Numerical evaluation of of finite part integrals. Development and comparison of Newton – Cotes type methods using local quadratic interpolation.

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Abstract: - Finite part integrals were first introduced by Hadamard in connection with hyperbolic partial differential equations. Since then they have been found useful in a number of engineering applications. In this paper we develop and compare simple Newton-Cotes type quadrature rules, which are also appropriate for the numerical solution of finite part integral equations in one dimension with a double pole singularity.

Key-Words: - Strongly singular integral, finite part integral.

1 Introduction

The formulation of certain classes of boundary value problems in terms of strongly singular integral equations is drawing increasing interest. Areas of applications are traditionally the Boundary element Method, fracture mechanics applications (e.g. problems involving cracks with loaded flanks), problems of electromagnetic scattering in cavities, etc. In all the above, the matter is to evaluate efficiently integrals of the type:

$$\fint_a^b \frac{f(x)}{(x-t)^m}dx, \quad t \in (a,b)$$

which is defined as follows:

$$\fint_a^b \frac{f(x)}{(x-t)^m}dx = \lim_{\varepsilon \to 0} \left\{ \begin{array}{l} \int_a^{x-\varepsilon} \frac{f(x)}{(x-t)^m}dx + \int_{x+\varepsilon}^b \frac{f(x)}{(x-t)^m}dx \\ -\varepsilon^{1-m}\varphi(x) \end{array} \right\}$$

$$\text{with } \varphi(x) := \sum_{k=0}^{m-2} \frac{\varepsilon^k}{m-k-1} \frac{f^{(k)}(x)}{k!\left[1+(-1)^{m-k}\right]}$$

2 Problem Formulation

Consider the following type of finite part integral:

$$I = \fint_a^b \frac{f(x)}{(x-t)^2}dx, \quad t \in (a,b) \tag{1}$$

Our goal is to establish a numerical scheme for the evaluation of the above integral, i.e. we seek a formula of the following type:

$$I = \sum_{j=1}^{N} w_j(x;t) f(x_j) + E_N \tag{2}$$

We propose two different methods to address the problem which are described in the following subsections.

In both methods we interpolate the density (or the modified density) function using piecewise continuous quadratic polynomials.

2.1 Direct density interpolation

In this method, we generate a uniform sequence of n integration points (n odd) and express the density function within the segment $[x_{2i-1}, x_{2i+1}]$ in the following way:

$$\begin{aligned} f^e(x) = {} & N_1^i(x) f(x_{2i-1}) + N_2^i(x) f(x_{2i}) + \\ & N_3^i(x) f(x_{2i+1}) \end{aligned} \tag{3}$$

where the local interpolation polynomials $N_j^i(x)$ have the following expressions:

$$N_1^i(x) = \frac{1}{\alpha_i}\bar{x}_i^2 - \frac{\alpha_i+1}{\alpha_i}\bar{x}_i + 1$$

$$N_2^i(x) = \frac{1}{\alpha_i(1-\alpha_i)}\left(\bar{x}_i^2 - \bar{x}_i\right)$$

$$N_3^i(x) = -\frac{1}{\alpha_i - 1}\left(\bar{x}_i^2 - \alpha_i \bar{x}_i\right), \quad i = 1,(1),n$$

$$\bar{x}_i := (x - x_{2i-1})/h_i, \quad h_i := x_{2i+1} - x_{2i-1},$$

$$\alpha_i := (x_{2i} - x_{2i-1})/h_i, \quad \alpha_i \in (0,1)$$

Introducing

$$\overline{t}_i := \left(t - x_{2i-1}\right) / h_i$$

the quadrature weights become:

$$w_1 = \frac{1}{h_i}\int_0^1 \frac{N_1^i\left(\overline{x}_i\right)}{\left(\overline{x}_1 - \overline{t}_1\right)^2} d\overline{x}_i, \quad w_{2n+1} := \frac{1}{h_i}\int_0^1 \frac{N_3^n\left(\overline{x}_i\right)}{\left(\overline{x}_n - \overline{t}_n\right)^2} d\overline{x}_i$$

$$w_{2i} := \frac{1}{h_i}\int_0^1 \frac{N_2^i\left(\overline{x}_i\right)}{\left(\overline{x}_i - \overline{t}_i\right)^2} d\overline{x}_i$$

$$w_{2i+1} := \frac{1}{h_i}\left(\int_0^1 \frac{N_3^i\left(\overline{x}_i\right)}{\left(\overline{x}_i - \overline{t}_i\right)^2} d\overline{x}_i + \int_0^1 \frac{N_1^{i+1}\left(\overline{x}_{i+1}\right)}{\left(\overline{x}_{i+1} - \overline{t}_{i+1}\right)^2} d\overline{x}_{i+1}\right)$$

Using the expressions of the interpolation polynomials, it is obvious that it suffices to calculate the following integrals (in the finite part sense):

$$I_1^{(i)} := \int_0^1 \frac{\overline{x}_i^2 d\overline{x}_i}{\left(\overline{x}_i - \overline{t}_i\right)^2}, \quad I_2^{(i)} := \int_0^1 \frac{\overline{x}_i d\overline{x}_i}{\left(\overline{x}_i - \overline{t}_i\right)^2}$$

$$I_3^{(i)} := \int_0^1 \frac{d\overline{x}_i}{\left(\overline{x}_i - \overline{t}_i\right)^2}$$

Direct calculation of the above yields:

$$I_1^{(i)} = \begin{cases} \dfrac{2\overline{t}_i - 1}{\overline{t}_i - 1} + 2\overline{t}_i \ln\left|\dfrac{1-\overline{t}_i}{\overline{t}_i}\right|, & \overline{t}_i \neq 0,1 \\ 1, & \overline{t}_i = 0 \\ 0, & \overline{t}_i = 1 \end{cases}$$

$$I_2^{(i)} = \begin{cases} \dfrac{1}{\overline{t}_i - 1} + \ln\left|\dfrac{1-\overline{t}_i}{\overline{t}_i}\right|, & \overline{t}_i \neq 0,1 \\ 0, & \overline{t}_i = 0 \\ 1, & \overline{t}_i = 1 \end{cases} \tag{4}$$

$$I_3^{(i)} = \begin{cases} \dfrac{1}{\overline{t}_i\left(\overline{t}_i - 1\right)}, & \overline{t}_i \neq 0,1 \\ -1, & \overline{t}_i = 0 \text{ or } 1 \end{cases}$$

Thus, the formulae for the quadrature weights become:

$$\begin{aligned} w_{2i} &= \frac{1}{h_i \alpha_i \left(\alpha_i - 1\right)}\left(I_1^{(i)} - I_2^{(i)}\right) \\ w_{2i+1} &= -\frac{1}{h_i\left(\alpha_i - 1\right)} I_1^{(i)} + \frac{\alpha_i}{h_i\left(\alpha_i - 1\right)} I_2^{(i)} + \\ &\quad \frac{1}{h_i \alpha_{i+1}} I_1^{(i+1)} - \frac{\alpha_{i+1} + 1}{h_i \alpha_{i+1}} I_2^{(i+1)} + \frac{I_3^{(i+1)}}{h_i} \end{aligned} \tag{5}$$

where $\alpha_i := \left(x_{2i} - x_{2i-1}\right) / h_i$

In the above formulae index i ranges from 0 to n and the modifications are obvious for the index end values.

2.2 Modified density interpolation

In this method we modify the density function by subtracting and adding $f(t)$ inside the integral in (1):

$$⨎_a^b \frac{f(x) - f(t)}{(x-t)^2} dx + f(t) \quad ⨎_a^b \frac{dx}{(x-t)^2} =$$

$$\int_a^b \frac{F(x;t)}{(x-t)^2} dx + f(t) \quad ⨎_a^b \frac{dx}{(x-t)^2}$$

The second integral can be calculated analytically:

$$⨎_a^b \frac{dx}{(x-t)^2} = \frac{b-a}{(b-t)(a-t)}$$

So we just have to numerically approximate the first integral, which -provided that f possesses a Holder continuous first derivative- is at most weakly singular.

Proceeding the same way as in subsection 2.1, we find the following results:

$$I_1^{(i)} = \begin{cases} \overline{t}_i + \dfrac{1}{2} + \overline{t}_i^2 \ln\left|\dfrac{1-\overline{t}_i}{\overline{t}_i}\right|, & \overline{t}_i \neq 0,1 \\ 1/2, & \overline{t}_i = 0 \\ 3/2, & \overline{t}_i = 1 \end{cases}$$

$$I_2^{(i)} = \begin{cases} 1 + \overline{t}_i \ln\left|\dfrac{1-\overline{t}_i}{\overline{t}_i}\right|, & \overline{t}_i \neq 0,1 \\ 1, & \overline{t}_i = 0 \text{ or } 1 \end{cases} \tag{6}$$

$$I_3^{(i)} = \begin{cases} \ln\left|\dfrac{1-\overline{t}_i}{\overline{t}_i}\right|, & \overline{t}_i \neq 0,1 \\ 0, & \overline{t}_i = 0 \text{ or } 1 \end{cases}$$

$$\begin{aligned} w_{2i} &= \frac{1}{\alpha_i\left(\alpha_i - 1\right)}\left(I_1^{(i)} - I_2^{(i)}\right) \\ w_{2i+1} &= -\frac{1}{\left(\alpha_i - 1\right)} I_1^{(i)} + \frac{\alpha_i}{\left(\alpha_i - 1\right)} I_2^{(i)} + \\ &\quad \frac{1}{\alpha_{i+1}} I_1^{(i+1)} - \frac{\alpha_{i+1} + 1}{\alpha_{i+1}} I_2^{(i+1)} + I_3^{(i+1)} \end{aligned} \tag{7}$$

In case that the singularity t does not coincide with any integration node, the values of the modified density are calculated directly, but when t coincides with an integration node ($t = x_j$), then the modified density tends to the value of the original density derivative at the location of the singularity. In the latter case, we approximate the derivative with a central difference scheme as follows:

$$f'(t)\big|_{t=x_j} = \begin{cases} \dfrac{f(x_{2k+1}) - f(x_{2k-1})}{2h_k} + O(h_k^2), & j = 2k \\[2ex] \dfrac{f(x_{2k+2}) - f(x_{2k})}{2\delta} + O(\delta^2), & j = 2k+1 \end{cases}$$

where $\delta := \alpha_{k+1} h_{k+1} + (1-\alpha_k) h_k$

Thus, the final numerical integration formulae for this method become:

$$I_{2n+1}^{num} = \begin{cases} \sum_{j=1}^{2n+1} \overline{w}_j f(x_j) + \overline{w}_{2n+2} f(t), & t \neq x_j \ \forall j \\[2ex] \sum_{j=1}^{2n+1} \overline{w}_j f(x_j), & t = x_j \end{cases} \tag{8}$$

where the expressions for the barred weights are given by:

$\bullet\, t \neq x_j$

$$\overline{w}_j = \begin{cases} \dfrac{w_j}{x_j - t}, & j = 1 \div 2n+1 \\[2ex] \dfrac{(b-a)}{(b-t)(a-t)} - \sum_{j=1}^{2n+1} \dfrac{w_j}{x_j - t} & j = 2n+2 \end{cases}$$

$\bullet\bullet\, t = x_j,\ j = 2k,\ k = 1, 2, \ldots, n$

$$\overline{w}_j = \begin{cases} \dfrac{w_j}{x_j - x_{2k}}, & j \neq 2k-1,\ 2k,\ 2k+1 \\[2ex] -\dfrac{1}{h_k}\left(\dfrac{w_{2k}}{2} + \dfrac{w_{2k-1}}{\alpha_k}\right), & j = 2k-1 \\[2ex] \dfrac{(b-a)}{(b-t)(a-t)} - \sum_{j=1, j\neq 2k}^{2n+1} \dfrac{w_j}{x_j - x_{2k}} & j = 2k \\[2ex] \dfrac{1}{h_k}\left(\dfrac{w_{2k}}{2} + \dfrac{w_{2k+1}}{1-\alpha_k}\right), & j = 2k+1 \end{cases} \tag{9}$$

$\bullet\bullet\, t = x_j,\ j = 2k+1,\ k = 1, 2, \ldots, n-1$

$$\overline{w}_j = \begin{cases} \dfrac{w_j}{x_j - x_{2k+1}}, & j \neq 2k,\ 2k+1,\ 2k+2 \\[2ex] \left(-\dfrac{w_{2k}}{(1-\alpha_k) h_k} - \dfrac{w_{2k+1}}{2\left[\alpha_{k+1} h_{k+1} + (1-\alpha_k) h_k\right]}\right), & j = 2k \\[2ex] \dfrac{(b-a)}{(b-t)(a-t)} - \sum_{j=1, j\neq 2k+1}^{2n+1} \dfrac{w_j}{x_j - x_{2k+1}} & j = 2k+1 \\[2ex] \left(\dfrac{w_{2k+1}}{2\left[\alpha_{k+1} h_{k+1} + (1-\alpha_k) h_k\right]} + \dfrac{w_{2k+2}}{\alpha_{k+1} h_{k+1}}\right), & j = 2k+2 \end{cases} \tag{10}$$

3 Numerical examples

In this section we present the results of the methods presented in sections 2.1 and 2.2 using the following examples ($a \geq 0$, $b > 0$):

(EX-1) $$⨎_{-a}^{b} \frac{x^3}{(x-t)^2} dx = \frac{b^2 - a^2}{2} + 2(b+a)t - t^3\left(\frac{1}{b-t} + \frac{1}{t+a}\right) + 3t^2 \ln\frac{b-t}{t+a}$$

(EX-2) $$⨎_{-a}^{b} \frac{x^5}{(x-t)^2} dx = \frac{b^4 - a^4}{4} + \frac{2t(b^3 + a^3)}{3} + \frac{3(b^2 - a^2)t^2}{2} t + 4(b+a)t^3 - t^5\left(\frac{1}{b-t} + \frac{1}{t+a}\right) + 5t^4 \ln\frac{b-t}{t+a}$$

(EX-3) $$⨎_{-1}^{2} \frac{|x|^{5/2} + x + 1}{x^2} dx = -\frac{5}{6} + \frac{4\sqrt{2}}{3} + \ln(2)$$

(EX-4) $$⨎_{0}^{1} \frac{\left[x(1-x)\right]^{\frac{3}{2}}}{(x-t)^2} dx = \frac{\pi}{2}\left[\frac{3}{4} - 6x(1-x)\right]$$

The method presented in section 2.1 (direct density interpolation) has been first applied in its original form using a uniform mesh and secondly by modifying the mesh in such a way that t is always the mid-node of some segment. It is obvious that this modification makes the method perform better, especially when the number of nodes is small. In fact we have a super-convergence behavior in this case.

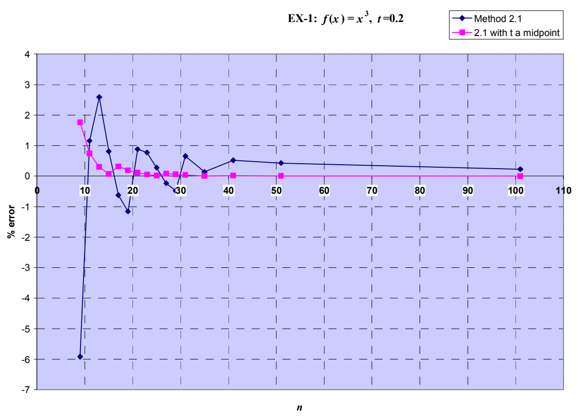

Fig.1: Performance of the method in 2.1 and its variant

For the first example, Fig. 1 shows the performance of the method presented in section 2.1 (in blue) and its modified version (purple), i.e. the one obtained by forcing t to be a mid-node of some segment. The modified version is remarkably better as its maximum error is below 2% (n = 9). The method presented in section 2.2 is not shown in Fig. 1, as it is exact for the specific case (as expected) and it would merely obscure the graph.

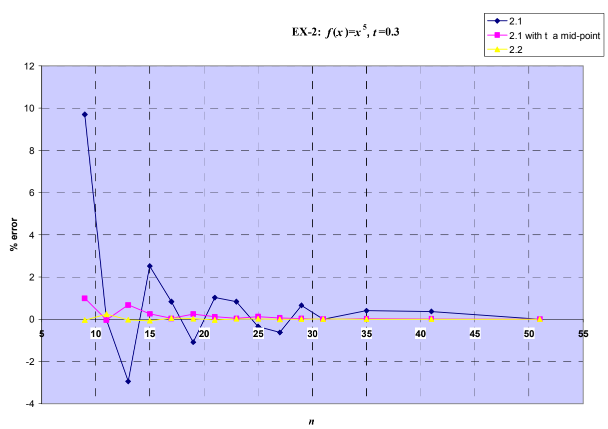

Fig. 2: All methods for EX-2, t=0.3

In Fig. 2 we present the results of all methods for EX-2. It is clear that the modified version of 2.1 behaves much better than its original counterpart. The method 2.2 has the best performance, as expected, since it is more accurate by construction (the modified density is a polynomial of 1 degree lower than the original density).

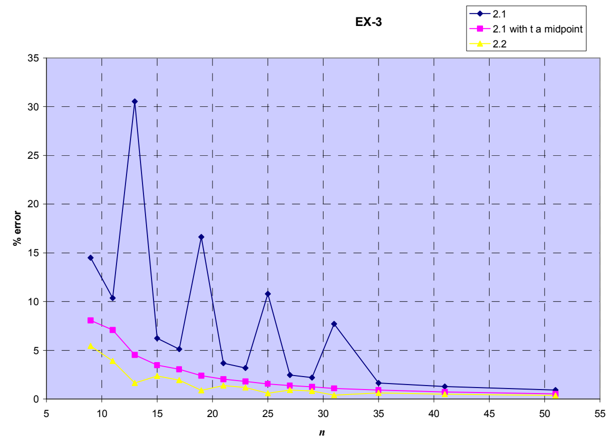

Fig. 3: All methods for EX-3

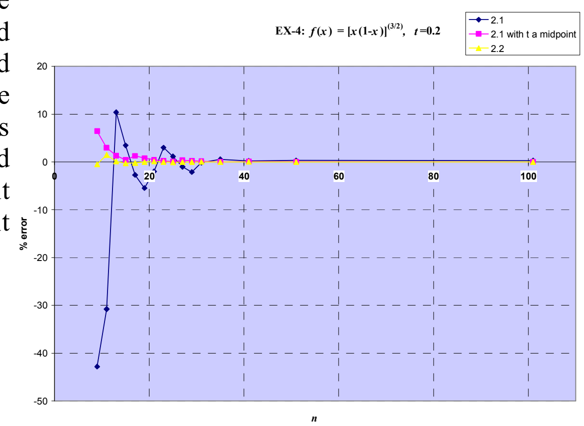

Fig. 4: All methods for EX-4, t = 0.5

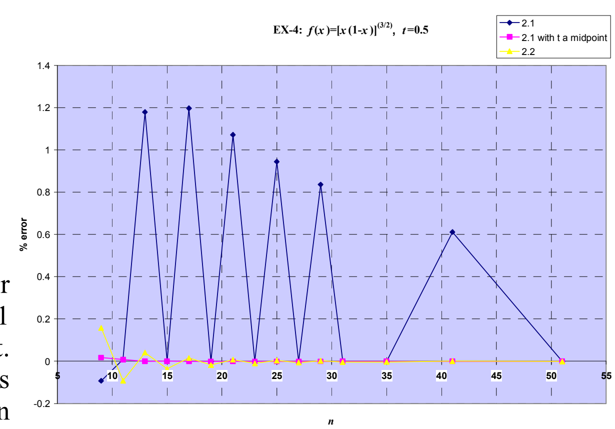

Fig. 5: All methods for EX-4, t = 0.2

For the example EX-3, the density belongs to the class $C^{5/2}\left[-1,2\right]$. Again modified 2.1 and 2.2 behave better. The absolute difference between the exact and the numerical values with n = 91 is 0.001. The same result is obtained in [2] using the double number of nodes (0.001 for n = 192).

Finally, in Figures 4 and 5 we present the results of all methods for EX-4, with two different choices for the location of the singularity. Again the modified version 2.1 and the method in 2.2 perform the best.

4 Conclusions

We have presented two Newton-Cotes type methods which are appropriate for the numerical evaluation of finite part integrals in one dimension with a double pole singularity. The methods are simple (no special polynomials required) and relatively straightforward and seem to behave satisfactorily in a number of cases. The methods are especially suitable for the solution of strongly singular integral equations.

Convergence and error analysis, as well as the application to the solution of the respective integral equations are under development.

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