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Numerical Evaluation of Multiple Integrals II

by Preston C. Hammer and Arthur H. Stroud

1. Introduction. In the first paper of this title [1], Hammer and Wymore introduced methods whereby integration formulas of the form

$$\int_R w(x)f(x)\,dx \doteq \sum a_i f(\xi_i) \tag{1}$$

which are known for special regions (in n-dimensional euclidean space E_n) may be used to determine formulas for other regions. They also showed, in some cases, how the symmetry of a region may simplify the task of finding integration formulas for the region.

To facilitate numerical integration over regions in higher dimensional spaces, we summarize the most important formulas (1) and review methods by which formulas for classes of regions may be obtained from them. These methods enable one to obtain formulas for regions which we consider too special to warrant particular formulas.

2. Regions with symmetry. In deriving numerical integration formulas it is possible to obtain explicit formulas with comparatively little effort when the region and the formula both are assumed to have certain kinds of symmetry. Formulas precise for polynomial functions involving minimal numbers of points can be derived, in principle, by solving simultaneous algebraic equations by general elimination procedures leading to polynomials which have as roots the solutions of the system. However, the manipulative work in achieving such solutions is forbidding in magnitude and can probably be done effectively only with high speed computers. Moreover, the solutions may turn out to be complex numbers and the determinations of approximate values for the solutions will involve the numerical solution of high degree polynomial equations. For example, the general seventh degree polynomial in three variables has 120 terms so that the determination of a numerical integration formula precise for all such polynomials over an arbitrary region R would lead to the problem of solving a system of 120 equations of algebraic (non-linear) character. In [1] it is shown that for certain symmetrical regions with a symmetrical formula the problem is reduced to seven simultaneous algebraic equations for which explicit solutions are easily derived. The problem of finding integrals of monomials to establish the equations to be solved also will be a difficult problem for many regions.

A set S in E_n is said to be *fully symmetrical* provided $x \in S$ implies that every

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point y obtainable from x by permutations and/or changes of sign of the coordinates of x is also in S. A function g defined on a fully symmetrical set S is said to be *fully symmetrical* provided $g(x) = g(y)$ whenever y may be obtained from x as above. A numerical integration formula of the form (1) is said to be *fully symmetrical* if the set of all evaluation points $\xi_1, \xi_2, \cdots$ forms a fully symmetrical set and the weight function $a_j = a(\xi_j)$ is a fully symmetrical function. In [1] full symmetry was indicated simply as symmetry. Full symmetry is defined here in reference to the coordinate system, but could readily be extended to include all sets which result from rigid motions of those included in the definition. For use in this paper the definition given is adequate.

Now let $w(x)$ be a fully symmetrical function on a fully symmetrical region R. If a fully symmetrical integration formula $\sum a_j f(\xi_j)$ is equal to $\int_R f(x)\, dx$ for all polynomials of at most degree k then, in principle, a fully symmetrical formula $\sum b_j f(\nu_j)$ may be found which gives the value of $\int_R w(x) f(x)\, dx$ for the same class of polynomials using the same algebraic manipulations as in finding a_j and ξ_j. That is, the algebraic form in which a_j and ξ_j appear is the same form as that in which b_j and ν_j appear. Since the existence of solutions of these equations may depend on the values of the constants it cannot be stated that b_j and ν_j can always be found if a_j and ξ_j were determined. This remark is important since for spherical regions weight functions $w(r)$ depending only on $r = |x|$ are common and such weight functions are fully symmetrical.

We anticipate that for many useful weight functions $w(r)$ there will be numerical integration formulas over the spherical shell involving the same number of points as formulas for $w = 1$.

3. Summary of numerical integration formulas. We summarize known formulas of the form (1) with $w(x) = 1$ for regions in euclidean spaces of dimension $\geqq 2$. We give formulas for cubes, spheres, and simplexes.

Tables 1 and 2 give certain fully symmetrical formulas for cubes and spheres respectively. The points in these formulas are divided into one or more fully symmetric subsets; each subset is generated by any one of its points (a generator). Below are generators for each fully symmetric subset occurring in the formulas of these tables. With the generators we give the number of points in the subset and the weight for each point in the subset.

Generator	Number of points	Weight
$(0, 0, 0, 0, \cdots, 0)$	1	a_0
$(\nu, 0, 0, 0, \cdots, 0)$	$2n$	a_1
$(\xi_1, \xi_1, 0, 0, \cdots, 0)$	$2n(n-1)$	b_1
$(\xi_2, \xi_2, 0, 0, \cdots, 0)$	$2n(n-1)$	b_2
$(\eta_1, \eta_1, \eta_1, 0, \cdots, 0)$	$\frac{4}{3}n(n-1)(n-2)$	c_1
$(\eta_2, \eta_2, \eta_2, 0, \cdots, 0)$	$\frac{4}{3}n(n-1)(n-2)$	c_2

With these generators we can obtain formulas of degree $\leqq 7$. (A formula is of degree k if it is exact for polynomials of at degree no greater than k.) The system of

TABLE 1. *Formulas for cubes*

1-2	2-cube	degree 3	4 points
	$\nu = 0.8164965809277260$		$a_1 = 1.0000000000000000$
2-2	2-cube	degree 5	9 points
			$a_0 = 0.7901234567901235$
	$\nu = 0.7745966692414834$		$a_1 = 0.4938271604938272$
	$\xi_1 = 0.7745966692414834$		$b_1 = 0.3086419753086420$
3-2	2-cube	degree 7	12 points
	$\nu = 0.9258200997725515$		$a_1 = 0.2419753086419753$
	$\xi_1 = 0.3805544332083157$		$b_1 = 0.5205929166673945$
	$\xi_2 = 0.8059797829185987$		$b_2 = 0.2374317746906302$
1-3	3-cube	degree 3	6 points
	$\nu = 1.0000000000000000$		$a_1 = 1.3333333333333333$
2-3	3-cube	degree 5	19 points
			$a_0 = 2.0740740740740741$
	$\nu = 0.7745966692414834$		$-a_1 = 0.2469135802469136$
	$\xi_1 = 0.7745966692414834$		$b_1 = 0.6172839506172840$
4-3	3-cube	degree 5	14 points
	$\nu = 0.7958224257542215$		$a_1 = 0.8864265927977839$
	$\eta_1 = 0.7587869106393281$		$c_1 = 0.3351800554016621$
5-3	3-cube	degree 7	27 points
			$a_0 = 0.7880734827442106$
			(0.9478945552646438)
	$\nu = 0.8484180114722525$		$a_1 = 0.4993690023077203$
	(1.2795818594182734)		(0.0424299394912215)
	$\xi_1 = 1.1064128986267175$		$b_1 = 0.0323037423340374$
	(0.7000972875523367)		(0.5032755687554778)
	$\eta_1 = 0.6528164721016912$		$c_1 = 0.4785084494251273$
	(0.8550442581681327)		(0.0947773728402868)
6-3	3-cube	degree 7	34 points
	$\nu = 0.9258200997725515$		$a_1 = 0.2957475994513032$
	$\xi_1 = 0.9258200997725515$		$b_1 = 0.0941015089163237$
	$\eta_1 = 0.7341125287521153$		$c_1 = 0.2247031747656014$
	$\eta_2 = 0.4067031864267161$		$c_2 = 0.4123338622714356$
1-n	n-cube	degree 3	$2n$ points
	$\nu = \sqrt{\frac{n}{3}}$		$a_1 = \frac{2^{n-1}}{n}$
2-n	n-cube	degree 5	$2n^2 + 1$ points
			$a_0 = \frac{2^{n-1}}{81}(25n^2 - 115n + 162)$
	$\nu = \sqrt{\frac{3}{5}}$		$a_1 = \frac{2^{n-1}}{81}(70 - 25n)$
	$\xi_1 = \sqrt{\frac{3}{5}}$		$b_1 = \frac{(25)2^{n-1}}{162}$

TABLE 2. *Formulas for spheres*

11-2	2-sphere	degree 3	4 points
	$\nu = 0.7071067811865475$		$a_1 = 0.7853981633974483$
12-2	2-sphere	degree 5	9 points
			$a_0 = 0.5235987755982989$
	$\nu = 0.7071067811865475$		$a_1 = 0.5235987755982989$
	$\xi_1 = 0.7071067811865475$		$b_1 = 0.1308996938995747$
13-2	2-sphere	degree 7	12 points
	$\nu = 0.8660254037844386$		$a_1 = 0.2327105669325773$
	$\xi_1 = 0.3229149920674005$		$b_1 = 0.3870777960062264$
	$\xi_2 = 0.6441713103894646$		$b_2 = 0.1656098004586446$
11-3	3-sphere	degree 3	6 points
	$\nu = 0.7745966692414834$		$a_1 = 0.6981317007977318$
12-3	3-sphere	degree 5	19 points
			$a_0 = 0.2792526803190927$
	$\nu = 0.6546536707079771$		$a_1 = 0.3257947937056082$
	$\xi_1 = 0.6546536707079771$		$b_1 = 0.1628973968528041$
14-3	3-sphere	degree 5	14 points
	$\nu = 0.6822591268536840$		$a_1 = 0.5523611797267854$
	(1.2387584445019331)		(0.5082460976245486)
	$\eta_1 = 0.6082048823194740$		$c_1 = 0.1093278908032098$
	(0.4189765704395655)		(0.4854803182764577)
15-3	3-sphere	degree 7	27 points
			$a_0 = 0.4156003482691997$
			(0.4441396821009518)
	$\nu = 0.8326956271382924$		$a_1 = 0.1994483077968051$
	(0.9410448241002225)		(0.0957384071760634)
	$\xi_1 = 0.7476506947169606$		$b_1 = 0.0380676101171267$
	(0.5460414781242386)		(0.2508385364520637)
	$\eta_1 = 0.4294549987784796$		$c_1 = 0.2649610860413550$
	(0.6604983415547611)		(0.0200197052755367)
11-n	n-sphere	degree 3	$2n$ points
	$\nu = \sqrt{\frac{n}{n+2}}$		$a_1 = \frac{1}{2n} I(1)^*$
12-n	n-sphere	degree 5	$2n^2 + 1$ points
			$a_0 = \frac{n^3 - 3n^2 - 10n + 36}{18n + 36} I(1)$
	$\nu = \sqrt{\frac{3}{n+4}}$		$-a_1 = \frac{n^2 - 16}{18n + 36} I(1)$
	$\xi_1 = \sqrt{\frac{3}{n+4}}$		$b_1 = \frac{n+4}{36n + 72} I(1)$

* $I(1) = \pi^{n/2}/\Gamma\left(\frac{n}{2} + 1\right)$

TABLE 3. *Formulas for the circle* $x_1^2 + x_2^2 \leq 1$

Points		Weights
17.	degree 5	7 points
(0.0000000000000000,	0.0000000000000000)	0.7853981633974483
(±0.8164965809277260,	0.0000000000000000)	0.3926990816987242
(±0.4082482904638630,	±0.7071067811865475)	0.3926990816987242
18.	degree 7	16 points
(±0.4247082002778669,	±0.1759198966061612)	0.1963495408493621
(±0.1759198966061612,	±0.4247082002778669)	0.1963495408493621
(±0.8204732385702833,	±0.3398511429799874)	0.1963495408493621
(±0.3398511429799874,	±0.8204732385702833)	0.1963495408493621
19.	degree 9	21 points
(0.0000000000000000,	0.0000000000000000)	0.3490658503988659
(±0.5505043204538557,	±0.2280263556769715)	0.2012527133278051
(±0.2280263556769715,	±0.5505043204538557)	0.2012527133278051
(±0.9192110607898046,	0.0000000000000000)	0.1012918735702551
(0.0000000000000000,	±0.9192110607898046)	0.1012918735702551
(±0.7932084745126058,	±0.4645097310495256)	0.0971672002859332
(±0.4645097310495256,	±0.7932084745126058)	0.0971672002859332
20.	degree 11	32 points
(±0.3357106870197288,	0.0000000000000000)	0.1090830782496456
(0.0000000000000000,	±0.3357106870197288)	0.1090830782496456
(±0.2373833033084449,	±0.2373833033084449)	0.1090830782496456
(±0.7071067811865475,	0.0000000000000000)	0.1161047224304262
(0.0000000000000000,	±0.7071067811865475)	0.1161047224304262
(±0.6125369400823741,	±0.3532683074300921)	0.1164805639842198
(±0.3532683074300921,	±0.6125369400823741)	0.1164805639842198
(±0.8157480497746617,	±0.4710132205252606)	0.0727157433213629
(±0.4710132205252606,	±0.8157480497746617)	0.0727157433213629
(±0.9419651451198933,	0.0000000000000000)	0.0727346698565653
(0.0000000000000000,	±0.9419651451198933)	0.0727346698565653
21.	degree 15	64 points
(±0.2584361661674054,	±0.0514061496288813)	0.0341505695624825
(±0.0514061496288813,	±0.2584361661674054)	0.0341505695624825
(±0.5634263397544869,	±0.1120724670846205)	0.0640242008621985
(±0.1120724670846205,	±0.5634263397544869)	0.0640242008621985
(±0.4776497869993547,	±0.3191553840796721)	0.0640242008621985
(±0.3191553840796721,	±0.4776497869993547)	0.0640242008621985
(±0.8028016728473508,	±0.1596871812824163)	0.0640242008621985
(±0.1596871812824163,	±0.8028016728473508)	0.0640242008621985
(±0.6805823955716280,	±0.4547506180649039)	0.0640242008621985
(±0.4547506180649039,	±0.6805823955716280)	0.0640242008621985
(±0.2190916025980981,	±0.1463923286035535)	0.0341505695624825
(±0.1463923286035535,	±0.2190916025980981)	0.0341505695624825
(±0.9461239423417719,	±0.1881957532057769)	0.0341505695624825
(±0.1881957532057769,	±0.9461239423417719)	0.0341505695624825
(±0.8020851487551318,	±0.5359361621905023)	0.0341505695624825
(±0.5359361621905023,	±0.8020851487551318)	0.0341505695624825

TABLE 4. *Formulas for the triangle and tetrahedron*

Triangle, degree 2		Triangle, degree 3	
$\left(\frac{1}{6}, \frac{1}{6}\right)$	$\frac{1}{6}$	$\left(\frac{1}{5}, \frac{1}{5}\right)$	$\frac{25}{96}$
$\left(\frac{4}{6}, \frac{1}{6}\right)$	$\frac{1}{6}$	$\left(\frac{3}{5}, \frac{1}{5}\right)$	$\frac{25}{96}$
$\left(\frac{1}{6}, \frac{4}{6}\right)$	$\frac{1}{6}$	$\left(\frac{1}{5}, \frac{3}{5}\right)$	$\frac{25}{96}$
		$\left(\frac{1}{3}, \frac{1}{3}\right)$	$\frac{-27}{96}$
Tetrahedron, degree 2		**Tetrahedron, degree 3**	
$\left(\frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}\right)$	$\frac{1}{24}$	$\left(\frac{1}{6}, \frac{1}{6}, \frac{1}{6}\right)$	$\frac{9}{120}$
$\left(\frac{5+3\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}\right)$	$\frac{1}{24}$	$\left(\frac{3}{6}, \frac{1}{6}, \frac{1}{6}\right)$	$\frac{9}{120}$
$\left(\frac{5-\sqrt{5}}{20}, \frac{5+3\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}\right)$	$\frac{1}{24}$	$\left(\frac{1}{6}, \frac{3}{6}, \frac{1}{6}\right)$	$\frac{9}{120}$
$\left(\frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5+3\sqrt{5}}{20}\right)$	$\frac{1}{24}$	$\left(\frac{1}{6}, \frac{1}{6}, \frac{3}{6}\right)$	$\frac{9}{120}$
		$\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$	$\frac{-16}{120}$

equations which a formula of either Table 1 or 2 satisfies can be obtained from the following system by making suitable omissions and substitutions. We use $I(f(x)) = \int_R f(x)\,dx$.

$$a_0 + 2na_1 + 2n(n-1)(b_1 + b_2) + \tfrac{4}{3}n(n-1)(n-2)(c_1 + c_2) = I(1)$$

$$2a_1\nu^2 + 4(n-1)(b_1\xi_1^2 + b_2\xi_2^2) + 4(n-1)(n-2)(c_1\eta_1^2 + c_2\eta_2^2) = I(x_1^2)$$

$$2a_1\nu^4 + 4(n-1)(b_1\xi_1^4 + b_2\xi_2^4) + 4(n-1)(n-2)(c_1\eta_1^4 + c_2\eta_2^4) = I(x_1^4)$$

$$4(b_1\xi_1^4 + b_2\xi_2^4) + 8(n-2)(c_1\eta_1^4 + c_2\eta_2^4) = I(x_1^2x_2^2)$$

$$2a_1\nu^6 + 4(n-1)(b_1\xi_1^6 + b_2\xi_2^6) + 4(n-1)(n-2)(c_1\eta_1^6 + c_2\eta_2^6) = I(x_1^6)$$

$$4(b_1\xi_1^6 + b_2\xi_2^6) + 8(n-2)(c_1\eta_1^6 + c_2\eta_2^6) = I(x_1^4x_2^2)$$

$$8(c_1\eta_1^6 + c_2\eta_2^6) = I(x_1^2x_2^2x_3^2)$$

Tables 1 and 2 give formulas for the cube with vertices $(\pm 1, \pm 1, \cdots, \pm 1)$ and for the sphere of radius 1 with centroid at the origin. The formulas have been numbered in the form $h - k$ where h is the formula number and k is the dimension of the space.

Formula 1 (for the n-cube) was first given by Tyler [3]. For $n > 3$ this formula has the disadvantage of having the points exterior to the cube. Stroud [4] has given a comparable formula with points interior to the cube for all n. Formula 3–2 was also given by Tyler and the two formulas given as formula 5–3 were given by Clerk-Maxwell (p. 66[1]). Formula 6–3 though containing more points may be more desirable than formulas 5–3, which have points exterior to the 3-cube.

Peirce has obtained formulas of arbitrarily high degree for both the circular annulus [5] and the spherical shell [6], all the points being interior to the regions. Table 3 gives certain of his formulas for the circle of unit radius with center at the origin. Formulas 17, 18, and 21 are members of the class of arbitrarily high degree. Formulas 19 and 20 are not of this class.

Hammer and Stroud [7] have given formulas of degrees 2 and 3 consisting of $n + 1$ and $n + 2$ points respectively for the n-simplex. Table 4 gives these formulas for the triangle with vertices (0, 0), (1, 0), (0, 1) and the tetrahedron with vertices (0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1).

4. Extensions of formulas. Because a formula for a particular region may not always be available, it is desirable to use the known formulas to as large an extent as possible. In this discussion we limit ourselves to formulas of the form (1). In general, however, we assume numerical integration includes every manner of obtaining estimates including contour integration, expansion of the integrand, evaluation in finite terms and so on.

We give the following five methods for extension of formulas:

1. Transformation from a region R to a region S when a formula for R is known. This is discussed in I. This method is limited in practice by the difficulty of finding transformations.

2. If the region is a cartesian product of two or more regions of lower dimension and formulas are known for all or some of the factor regions the work of determining a formula is reduced as shown in I. For example, with formulas for the line segment and Peirce's formulas for the circular annulus formulas for truncated cylindrical shells may be determined.

3. If a region is a finite cone based on a region for which a formula is given a formula may be determined for the cone using the theory and tables given by Hammer, Marlowe and Stroud and by Fishman [8, 9].

4. Decompositions of regions into subregions for which formulas are known. For example, polygonal regions may be treated with the triangle formulas of Hammer, Marlowe, and Stroud. When feasible one may "subtract" to obtain estimates for integrals over regions representable as differences between regions for which formulas are available.

5. Approximate the region with a suitable region for which the integral may be approximated. Thus bounded planar regions may be approximated by polygonal regions.

Decompositions of a region into simplexes or cubes and the factoring of a region into cartesian factors both have practical limitations for higher dimensions. The number of simplexes of equal volume in the n-cube, for example, is $n!$. The cartesian product methods multiply the numbers of points so that it is not feasible to develop formulas for the hypercube by cartesian product methods if the dimension is great.

It is our impresson that triangulation will not be very useful except for 2 and 3 dimensions. Cartesian product methods may be useful up to, say, dimension 30 if one starts with efficient 3-dimensional factor formulas and uses a high-speed calculator.

With the above remarks in mind it is clear that the limitations on the classical type formulas are not as severe as some had thought and it appears as if the necessity for Monte-Carlo methods in dimensions of order 10 or less definitely will decrease. On the other hand the difficulty of error analysis will still mean that in the actual applications even the classical formulas will require empirical error estimates.

5. Concluding remarks. We have given here certain numerical integration formulas and indicated the extent of some not given. While the literature of the subject seems to be rather small, we cannot claim completeness in that regard. Bourget [10] discusses means of generating numerical integration formulas using orthogonal polynomials for the circular disk. While his method gives a number of points comparable to that of Peirce, the connection between the two has yet to be established. Since Peirce's results are more general (applicable to the annulus), more available, and his approach simpler, we have presented them.

Appell and Kampe de Feriet [11] discuss the use of orthogonal polynomials for numerical integration over the circular disk. Their applications are not as extensive as those of Bourget but the discussion is simpler. The thesis of Angelescu [12] we have yet to study. Thacher [13] gives methods of deriving formulas for the hypercube of degrees 2 and 3. His matrix methods provide an interesting point of view. The paper [14] of Lauffer contains formulas for the simplex based on a regular lattice of points in the simplex. The degree may be arbitrarily large.

Formulas with non-constant weight functions have not been derived. We have indicated that such formulas for symmetrical weight functions might be achieved but the presentation of such tables should hinge on the indicated usefulness of particular weight functions.

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Appendix A. *Integration formulas and interpolating polynomials.* In the one-dimensional case certain numerical integration formulas may be considered as giving the integral of an interpolating polynomial agreeing with the integrand at the points of evaluation. For example, this is true of the Gauss formulas and of Simpson's rule for one step of two subintervals. In higher dimensions formulas may not always be interpreted as integrals of interpolating polynomials agreeing with the integrand at the evaluation points. For example, one may obtain a numerical integration formula for the square which is exact for every polynomial of the form $\sum \sum c_{ij}x^iy^j$, $0 \leqq i + j \leqq 7$, and which has 36 evaluation points in a regular square lattice array. However, if this formula is applied to a non-polynomial integrand function, the approximate value usually cannot be interpreted as the integral of a seventh degree polynomial agreeing with the integrand at the 36 points. This is true since it is generally impossible to determine a seventh degree polynomial assuming arbitrarily specified values at 36 points of a square lattice as these points lie on a sixth degree algebraic curve. This situation is summarized in the following theorem.

Theorem 1. Let P be a linear space of functions (of n variables) which has m linearly independent functions as a basis. Let $x_1, \cdots, x_m$ be m points in E_n and let $c_1, \cdots, c_m$ be m arbitrary real numbers. A necessary and sufficient condition that there always exist a function $p \in P$ such that $p(x_i) = c_i$ $(i = 1, \cdots m)$ is that there exist no $f \in P$ $(f \neq 0)$ such that $f(x_i) = 0$ $(i = 1, \cdots, m)$. That is, $x_1, \cdots, x_m$ must be independent with regard to P.

The example and theorem 1 indicate that certain types of error analysis depending on interpolation are not applicable for certain formulas in higher dimensions.

Cartesian product formulas, however, may be considered as integrals of interpolating polynomials provided the formulas from which they are derived can be considered in this manner. More precisely, let $L_1 : [f_1, \cdots, f_m]$ and $L_2 : [g_1, \cdots, g_n]$ be two linear function spaces with the linearly independent bases $f_1, \cdots, f_m$ and $g_1, \cdots, g_n$ respectively and let f_i be defined for all $x \in R$ and g_h for all $y \in S$. Further, let $x_1, \cdots, x_m$ in R and $y_1, \cdots, y_n$ in S be points such that the matrices $F = (f_i(x_j))$ and $G = (g_h(y_k))$ are non-singular. Then for each set of mn constants c_{jk} there exists a unique function $h \in L_1 \times L_2$ such that $h(x_j, y_k) = c_{jk}$ $(j = 1, \cdots, m;\ k = 1, \cdots, n)$. The proof of this follows from the relation $| F \times G | = | F |^n \, | G |^m$ (see MacDuffee [2], p. 81).