome, but trivial enough; we leave it as an exercise to the interested reader. So the formulae (1)–(20) are proved formally.

At last, the restrictions on β and the a_k ’s are chosen such that all arguments of the logarithms and algebraic functions in the r.h.s. of (1)–(20) were positive. Thus, taking into consideration finiteness of integration regions C_n and S_n , the restrictions are the ‘minimal’ reality and finiteness conditions for the integral in \mathbb{R}^n ; they ensure n -dimensional integral existence. This completes the proof. \square

5 Speed-up due to using the explicit formulae for integrals

It is natural to expect that a significant speed-up due to using of symbolic sums can be gained only at high enough dimensionality of space to integrate, but that is completely false. In fact, a speed-up of order 10^2 - 10^4 even for triple integrals is rather a rule than an exception. For example, the following innocent integral can be computed via the corresponding symbolic sum 28000 times faster than via straightforward integration [6]:

$$\int_0^\infty \int_0^\infty \int_0^\infty \frac{(x_0 + \vec{x} \cdot \vec{x})^3}{(c_0 + \vec{x} \cdot \vec{x})^7} dx_1 dx_2 dx_3.$$

Apart from their intrinsic value as new examples of analytic integration, the discovered formulae (1)–(20) enable us to gain a dramatic speed-up in multiple integrals computation using the corresponding symbolic sums because they involves the fast operations only; the slowest of these operations is symbolic differentiation which runs efficiently in all CASs. Our experiments with the formulae show that the higher dimension of space to integrate the greater speed-up.

The other aspect of this research is an opportunity of fast numeric high-precision evaluation of certain class of integrals in high-dimensional spaces (say, in 1000- or 10000-dimensional) [5]. This can be used for approximation of some *continual* integrals which are of great interest for quantum mechanics; the question is under study now [6].

We suggest to use both the standard tabular explicit formulae for n -dimensional integrals as well as the formulae (1)–(20), after some independent reproving, for using a lookup technique or *for the mathematical data base extension of computer algebra systems*.

6 Two conjectures

Let unit n -cube C_n and the unit n -simplex S_n be integration regions in \mathbb{R}^n , the integrand has structure $f(\beta + \vec{a} \cdot \vec{x})$ and n -dimensional integral can be expressed via finite sums. Then two following conjectures are supported by 44 computed integrals [3], [4], [5], [6]:

$$(C1) \int_{C_n} \dots \int f(\beta + \vec{a} \cdot \vec{x}) d\Omega_n = V(n, \beta, \vec{a}) + \frac{1}{c_1(n \pm c_2)! \prod_{i=1}^n a_i} \sum_{\tau \in U_n} (-1)^{(n+\text{rank}(\tau))} \sum_j \mathcal{L}_j(\beta + \tau, n) \mathcal{R}_j(\beta + \tau, n),$$

$$(C2) \int_{S_n} \dots \int f(\beta + \vec{a} \cdot \vec{x}) d\Omega_n = \frac{1}{c_1(n \pm c_2)!} \left(V(n, \beta, \vec{a}) + \sum_{\tau \in Y_n} \frac{\sum_j \mathcal{L}_j(\beta + \tau, n) \mathcal{R}_j(\beta + \tau, n)}{\prod_{j=1}^n (\tau - (1 - \delta_{\tau a_j}) a_j)} \right),$$

where $V(n, \beta, \vec{a})$ is either an n -fold sum or zero, $\mathcal{L}_j(z, n)$ is a polynomial in z and $c_1, c_2 \in \mathbb{N}$.

7 Open questions for future work

At least, there are three questions: 1) What is the exact class of integrands for which there exists a 'closed-form' expression for n -dimensional integral (involving finite sums only) ? 2) What are the most general existence conditions for integrals (1)–(20) if $\beta \in \mathbb{C}$, $a_j \in \mathbb{C}$? 3) Is it possible to calculate some non-tabular integrals involving special functions different from the error function and the parabolic cylinder function? We have a precursory data; in the next paper we hope to answer this question affirmatively by combining the technique described in this work and that developed in [2] which is based on an approach using the Meijer G function and enables us to integrate functions of hypergeometric type.

Acknowledgements

The author is grateful to Dr. A. Rich and Dr. D. Stoutemyer of Soft Warehouse, Inc. for permanent supporting him with the most recent DERIVE copies; our work is based significantly on its outstanding integrator.

References

- [1] Abramowitz, M. and Stegun, I. A. Handbook of Mathematical Functions, Dover, N. Y., 1970
- [2] Adamchik, V. S. and Marichev, O. I., The Algorithm for Calculating Integrals of Hypergeometric Type Functions and Its Realization in REDUCE system, in *Proceedings of the International Symposium on Symbolic and Algebraic Computation '90*, ed by Watanabe, S. and Nagata, M., Addison-Wesley, New York, 1990, pp. 212-224
- [3] Bondarenko, V. V., Computer Algebra System Aided Evaluation of Some Definite n -fold Integrals with Undetermined n , accepted and invited by the Poster Committee for *the International Symposium on Symbolic and Algebraic Computation '95* Poster Session, University of Concordia, Montreal, 1995
- [4] Bondarenko, V. V., Exact Evaluation of Definite n -dimensional Integrals with Undetermined a priori Integer n , accepted and invited by the Poster Committee for *the International Symposium on Symbolic and Algebraic Computation '96* Poster Session, Eidgenössische Technische Hochschule, Zürich, 1996
- [5] Bondarenko, V. V., On Fast High-Precision Evaluation of Some Multi-Dimensional Integrals, in *Proceedings of the International Workshop on New Computer Technologies in Control Systems '95*, ed by Dmitriev, M. G. and Sachkov, Yu. L., Pereslavl-Zalessky, 1995
- [6] Bondarenko, V. V., On Exact Evaluation of Indefinite and Definite n -dimensional Multiparametric Integrals of a Class of Elementary and Special Functions: The Method and Tables, in progress
- [7] Bronstein, M., Integration of Elementary Functions, *Journal of Symbolic Computation*, 9, 1990, pp. 117-173
- [8] Dwight, H. D., Tables of Integrals and other mathematical data, The Macmillan Company, N.Y., 1961
- [9] Erdélyi, A., Higher Transcendental Functions, vol. 1-2-3, R. E. Krieger Publishing Company, Inc., Malabar, Florida, 1981
- [10] Gradshteyn, I. S. and Ryzhik, I. M., Tables of Integrals, Sums, Series and Products, Nauka, Moscow, 1971
- [11] Gröebner, W. and Hofreiter, N., Integraltafel, Teil I, Unbestimmte Integrale, Wien und New York, Springer-Verlag, 1975
- [12] Gröebner, W. and Hofreiter, N., Integraltafel, Teil II, Bestimmte Integrale, Wien und Innsbruck, Springer-Verlag, 1958
- [13] D. Bierens de Haan, *Nouvelles Tables d'Intégrales Définies* edition of 1867 corrected, with an English translation of the Introduction by J. F. Ritt, G. E. Stechert & Co. , N.Y., 1939
- [14] Luke, Y. L., Mathematical Functions and their Approximations, Academic Press, 1975
- [15] Prudnikov, A. P., Brychkov, Yu. A., Marichev, O. I., Integrals and Series. Vol. 1: Elementary functions, Gordon and Breach, N. Y., London, Tokyo, 1988
- [16] Prudnikov, A. P., Brychkov, Yu. A., Marichev, O. I., Integrals and Series. Vol. 2: Special functions, Gordon and Breach, N. Y., London, Tokyo, 1988
- [17] Prudnikov, A. P., Brychkov, Yu. A., Marichev, O. I., Integrals and Series. Vol. 3: More special functions, Gordon and Breach, N. Y., London, Tokyo, 1989

- [18] Rich, A. D. and Stoutemyer, D. R., DERIVE version 3: User manual: A Mathematical Assistant for Your Personal Computer, 1995
- [19] Salvy, B. and Zimmermann, P., Gfun: A Maple Package for the Manipulation of Generating and Holonomic Functions in One Variable. MapleV Share Library, March 4 1992
- [20] Sloane, N. J. A., A Handbook of Integer Sequences, Academic Press, 1973
- [21] Tsikh, A. K., Multi-dimensional Residues with Applications, Nauka, Novosibirsk, 1988 (in Russian)
- [22] Takayama, N., Gröbner Basis, Integration and Transcendental Functions, in *ISSAC '90 proceedings of the International Symposium on Symbolic and Algebraic Computation*, ed by Watanabe, S. and Nagata, M., Addison-Wesley, 1990, pp 152-156
- [23] Wilf, H. S. and Zeilberger, D., An Algorithmic Proof Theory for Hypergeometric (Ordinary and "q") Multisum / Integral Identities, *Inventiones Mathematicæ*, 108, 1992, pp. 575-633