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On Abstract Numerical Integrations

John J. Sopka*

National Bureau of Standards, Boulder, Colo.

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Let X be a space of functions, say $X \subset C(K)$, K locally compact Hausdorff, let $l \epsilon X^*$ be an integral on X and let $M^* \subset X^*$ be a given subspace of "simple" functionals, then it is desired to obtain an $\bar{l} \epsilon M^*$ for given n, $\bar{l} \epsilon M_n^* \subset M^*$; M_n^* being a suitable n dimensional subspace determined so that $l - \bar{l}$ annihilates a given finite dimensional subspace $X_1 \subset X$. In this general context, the abstract analysis of numerical integration is developed and certain specific applications are made.

Key Words: Numerical integrations, abstract Gaussian quadrature methods.

1. Introduction

In the development of numerical integration formulas, one is given a function space X, say $X \subset C(K)$, where K is some locally compact Hausdorff space, and an integral $l \epsilon X^*$. It is then desired to find an $\bar{l} \epsilon M^* \subset X^*$, where M^* is a subspace generated by a family of "simple" integrals $\{x_\alpha^*\}$ such that $\bar{l}$ can be said to approximate l in some given sense.

In ordinary quadrature, the family $\{x_\alpha^*\}$ are given by $x_\alpha^* f = f(x_\alpha) \, \forall \, f \epsilon C(K)$ where $x_\alpha \epsilon K$. An element $\bar{l} \epsilon M^*$ is said to approximate the given integral l if $l - \bar{l} \epsilon X_\omega^\perp$ where $X_\omega^\perp$ is the subspace in X^* of all annihilators of a given subspace $X_\omega \subset X$.

The following paper summarizes the essential mathematical structure of numerical integration methods with the purpose of extending systematically the class of such methods.

2. General Analysis

Let $X \subset C(K)$ and let $X_0 \subset X$ be a subspace $\ni$ dim $X_0 = n$ and X_0 is generated by a given set of n "basis" functions $\{f_k\}$. In X^* take M^* a subspace generated by a given family $\{x_\alpha^*\}$ of linearly independent functionals with the properties: M^* is total over X_0 and $\{x_\alpha^*\} \cap X_0^\perp$ is void where $X_0^\perp = \{l;\ l \epsilon X^*,\ lf = 0,\ f \epsilon X_0\}$. If $M_n^* \subset M^*$ designates a subspace generated by n of the x_α^*, say $\{x_{\alpha i}\}\ i = 1 \ldots n$ so that dim $M_n^* = n$, then one has $X^* = X_0^\perp \dot{+} M_n^*$ since the deficiency of $X_0^\perp =$ dim $X_0 = n$. Also M_n^* is total over X_0 as is readily seen.

If $l \epsilon X^*$ is a given integral, then $\exists\ \bar{l} \epsilon M_n^* \ni l = \bar{l} + l_0^\perp$ where $l_0^\perp \epsilon X_0^\perp$ and $\exists$ such an $\bar{l}$ for each subspace M_n^* as defined above. For any such given subspace M_n^* $\exists\ l_i\ \epsilon M_n^*\ i = 1 \ldots n \ni l_i f_k = \delta_{ik}\ i, k = 1 \ldots n\ \delta_{ik} = 1$ $i = k$, $\delta_{ik} = 0\ i \neq k$. This follows from M_n^* being total over X_0.

Thus one can write: $l = \sum_i l(f_i)\, l_i + l_0^\perp,\ l_0^\perp \epsilon X_0^\perp$ and

$l_i = \sum_j \gamma_{ij} x_j^*$ where $x_j^* = x_{\alpha,j}^*$.

Then $$l = \sum_i \sum_j (l f_i) \gamma_{ij} x_j^* + l_0^\perp$$

or $$\bar{l} = l - l_0^\perp = \sum_j \left(\sum_i l f_i \gamma_{ij} \right) x_j^*. \qquad (1)$$

The functional $\bar{l}$ therefore depends on the selected set $\{x_{\alpha i}^*\}$, that is on M_n^*, on the $l f_i$ and on the coefficients $\gamma_{ij}\ i, j = 1 \ldots n$.

The relations $\sum_j \gamma_{ij} x_j^* f_k = \delta_{ik} i,\ k = 1 \ldots n$ can be put in matrix form: $\Gamma \Gamma_0 = I$ where I is the identity matrix, $\Gamma = (\gamma_{ij})\ \Gamma_0 = (x_j^* f_k)$. Now Γ_0 is nonsingular for any given M_n^* since M_n^* total over X_0 implies that $\sum_{k=1}^{n} \tau_k x_j^* f_k = 0\ j = 1 \ldots n$ is possible only when $\tau_k = 0$ $k = 1 \ldots n$. Hence the matrix $\Gamma = \Gamma_0^{-1}$ is determined once Γ_0 is known.

If the $\{f_k\}$ are such that the $l f_k$ are readily evaluated then the problem of determining $\bar{l}$ is that of specifying M_n^* or a corresponding basis $\{x_{\alpha i}^*\}$. Under the conditions imposed thus far with dim $X_0 =$ dim $M_n^* = n$ $\bar{l}$ will not in general be unique without additional conditions on X and/or the M_n^*.

3. Specific Cases

In certain quadrature procedures, such as the Newton-Cotes formulas, M_n^* is specified a priori by choosing the $x_{\alpha i}^*$. The subspace X_0 in these cases is such that the $l f_i$ are easily calculated and thus $\bar{l}$

*Consultant-Mathematics, National Bureau of Standards, Boulder, Colo.

is determined. For instance, the Parabolic Rule has $l = \int_{x_1}^{x_3} dx$, where X_0 is the space over the Reals generated by the $f_k = x^{k-1}$, $k=1,2,3$ and $x_{\alpha i}^* f = f(x_i)$ for given real numbers x_1, $x_2 = \frac{1}{2}(x_1 + x_3)$, x_3.

In Gaussian quadrature methods, the following additional conditions limit the choice of M_n^*. Consider a subspace $X_1 \subset X$, where $X_1 \supset X_0$ and X_1 has generators $\{f_k'\}$, $k=1 \ldots p$, $p>n$, $f_k' = f_k$ for $k=1 \ldots n$. Now if T is a linear transformation on $X \ni f_k' = Tf_{k-1}' = T^{k-1}f_1'$. Then T induces a linear transformation Q on X^* given by $Qlf = lf = lTf$, $\forall l \epsilon X^*$, $f \epsilon X$. Consequently $x_j^* f_k' = (Qx_j^*)f_{k-1}' = (Q^{k-1}x^*)f_1'$ and one can write:

$$\bar{l}f_k = \sum_j \left(\sum_i lf_i\gamma_{ij}\right) Q^{k-1}x_j^* f_1 \text{ for } k=1 \ldots p. \tag{2}$$

Since the matrix $\Gamma_0 = (x_j^* f_k) = (Q^{k-1}x_j^* f_1)$ for j, $k=1 \ldots n$ is nonsingular, the n-tuple $(Q^n x_j^* f_1)$ $j=1 \ldots n$ corresponding to

$$\bar{l}f_{n+1} = \sum_j \left(\sum_i lf_i\gamma_{ij}\right) Q^n x_j^* f_1$$

is linearly dependent on the rows of Γ_0, i.e.

$$Q^n x_j^* f_1 = \sum_{k=1}^{n} \beta_k Q^{k-1} x_j^* f_1 \qquad j=1 \ldots n. \tag{3}$$

This gives the relationship

$$\bar{l}f_{n+1}' = \sum_{k=1}^{n} \beta_k \bar{l} f_k'. \tag{4}$$

Now, if for $M_{n\perp}^* = \{f;\ f\epsilon X_1,\ x_j^* f = 0,\ j=1 \ldots n\}$ one also assumes: $TM_{n\perp}^* \subset M_{n\perp}^*$ that is, $x_j^* f = 0$ implies $x_j^* Tf = 0 = Qx_j^* f$ for $j=1 \ldots n$ then this condition, plus the statement:

$$\left(Q^n - \sum_{1=1}^{n} \beta_k Q^{k-1}\right) x_j^* f_1' = 0 \qquad j=1 \ldots n \tag{5}$$

will imply that

$$\left(Q^{n+q} - \sum_{k=1}^{n} \beta_k Q^{k+q-1}\right) x_j^* f_1' = 0 \qquad j=1 \ldots n, \forall q \tag{6}$$

Taking $q=0, 1 \ldots n-1$ one gets the n equations

$$\bar{l}f_{n+1+q}' = \sum_{k=1}^{n} \beta_k \bar{l} f_{k+q}'. \tag{7}$$

In Gaussian quadrature, the stronger condition $l - \bar{l} \epsilon X_1^{\perp} \subset X_0^{\perp}$ is imposed. Thus, if $l - \bar{l} \epsilon X_1^{\perp}$, if the f_{k+q}' are such that the lf_{k+q}' are readily obtained and if the matrix $L = (lf_{k+q}')$, $k=1 \ldots n$, $q=0 \ldots n-1$ is nonsingular then the β_k can be obtained uniquely. Given the β_k, solution for the $x_j^* f_1'$ $j=1 \ldots n$ follows from the relations (5) when they are solvable. Determination of the functionals x_j^* $j=1 \ldots n$ proceeds from the values of the $x_j^* f_1$ when the x_j^* are sufficiently simple, for example, a one parameter family like those in the examples below.

Now, $L = (lf_{k+q}')$ is nonsingular if and only if $\nexists$ scalars

$$\epsilon_k \neq 0,\ k=1 \ldots n \ni l\left(\sum_{k=1}^{n} \epsilon_k f_{k+q}\right) = 0$$

$$q=0 \ldots n-1.$$

Since these last relations can be written as:

$$l\left(\sum_{k=1}^{n} \epsilon_k T^{k-1+q} f_1\right) = l\left(T^q\left(\sum_{k=1}^{n} \epsilon_k T^{k-1}\right) f_1\right) = 0 \tag{8}$$

one has, in this general context, an orthogonality condition stating that no $n-1$ degree "polynomial" in T is orthogonal in this sense to all $n-1$ degree polynomials in T. The n-equations (7) can also be written as:

$$l\left(T^q\left(T^n - \sum_{k=1}^{n} \beta_k T^{k-1}\right) f_1\right) = 0 \qquad q=0 \ldots n-1 \tag{9}$$

which states that the n degree polynomial $T^n - \sum_{k=1}^{n} \beta_k T^{k-1}$ is orthogonal, in this sense, to all $n-1$ degree polynomials in T.

Thus if X_0, X_1, M_n^* satisfy the conditions imposed, it was seen in the general section above that $\exists\, \bar{l} \epsilon M_n^* \ni l - \bar{l} \epsilon X_0^{\perp}$. The preceding discussion shows that if $l - \bar{l} \epsilon X_1^{\perp}$ then (9) follows. Conversely, if $\exists\, \beta_k \ni (9)$ holds one shows directly $l - l \epsilon X_1^{\perp}$ using (5) and (6). Consequently one has the following statement analogous to the ordinary Gaussian quadrature theorem [1] which is usually stated in terms of classical orthogonal polynomials: If X_0, X_1, M_n^* satisfy all the conditions imposed above then $\exists\, \bar{l} \epsilon M_n^* \ni l - \bar{l} \epsilon X_1^{\perp}$ if and only if $\exists$ an n degree "polynomial" $T^n - \sum_{k=1}^{n} \beta_k T^{k-1}$ orthogonal as in (9) to all polynomials in T of degree $< n$.

4. Applications

In ordinary Gaussian quadrature, the above specializes to the case where $X_0 = \{x^{i-1};\ i=1 \ldots n\}$, $X_1 = \{x^{i-1};\ i=1 \ldots 2n\}$, and the $\{x_\alpha^*\}$ are defined by $x_\alpha^* f = f(x_\alpha)$. Then the other Gaussian conditions are seen to hold when T is $\ni (Tf)(x) = f(x)x$.

An interesting nonclassical application is to $l = \int_0^1 dx$ on the space $X = C_0(K) = \{f;\ f \epsilon C(K),\ K=[0,1], f(0) = f(1) = 0\}$. The natural basis functions here are $\sin \pi kx$ or the equivalent functions $f_k(x) = \sin \pi x (\cos \pi x)^{k-1}$.

Take X_0, X_1; with this basis and x_α^* defined by $x_\alpha^* f = f(x_\alpha)$, $x_\alpha \epsilon [0, 1]$. Take $T \ni Tf(x) = f(x) \cos \pi x$ then $TM_{n\perp}^* \subset M_{n\perp}^*$ and one gets:

$$\bar{l} = 0.39\,(x_1^* + x_2^*) \qquad \text{for } n=2$$

$$\bar{l} = 0.205\,(x_1^* + x_3^*) + 0.247\,(x_2^* + x_4^*) \qquad \text{for } n=4$$

$$\bar{l} = 0.18502\,(x_1^* + x_2^*) + 0.12306\,(x_3^* + x_4^*) + 0.16882\,(x_5^* + x_6^*) \qquad \text{for } n=6.$$

Another application is to $l = \int_0^\infty k(x)dx$ for some weight function $k(x)$ e.g., $k(x) = e^{-x^2}$. Here $K = [0, \infty]$

$$X = \left\{ f;\ f \epsilon C(K),\ lf \text{ exists}, \int_0^x f(t)dt \text{ exists and is easily obtained for arbitrary } x \epsilon K \right\}.$$

Take $f_k'(x) = kx^{k-1}$, let $x_j^* f = k(\xi_j) \int_{x_{j-1}}^{x_j} f(x)dx$. For $x_0 = 0$ $x_{j-1} < \xi_j < x_j$ and take T given by $Tf(x) = xf(x) + \int_0^x f(t)dt$ then $TM_{n\perp}^* \subset M_{n\perp}^*$ and one gets:

$$\bar{l} = 0.922 \int_{x_0}^{x_1} dx + 0.195 \int_{x_1}^{x_2} dx \qquad \text{for } n=2.$$

where $x_0 = 0$, $x_1 = 0.754$, $x_2 = 1.734$

$$\bar{l} = 0.9798 \int_{x_0}^{x_1} dx + 0.6188 \int_{x_1}^{x_2} dx + 0.1386 \int_{x_2}^{x_3} dx + 0.0051 \int_{x_3}^{x_4} dx \qquad \text{for } n=4$$

where $x_0 = 0$, $x_1 = 0.4239$ $x_2 = 1.014$ $x_3 = 1.792$ $x_4 = 2.640$

$$\bar{l} = 0.99200 \int_{x_0}^{x_1} dx + 0.81425 \int_{x_1}^{x_2} dx + 0.41032 \int_{x_2}^{x_3} dx + 0.09445 \int_{x_3}^{x_4} dx + 0.00702 \int_{x_4}^{x_5} dx + 0.00008 \int_{x_5}^{x_6} dx \qquad \text{for } n=6$$

where $x_0 = 0$ $x_1 = 0.27779$ $x_2 = 0.68991$ $x_3 = 1.2090$ $x_4 = 1.8138$ $x_5 = 2.5104$ $x_6 = 3.3556$.

Greater detail on the development of such formulas and their utility will be given in a subsequent paper.

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