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Approximate Formulas for the Mean Value of a Function over a Tetrahedron

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Formulas to express the mean value of a polynomial of degree up to 5 over a tetrahedron by a linear combination of the values of the polynomial at the least set of points within the tetrahedron are established and applied to a few functions to estimate errors comprised.

§ 1. Introduction

There are several formulas for a line integral, for example, Simpson's, Gauss', Tchebyschef's and others. In space the shape of a domain of integration may vary infinitely. If the domain of integration is a cube, a triple application of one of the above-mentioned formulas may be useful. However if the domain of integration is a polyhedron, there seems to be no formula for fairly general use.

As is well-known, a polyhedron can be divided into a set of simplexes, that is, tetrahedrons.

Therefore an integral over a polyhedron may be represented by the sum of integrals over constituent tetrahedrons. Hence it is fundamental to establish an approximate formula for an integral over a tetrahedron.

Since a continuous function can be approximated by a polynomial suitably chosen, we seek an exact integration formula for a polynomial of degree up to 5.

A polynomial of degree 5 in three variables x, y and z has $1+3+6+10+15+21=56$ arbitrary coefficients. So it seems possible to get a formula

$$\int Pdxdydz\Big/\int dxdydz=\sum_{k=1}^{14} A_k P(x_k, y_k, z_k) \tag{1}$$

with suitably chosen weights A_k and points (x_k, y_k, z_k), because the number of weights and coordinates to be chosen is equal to $(1+3)\times 14=56$. This conjecture proves right in the following. The number of chosen points cannot be less than 14.

§2. Symmetrization

We take the origin of a coordinate system at a vertex of a tetrahedron and x, y, z-axes along the three edges issuing from the vertex so that we may have coordinates of four vertices

$$(0, 0, 0),\ (1, 0, 0),\ (0, 1, 0) \text{ and } (0, 0, 1)\,.$$

A polynomial P of degree N may be represented as

$$P=\sum b_{lmn}x^l y^m z^n \tag{2}$$

l, m and n running from 0 to N while satisfying the condition $l+m+n\leqq N$. This representation, however, complicates the ensuing calculations, so we replace it by a more convenient representation

$$P=\sum a_{hklm}\frac{x^h}{h\,!}\cdot\frac{y^k}{k\,!}\cdot\frac{z^l}{l\,!}\cdot\frac{t^m}{m\,!} \tag{3}$$

$$h+k+l+m=N\,,\quad t=1-x-y-z\,.$$

In this representation P has the same number of arbitrary coefficients as in the previous representation.

We denote the mean value of a quantity Q over the tetrahedron by $\langle Q\rangle$, or

$$\langle Q\rangle=\iiint Q dxdydz\Big/\iiint dxdydz \tag{4}$$

the domain of integration being the tetrahedron, or,

$$x,\ y,\ z>0\,,\quad 1-x-y-z>0\,.$$

If Q is taken to be $x^h y^k z^l(1-x-y-z)^m$, the use of a formula

$$\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}e^{xs}\frac{ds}{s^{m+1}}=\begin{cases}\dfrac{x^m}{m\,!} & x>0,\quad \sigma>0\\[2ex] 0 & x<0\end{cases} \tag{5}$$

gives

$$\iiint Q dxdydz=\iiint x^h y^k z^l t^m dxdydz$$

$$=\iiint x^h y^k z^l(1-x-y-z)^m dxdydz$$

$$=\frac{m\,!}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{ds}{s^{m+1}}\iiint_0^\infty x^h y^k z^l e^{s(1-x-y-z)}\,dxdydz$$

$$=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{ds}{s^{m+1}}e^s\cdot\frac{h\,!\,k\,!\,l\,!\,m\,!}{s^{h+k+l+3}}=\frac{h\,!\,k\,!\,l\,!\,m\,!}{(h+k+l+m+3)\,!}\,. \tag{6}$$

Setting of $h=k=l=m=0$ shows the second integral in (4) to be $1/3\,!$. Hence

$$\langle x^h y^k z^l t^m\rangle=\frac{h\,!\,k\,!\,l\,!\,m\,!\,3\,!}{(h+k+l+m+3)\,!} \tag{7}$$

and

$$\langle P\rangle=\frac{3\,!}{(N+3)\,!}\sum a_{hklm}\,. \tag{8}$$

Therefore any variable among four variables x, y, z and t plays the same part. So we represent hereafter a point rather by (x, y, z, t) than by (x, y, z).

A point $(\alpha, \beta, \gamma, \delta)$ lies within the tetrahedron, when four coordinates α, β, γ and δ satisfy the following conditions

$$\alpha\geqq 0\,,\quad \beta\geqq 0\,,\quad \gamma\geqq 0\,,\quad \delta\geqq 0 \quad\text{and}\quad \alpha+\beta+\gamma+\delta=1\,. \tag{9}$$

If a point $(\alpha, \beta, \gamma, \delta)$ falls in a set of points (x_k, y_k, z_k, t_k) to give a formula

$$\langle Q\rangle=\sum_k A_k Q(x_k, y_k, z_k, t_k) \tag{10}$$

it seems probable that any point with four coordinates α, β, γ and δ in all possible orders may fall equally in the set of points. Points with the same coordinates in a different order may be called conjugate points. They are classified by the types as follows.

T type	$g(T)$ number of conjugate points	$f(T)$ number of parameters	
$(\alpha, \beta, \gamma, \delta)$	24	4	
$(\alpha, \beta, \gamma, \gamma)$	12	3	
$(\alpha, \alpha, \gamma, \gamma)$	6	2	(11)
$(\alpha, \beta, \beta, \beta)$	4	2	
$(\alpha, \alpha, \alpha, \alpha)$	1	1	

The α, β, γ and δ here are assumed to differ one from another. It is to be noted that while the condition $\alpha+\beta+\gamma+\delta=1$ reduces the number of independent parameters assigned to a type by one, the weight A assigned to the type increases it by one. The last type $(\alpha, \alpha, \alpha, \alpha)$ refers to the barycenter.

The assumption that the right side expression in (10) consists of terms taken at sets of conjugate points allows to regard $Q(x, y, z, t)$ as a symmetric polynomial in x, y, z and t. Symmetric polynomials may be expressed with s_1, s_2, s_3 and s_4 defined by the relation $\rho^4-s_1\rho^3+s_2\rho^2-s_3\rho+s_4=(\rho-x)(\rho-y)(\rho-z)(\rho-t)$ and s_1 is equal to 1, so that symmetric polynomials may be expressed with s_2, s_3 and s_4.

In the following, independent symmetric polynomials are listed for degree N together with $S(N)$ the number of independent symmetric polynomials of degree up to N, $C(N)$ the number of coefficients a_{hklm} for $h+k+l+m=N$ and $P(N)$ the number of points needed in the formula (10).

N	Symm. Polynom.	$S(N)$	$C(N)$	$P(N)$
0	1	1	1	
1	1	1	4	1
2	s_2	2	10	3
3	s_3	3	20	5
4	$s_2^2,\ s_4$	5	35	9
5	s_2s_3	6	56	14
6	$s_2^3,\ s_2s_4,\ s_3^2$	9	84	21
7	$s_2^2s_3,\ s_3s_4$	11	120	30
8	$s_2^4,\ s_2^2s_4,\ s_2s_3^2,\ s_4^2$	15	165	42
9	$s_2^3s_3,\ s_2s_3s_4,\ s_3^3$	18	220	55

the $P(N)$ being the minimum integer not less than $C(N)/4$.

If the formula (10) prevails for polynomials of degree N, it should do so for symmetric polynomials listed above of degree up to N. Therefore the formula (10) must satisfy $S(N)$ conditions, consequently it must include $S(N)$ parameters. If points chosen in (10) are classified by types T, the sum of $g(T)$, that is, the number of conjugate points of type T, over types T's, must be equal to $P(N)$, and the sum of $f(T)$, that is, the number of parameters of type T, over types T's, must be equal to $S(N)$, or

$$P(N)=\sum_T g(T)\,, \qquad S(N)=\sum_T f(T)$$

or in vector form

$$\begin{pmatrix}P(N)\\S(N)\end{pmatrix}=\sum_T\begin{pmatrix}g(T)\\f(T)\end{pmatrix}. \tag{13}$$

Possible partitions of $(P(N), S(N))$ into $(g(T), f(T))$'s are as follows.

$$\begin{array}{ll}
N & \\
3 & \begin{pmatrix}5\\3\end{pmatrix}=\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}1\\1\end{pmatrix}\\
4 & \begin{pmatrix}9\\5\end{pmatrix}=\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}1\\1\end{pmatrix}\\
5 & \begin{pmatrix}14\\6\end{pmatrix}=\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}\\
6 & \begin{pmatrix}21\\9\end{pmatrix}=\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}1\\1\end{pmatrix}\\
7 & \begin{pmatrix}30\\11\end{pmatrix}=\begin{pmatrix}12\\3\end{pmatrix}+\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}\\
8 & \begin{pmatrix}42\\15\end{pmatrix}=\begin{pmatrix}12\\3\end{pmatrix}+\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}\\
9 & \begin{pmatrix}55\\18\end{pmatrix}=\begin{pmatrix}12\\3\end{pmatrix}+\begin{pmatrix}12\\3\end{pmatrix}+\begin{pmatrix}12\\3\end{pmatrix}+\begin{pmatrix}6\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}4\\2\end{pmatrix}+\begin{pmatrix}1\\1\end{pmatrix}
\end{array} \tag{14}$$

§ 3. Cases $N=1, 2, 3, 4$ and 5

For the case $N=1$, the mean value of a polynomial of degree 1 is expressed as the value of the polynomial at the barycenter of the tetrahedron as is easily suspected and proved.

$$\langle Q\rangle_1 = Q\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right). \tag{15}$$

For the case $N=2$, the partition of (3,2) is not possible. However the mean of a polynomial of degree 2 can be expressed by the linear combination of the values of the polynomial at 4 barycenters of 4 faces and 6 midpoints of 6 edges, or

$$\langle Q\rangle_2 = \frac{1}{10}\sum_{\text{perm}} Q\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0\right) + \frac{1}{10}\sum_{\text{perm}} Q\left(\frac{1}{2}, \frac{1}{2}, 0, 0\right) \tag{16}$$

each $\sum$ ranging over all possible permutations among four coordinates.

For the case $N=3$, we have the partition

$$\binom{5}{3} = \binom{4}{2} + \binom{1}{1}$$

and

$$\langle Q\rangle = A\sum_{\text{perm}} Q(\alpha, \alpha, \alpha, 1-3\alpha) + BQ\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right).$$

The substitution of Q by s_1, s_2 and s_3 gives the conditions

$$\langle 1\rangle = 1 = A\cdot 4 + B$$

$$\langle s_2\rangle = \frac{3}{10} = 4A(3\alpha - 6\alpha^2) + B\cdot\frac{3}{8}$$

$$\langle s_3\rangle = \frac{1}{30} = 4A(3\alpha^2 - 8\alpha^3) + B\cdot\frac{1}{16}$$

which determine A, B and α

$$A = \frac{9}{20}, \quad B = -\frac{4}{5}, \quad \alpha = \frac{1}{6},$$

or

$$\langle Q\rangle_3 = \frac{9}{20}\sum_{\text{perm}} Q\left(\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{2}\right) - \frac{4}{5}Q\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right). \tag{17}$$

For the case $N=4$, the partition

$$\binom{9}{5} = \binom{4}{2} + \binom{4}{2} + \binom{1}{1}$$

gives

$$\langle Q\rangle_4 = A\sum_{\text{perm}} Q(\alpha, \alpha, \alpha, 1-3\alpha) + B\sum_{\text{perm}} Q(\beta, \beta, \beta, 1-3\beta)$$
$$+ CQ\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right). \tag{18}$$

The substitution of 1, s_2, s_3, s_4 and s_2^2 for Q leads to the equations

$$\begin{aligned}
1 &= 4A + 4B + C \\
\langle s_2\rangle = \frac{3}{10} &= 4A(3\alpha-6\alpha^2)+4B(3\beta-6\beta^2)+C\cdot\frac{3}{8} \\
\langle s_3\rangle = \frac{1}{30} &= 4A(3\alpha^2-8\alpha^3)+4B(3\beta^2-8\beta^3)+C\cdot\frac{1}{16} \\
\langle s_4\rangle = \frac{1}{840} &= 4A(\alpha^3-3\alpha^4)+4B(\beta^3-3\beta^4)+C\cdot\frac{1}{64} \\
\langle s_2^2\rangle = \frac{13}{140} &= 4A(3\alpha-6\alpha^2)^2+4B(3\beta-6\beta^2)^2+C\cdot\frac{9}{64}\,.
\end{aligned} \tag{19}$$

The elimination of C, A and B gives two equations

$$126\,\alpha\beta-21(\alpha+\beta)+5=0$$

$$\frac{598}{21}=\frac{1}{\alpha-\beta}\left\{\frac{1-6\beta}{(1-4\alpha)^2}+\frac{6\alpha-1}{(1-4\beta)^2}\right\}$$

from which is derived the equation to $x=21\,\alpha\beta$

$$536\,x^2-1268\,x+599=0\,.$$

In turn, it gives

$$\alpha=0.33045\ 72443\,,\qquad \beta=0.09398\ 38416 \tag{20}$$

and

$$A=0.14837\ 78971\,,\qquad B=0.08892\ 36899\,,\qquad C=0.05079\ 36508\,.$$

For the case $N=5$, the partition

$$\binom{14}{6}=\binom{6}{2}+\binom{4}{2}+\binom{4}{2}$$

gives

$$\langle Q_5\rangle=A\sum_{\text{perm}}Q(\alpha,\alpha,\alpha,1-3\alpha)+B\sum_{\text{perm}}Q(\beta,\beta,\beta,1-3\beta)+C\sum_{\text{perm}}Q\left(r\,,\ r\,,\ \frac{1}{2}-r\,,\ \frac{1}{2}-r\right). \tag{21}$$

The substitution of 1, s_2, s_2^2, s_3, s_2s_3, and s_4 for Q gives 6 equations

$$\begin{aligned}
&\lambda &&+\mu &&+\nu &&=840 \\
&\lambda(3\alpha-6\alpha^2) &&+\mu(3\beta-6\beta^2) &&+\nu\left(\frac{1}{4}+2c\right) &&=252 \\
&\lambda(3\alpha-6\alpha^2)^2 &&+\mu(3\beta-6\beta^2)^2 &&+\nu\left(\frac{1}{4}+2c\right)^2 &&=78 \\
&\lambda(3\alpha^2-6\alpha^3) &&+\mu(3\beta^2-6\beta^3) &&+\nu c &&=28
\end{aligned} \tag{22}$$

$$\begin{array}{llll} \lambda(3\alpha-6\alpha^2)(3\alpha^2-8\alpha^3) & +\mu(3\beta-6\beta^2)(3\beta^2-8\beta^3) & +\nu\left(\frac{1}{4}+2c\right)c & =9 \\ \lambda(\alpha^3-3\alpha^4) & +\mu(\beta^3-3\beta^4) & +\nu c^2 & =1 \end{array}$$

where $\lambda=840\times 4A$, $\mu=840\times 4B$ and $\nu=840\times 6C$.

The elimination of ν and c leads to

$$\begin{aligned} &\xi^3\lambda+\eta^3\mu=56 \\ &\xi^4\lambda+\eta^4\mu=40 \\ &\xi^5\lambda+\eta^5\mu=24 \qquad (23) \\ &9(168-\xi^2\lambda-\eta^2\mu)^2=96(840-\lambda-\mu) \end{aligned}$$

where $\xi=1-4\alpha$ and $\eta=1-4\beta$. The first and second equations give the relations

$$\lambda=\frac{56\eta-40}{\xi^3(\eta-\xi)}, \qquad \mu=\frac{56\xi-40}{\eta^3(\xi-\eta)}$$

which yield, by way of the third equation,

$$7\xi\eta-5(\xi+\eta)+3=0 .$$

In terms of unknowns $\xi\eta=q$ and $\xi+\eta=p$, one gets

$$7q-5p+3=0$$

and

$$9\left(168-\frac{56p-40}{q}\right)^2=96\left(840-\frac{56p(p^2-2q)-40(p^2-q)}{q^3}\right) .$$

The elimination of p leads to the equation

$$259q^3+273q^2-23q-9=0 .$$

Final results are as follows.

$$\begin{array}{lll} \alpha=0.09273\ 52503 & \lambda=246.93663\ 50 & A=0.07349\ 30431 \\ \beta=0.31088\ 59192 & \mu=378.63143\ 48 & B=0.11268\ 79270 \qquad (24) \\ \gamma=0.45449\ 62795 & \nu=241.43194\ 02 & C=0.04254\ 60199 \end{array}$$

§ 4. Comparison with a crude formula

A crude formula may be to replace the mean value of a function $g(\mathbf{r})$ by the average of the values of $g(\mathbf{r})$ at four vertices of the tetrahedron. The division of the tetrahedron into m^3 tetrahedrons formed with four sets of equidistant planes parallel to four faces of the tetrahedron and the replacement of the mean value of $g(\mathbf{r})$ in each of m^3 tetrahedrons by the average of values of $g(\mathbf{r})$ at four vertices of each tetrahedron give a formula

$$\langle g(\mathbf{r})\rangle=1/m^3\cdot\sum w(\mathbf{s})g(\mathbf{s}) \qquad (25)$$

where $\mathbf{s}$ ranges over lattice points

$$\mathbf{s}=(i/m,\ j/m,\ k/m)$$
$$i,\ j,\ k=0,\ 1,\ 2,\ \cdots,\ m$$
$$i+j+k\leqq m$$

and the weight $w(\mathbf{s})$ is equal to

1/4	when $\mathbf{s}$ is at a vertex,
7/6	when $\mathbf{s}$ is on an edge,
3	when $\mathbf{s}$ is on a face,
6	when $\mathbf{s}$ is inside,

of the tetrahedron. This formula is exact when the function $g(\mathbf{r})$ is continuous and linear in each of m^3 tetrahedrons.

Comparison of the formulas (15), (16), (17), (18), (21) with (25) for $m=1, 2, 3, 4, 5$ is given below in connection with three functions e^{-x}, $1/(1+x)$ and $1/(1+x^2)$.

For $Q=e^{-x}$, the mean value of Q turns out to be

$$\langle Q\rangle=3(1-2/e)=0.79272\ 33$$

and approximate values are

$\langle Q\rangle_1=0.77880\ 08$	$(25)_1=0.84196\ 76$
$\langle Q\rangle_2=0.79691\ 86$	$(25)_2=0.80810\ 31$
$\langle Q\rangle_3=0.79264\ 85$	$(25)_3=0.79988\ 02$
$\langle Q\rangle_4=0.79275\ 62$	$(25)_4=0.79677\ 97$
$\langle Q\rangle_5=0.79272\ 30$	$(25)_5=0.79533\ 60$.

For $Q=1/(1+x)$,

$$\langle Q\rangle=3(4\log 2-2.5)=0.81776\ 61$$

$\langle Q\rangle_1=0.8$	$(25)_1=0.875$
$\langle Q\rangle_2=0.825$	$(25)_2=0.83854\ 16$
$\langle Q\rangle_3=0.81714\ 28$	$(25)_3=0.82777\ 77$
$\langle Q\rangle_4=0.81792\ 70$	$(25)_4=0.82356\ 76$
$\langle Q\rangle_5=0.81775\ 66$	$(25)_5=0.82153\ 17$.

For $Q=1/(1+x^2)$,

$$\langle Q\rangle=3(1-\log 2)=0.92055\ 84$$

$\langle Q\rangle_1=0.94117\ 64$	$(25)_1=0.875$
$\langle Q\rangle_2=0.91$	$(25)_2=0.89687\ 50$
$\langle Q\rangle_3=0.92057\ 24$	$(25)_3=0.90918\ 80$
$\langle Q\rangle_4=0.92059\ 03$	$(25)_4=0.91402\ 11$
$\langle Q\rangle_5=0.92052\ 77$	$(25)_5=0.91633\ 46$

$\langle Q\rangle_5$ is obtained from the values of the function at 14 points, whereas $(25)_5$ is obtained from the values of the function at 56 points. The formulas $\langle Q\rangle_m$ are far more accurate than the formula (25). Errors committed by formula $\langle Q\rangle_m$ may be estimated as

$$|\text{error}|<\frac{3M}{(m+1)!\,(m+4)}$$

with the aid of Taylor's theorem, where M denotes the maximum value of

$$\left|\left(\frac{\partial}{\partial x}\right)^i\left(\frac{\partial}{\partial y}\right)^j\left(\frac{\partial}{\partial z}\right)^k Q(x,\,y,\,z)\right|,\qquad i+j+k=m+1$$

over the tetrahedron.

For a function that shows abrupt jumps, $M=\infty$. So formulas $\langle Q\rangle_m$ might yield poorer results than the formula (25) where domains of abrupt changes will be diminished with increasing m. For $Q=\epsilon(1/2-x)$, where $\epsilon(x)=0$ for $x>0$ and $\epsilon(x)=0$ for $x<0$, comparison is as follows

$\langle Q\rangle=0.875$	
$\langle Q\rangle_1=1$	$(25)_1=0.75$
$\langle Q\rangle_2=0.85$	$(25)_2=0.75$
$\langle Q\rangle_3=0.775$	$(25)_3=0.86111\ 11$
$\langle Q\rangle_4=0.91107\ 63$	$(25)_4=0.84375$
$\langle Q\rangle_5=0.79886\ 86$	$(25)_5=0.87$

In conclusion one may say that formulas $\langle Q\rangle_m$ are far superior to formula (25) for a smooth function whereas the latter is preferable to the former for applying to functions that show abrupt jumps.