CALCULATION OF NUMERICAL INTEGRATION OF MULTIPLE DIMENSIONS BY DISSECTION INTO SIMPLICES*

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Abstract

In this paper, we introduce a method of numerical integration on a polytope of multiple dimensions. Its basic idea is to cut a polytope into some simplices and sum the integral values on the simplices. We give the integral formulae, the expressions to estimate the error and the method for cutting a polytope into simplices. Some examples are provided to explain the adaptability of the method.

I. Introduction

For numerical integration in higher dimensions with certain complicated regions of integration and integrands it is too difficult to obtain a very precise result, because that generally requires a very large amount of computation. Some commonly used methods[1] are the network method of number theory and the Monte Carlo methods. The former has its advantage when the integrand belongs to the $E_s^\alpha(c)$ class of functions on a unit cube[2]. The Latter[3] are relatively good when high precision is not required. Their computational formulae and programs are not very complicated, but it is too difficult to obtain a precise result. In practice, sometimes we could not improve the computational precision even by one significant digit, although astonishingly large amount of additional computation is done.

In this paper, we try to study the numerical integration for an n-dimensional polytope, whose boundary consists of $(n-1)$-dimensional hyperplanes. For the integral on this kind of region we give a numerical method with relatively high precision. Its basic idea is to separate the polytope into simplices. We can adopt the centroid method of numerical integration[4] to compute the integrals on the simplices and then sum the integrals to obtain the integral on the polytope. Compared with the other methods, its computational precision is relatively high and its computational amount relatively small. For some cases the advantage of the integration method of dissection into simplices is without comparison.

II. Numerical Integration on a Simplex

Definition 2.1. *In R^n (n-dimensional Euclidean space) the convex span of $r+1$ $(r\leq n)$ affinely independent points is an r-dimensional simplex, denoted by $r-S$. These $r+1$ independent points are the vertices of $r-S$*[5].

Assume the i-th vertex is denoted by

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$$X_i=\{x_{i1},\ x_{i2},\ \cdots,\ x_{in}\}.$$

Then, its $r+1$ vertices define a matrix

$$M=\begin{bmatrix} 1 & x_{01} & x_{02} & \cdots & x_{0n} \\ 1 & x_{11} & x_{12} & \cdots & x_{1n} \\ \vdots & & & & \\ 1 & x_{r1} & x_{r2} & \cdots & x_{rn} \end{bmatrix}.$$

From the properties of the affinely independent points, we have

$$\text{rank } M=r+1.$$

Let

$$S_r=S_r(X_0,\ X_1,\ \cdots,\ X_r)$$

be the closed region of a $r-S$. Let $|S_r|$ denote the Euclidean measurement volume of $r-S$[6]. Then

$$|S_r|=\frac{1}{r!}\,[\det(MM^{\tau})]^{\frac{1}{2}}. \tag{2.1}$$

If $r=n$,

$$|S_n|=\frac{1}{n!}\det M. \tag{2.2}$$

The centroid point of a $r-S$ is denoted by $\bar{X}$.

$$\bar{X}=\frac{1}{r+1}\sum_{i=0}^{r}X_i, \tag{2.3}$$

which satisfies

$$\int_{S_r}(X-\bar{X})dX=0.$$

Assume

$$I=\int_{S_r}f(X)dX. \tag{2.4}$$

When $f(X)$ has a continuous $(p+1)$-th derivative with respect to X, we can use the Taylor expansion; then

$$I=|S_r|f(\bar{X})+\frac{1}{2!}\int_{S_r}\left[(X-\bar{X})^{\tau}\frac{\partial}{\partial X}\right]^2 f(\bar{X})dX+\cdots$$
$$+\frac{1}{P!}\int_{S_r}\left[(X-\bar{X})^{\tau}\frac{\partial}{\partial X}\right]^p f(\bar{X})dX+\frac{1}{(p+1)!}\int_{S_r}\left[(X-\bar{X})^{\tau}\frac{\partial}{\partial X}\right]^{p+1} f(\xi)dX,$$

where

$$\frac{\partial\cdot}{\partial X}=\begin{bmatrix}\dfrac{\partial\cdot}{\partial x_1}\\ \dfrac{\partial\cdot}{\partial x_2}\\ \vdots \\ \dfrac{\partial\cdot}{\partial x_n}\end{bmatrix}.$$

We simplify this to

$$I=|S_r|f(\bar{X})+\sum_{i=2}^{p}T_i+R_{p+1}, \tag{2.5}$$

where
$$T_i=\sum_{\nu}^{|\nu|=i}\frac{m(\nu)}{\nu!}\left.\frac{\partial^i f(X)}{\partial x_1^{\nu_1}\partial x_2^{\nu_2}\cdots\partial x_n^{\nu_n}}\right|_{X=\bar{X}},$$

$$|\nu|=\nu_1+\nu_2+\cdots+\nu_n,$$
$$\nu!=\nu_1!\nu_2!\cdots\nu_n!,$$
$$m(\nu)=\int_{S_r}(X_1-\bar{X}_1)^{\nu_1}\cdots(X_n-\bar{X}_n)^{\nu_n}dX,$$
$$R_{p+1}=\frac{1}{(p+1)!}\int_{S_r}\left[(X-\bar{X})^{\tau}\frac{\partial}{\partial X}\right]^{p+1}f(\xi)dX.$$

Obviously,

$$|R_{p+1}|\leqslant\frac{1}{(p+1)!}\int_{S_r}[|X-\bar{X}|^{\tau}\cdot E]^{p+1}B_{p+1}dX, \tag{2.6}$$

where E denotes an identity vector, and B_{p+1} is the upper bound of the norm of the $(p+1)$-th derivative of $f(X)$ with respect to X;

$$|R_{p+1}|\leqslant\frac{1}{(p+1)!}|S_r|R^{p+1}B_{p+1}, \tag{2.7}$$

where

$$R=\max_{X\in S_r}[|X-\bar{X}|^{\tau}\cdot E]. \tag{2.8}$$

If $\tilde{I}_p$ denotes the approximation of $(p+1)$-th degree of I, we have

$$\tilde{I}_p=|S_r|f(\bar{X})+\sum_{i=2}^{p}T_i \tag{2.9}$$

and

$$|I-\tilde{I}_p|=|R_{p+1}|.$$

To calculate $\tilde{I}_p$, obtaining the values of $m(\nu)$ is a key step. There are some formulae for it in [4]:

$$m(\nu)=\frac{|S_r|r!\nu!}{(p+r)!}\left\{\mathscr{C}(t^{\nu})\exp\left[\frac{1}{2}W_2+\frac{1}{2}W_3+\cdots\right]\right\}, \tag{2.10}$$

where

$$P=|\nu|,$$
$$W_i=\sum_{k=0}^{r}\left\{\sum_{i=0}^{n}(x_{kj}-\bar{x}_j)t_j\right\}^i$$

and $\mathscr{C}(t^{\nu})\left\{\exp\left[\frac{1}{2}W_2+\frac{1}{2}W_3+\cdots\right]\right\}$ is the coefficient of the term t^{ν} in $\exp\left[\frac{1}{2}W_2+\frac{1}{2}W_3+\cdots\right]$.

When $1\leqslant p\leqslant 3$, we simplify (2.10) by

$$m(\nu)=\frac{|S_r|r!(p-1)!S(\nu)}{(p+r)!}, \tag{2.11}$$

where

$$S(\nu)=\sum_{k=0}^{r}(X_k-\bar{X})^{\nu}=\sum_{k=0}^{r}(x_{k1}-\bar{x}_1)^{\nu_1}\cdots(x_{kn}-\bar{x}_r)^{\nu_n}.$$

When $r=2$, there is a simple result

$$m(\nu)=|S_r|C_pS(\nu), \tag{2.12}$$

$$C_2=\frac{1}{12},$$
$$C_3=C_4=\frac{1}{30},$$
$$C_5=\frac{2}{105}.$$

In the above we have given the approximation expression of numerical integration on a simplex (when $f(X)$ has a continuous $(p+1)$-th derivative with respect to X) and the upper bound of the truncation error. In practice, according to the properties of the function $f(X)$ and our required precision, we can decide on the appropriate approximation degree P. Generally speaking, we choose $1\leqslant p\leqslant 3$.

III. How to Cut a Polytope into Simplices

In R^n the closed region surrounded by $(n-1)$-dimensional hyperplanes is a n-dimensional polytope denoted by $n-P$. The convex region which is a polytope is called a convex polytope, which is the convex span of a set having a finite number of points. For the problem of cutting a polytope into simplices we have the following propositions[5,7,8,9].

Proposition 1. An n-dimensional polytope can be separated into the union of disjoint n-dimensional convex polytopes. By "Disjoint" is meant that the common part consists of at most $(n-1)$-dimensional regions.

Proposition 2. Any convex polytope has interior points; in particular, the centroid of all vertices is one of them.

Proposition 3. An n-dimensional convex polytope can be separated into the union of disjoint n simplices.

[8, 9] have given and proved some methods for cutting a polytope. In the following we will show the procedure of programming of the method introduced in [8].

1. From the boundary conditions of the convex polytope $n-P$, the set of all the vertices of $n-P$ denoted by $n-PV$ is found.

2. An interior point O_n of $n-P$ is chosen. (O_n can be located in the boundary of $n-P$ and may be a vertex of $n-P$) O_n will be the common vertex of all the separation simplices.

3. All the vertices of set $n-PV$ are divided into n_k subsets denoted by $(n-1)-PV_1$, $(n-1)-PV_2$, $\cdots$, $(n-1)-PV_{nk}$. Each subset corresponds to a surface of $n-P$ which is an $(n-1)$-dimensional convex polytope. All the members of a subset $(n-1)-PV_i$ are the vertices of the convex polytope $(n-1)-P_i$ corresponding to $(n-1)-PV_i$. n_k equals to subtraction of the boundary number in which O_n is located from that of $n-P$.

4. Substituting n by $n-1$, we repeat step 2 and 3 for all the n_k subsets.

5. Go on in this way until all the subsets have only two points. The procedure will be stoped. Then, the convex polytope $n-P$ divides into the simplices whose vertices are found.

Proposition 4. An n-dimensional polytope can be separated into the union of disjoint n simplices.

IV. Error Estimation of the Integration

Since a polytope can be separated into disjoint simplices, the integration on the polytope is calculated by the sum of the integrations on each simplex. The error estimation of the integration on the polytope is obtained by the sum of those on all the simplices.

If we denote the radius of set A by $d(A)$,

$$d(A)=\text{lub}\{d(X, Y)\mid X, Y\in A\}.$$

From (2.7), if $f(X)\in C^{p+1}$, the error R_{p+1} of integration on a simplex S_n satisfies

$$|R_{p+1}|\leqslant\frac{1}{(p+1)!}|S_n|(\sqrt{n}d)^{p+1}B_{p+1}, \tag{4.1}$$

where d is the radius of S_n.

As integration on a polytope $n-P$ can be dissected into integrations on simplices and the error of the integration on a simplex satisfies (4.1), the error on the polytope $n-P$ satisfies

$$|R'|\leqslant\frac{1}{(p+1)!}|S'|(\sqrt{n}d')^{p+1}B', \tag{4.2}$$

where $|S'|$ is the volume of $n-P$, and B' is the upper bound of the norm of the $(p+1)$-th derivative of $f(X)$ with respect to X.

$$d'=\max_i\{d_i\},$$

where d_i is the radius of i-th simplex contained in $n-P$.

In (4.2) all the elements except d' are independent of the dissection. If we do not intend to improve the precision of the integration by increasing p, the only way is to decrease d'. Obviously, provided d' is small enough we can make R' arbitrarily small.

We can adopt the following way to reduce the value of d'. The polytope $n-P$ is covered by a cube whose side is divided into k identical parts to obtain 2^n_k subcubes. Each of them covers a part of the polytope $n-P$ denoted by $n-P_i$ $(i=1, 2, \cdots, n_k)$. We divide $n-P_i$ into simplices. Then the ratio of the error R'_1 to the original error R'_0 is

$$\frac{|R'_1|}{|R'_0|}\approx k. \tag{4.3}$$

V. Examples

In the following we will give two examples——calculation of the coefficient of quantization of the lattice quantizers[10]——to show the advantages of the method. In the two examples incomparable results are obtained by dissection into simplices. We do not want to show that the method of dissection into simplices is better than the others for any cases, but it is a good method in some situations.

Example 1. Calculate

$$C_4=\frac{1}{4}\int_{P_4}\|X\|^2dX/|P_4|^{1.5}, \tag{5.1}$$

where P_4 is a symmetric polytope with the center at origin in R^4, that is,

$$P_4=\{X\mid\sum_{i=1}^{4}|x_i|\leqslant 2; |x_i|\leqslant 1, i=1, 2, 3, 4\}. \tag{5.2}$$

The symmetry about each quadrant and axis is used to compute the integration. By the above-mentioned method, the program automatically divides the polytope into 3 kinds of simplices whose corresponding matrices are the following

$$M_{41}=\begin{bmatrix}1&0&0&0&0\\1&1&0&0&0\\1&1&0&0&1\\1&1&0&1&0\\1&1&1&0&0\end{bmatrix},$$

$$M_{42}=\begin{bmatrix}1&0&0&0&0\\1&0.5&0.5&0.5&0.5\\1&1&0&0&1\\1&1&0&1&0\\1&1&1&0&0\end{bmatrix},$$

$$M_{43}=\begin{bmatrix}1&0&0&0&0\\1&0.5&0.5&0.5&0.5\\1&0&0&1&1\\1&0&1&0&1\\1&0&1&1&0\end{bmatrix}.$$

The integral on the polytope is 64 times as much as the sum of the integrals on 3 simplices. Since the integrand is of second-order, we need to consider the second-order moments and to obtain the truncation error 0. For the integration on a simplex the following formulae are used.

$$\int_S \|X\|^2 dX = |S|\,\|\bar{X}\|^2 + \frac{|S|}{30}\sum_{i=0}^{4}\sum_{k=1}^{4}(x_{ik}-\bar{x}_k)^2, \tag{5.4}$$

where S denotes a simplex, $|S|$ is its volume, and $\bar{X}$ is the centroid of the simplex. Then, we have

$$C_4=0.0766032.$$

Since (5.4) is a correct integration formula for the problem, the error of the above result is due to the rounding off.

We treat the problem using the Monte Carlo methods (IBM 4341, Fortran). The result has only three significant digits and we could not improve it (see Table 1).

Example 2. Calculate

$$C_8=\frac{1}{8}\int_{P_8}\|X\|^2 dX/|P_8|^{1.25}, \tag{5.5}$$

where

$$P_8=\{X\,|\,|x_i|<1,\ i=1,2,\cdots,8;\ \sum_{j=1}^{4}|x_{ij}|\leqslant 2,\ i=1,2,\cdots,14\}. \tag{5.6}$$

The correspondence between ij and k is given by Table 3. This 8-dimensional polytope region is surrounded by 240 7-dimensional hyperplanes with symmetric center at the origin. We use the same may with above example 1 and the methods mentioned in Sections 2 and 3 to obtain

$$C_8=0.0716821.$$

For this problem we use the Monte Carlo methods and the network method of number theory (PDP 11/45, Fortran). Two significant digits are obtained and we could not get more (see Table 2).

Table 1 Example 1

Method	CPU time (seconds)	Precision
dissection into simplices	1.13	6 significant digits
Monte Carlo methods	5.44 or more	within 3 significant digits

Table 2 Example 2

Method	CPU time (minutes)	Precision
dissection into simplices	3.53	6 significant digits
Monte Carlo methods	6.75 or more	within 2 significant digits
number theory network	5.64 or more	

Table 3

i	$j=1$	$j=2$	$j=3$	$j=4$
		$ij=k$		
1	1	2	3	5
2	2	3	4	6
3	3	4	5	7
4	1	4	5	6
5	1	2	4	6
6	2	5	6	7
7	1	3	6	7
8	4	6	7	8
9	1	5	7	8
10	1	2	6	8
11	2	3	7	8
12	3	5	7	8
13	1	3	4	8
14	2	4	5	8

VI. Conclusion

The method is suitable for calculating integration on a polytope, especially for the integrand having small values for over 3rd or 4th derivative. Thereby we will obtain an incomparable good result. Its drawback is that the dissection into simplices causes complication in programming.

References

[1] A. H. Stroud, Approximate Calculation of Multiple Integrals, Englewood Cliffs, N. J., Prentice-Hall, 1971.

[2] Hua Luo-geng, Wang Yuan, Application of Number Theory in Approximation Analysis (in Chinese), Science Press, 1978.

[3] J. M. Hammersley, D. C. Hanelscomb, Monte Carlo Methods, Lexington Books, 1973.

[4] I. J. Good, R. A. Gaskins, The centroid method of numerical integration, *Numer. Math.*, 16 (1971), 343—359.

[5] P. T. Kelly, M. L. Weiss, Geometry and Convexity, John Wiley & Sons, Inc., 1979.

[6] D. M. Y. Sommerville, An Introduction to the Geometry of N Dimensions, Dover Publications, Inc., New York, 1958.

[7] H. S. M. Coxeter, Regular Polytopes, MacMillan Co., New York, 1963.

[8] Wang Cheng-shu, Cut a Polytope, to be published.

[9] H. Tverberg, How to cut a polytope into simplices, *Geometriae Dedi cata*, **3** (1974), 239—240.

[10] A. Gersho, Asymptotically optimal block quantization, *IEEE Trans. Inform. Theory*, **25** (1979), 378—380.