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Problems of optimization of numerical mathematics

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PROBLEMS OF OPTIMIZATION OF NUMERICAL MATHEMATICS.

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1. Modern computational techniques are putting forward new problems in numerical analysis. At present numerical mathematics can be considered as a set od constructive mathematical methods transforming given information into desired ones (see e.g. BABUŠKA [1966], HENRICI [1964], BABUŠKA, SOBOLEV [1965], BABUŠKA, PRÁGER, VITÁSEK [1966]). The classic concepts as for example that of method are beginning to have new meaning. The first place is being occupied by algorithms and the methods are rather comprehend as a class of algorithms of certain kind. Concerning algorithms the following requirements arise:

a) sufficient generality of algorithms

this requires the algorithm to be applicable to a sufficiently wide class of problems. For example the algorithm of integration by Cotes' formulae of highest order is not sufficiently general as it is applicable only to the narrow class of analytic functions.

b) Sufficient universal efficiency;

this means that the algorithm should treat the given informations „approximately" as well as the optimal algorithm (see below).

c) sufficiently good realizability

By realizability we mean, that the fact, that the computer does not work in the field of real numbers (the rounding off) should not have a great effect on the result. Especially this is the problem of numerical stability (see BABUŠKA, PRÁGER, VITÁSEK [1966]).

In this paper we will study some aspects concerning the universal efficiency. In order to illustrate this problem we will restrict us here only to very special cases.

2. Let a Banach space B be given and let $\varphi \in B^*$. Our task will be to calculate the value $\varphi(f)$ for a given $f \in B$. The principal idea of (linear) numerical methods of calculation of the value of the functional φ is the following. A matrix of functionals $\Phi \equiv \{\varphi_j^{(n)}\}$, $j = 1, \ldots, n$, $n = 1, 2, \ldots$, $\varphi_j^{(n)} \in B^*$, is given (these functionals will be called *calculable functionals*). Now it is necessary to construct the functionals $\varphi_n = \sum_{j=1}^{n} C_j^{(n)} \varphi_j^{(n)}$ in such a way that $\varphi_n(f) \to \varphi(f)$ for $n \to \infty$. In practical cases we take $\varphi_n(f) \approx \varphi(f)$ for sufficiently great n. There is a number of problems connected with this task.

1) Problem of the estimate for the upper bound of error.

Here the upper bound of the quantity $\varepsilon_n(\varphi, \varphi_n, B) = \|\varphi - \varphi_n\|_{B^*}$ is to be estimated.

This problem bears in fact a classic character and is intensively investigated at present (especially it concerns not only the estimate of order, but also of the corresponding constants); in the case of integration of periodic functions see e.g. SOBOLEV [1965], [1967], JAGERMAN [1966], AGAHANOV [1965], EHLICH [1966], BABUŠKA [1965], ČARUŠNIKOV [1966] and others.

2) Problem of the estimate for the lower bound of error.

Here the lower bound of the quantity

$$\eta_n(\varphi, \Phi, B) = \inf_{\alpha_k^{(n)},\, k = 1, \ldots, n} \|\varphi - \sum_{k=1}^{n} \alpha_k^{(n)} \varphi_k^{(n)}\|_{B^*}$$

is to be estimated. Also this question is intensively studied at present. See e.g. SOBOLEV [1965], [1967], BABUŠKA, SOBOLEV [1965], BACHVALOV [1963] and many others. The quantity gives the maximal accuracy at obtainable on the ground of given information.

3) Problem of the optimal formula.

The task is to construct the functionals φ_n in such a way that

$$\varepsilon_n(\varphi, \varphi_n, B) = \eta_n(\varphi, \Phi, B)$$

See e.g. BABUŠKA, SOBOLEV [1965], SOBOLEV [1965], [1967], GOLOMB, WEINBERGER [1959] etc. The concrete construction of optimal formulae is very difficult and is known only in special cases. In connection with these difficulties formulae are studied, which are asymptotically optimal or optimal by order. See e.g. BABUŠKA, SOBOLEV [1965], SOBOLEV [1965]. From the point of view of numerical practice the problem of optimal formulae encounters some difficulties. Beyond the difficulties connected with the construction of optimal formulae there is also the problem of how to choose the space B in a concrete case. We will now illustrate the practical importance of this problem by a simple example.

Let
$$\varphi(f) = \int_0^1 f(x)\,\mathrm{d}x$$

Let Φ be a matrix of the functional,such that $\varphi_{n+1}(f) = \frac{1}{n} \sum_{s=0}^{n} a_s^{(n)} f\left(\frac{s}{n}\right)$ holds. If $\|f\|_B^2 = f^2(0) + \int_0^1 (f')^2\,\mathrm{d}x$, then the optimal formula will be the trapezoid-rule. At the same time it is known, that the trapezoid-rule is scarcely used in practice.

The question of how to lower the risk of choosing the space B in a concrete case is the question of universality of the formula.

4) Problem of universal optimality by order.

Let $\mathfrak{A}$ be a given system of Banach spaces B embedded in a Banach space B_0. Let us have a matrix of calculable functionals $\varphi_j^{(n)} \in B_0^*$ and a matrix of coefficients $\Psi = \{C_j^{(n)}\}$, $j = 1, \ldots, n$; $n = 1, 2, \ldots\ldots$ We will use the following notation:

$$\mathfrak{A}_{\Psi}^{\Phi,\varphi} = E\left[B \in \mathfrak{A},\ \frac{\|\varphi - \sum_{j=1}^{n} C_j^{(n)} \varphi_j^{(n)}\|_{B^*}}{\eta_n(\varphi, \Phi, B)} \leq C(B)\right]$$

[where $C(B)$ depends on B, φ, Φ, Ψ but not on n]. We will say that the formula $\varphi_n = \sum_{j=1}^{n} C_j^{(n)} \varphi_j^{(n)}$ is universally optimal by order with respect to $\mathfrak{A}_{\Psi}^{\Phi,\varphi}$. Further let us have two formulae given by the matrices $\Psi_i = \{{}^iC_j^{(n)}\}$, $i = 1, 2. \dots$ [i.e. $\varphi_{n,i} = \sum_{j=1}^{n} {}^iC_j^{(n)}\varphi_j^{(n)}$]. We will say that the formula given by with the matrix Ψ_1 is comparable or better or not worse respect to $\mathfrak{A}$ than the formula given by the matrix Ψ_2, if $\mathfrak{A}_{\Psi_1}^{\Phi,\varphi} \supseteq \mathfrak{A}_{\Psi_2}^{\Phi,\varphi}$ or $\mathfrak{A}_{\Psi_1}^{\Phi,\varphi} \supset \mathfrak{A}_{\Psi_2}^{\Phi,\varphi}$ or $\mathfrak{A}_{\Psi_1}^{\Phi,\varphi} \supseteq \mathfrak{A}_{\Psi_2}^{\Phi,\varphi}$, respectively. The problem of universal optimality lies in

a) characterization of $\mathfrak{A}_{\Psi}^{\Phi,\varphi}$ for a given formula,

b) characterization of $\mathfrak{A}$ in such a that the best formula exist,

c) construction of an algorithm leading to this best formula and an estimate of the quantities η_n and $C(B)$ as functions of B.

3. In this part we will give some illustrative assertions concerning the universal optimality. Let us have the task to calculate a functional over the Hilbert space of periodic functions and let us ask, what is (in the intuitive sense) understood the concept of this space. Its intuitive meaning can be perhaps expressed in the following manner.

Definition 1. *We will say that a Hilbert space H of 2π-periodic complex functions has the property P, if the following properties are fullfiled.*

P_1: *H is dense in $C_{2\pi}$.*

P_2: if *$f \in H$ then also $g(x) = f(x + c) \in H$ for every real c and $||f|| = ||g||$.*

P_3: *H is imbedded in $C_{2\pi}$.*

Now the following theorem holds.

Theorem 1.[1)]

Let H have the property P. Then

1) $e^{ikx} \in H$, $k = \dots, -1, 0, 1, \dots$;

2) $(e^{ikx}, e^{ilx}) = \lambda_k^2$ for $k = l$
$= 0$ *for* $k \neq l$;

3) $\sum_{m=-\infty}^{+\infty} \lambda_k^{-2} < \infty$.

It is easy to prove also the inverse theorem.

Theorem 2.

Let K be the set of all sequences Λ, $\Lambda \equiv \{\dots, \lambda_{-1}, \lambda_0, \lambda_1, \dots\}$ for which $\lambda_k > 0$, $k = \dots, -1, 0, 1, \dots$ and $\Sigma\, \lambda_k^{-2} < \infty$.

Let M be a linear space of all trigonometric polynomials with the scalar product
$(e^{ikx}, e^{ilx}) = \lambda_k^2$ *for* $k = l$
$= 0$ *for* $k \neq l$.

Let H_Λ denote the complete envelope of M in the given norm; then H_Λ has the property P.

1) It was M. PRÁGER who has drawn my attention to this theorem.

Now we will introduce various systems of spaces with the property P.
Let $\mathfrak{A}$ be the system of all Hilbert spaces with the property P.
Let $\mathfrak{A}_1$ be of all H_Λ, $\Lambda \in K_1 \subset K$, such that if $\Lambda \in K_1$, then

1) $\lambda_k = \lambda_{-k}$, $\quad k = 0, 1, 2, \ldots$
2) $\lambda_{k+1} \geq \lambda_k \quad k \geq 0$
3) $\displaystyle\sum_{t=0}^{\infty} \frac{\lambda^2[\alpha n]}{\lambda^2[\alpha n] + t(2n+1)} \leq D, \quad 0 \leq \alpha \leq 4.$

D does not depend on n (but depends on Λ.)

Let $\mathfrak{A}_2$ be the system of all H_Λ, $\Lambda \in K_2 \subset K_1$ satisfying.

$$\lambda_k \leq C + |k|^\beta, \quad \beta > 0 .$$

Now let $\quad \Phi \equiv \{\varphi_j^{(n)}\}, \quad j = 1, 2, \ldots, 2n+1, \quad n = 1, 2, \ldots$

$$\varphi_j^{(n)}(f) = f\left(\frac{2\pi}{2n+1} j\right)$$

be a matrix of calculable functionals and let us turn to the problem of computation of the functional

$$\varphi(f) = \frac{1}{2\pi} \int_0^{2\pi} f(x)\, \zeta(x)\, dx, \quad \zeta(x) \in L_2 .$$

Then the formula becomes[2)]

$$\varphi_n(f) = \sum_{j=1}^{2n+1} C_j^{(n)}(\zeta)\, \varphi_j^{(n)}$$

Now the question is how to choose the coefficients $C_j^{(n)}(\zeta)$. The following theorem holds.

Theorem 3.

A necessary and sufficient condition that there should exist such $C_j^{(n)}(\zeta)$ that the formula

$$\varphi_n(f) = \sum_{j=1}^{2n+1} C_j^{(n)}(\zeta)\, \varphi_j^{(n)}$$

should be universally optimal by order with respect to $\mathfrak{A}$, is that $\zeta(x)$ should be a trigonometric polynomial. The coefficients are uniquelly determined except for a finite number of indices n and are given by

$$*C_j^{(n)} = \frac{1}{2n+1}\, \zeta\left(\frac{2\pi}{2n+1} j\right)$$

If $\zeta(x)$ is a more general function, then it follows from theorem **3** that

[2)] To simplify formally the following assertions we have restricted us to an odd number of points used.

a formula, which would be universally optimal by order with respect to $\mathfrak{A}$ does not exist. In connection with what has been said above the question arises whether it is possible to restrict the system of spaces $\mathfrak{A}$ in such a way that universally optimal — by — order formula should exist. This is solved by the following theorem.

Theorem 4.

If $\zeta(x) \in L_2$, then $^*C_j^{(n)}(\zeta)$ exist so that the formula

$$\varphi_n(f) = \sum_{j=1}^{2n+1} {}^*C_j^{(n)}(\zeta)\, \varphi_j^{(n)}$$

is universally optimal by order with respect to $\mathfrak{A}_1$. Except for a finite number of indices n, the coefficients are uniquelly determined and we have

$$^*C_j^{(n)} = \frac{1}{2n+1} S_n \left(\frac{2\pi}{2n+1} j\right)$$

where
$$S_n = \sum_{k=-n}^{+n} d_k e^{ikx} \quad \textit{and} \quad \zeta(x) = \sum_{k=-\infty}^{+\infty} d_k e^{ikx} .$$

By theorem 3 and 4 the universally optimal — by — order formula is uniquelly determined. It is clear that should we further restrict the system of spaces $\mathfrak{A}$, then the formula can be determined non uniquelly. In this connection the following theorem holds.

Theorem 5.

Let $\zeta(x) \in L_2$. Then the formula given by theorem 4 is not the only formula universally optimal by order with respect to $\mathfrak{A}_2$.

Returning once more to the formula given by theorem 4 we see that it is not optimal in any $H \in \mathfrak{A}_1$ but is universally optimal by order. It is also easy to see that in fact this formula is obtainable by means of the classic (interpolation) method using trigonometric polynomials. From this point of view the connection between the classic (interpolation) theory of quadrature formulae and the theory based on optimization of formulae is well visible. But we will not go further in the study of this problem.

Using the simplest examples, I have given some typical theorems concerning the form of the universal optimality by order. This problem can of course be substantionally extended to include the problem of calculation of functionals as well as operators.

4. In the conclusion let us give some numerical results. Let us compute

$$I = \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} e^{\alpha \sin x} \cos x \, dx$$

for different values of α.

As the integrand is obviously a 2π-periodic function, I can be written in the form

$$I = \int_{-\pi}^{+\pi} e^{\alpha \sin x}\, \zeta(x)\, \mathrm{d}x$$

where $\zeta(x) = \cos x \qquad \text{for } |x| < \frac{\pi}{2}$

$$\zeta(x) = 0 \qquad \text{for } \frac{\pi}{2} \leq x \leq \pi, \quad -\pi \leq x \leq -\frac{\pi}{2}$$

$\Big($here we make use of the symetry of $f = e^{\alpha \sin x}$ with respect to the point $x = \pm\frac{\pi}{2}\Big)$. Now the integrand has the form studied in theorem 4. In the following Table together with various formulae the quadrature error is given in dependence on the number of vaules of the function $e^{\alpha \sin x}$ (for $\alpha = 1, 5, 7$) used in the calculation. Besides the trapezoid-rule and the Simpson formula also the Romberg formula (see Bauer, Rutishauser, Stiefl [1963]) according to Bauman algorithm [1961] is given under the notation Romberg. Two other modified methods are given as Romberg 1 and Romberg 2. The formula Romberg 1 is that of Bulirsch—Romberg (see Bulirsch [1964]) and the formula Romberg 2 is that of Bulirsch—Stoer (see Bulirsch, Stoer [1965]). The last one is given for comparison although it is not a linearone.

The computation has been carried out on the *ICT* **1900** with a double precission of word.

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Number of points	1	2	3	4	5	6
4	0.17 0	−0.40 −1	0.76 −3	0.19 −2	−0.12 0	−0.11 −1
6	0.72 −1	−0.62 −2	0.26 −5		0.12 −1	−0.11 −1
8	0.40 −1	−0.16 −2	0.63 −8	−0.85 −5	0.57 −3	0.93 −3
10	0.26 −1	−0.61 −3	0.11 −10			
12	0.18 −1	−0.28 −3	0.15 −13		−0.15 −3	−0.53 −4
14	0.13 −1	−0.15 −3	0.15 −16			
16	0.99 −2	−0.87 −4	−0.54 −19	−0.38 −7	0.71 −5	−0.44 −6
18	0.79 −2	−0.54 −4	0.60 −18			
20	0.64 −2	−0.35 −4	0.16 −18			
22	0.53 −2	−0.24 −4	−0.16 −18			
24	0.44 −2	−0.17 −4	−0.54 −19		−0.12 −6	0.27 −7
26	0.38 −2	−0.12 −4	−0.49 −18			
28	0.32 −2	−0.90 −5	−0.27 −18			
30	0.28 −2	−0.69 −5	−0.27 −18			
32	0.25 −2	−0.53 −5	−0.54 −19	0.12 −9	−0.70 −10	−0.19 −9
34	0.22 −2	−0.41 −5	−0.16 −18			
36	0.20 −2	−0.33 −5	0.54 −19			
38	0.18 −2	−0.27 −5	0.54 −19			
40	0.16 −2	−0.22 −5	0.16 −18			
42	0.14 −2	−0.18 −5	0.16 −18			
44	0.13 −2	−0.15 −5	0.38 −18			
46	0.12 −2	−0.12 −5	0.38 −18			
48	0.11 −2	−0.10 −5	0.16 −18		0.17 −10	−0.76 −12
50	0.10 −2	−0.88 −6	0.38 −18			
52	0.94 −3	−0.75 −6	0.38 −18			
54	0.87 −3	−0.65 −6	0.38 −18			
56	0.81 −3	−0.56 −6	0.38 −18			
58	0.76 −3	−0.49 −6	0.38 −18			
60	0.71 −3	−0.42 −6	0.38 −18			
62	0.66 −3	−0.37 −6	0.38 −18			
64	0.62 −3	−0.33 −6	0.60 −18	−0.62 −13	−0.13 −12	0.12 −14

Table *1. The calculation of I for* $\alpha = 1$ *according to various formulae.* 1) *trapezoid-rule,* 2) *Simpson formula,* 3) *universal formula,* 4) *Romberg formula,* 5) *Romberg formula 1,* 6) *Romberg formula 2.*

Number of points	1	2	3	4	5	6
4	0.98 1	0.37 1	0.20 1	−0.95 0	0.88 1	−0.21 2
6	0.37 1	−0.12 1	0.11 0		−0.65 1	−0.21 2
8	0.20 1	−0.61 0	0.51 −2	0.35 −1	−0.39 0	0.15 1
10	0.13 1	−0.21 0	0.19 −3			
12	0.86 0	−0.84 −1	0.57 −5		0.39 0	0.24 0
14	0.63 0	−0.41 −1	0.13 −6			
16	0.48 0	−0.23 −1	0.25 −8	−0.26 −3	−0.35 −1	−0.48 −1
18	0.38 0	−0.14 −1	0.39 −10			
20	0.31 0	−0.88 −2	0.51 −12			
22	0.25 0	−0.59 −2	0.55 −14			
24	0.21 0	−0.41 −2	0.49 −16		0.52 −3	−0.56 −3
26	0.18 0	−0.30 −2	−0.26 −17			
28	0.16 0	−0.22 −2	−0.30 −17			
30	0.14 0	−0.17 −2	−0.26 −17			
32	0.12 0	−0.13 −2	0.00 0	0.22 −6	0.50 −4	0.44 −4
34	0.11 0	−0.99 −3	−0.13 −17			
36	0.94 −1	−0.79 −3	−0.43 −18			
38	0.85 −1	−0.63 −3	0.87 −18			
40	0.76 −1	−0.51 −3	0.87 −18			
42	0.69 −1	−0.42 −3	0.87 −18			
44	0.63 −1	−0.35 −3	0.22 −17			
46	0.58 −1	−0.29 −3	0.87 −18			
48	0.53 −1	−0.25 −3	0.17 −17		−0.20 −5	0.65 −8
50	0.49 −1	−0.21 −3	0.22 −17			
52	0.45 −1	−0.18 −3	0.13 −17			
54	0.42 −1	−0.15 −3	0.22 −17			
56	0.39 −1	−0.13 −3	0.26 −17			
58	0.36 −1	−0.12 −3	0.26 −17			
60	0.34 −1	−0.10 −3	0.30 −17			
62	0.32 −1	−0.88 −4	0.87 −18			
64	0.30 −1	−0.77 −4	0.35 −17	0.45 −9	0.23 −7	−0.64 −9

Table 2. *The calculation of I for $\alpha = 5$ according to various formulae.* 1) *trapezoid-rule,* 2) *Simpson formula,* 3) *universal formula,* 4) *Romberg formula,* 5) *Romberg formula* 1, 6) *Romberg formula* 2.

Number of points	1	2	3	4	5	6
4	0.77 2	0.52 2	0.21 2	−0.11 2	0.98 2	0.57 3
6	0.29 2	−0.39 1	0.21 1		−0.23 2	0.57 3
8	0.15 2	−0.58 1	0.15 0	0.32 0	−0.19 2	0.22 2
10	0.94 1	−0.25 1	0.97 −2			
12	0.64 1	−0.99 0	0.52 −3		0.49 1	0.36 1
14	0.47 1	−0.46 0	0.22 −4			
16	0.36 1	−0.25 0	0.79 −6	−0.80 −3	−0.79 −1	−0.52 0
18	0.28 1	−0.15 0	0.23 −7			
20	0.23 1	−0.92 −1	0.56 −9			
22	0.19 1	−0.62 −1	0.12 −10			
24	0.16 1	−0.43 −1	0.21 −12		−0.40 −1	−0.25 −1
26	0.13 1	−0.31 −1	0.32 −14			
28	0.12 1	−0.23 −1	0.24 −16			
30	0.10 1	−0.17 −1	−0.12 −16			
32	0.88 0	−0.13 −1	0.52 −17	−0.12 −4	0.26 −2	0.15 −1
34	0.78 0	−0.10 −1	0.87 −18			
36	0.70 0	−0.81 −2	0.35 −17			
38	0.63 0	−0.65 −2	0.11 −16			
40	0.57 0	−0.53 −2	0.95 −17			
42	0.51 0	−0.43 −2	0.61 −17			
44	0.47 0	−0.36 −2	0.19 −16			
46	0.43 0	−0.30 −2	0.69 −17			
48	0.39 0	−0.25 −2	0.15 −16		−0.60 −4	0.41 −5
50	0.36 0	−0.21 −2	0.21 −16			
52	0.33 0	−0.18 −2	0.16 −16			
54	0.31 0	−0.16 −2	0.17 −16			
56	0.29 0	−0.14 −2	0.23 −16			
58	0.27 0	−0.12 −2	0.21 −16			
60	0.25 0	−0.10 −2	0.26 −16			
62	0.24 0	−0.89 −3	0.87 −17			
64	0.22 0	−0.79 −3	0.30 −16	0.29 −7	0.36 −6	−0.37 −7

Table 3. *The calculation of I for α = 7 according to various formulae.* 1) *trapezoid-rule,* 2) *Simpson formula,* 3) *universal formula,* 4) *Romberg formula,* 5) *Romberg formula* 1, 6) *Romberg formula 2.*