

Methods for computing singular and nearly singular integrals*

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Abstract. Many scientific problems are formulated in terms of singular integrals. We describe a simple method for computing such integrals. Our approach is to replace a singularity, or near singularity, with a regularized version, compute a sum in a standard way, and then add correction terms, which are found by asymptotic analysis near the singularity. We have used this approach for a single-layer potential on a doubly periodic surface, evaluated at a grid point on the surface. The quadrature rule so developed was used to design a convergent boundary integral method for three-dimensional water waves. In related work we have developed a method for computing a double-layer potential on a curve, evaluated at a point near the curve. Thus values of harmonic functions, with prescribed boundary conditions on a curve, can be calculated at grid points inside or outside, with only slightly extra effort for those points near the boundary. This procedure may be useful for computing fluid flow with moving boundaries.

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We describe a simple and efficient approach to computing singular and nearly singular integrals. We emphasize two cases. The first is a single-layer potential on a surface in 3D, evaluated at a grid point in a coordinate system on the surface. This approach has been used to design a convergent boundary integral method for time-dependent, three-dimensional water waves [1]. The second case is a layer potential on a curve in the plane, evaluated at a point near the curve but not on it. When a problem is solved in the boundary integral or boundary element formulation, it is a separate task to find required field quantities away from the boundary. For points near the boundary, the integrals are nearly singular, that is, the integrands have large derivatives. The need for methods to compute such integrals has often been noted. In the work [2] with Ming-Chi Lai we developed a method using the approach described here. As an application, we compute harmonic functions with conditions prescribed on a general smooth

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boundary; an integral formulation can be used to compute values at points which are near the boundary. This method could be applied to computations of fluid flow with moving boundaries. For example, the pressure change due to a force on a boundary can be written in terms of single- and double-layer potentials.

Our strategy is to replace the singularity, or near singularity, with a regularized version, compute a trapezoidal sum, which may be inaccurate, and then add correction terms. The regularization corresponds to the ‘blobs’ in vortex methods, which are used to regularize the singular integral giving the velocity from the vorticity. The correction terms are found by asymptotic analysis near the singularity. They account for the discretization error as well as the error introduced by smoothing. Because the corrections are local, the full computation could be done efficiently using a fast summation method.

For a smooth function, integrated without boundaries, the trapezoidal rule on a regular grid is high-order accurate. For integrands with singularities such as those in the fundamental solution of the Laplacian, the situation is very different. The error is not high order, but there is a regular expansion which can be exploited. To illustrate this, we compare

$$I = \int_{R^2} \frac{f(x)}{|x|} dx, \quad S = \sum_{j \neq 0} \frac{f(jh)}{|jh|} h^2 \tag{1}$$

where f is smooth and rapidly decreasing, $j = (j_1, j_2)$ is a pair of integers, and h is the grid size. (We can think of this as a special case of a single-layer potential on a flat surface.) In this case the error is $O(h)$. However, we know the form of the error more precisely:

$$I = S + c_0 f(0)h + O(h^3) \tag{2}$$

where c_0 is a particular constant, $c_0 \approx 3.900\,265$. Thus we can correct the sum so that the error is $O(h^3)$, a great improvement. Such constants are hard to find; their identity is connected with number theory [3]. In applications, we will have similar integrals but with different constants. For a single-layer potential on a surface, we might discretize with a regular grid in local coordinates $\alpha = (\alpha_1, \alpha_2)$. In that case the singularity $1/|x|$ will be replaced by $1/\sqrt{q(\alpha)}$ with $q(\alpha) = g_{11}\alpha_1^2 + 2g_{12}\alpha_1\alpha_2 + g_{22}\alpha_2^2$, and the constant c_0 will depend on the g_{ij} , which vary with the point of evaluation. Special cases can be useful: Lowengrub *et al* [4] designed a good method for 2D inviscid flow in the vorticity formulation by making a linear coordinate transformation to allow for shear. They found the appropriate constants for that case.

The example above illustrates an important general principle [5, 6] for the error in a quadrature rule applied to a homogeneous singularity: let $K(x)$ be homogeneous on R^d of degree m (i.e., $K(ax) = a^m K(x)$ for $a > 0$), and let $f(x)$ be smooth and rapidly decreasing. Then,

$$\sum_{n \neq 0} K(nh) f(nh) h^d - \int_{R^d} K(x) f(x) dx = h^{d+m} (c_0 f(0) + C_1 h + C_2 h^2 + \dots).$$

Here c_0 depends only on K , but C_1, C_2, \dots depend on f as well. For example, a $1/r$ singularity in the plane leads to an $O(h)$ error, as above. To make this principle more useful, we have extended it to regularized singularities and to the nearly singular case [1, 2]. We replace the kernel $K(x)$ with a regularized version $K_h(x) = K(x)s(x/h)$ where $s(x) \rightarrow 1$ rapidly as $x \rightarrow \infty$ and s is chosen so that K_h is smooth for all x . Because K is homogeneous, we have $K_h(x) = h^m K_1(x/h)$. In this case the same principle holds, but with different constants. This is surprising, since the smoothing factor is rapidly varying, but it is possible because of the homogeneity. The dependence on x/h can be thought of as a quadrature rule. In the regularized case, the constant c_0 can be identified using the Poisson summation formula; it is an infinite sum of values of \hat{K}_1 . If we choose the smoothing wisely, the terms are rapidly decreasing, and only a few are needed.

In [1] we want to compute a single-layer potential on a doubly periodic surface. The kernel is the Green function $G(x) = -1/4\pi|x|$. We replace it with the regularized version

$$G_h(x) = -(4\pi|x|)^{-1}(\text{erf}(\rho) + 2\pi^{-1/2}\rho \exp(-\rho^2)), \quad \rho = |x|/h$$

where erf is the error function. The first term removes the singularity; the second term is added to reduce the smoothing error to $O(h^3)$ by setting a certain moment to zero. (For simplicity here we have set the smoothing parameter to h .) We use local coordinates $\alpha = (\alpha_1, \alpha_2)$. The trapezoidal sum over a regular grid has error $O(h)$, but we find that it can be improved to $O(h^3)$ in the manner described. Assume that the singularity is at $x = 0$, corresponding to $\alpha = 0$; there are extra error terms because of the coordinate mapping, but the important contribution comes from making the approximation $G(x(\alpha)) \approx G(J\alpha)$, where $J = \partial x/\partial\alpha$ at $\alpha = 0$. Consequently, we find

$$\int_{\mathbb{R}^2} G_h(x(\alpha))f(\alpha) \, d\alpha = \sum G_h(x(jh))f(jh)h^2 - c_0f(0)h + O(h^3) \tag{3}$$

with

$$c_0 = 2\pi \sum_{n \neq 0} (G_1 \circ J)^{\wedge}(2\pi n) = 2\pi(\det g^{ij})^{1/2} \sum_{n \neq 0} \Gamma(2\pi\sqrt{g^{ij}n_in_j}),$$

$$\Gamma(k) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \hat{G}_1(k, 0, \ell) \, d\ell.$$

Here $g_{ij} = (\partial x_i/\partial\alpha)(\partial x_j/\partial\alpha)$ and g^{ij} is the inverse matrix. With G_h as chosen, Γ can be found explicitly, so the constant can be computed as a sum with a Gaussian rate of decay. The formula, resulting from local analysis, depends on the geometry of the surface near the singularity. The resulting quadrature rule has a sign condition, as an operator on discrete functions, analogous to that of the exact single-layer potential. This property is important for the numerical stability of the method in [1]; it helps to maintain wavelike behaviour in the error, i.e., oscillations in time rather than rapidly growing exponentials. Using this technique we designed a version of the boundary integral method for time-dependent, doubly periodic, 3D water waves, and proved that the method converges [1]. Another approach has been developed by Hou and Zhang [7].

To describe the technique in [2] for nearly singular integrals, we consider a double-layer potential on a smooth closed curve in the plane. Suppose the curve is parametrized as $x(\alpha)$ and we wish to compute the potential at a point y . If y is on the curve, the integrand is smooth, and the integration is routine. However, if y is off the curve but nearby, the singularity in ∇G reappears. We can subtract as usual, to reduce the near singularity, and then compute

$$\int_0^L N(\alpha) \nabla G(x(\alpha) - y)[f(\alpha) - f(\alpha_0)] \, d\alpha$$

where y is along the normal line at $x(\alpha_0)$. The integrand is bounded but not smooth; it has a factor like $\alpha b/(\alpha^2 + b^2)$, where $b = |y - x(\alpha_0)|$. The trapezoidal sum for this integral, with points equally spaced in α , is only $O(h)$ accurate, uniformly with respect to y . This fact can be understood from the principle above, since the singular factor is of degree zero in α and b together. However, the sum can be corrected by a simple formula to $O(h^2)$, even without smoothing. We believe, nonetheless, that smoothing is still desirable, because the smoothing errors are more predictable than the quadrature errors. In [2] we use $\nabla G_\delta = (1 - \exp(r^2/\delta^2)) \nabla G$ with smoothing radius $\delta = O(h)$. Local analysis is used to identify the largest errors due to smoothing and discretization. For the trapezoidal sum with this regularized kernel, the smoothing error is $O(\delta^2)$ and the discretization error is $O(h)$. In this nearly singular case, it seems that the smoothing error cannot be corrected by imposing moment conditions on the smoothing factor, as for free space. Nonetheless, the principal contribution to the smoothing error can be found analytically. The discretization error can again be found using the Poisson

summation formula. After these corrections, the smoothing error is reduced to $O(\delta^3)$ and the discretization error is $O(h^2)$; see [2] for the formulae. These estimates are uniform for points near the curve. In our test problems the errors are fairly insensitive to the choice of δ/h ; the corrections for smoothing and discretization complement each other. In practice we find that the smoothing error dominates if δ is not very small. For example, for a double-layer potential on the unit circle with $f(\alpha) = 2\sin 3\alpha$, with $\delta = 2h$, we find that the relative error at a typical angle, at distance about $h/3$ from the circle is about $0.7h^3$. Examples with ellipses (for which exact solutions can be found) are similar to those for the circle.

The method for computing singular integrals leads to a natural method for solving boundary value problems for harmonic functions. Suppose that we have a region in the plane whose boundary is a smooth, closed curve, and we wish to find a harmonic function with prescribed boundary values at points on a rectangular grid inside or outside; the grid need not be fitted to the boundary. We can write the problem in classical form as an integral equation of the second kind for the strength μ of a double-layer potential on the boundary. It is not hard to solve the integral equation, since the kernel is smooth. Once we know μ , the harmonic function is represented as a known double-layer potential which can be calculated at any point in the manner described. In practice it is useful to proceed as in Mayo [8] (also cf [9]): compute values carefully near the boundary; form a discrete Laplacian near the boundary, and extend it to be zero away; then use a fast Poisson solver to find values at all grid points. Test problems were done in this way in [2]. Convergence better than $O(h^2)$ was found with the nine-point Laplacian. Because of the simplicity and efficiency of this approach, it might be useful for computational methods of fluid flow with moving boundaries. In that situation the present approach can be accurate even with the limited information on the boundary.

The method for nearly singular integrals developed in [2] has been used by Cortez [10] in computing Stokes flow due to concentrated forces. A related correction of a singular integral was derived by Nitsche [11] for axisymmetric vortex sheets near the axis of symmetry.

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