Automatic differentiation for the evaluation of singular integrals in two-dimensional boundary element computations

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Abstract

In the evaluation of the logarithmic singular integrals which arise in two-dimensional boundary element computations a variety of approaches may be adopted. For linear elements the integrals may be performed analytically. For quadratic elements an approximate method is required and the most common technique is to use a special logarithmic numerical quadrature. A second approach uses a transformation in such a way that the Jacobian is zero at the singular point removing the singularity, conventional Gauss quadrature may then be used. A third possibility is to expand the Jacobian as a Taylor series up to the first or second order term. Then by subtracting out the singularity two integrals remain, one may be integrated analytically and the other by standard Gauss quadrature. We consider the problem of evaluating the Taylor series for the Jacobian as a sequence of numerical coefficient values, to an arbitrary order, without the explicit formation of symbolic formulae to represent them. The integral then becomes a finite sum of numerical coefficients multiplied by terms which may be integrated analytically. The accuracy of the value of the singular integral is determined by the degree of approximation in the Taylor series and does not depend on a numerical quadrature. This approach is ideally-suited to the process of automatic differentiation and we use fortran90 which supports the definition of suitable data types and operator overloading for the implementation of the technique.

Introduction

In the development of the system of equations which arise in the collocation approach to the boundary element method it is necessary to perform integrations over target elements where the integration is a function of \( R \), the distance from the base node to the target element. Very similar integrals occur in other approaches such as Galerkin, so we shall develop the ideas in terms of the collocation method. When the base node is not in the target element then the integrals occurring are either non-singular or quasi-singular, the latter occurring if \( R \) is small which may be the case in regions with high aspect ratio.
If the base node is in the target element then the integrals are singular. The singular integrals may have a removable singularity e.g. $O(R \ln R)$; a weak singularity e.g. $O(\ln R)$; a strong singularity e.g. $O(1/R)$; or a hyper-singularity e.g. $O(1/R^2)$.

The non-singular integrals are straightforward and are almost always evaluated using Gauss-Legendre quadrature. The quasi-singular integrals are usually evaluated using a higher order Gauss-Legendre formula paying particular attention to the distance of the nearest node outside the element. However, there are some schemes which are specifically designed to reduce the influence of a near-by singularity\(^1\).

The evaluation of the singular integrals has been the subject of much attention and an excellent account is given by Hall\(^3\) in which six approaches are described: The use of exact integrals is possible in only the simplest cases\(^4\) but they have been used from the earliest days of the method\(^5\). In a singularity subtraction approach a suitable term is added to and subtracted from the integrand in such a manner that on re-arrangement there are two terms to evaluate; one which has a removable singularity and may be evaluated using Gauss-Legendre quadrature, the other which may be integrated analytically. In some circumstances strongly-singular integrals may be avoided altogether by a row-sum technique applied to the system equation coefficient matrix\(^6\). A third approach is to use a transformation method so that the Jacobian has a zero at the singular point\(^7\). For some very special singular integrands there are specific quadrature rules which may be used directly e.g. integrands with a logarithmic singularity may be evaluated using a special logarithmic Gauss quadrature\(^8\). Finally, a sixth possibility is to use a Taylor series approximation\(^9\). In this approach the subtraction method is used to isolate the singularity, the ‘suitable’ term being a Taylor polynomial for the regular function in the integrand. The major problem is that, except for very simple situations, it is difficult, both in terms of accuracy and computation time, to calculate more than the first few polynomials.

Automatic differentiation (AD) provides an efficient process for finding Taylor polynomials\(^9\) without the explicit process of differentiating the functions involved. The problem may be considered as that of obtaining a sequence of numerical coefficients, to an arbitrary order, without the formation of symbolic formulae to represent them. The integral then becomes a finite sum of numerical coefficients multiplied by terms which may be integrated analytically. The accuracy of the value for the singular integral is determined by the degree of the Taylor polynomial and does not depend on a numerical quadrature. In the next section we consider an AD approach to the evaluation of the weakly-singular, $O(\ln R)$, integrals which occur in two-dimensional potential problems and which are of the form

\[
\int_{-1}^{1} f(\xi) \ln|\xi| d\xi \quad \text{and} \quad \int_{-1}^{1} f(\xi) \ln(1 \pm \xi) d\xi
\]
involving logarithmic singularities. For constant or linear elements these integrals are easily evaluated analytically. For subparametric elements with linear geometry and continuous or discontinuous quadratic potential variation it is also possible to evaluate the singular integrals exactly. For isoparametric quadratic or higher-order elements a numerical approximation method is required.

**Automatic differentiation for singular integrals**

We shall consider the quadratic element with nodes 1, 2 and 3 whose position vectors are

\[ \mathbf{r}_1 = (x_1, y_1), \quad \mathbf{r}_2 = (x_2, y_2), \quad \mathbf{r}_3 = (x_3, y_3) \]

with the local co-ordinate \( \{\xi:-1 < \xi < 1\} \) and Lagrange quadratic interpolation polynomials

\[
L_1(\xi) = \frac{1}{2} \xi (\xi - 1), \quad L_2(\xi) = 1 - \xi^2, \quad L_3(\xi) = \frac{1}{2} \xi (\xi + 1)
\]

The equation which defines the geometry of the element is given by

\[
\mathbf{r}(\xi) = \sum_{i=1}^{3} L_i(\xi) \mathbf{r}_i
\]

(1)

If \( \mathbf{R}_j(\xi) = \mathbf{r}(\xi) - \mathbf{r}_j \) is the position vector of a point, \( \mathbf{r}(\xi) \), in the element, relative to the base node, \( \mathbf{r}_j \), then we require the evaluation of the following nine singular integrals:

\[
I_{ij} = \int_{-1}^{1} L_i(\xi) J(\xi) \ln R_j(\xi) d\xi \quad i, j = 1, 2, 3
\]

(2)

where \( J(\xi) \) is the Jacobian of the transformation given by

\[
J(\xi) = [\mathbf{r}'(\xi), \mathbf{r}''(\xi)]^T
\]

Suppose that the singularity occurs when \( \xi = \xi_0 \) i.e. \( \mathbf{r}(\xi_0) = \mathbf{r}_j \) then

\[
R_j(\xi) = |\mathbf{r}(\xi) - \mathbf{r}_j| = |\mathbf{r}'(\xi_0) \Delta \xi + \frac{1}{2} \mathbf{r}''(\xi_0) \Delta \xi^2|^\frac{1}{2}
\]

\[
= |\Delta \xi \left( d_0 + \Delta \xi d_1 + \Delta \xi^2 d_2 \right)^\frac{1}{2}
\]

\[
= |\Delta \xi \left[ R_d(\xi) \right]^\frac{1}{2}
\]

where

\[
\Delta \xi = \xi - \xi_0
\]

and

\[
d_0 = \mathbf{r}'(\xi_0) \cdot \mathbf{r}''(\xi_0)
\]

\[
d_1 = \mathbf{r}'(\xi_0) \cdot \mathbf{r}''(\xi_0)
\]

\[
d_2 = \frac{1}{4} \mathbf{r}''(\xi_0) \cdot \mathbf{r}''(\xi_0)
\]

\[
R_d(\xi) = d_0 + \Delta \xi d_1 + \Delta \xi^2 d_2
\]
Also \[ J(\xi) = \left[r'(\xi), r''(\xi)\right]^\frac{1}{2} \]
\[ = \left[d_0 + 2d_1 \Delta \xi + 4d_2 \Delta \xi^2\right]^\frac{1}{2} \]

We develop all the terms in the integrand (2) as Taylor polynomials. This approach is similar to the direct factorisation technique described by Smith and Mason\(^a\).

The interpolation polynomials are easily written as third degree Taylor polynomials as follows:
\[ L_i(\xi) = L_i(\xi_0) + L_i'(\xi_0) \Delta \xi + \frac{1}{2} L_i''(\xi_0) \Delta \xi^2 \]
\[ = l_0 + l_1 \Delta \xi + l_2 \Delta \xi^2 \quad \text{say} \]

The Jacobian, \( J(\xi) \), and the term \( \ln R_d(\xi) \) may be expanded as an \( n^{th} \) degree polynomial
\[ J(\xi) \approx j_0 + j_1 \Delta \xi + j_2 \Delta \xi^2 + \ldots + j_n \Delta \xi^n \]
and
\[ \ln R_d(\xi) \approx b_0 + b_1 \Delta \xi + b_2 \Delta \xi^2 + \ldots + b_n \Delta \xi^n \]

Now we form the product of the two Taylor polynomials for \( L_i(\xi) \) and \( J(\xi) \) as
\[ L_i(\xi) J(\xi) = (l_0 + l_1 \Delta \xi + l_2 \Delta \xi^2)(j_0 + j_1 \Delta \xi + j_2 \Delta \xi^2 + \ldots + j_n \Delta \xi^n) \]
\[ \approx a_0^{(1)} + a_1^{(1)} \Delta \xi + \ldots + a_n^{(1)} \Delta \xi^n \] \hspace{1cm} (3)

where we truncate the product at the \( O(\Delta \xi^n) \) term.

Similarly we determine
\[ L_i(\xi) J(\xi) \ln[R_d(\xi)] = (l_0 + l_1 \Delta \xi + l_2 \Delta \xi^2)(j_0 + j_1 \Delta \xi + \ldots + j_n \Delta \xi^n) \times \]
\[ \frac{1}{2} (b_0 + b_1 \Delta \xi + \ldots + b_n \Delta \xi^n) \]
\[ \approx a_0^{(2)} + a_1^{(2)} \Delta \xi + \ldots + a_n^{(2)} \Delta \xi^n \] \hspace{1cm} (4)

The approximate value of the integral may now be obtained from
\[ I_{ij} = \int \sum_{-n}^{n} a_k^{(1)} |\Delta \xi|^n \ln|\Delta \xi| d\xi + \int \sum_{-n}^{n} a_k^{(2)} |\Delta \xi|^n d\xi \]
\[ = \sum_{k=0}^{n} \left( a_k^{(1)} \alpha_k + a_k^{(2)} \beta_k \right) \] \hspace{1cm} (5)

where
\[ \alpha_k = \int_{-1}^{1} |\Delta \xi|^n \ln|\Delta \xi| d\xi \]
\[ \beta_k = \int_{-1}^{1} |\Delta \xi|^n d\xi \]
There are three cases to consider:

(i) Singularity at \( r_1 \), i.e. \( \xi_0 = -1 \)

\[
\alpha_k = \frac{2^{k+1}}{k+1} \left( \ln 2 - \frac{1}{k+1} \right)
\]

\[
\beta_k = \frac{2^{k+1}}{k+1}
\]

(ii) Singularity at \( r_2 \), i.e. \( \xi_0 = 0 \)

\[
\alpha_k = \begin{cases} 
0 & \text{k odd} \\
-\frac{2}{(k+1)^2} & \text{k even}
\end{cases}
\]

\[
\beta_k = \begin{cases} 
0 & \text{k odd} \\
\frac{2}{k+1} & \text{k even}
\end{cases}
\]

(iii) Singularity at \( r_3 \), i.e. \( \xi_0 = +1 \)

\[
\alpha_k = \frac{(-2)^{k+1}}{k+1} \left( \ln 2 - \frac{1}{k+1} \right)
\]

\[
\beta_k = \frac{(-2)^{k+1}}{k+1}
\]

The Taylor polynomials used to obtain the expansions in equations (3) and (4) are a sequence of truncated Taylor series and the convergence of the sequence as \( n \) increases requires that \( |\Delta \xi| < \rho \) where \( \rho \) is the radius of convergence of the series. This condition implies a restriction on the placement of the position vectors \( r_1, r_2 \) and \( r_3 \) and before attempting to develop the Taylor polynomial we must ensure that \( r_2 \) is suitably placed. Clearly, we would like \( \rho \) to be as large as possible since the larger the value of \( \rho \) the more rapid is the rate of convergence. Crann et al.\(^{15}\) show that is sufficient that \( \left| r_2 - \frac{1}{2} (r_1 + r_3) \right| \) is small compared with \( \min \left\{ \frac{1}{2} |r_1 - r_2|, \frac{1}{2} |r_3 - r_2| \right\} \). We define the parameter \( \rho_{\text{test}} \), as an estimate of \( \rho \), by

\[
\rho_{\text{test}} = \min \left\{ \frac{1}{2} |r_1 - r_2|, \frac{1}{2} |r_3 - r_2| \right\}
\]

and use the value of \( \rho_{\text{test}} \) to determine whether or not convergence is satisfactory. From a practical point of view a value of \( \rho_{\text{test}} \) greater than about 3 is likely to be satisfactory and for any reasonable discretisation this will always be the case e.g. even a very crude discretisation of a quadrant of a circle of unit radius into two equal quadratic elements has \( \rho_{\text{test}} = 3.8 \).

**Numerical examples**

The examples in this section were developed using fortran90 with suitable data types for the Taylor polynomials and operator overloading to define operations on the polynomials\(^{15}\).
**Example 1**

This example is considered by Smith\(^6\), the element has nodal coordinates

\[ \mathbf{r}_1 = (0.1, 0.1), \quad \mathbf{r}_2 = (0.2, 0.2 + \alpha), \quad \mathbf{r}_3 = (0.3, 0.3) \]

with \( \alpha = 0, 0.02, 0.04, 0.1 \).

In Tables 1(a)-(d) we compare the results for the integral \( I_{ij} \) using Taylor polynomials of degree 6 and 20 with that obtained using a very accurate numerical approximation to the exact value obtained using the adaptive numerical quadrature procedure available in the symbolic computation package Maple\(^\text{TM} \). Also shown are the values calculated by Smith\(^6\) using Crow’s quadrature method\(^7\) and Gauss/log-Gauss 4 and 10 point quadratures.

<table>
<thead>
<tr>
<th>( x )-coordinate</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
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<td>0.1</td>
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<tr>
<td>Maple</td>
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<td>0.3952628</td>
<td>0.0516752</td>
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<td>Taylor - 20</td>
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<td>0.3952628</td>
<td>0.0516752</td>
</tr>
</tbody>
</table>

Table 1(a): Values of \( |I_{ij}| \) with \( \alpha = 0 \), \( \rho_{\text{test}} = \infty \)

<table>
<thead>
<tr>
<th>( x )-coordinate</th>
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<th>0.3</th>
</tr>
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<td>0.2182665</td>
<td>0.3868546</td>
<td>0.0378033</td>
</tr>
<tr>
<td>Taylor - 6</td>
<td>0.2176048</td>
<td>0.3884189</td>
<td>0.0368806</td>
</tr>
<tr>
<td>Taylor - 20</td>
<td>0.2182667</td>
<td>0.3868547</td>
<td>0.0378031</td>
</tr>
</tbody>
</table>

Table 1(b): Values of \( |I_{ii}| \) with \( \alpha = 0.02 \), \( \rho_{\text{test}} = 3.91 \)
The accuracy of the method decreases as $\rho_{\text{test}}$ decreases as expected, and the results indicate that $\rho_{\text{test}} > 2$ yields satisfactory values.

**Example 2**

Consider the curved element with nodes

\[
\mathbf{r}_1 = (1.0, 0.0), \quad \mathbf{r}_2 = (0.5 + \alpha \sqrt{2}, 0.5 + \alpha \sqrt{2}), \quad \mathbf{r}_3 = (0.0, 1.0)
\]

Crann *et al.*\(^{15}\) provide details of the results for the following nine values:

\[
\alpha = 0.0, \ 0.001, \ 0.01, \ 0.05, \ 0.08, \ 0.1, \ 0.2, \ 0.5, \ 1.0
\]

using Taylor polynomials of degree 6 and 20 and compare the results with those obtained using the adaptive numerical quadrature procedure in *Maple™*. 

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<table>
<thead>
<tr>
<th>$x$ – coordinate</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
</tr>
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<tbody>
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<td>$y$ – coordinate</td>
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<td>0.3</td>
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<tr>
<td><em>Maple</em></td>
<td>0.2438544</td>
<td>0.3806926</td>
<td>0.0270271</td>
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<td>Smith</td>
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<td>Taylor - 6</td>
<td>0.2406218</td>
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<td>0.2438514</td>
<td>0.3807016</td>
<td>0.0270217</td>
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Table 1(c): Values of $|I_{ij}|$ with $\alpha = 0.04$, $\rho_{\text{test}} = 2.15$

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<th>$x$ – coordinate</th>
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<th>0.2</th>
<th>0.3</th>
</tr>
</thead>
<tbody>
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<td>$y$ – coordinate</td>
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<td>0.3</td>
<td>0.3</td>
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<td>Smith</td>
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<tr>
<td>Taylor - 6</td>
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<tr>
<td>Taylor - 20</td>
<td>0.3287444</td>
<td>0.3169090</td>
<td>0.0330741</td>
</tr>
</tbody>
</table>

Table 1(d): Values of $|I_{ij}|$ with $\alpha = 0.1$, $\rho_{\text{test}} = 1.12$
In Table 2 we show the root mean square errors
\[
\left( \frac{1}{9} \sum_{i,j=1}^{3} (\hat{I}_{ij} - I_{ij})^2 \right)^{\frac{1}{2}}
\]
where \(\hat{I}_{ij}\) is the approximate value of \(I_{ij}\) for values of \(\rho_{test} > 1\).

<table>
<thead>
<tr>
<th>(\rho_{test})</th>
<th>Taylor – 6</th>
<th>Taylor – 20</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\infty)</td>
<td>0</td>
<td>0</td>
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<tr>
<td>176</td>
<td>1.2E – 7</td>
<td>1.2E – 7</td>
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<tr>
<td>17.7</td>
<td>1.5E – 6</td>
<td>1.3E – 7</td>
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<td>3.57</td>
<td>1.6E – 4</td>
<td>7.2E – 8</td>
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<td>2.27</td>
<td>5.2E – 3</td>
<td>1.1E – 5</td>
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<td>1.84</td>
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<tr>
<td>1.02</td>
<td>4.3E – 2</td>
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</table>

Table 2: RMS errors for various values of \(\rho_{test}\)

We notice that when \(\rho_{test} < 2\) the errors are too large. When \(\rho_{test} \approx 3.6\)
the 6\(^{th}\) degree Taylor polynomial is unsatisfactory but the 20\(^{th}\) degree Taylor
polynomial is suitable. For \(\rho_{test} \geq 17.7\) both series yield satisfactory results.

**Conclusions**

The Taylor polynomial method in a fortran90 environment provides a suitable
approach for evaluating quadratic boundary element singular integrals which
occur in potential problems. We have seen that in terms of accuracy it
compares well with alternative methods. However, the attraction of the
method lies in the fact that the Taylor coefficients are obtained without a direct
evaluation of derivatives. Indeed, the approach offers a possibility for
evaluating the significantly more difficult singular integrals which occur in
more complicated situations.
References


