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Two methods for discretizing a delta function supported on a level set

John D. Towers *

MiraCosta College, 3333 Manchester Avenue, Cardiff-by-the-Sea, CA 92007-1516, USA

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Abstract

This paper presents two new methods for discretizing a Dirac delta function which is concentrated on the zero level set of a smooth function u: $\mathbf{R}^n \mapsto \mathbf{R}$. The function u is only known at the discrete set of points belonging to a regular mesh covering $\mathbf{R}^n$. These two methods are used to approximate integrals over the manifold defined by the level set. Both methods are conceptually simple and easy to implement. We present the results of numerical experiments indicating that as the mesh size h goes to zero, the rate of convergence is at least $O(h)$ for the first method, and $O(h^2)$ for the second method. We perform a limited analysis of the proposed algorithms, including a proof of convergence for both methods.

Keywords: Delta function; Level set method; Discretization; Convergence

1. Introduction

In this paper, we consider the problem of approximating an integral of the form

$$\mathscr{I} := \int_\Gamma f(\vec{x})\,\mathrm{d}s, \tag{1}$$

where $\vec{x} = (x^1, \ldots, x^n) \in \mathbf{R}^n$, f: $\mathbf{R}^n \mapsto \mathbf{R}$, and Γ is a manifold of codimension one defined by the zero level set of a function u: $\mathbf{R}^n \mapsto \mathbf{R}$. When the function u is only defined at the discrete set of mesh points of a regular grid, it is impractical to define the manifold parametrically. In this situation, it is common practice [3] to replace the integral above by an integral of the form

$$\int_{\mathbf{R}^n} f(\vec{x})\delta(u(\vec{x}))\|\nabla u(\vec{x})\|\,\mathrm{d}\vec{x}, \tag{2}$$

where $\delta(\cdot)$ denotes the Dirac delta function. (See [12] for a proof that the two integrals are equal.) One then approximates the integral (2) using the available grid-defined quantities. Clearly this requires some sort

* Tel.: +1 760 944 4449x7739.
E-mail address: john.towers@cox.net.
URL: http://www.miracosta.edu/home/jtowers/.

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of discretization of the quantity $\delta(u(\vec{x}))$. This paper proposes two new methods for accomplishing this discretization.

The problem described in the previous paragraph arises naturally in the level set method, which is a very effective technique for computing the evolution of interfaces, originally devised by Osher and Sethian [4]. In a level set application, the interface would be the manifold Γ of the previous paragraph, defined implicitly as the zero level set of the function u. Defining Γ implicitly in this way has the important advantage that it is unnecessary to track the interface as a distinct entity. The level set function u is evolved with time in accordance with the geometry or physics of the application, generally by numerically solving a partial differential equation on a regular mesh. In the process, the zero level set Γ (the interface) is automatically evolved in the desired manner. This approach easily captures topology changes that would be difficult to handle by attempting to track the interface in isolation. The problem of volume-preserving mean curvature motion provides a simple example of how integrals of the form (1) are encountered in this setting [5]. For this flow, the level function u evolves according to

$$\partial u/\partial t = (\kappa - \bar{\kappa})\|\nabla u\|, \tag{3}$$

where $\kappa = \nabla \cdot (\nabla u/\|\nabla u\|)$ is the mean curvature and $\bar{\kappa}$ is the average mean curvature, defined by

$$\bar{\kappa} = \int_\Gamma \kappa \, \mathrm{d}s \Big/ \int_\Gamma \mathrm{d}s. \tag{4}$$

Let $\{\vec{x}_{\mathbf{k}} = (x^1_{k_1}, \ldots x^n_{k_n}) : \mathbf{k} := (k_1, \ldots, k_n) \in \mathbf{Z}^n\}$ denote the set of mesh points of the regular grid. For simplicity of notation, we assume that the mesh spacing h is the same in all directions, $x^i_{k_i} = k_i h$, $k_i \in \mathbf{Z}$. If $v_{\mathbf{k}} = v(\vec{x}_{\mathbf{k}})$ is a function defined at each meshpoint $\vec{x}_{\mathbf{k}}$, we define the discrete gradient operator ∇^h via

$$\nabla^h v_{\mathbf{k}} = \sum_{m=1}^{n} \left(\frac{v(\vec{x}_{\mathbf{k}} + h\vec{e}_m) - v(\vec{x}_{\mathbf{k}} - h\vec{e}_m)}{2h} \right) \vec{e}_m, \tag{5}$$

where $\{\vec{e}_1, \ldots, \vec{e}_n\}$ is the standard basis for $\mathbf{R}^n$. Similarly, we define the discrete Laplacian Δ^h by

$$\Delta^h v_{\mathbf{k}} = \sum_{m=1}^{n} \frac{v(\vec{x}_{\mathbf{k}} + h\vec{e}_m) - 2v(\vec{x}_{\mathbf{k}}) + v(\vec{x}_{\mathbf{k}} - h\vec{e}_m)}{h^2}. \tag{6}$$

We approximate the integral $\mathscr{I}$ appearing in (1) using

$$\mathscr{I}^h := h^n \sum_{\mathbf{k} \in \mathscr{S}} f(\vec{x}_{\mathbf{k}}) \delta^h(\vec{x}_{\mathbf{k}}; u) \|\nabla^h u_{\mathbf{k}}\|, \tag{7}$$

where $\delta^h(\vec{x}_{\mathbf{k}}; u)$ is a discretized version of the delta function $\delta(u(\vec{x}_{\mathbf{k}}))$, and $\mathscr{S}$ is a subset of $\mathbf{Z}^n$ containing those indices $\mathbf{k}$ where $f(\vec{x}_{\mathbf{k}})\delta^h(\vec{x}_{\mathbf{k}}; u) \neq 0$. We propose two methods for computing $\delta^h(\vec{x}_{\mathbf{k}}; u)$.

To explain the first method, we start from the formal relationship

$$\nabla H(u(\vec{x})) = H'(u(\vec{x}))\nabla u(\vec{x}). \tag{8}$$

Here H denotes the Heaviside function,

$$H(z) = \begin{cases} 0, & z < 0, \\ 1, & z > 0. \end{cases} \tag{9}$$

Taking the inner product in (8) with $\nabla u(\vec{x})$ gives

$$\nabla H(u(\vec{x})) \cdot \nabla u(\vec{x}) = H'(u(\vec{x}))\|\nabla u(\vec{x})\|^2. \tag{10}$$

Solving for $H'(u(\vec{x}))$, and recalling that $H'(\cdot) = \delta(\cdot)$ yields the following formula:

$$\delta(u(\vec{x})) = \frac{\nabla H(u(\vec{x})) \cdot \nabla u(\vec{x})}{\|\nabla u(\vec{x})\|^2}. \tag{11}$$

We then discretize (11) to obtain

Method 1

$$\delta_1^h(\vec{x}_{\mathbf{k}};u) := \frac{\nabla^h H^h(u_{\mathbf{k}})\cdot\nabla^h u_{\mathbf{k}}}{\left\|\nabla^h u_{\mathbf{k}}\right\|^2}. \tag{12}$$

Here $u_{\mathbf{k}} = u_{k_1,\ldots,k_n} = u(x^1_{k_1},\ldots,x^n_{k_n})$, and H^h is a possibly regularized version of the Heaviside function, with the smoothing parameter (appearing as a superscript) dependent upon the mesh size h. Our basic assumption concerning H^h is

Assumption 1. $H^h(z)$ is bounded uniformly for $h \geqslant 0$, and for some $\alpha \geqslant 0$,

$$H^h(z) = H(z) \quad \text{for } |z| > \alpha h. \tag{13}$$

Method 1 is generally first order accurate, whether we use H itself or a regularized version H^h. However, with a certain amount of regularization, this method sometimes performs very well – it appears to converge like $O(h^2)$ on some of the numerical examples appearing in Section 5.

With the same type of approach used to derive (11), it is possible to derive yet another formal representation of $\delta(u)$. This time, we start with $I(z) = \int_0^z H(\zeta)\,d\zeta$, and the relationship

$$\nabla I(u) = H(u)\nabla u. \tag{14}$$

We are suppressing for now the dependence on the spatial variable $\vec{x}$. Next we apply the operator $\nabla\cdot$ to both sides of this relationship, which yields

$$\Delta I(u) = H(u)\Delta u + \delta(u)\|\nabla u\|^2. \tag{15}$$

Solving for $\delta(u)$ in (15) gives our second formal relationship for a delta function

$$\delta(u) = \frac{\Delta I(u) - H(u)\Delta u}{\|\nabla u\|^2}, \quad H(u) = \frac{\nabla I(u)\cdot\nabla u}{\|\nabla u\|^2}. \tag{16}$$

To get the second of these relationships, we have solved (14) for $H(u)$ in the same way that we solved (8) for $\delta(u)$.

Combining both equations in (16), and then discretizing yields

Method 2

$$\delta_2^h(\vec{x}_{\mathbf{k}},u) := \frac{\Delta^h I(u_{\mathbf{k}})}{\left\|\nabla^h u_{\mathbf{k}}\right\|^2} - \frac{(\nabla^h I(u_{\mathbf{k}})\cdot\nabla^h u_{\mathbf{k}})\Delta^h u_{\mathbf{k}}}{\left\|\nabla^h u_{\mathbf{k}}\right\|^4}. \tag{17}$$

In contrast to Method 1, where we use a smoothed Heaviside function H^h to improve accuracy, we are not proposing any parameter dependent regularization for the function I used in Method 2. In certain simplified cases analyzed in Sections 3 and 4, we are able to prove that using Method 2, $\mathscr{I}^h \to \mathscr{I}$ at a rate of $O(h^2)$. Our numerical experiments seem to indicate that if u and f are sufficiently smooth, this second order rate of convergence holds in general.

One technical detail that deserves comment at this point is that the formulas (12) and (17) are undefined if $\|\nabla^h u(\vec{x}_{\mathbf{k}})\| = 0$. We will always assume that $\|\nabla u(\vec{x})\|$ is bounded away from zero for $\vec{x}$ near Γ. It follows that both $\delta_1^h(\vec{x}_{\mathbf{k}},u)$ and $\delta_2^h(\vec{x}_{\mathbf{k}},u)$ are zero if $\vec{x}_{\mathbf{k}}$ is more than an $O(h)$ distance from Γ, and so the vanishing denominators are harmless. To be more precise, we can simply define $\delta_i^h(\vec{x}_{\mathbf{k}},u) = 0$ if $\|\nabla^h u(\vec{x}_{\mathbf{k}})\| = 0$. This logic is consistent with our computer implementations, which include a check like this to avoid division by zero.

As mentioned above, although Method 1 converges to the correct solution if we simply use the Heaviside function H without any smoothing, we find that better results are obtained with a certain amount of regularization. In a number of the numerical examples appearing in Section 5 we use $H^h = H^{C,\epsilon}$, where

$$H^{C,\epsilon}(z) = \begin{cases} 0, & z < \epsilon, \\ \frac{1}{2} + \frac{z}{2\epsilon} + \frac{1}{2\pi}\sin\left(\frac{\pi z}{\epsilon}\right), & -\epsilon \leqslant z \leqslant \epsilon, \\ 1, & \epsilon < z. \end{cases} \tag{18}$$

and $\epsilon = 1.5h$. The C appearing in the superscript refers to the fact that $H^{C,\epsilon}(z)$ is the approximate Heaviside function associated with the cosine approximation to the delta function:

$$\delta^{C,\epsilon}(z) = \begin{cases} \frac{1}{2\epsilon}\left(1 + \cos\left(\frac{\pi z}{\epsilon}\right)\right), & |z| < \epsilon, \\ 0, & |z| \geqslant \epsilon. \end{cases} \tag{19}$$

We also use the approximate Heaviside function $H^h = H^{L,\epsilon}$ defined by

$$H^{L,\epsilon}(z) = \begin{cases} 0, & z \leqslant \epsilon, \\ \frac{1}{2} + \frac{1}{\epsilon}\left(z - \frac{\text{sign}(z)z^2}{2\epsilon}\right), & |z| < \epsilon, \\ 1, & z \geqslant \epsilon, \end{cases} \tag{20}$$

and $\epsilon = 1.0h$. The approximate Heaviside function $H^{L,\epsilon}$ is associated with the linear hat approximate delta function:

$$\delta^{L,\epsilon}(z) = \begin{cases} \frac{1}{\epsilon}\left(1 - \left|\frac{z}{\epsilon}\right|\right), & |z| < \epsilon, \\ 0, & |z| \geqslant \epsilon. \end{cases} \tag{21}$$

A possible concern is the so-called bandwidth (the number of meshpoints surrounding the level set where we require that u be defined) of our proposed algorithms. Assume for the present discussion that the level set function u is a signed distance function. This means that $u(\vec{x})$ represents the distance from the point $\vec{x}$ to the closest point on the manifold Γ, modulo a plus or minus sign, which can be used to determine which side (i.e., inside or outside) of the manifold Γ the point $\vec{x}$ is on. There are a number of advantages to having u be a signed distance function [3]. Moreover, in many implementations of the level set method, the functions f and u are only defined at a small number of meshpoints surrounding the level set $u = 0$ [3,7]. In order to be of practical value, our algorithm should not require that u be defined for points very far from Γ. In fact, for Method 1, if Assumption 1 holds, a bandwidth of $\lceil 2\alpha \rceil + 2$ meshpoints is required. In our numerical examples, we use either $\alpha = 1.5$ (when using $H^{C,\epsilon}$) implying a bandwidth of five meshpoints, or $\alpha = 1.0$ (when using $H^{L,\epsilon}$), implying a bandwidth of four meshpoints. By way of comparison, if one were to use a smoothed delta function with support of $[-1.5h, 1.5h]$ in a pointwise manner, a bandwidth of only three meshpoints would be required. In the case where u is not a distance function, it is not possible to give a precise description of the bandwidth for Method 1 without specifying more about u and its partial derivatives. For Method 2, the bandwidth is four mesh points, whether or not u is a signed distance function.

The methods presented in this paper do not require that u be a distance function. Our numerical experiments indicate that the approximations converge like $O(h)$ or better for Method 1, and $O(h^2)$ for Method 2, whether or not u is a distance function, but that using a distance function usually (but not always – see Example 3 of Section 5) leads to smaller errors. Engquist, Tornberg, and Tsai [2] also observed better performance for their algorithms when u is a distance function.

An alternative to the methods proposed in this paper is to simply use an approximate delta function such as $\delta^{L,\epsilon}$ or $\delta^{C,\epsilon}$ in a pointwise manner, and this seems to be common practice [1–3,6]. Usually the value of the smoothing parameter ϵ is set to h or $1.5h$ or $2h$. Tornberg and Engquist [11] showed that for $\delta^{C,\epsilon}$ in one dimension, this approach leads to a consistent approximation (meaning that the approximation converges to the true solution as $h \to 0$) for integrals like (1), but only if ϵ is one of a set of discrete values. This is not a serious restriction in one dimension. However, they also demonstrated the much more serious problem that in more than one dimension, both $\delta^{L,\epsilon}$ and $\delta^{C,\epsilon}$ generally yield inconsistent approximations. In [10], Tornberg and Engquist studied this problem further, including numerical experiments demonstrating clearly the lack of consistency mentioned above. In [2], Engquist, Tornberg, and Tsai proposed two methods for overcoming this lack of consistency. Their first method is based on an approximate product formula for multidimensional delta functions, along with the linear hat approximate delta function $\delta^{L,\epsilon}$. They proved that this method is at least first order accurate for integrals like (1), and numerical experiments indicate that it is actually second order accurate. Their second method, which is first order accurate, is also based on the linear hat delta function. It allows the smoothing parameter ϵ to vary spatially depending on the local behavior of the level function u, and is simpler than their algorithm based on the approximate product rule.

The subject of this paper has also been studied by Smereka [8], who proposed both a first and second order method for two- and three-dimensional problems. This approach is derived from a technique for solving elliptic problems with discontinuous coefficients. It has the advantage that the support of the resulting approximate delta function is at most that of a single mesh width.

The rest of the paper is organized as follows. In Section 2, we prove that if u and f satisfy certain regularity conditions, both Methods 1 and 2 converge to the integral $\mathscr{I}$ as $h \to 0$. The results in Section 2 do not provide any information about rates of convergence. In Section 3, we carry out an analysis of the one-dimensional versions of the algorithms, this time obtaining rates of convergence. In Section 4, we show that for the greatly simplified case where u is linear and f has compact support, our one-dimensional rate of convergence results from Section 3 carry over to the two-dimensional setting. In Section 5 we present the results of some numerical experiments, borrowing heavily from the examples in Engquist, Tornberg, and Tsai [2], and also from Smereka [8].

2. Convergence in several dimensions

As mentioned previously, for the case of several dimensions, approximations to the integral $\mathscr{I}$ based on seemingly reasonable pointwise approximations to a delta function may not converge to $\mathscr{I}$ as $h \to 0$.

In this section, we prove that using either Method 1 or Method 2 to approximate $\delta(u(\vec{x}))$, the approximation $\mathscr{I}^h$ converges to the integral $\mathscr{I}$ as $h \to 0$. We do not attempt to prove a rate of convergence in the multidimensional setting considered in this section. In Sections 3 and 4 we study the rate of convergence for very much simplified problems.

For this section, our underlying regularity assumption concerning the data f and u is as follows:

Assumption 2. There is a bounded open rectangle $\Omega := \Pi_{i=1}^{n}(-X^i, X^i)$ containing Γ such that $u \in C^2(\overline{\Omega})$, $f \in C^1(\overline{\Omega})$. For each subset $S \subseteq \mathbf{R}$, let $U_S := \{\vec{x} \in \overline{\Omega} : u(\vec{x}) \in S\}$. With this notational convention, we further assume that for some $R > 0$, $\rho > 0$,

$$\begin{aligned} &\text{for } r \in [-R, R], \emptyset \neq U_{\{r\}} \subseteq \Omega, \\ &\|\nabla u\| \geqslant \rho \text{ for } \vec{x} \in U_{[-R,R]}. \end{aligned} \tag{22}$$

Remark 2.1. The purpose of the first condition in (22) is to ensure that the support of the approximate delta function δ_i^h $(i = 1, 2)$ is contained entirely within the computational domain. Since $\partial\Omega$ and $U_{[-R,R]}$ are compact and (by the first condition in (22)) disjoint, we are ensured that

$$\mathrm{d}(U_{[-R,R]}, \partial\Omega) := \inf\{\|\vec{y} - \vec{x}\| : \vec{y} \in U_{[-R,R]}, \vec{x} \in \partial\Omega\} > 0. \tag{23}$$

The purpose of the second condition in (22) is to guarantee that the formula for δ_i^h is well defined near Γ (recall that $\|\nabla^h u_{\mathbf{k}}\|$ appears in the denominator). In addition, this condition guarantees that each set of the form $U_{[r,s]}$ with $-R \leqslant r < s \leqslant R$ is a so-called oriented manifold with boundary [9], making it possible to apply the divergence theorem to certain integrals that will appear in the proofs of Theorems 2.1 and 2.2.

To specify the set $\mathscr{S}$ appearing in (7) that we will use in this section, let $K^i := \lfloor X^i/h \rfloor - 1$, and define

$$\mathscr{S} := \{\mathbf{k} = (k_1, \ldots, k_n) : -K^i \leqslant k_i \leqslant K^i,\ i = 1, \ldots, n\}. \tag{24}$$

The proofs of Theorems 2.1 and 2.2 use a certain modified version $\tilde{f}$ of the function f. To construct $\tilde{f}$, we start with the observation that there exists a C^∞ function μ: $\mathbf{R} \mapsto [0,1]$ such that $\mu(r) = 1$ for $-R/2 \leqslant r \leqslant R/2$ and $\mu(r) = 0$ for $|r| \geqslant R$. Let $\rho(\vec{x}) = \mu(u(\vec{x}))$. Due to Assumption 2, $\rho \in C^2(\mathbf{R}^n)$, and ρ has compact support. More specifically, $\mathrm{supp}(\rho) \subseteq U_{[-R,R]}$, and $\rho = 1$ on the set $U_{[-R/2,R/2]}$ containing Γ. Equipped with the function ρ, we define $\tilde{f}(\vec{x}) = \rho(\vec{x})f(\vec{x})$, and observe that $\tilde{f} \in C^1(\mathbf{R}^n)$, and $\tilde{f}(\vec{x}) = f(\vec{x})$ for $\vec{x} \in U_{[-R/2,R/2]}$. In addition, $\tilde{f}$ has compact support; in fact $\mathrm{supp}(\tilde{f}) \subseteq U_{[-R,R]}$.

We can finally state our convergence theorem for Method 1.

Theorem 2.1. *Suppose that Assumption 2 holds. Let $H^h(z)$ denote an approximation to the Heaviside function $H(z)$ satisfying Assumption 1. Assume that $\delta_1^h(\vec{x}_{\mathbf{k}}; u)$ defined by (12) (i.e., Method 1) is used in (7) defining the*

approximation $\mathscr{I}^h$. Finally assume that the set $\mathscr{S}$ is defined by (24). Then $\mathscr{I}^h$ converges to the integral $\mathscr{I}$ in (1) as $h \to 0$.

Remark 2.2. Although Assumption 1 allows for other possibilities, we have in mind the two versions of $H^h(z)$ that we have used in our numerical experiments. Specifically, we single out $H^{C,\epsilon}(z)$ with $\epsilon = 1.5h$ and $H^{L,\epsilon}(z)$ with $\epsilon = 1.0h$. Clearly both of these approximations satisfy the conditions of Assumption 1.

Proof. To keep the notation simple, we will carry out the proof in $\mathbf{R}^2$. It will become clear that the proof remains valid in $\mathbf{R}^n$. Let $\Omega = (-X, X) \times (-Y, Y)$, and consistent with (24), let $J = \lfloor X/h \rfloor - 1$, $K = \lfloor Y/h \rfloor - 1$. In $\mathbf{R}^2$, the approximation formula (7) becomes

$$\mathscr{I}^h := h^2 \sum_{j=-J}^{J} \sum_{k=-K}^{K} f_{j,k} \delta_1^h((x_j, y_k); u) \|\nabla^h u_{j,k}\|. \tag{25}$$

Here we are using the abbreviations $f_{j,k} = f(x_j, y_k)$, $u_{j,k} = u(x_j, y_k)$, and the set $\mathscr{S}$ appearing in (7) and (24) is $\{(j,k): -J \leqslant j \leqslant J, -K \leqslant k \leqslant K\}$.

Let $\sigma := \|\nabla u\|_{L^\infty(\overline{\Omega})}$, and define $\tilde{X}^h = (J-1)h$, $\tilde{Y}^h = (K-1)h$. For h sufficiently small,

$$\delta_1^h((x_j, y_k); u) = 0 \text{ for } |u_{j,k}| > (\alpha + \sigma)h, \tag{26}$$

$$U_{[-(\alpha+\sigma)h,(\alpha+\sigma)h]} \subseteq U_{[-R/2,R/2]} \subseteq U_{[-R,R]} \subseteq (-\tilde{X}^h, \tilde{X}^h) \times (-\tilde{Y}^h, \tilde{Y}^h), \tag{27}$$

$$\text{for } -K \leqslant k \leqslant K,\ \tilde{f}_{j,k} = 0 \quad \text{if } j = \pm J,\ \pm(J+1), \tag{28}$$

$$\text{for } -J \leqslant j \leqslant J,\ \tilde{f}_{j,k} = 0 \quad \text{if } k = \pm K,\ \pm(K+1). \tag{29}$$

Assertion (26) is readily verified using Assumption 1, and the fact that if $\vec{x}$ and $\vec{y}$ are a pair of points in the (convex) set Ω, then $\|u(\vec{x}) - u(\vec{y})\| \leqslant \sigma \|\vec{x} - \vec{y}\|$. The only portion of the (27) requiring verification is the set inclusion $U_{[-R,R]} \subseteq (-\tilde{X}^h, \tilde{X}^h) \times (-\tilde{Y}^h, \tilde{Y}^h)$, and this is a consequence of (23). Finally, (28) and (29) follow from (27), along with the fact that $\tilde{f}_{j,k} = 0$ for $(x_j, y_k) \notin U_{(-R,R)}$.

From (26) and (27), along with the fact that $\tilde{f}_{j,k} = f_{j,k}$ for $(x_j, y_k) \in U_{[-R/2,R/2]}$, it is clear that as soon as h is so small that $(\alpha + \sigma)h < R/2$, we will have $\delta_1^h((x_j, y_k); u) = 0$ on the set where $\tilde{f}_{j,k}$ differs from $f_{j,k}$. Thus for h sufficiently small, we can replace (25) by

$$\mathscr{I}^h := h^2 \sum_{j=-J}^{J} \sum_{k=-K}^{K} \tilde{f}_{j,k} \delta_1^h((x_j, y_k); u) \|\nabla^h u_{j,k}\|. \tag{30}$$

Let

$$(p_{j,k}, q_{j,k}) = \tilde{f}_{j,k} \frac{(D_0^x u_{j,k}, D_0^y u_{j,k})}{\|(D_0^x u_{j,k}, D_0^y u_{j,k})\|}, \tag{31}$$

where

$$\begin{aligned} D_0^x u_{j,k} &= (u_{j+1,k} - u_{j-1,k})/2h, \\ D_0^y u_{j,k} &= (u_{j,k+1} - u_{j,k-1})/2h. \end{aligned} \tag{32}$$

Note that due to our assumption that $\|\nabla u\| \geqslant \rho$ for $\vec{x} \in U_{[-R,R]}$, and the fact that $\tilde{f}_{j,k}$ vanishes for $|u_{j,k}| \geqslant R$, the quantity appearing in (31) is bounded and well-defined in spite of the denominator term $\|(D_0^x u_{j,k}, D_0^y u_{j,k})\|$.

Substituting (12) and (31) into (25) we can equivalently write

$$\mathscr{I}^h = h^2 \sum_{k=-K}^{K} \sum_{j=-J}^{J} p_{j,k} D_0^x H^h(u_{j,k}) + h^2 \sum_{j=-J}^{J} \sum_{k=-K}^{K} q_{j,k} D_0^y H^h(u_{j,k}). \tag{33}$$

We now sum by parts in (33). Specifically, we sum by parts in j (with k fixed) in the first sum, and sum by parts in k (with j fixed) in the second sum. Due to (28) and (29), there are no boundary contributions, and the result is

$$\mathscr{I}^h = -h^2 \sum_{k=-K}^{K} \sum_{j=-J}^{J} H^h(u_{j,k}) D_0^x p_{j,k} - h^2 \sum_{j=-J}^{J} \sum_{k=-K}^{K} H^h(u_{j,k}) D_0^y q_{j,k}. \tag{34}$$

Let $R_{j,k}(x,y)$ denote the characteristic function for the rectangle $[x_j - h/2, x_j + h/2) \times [y_k - h/2, y_k + h/2)$, and define

$$\mathscr{H}^h(x,y) = \sum_{j=-J}^{J} \sum_{k=-K}^{K} R_{j,k}(x,y) H^h(u_{j,k}), \tag{35}$$

$$P^h(x,y) = \sum_{j=-J}^{J} \sum_{k=-K}^{K} R_{j,k}(x,y) D_0^x p_{j,k}, \tag{36}$$

$$Q^h(x,y) = \sum_{j=-J}^{J} \sum_{k=-K}^{K} R_{j,k}(x,y) D_0^y q_{j,k}. \tag{37}$$

In terms of these quantities, (34) becomes

$$\mathscr{I}_h = -\int\int_{\Omega^h} \mathscr{H}^h(x,y) P^h(x,y)\,\mathrm{d}x\,\mathrm{d}y - \int\int_{\Omega^h} \mathscr{H}^h(x,y) Q^h(x,y)\,\mathrm{d}x\,\mathrm{d}y. \tag{38}$$

Here $\Omega^h := [-(J+1/2)h, (J+1/2)h) \times [-(K+1/2)h, (K+1/2)h)$. Note that $\Omega^h \subseteq \Omega$, and that Ω^h approximates the set Ω in the sense that the characteristic function of Ω^h converges boundedly a.e. to the characteristic function of Ω.

Our immediate goal is to apply the bounded convergence theorem to each of the integrals on the right side of (38). Clearly,

$$P^h(x,y) \to \partial_x \left(\tilde{f}(x,y) \frac{u_x(x,y)}{\|\nabla u(x,y)\|} \right), \quad Q^h(x,y) \to \partial_y \left(\tilde{f}(x,y) \frac{u_y(x,y)}{\|\nabla u(x,y)\|} \right) \tag{39}$$

boundedly at each point $(x,y) \in \Omega$. Concerning the convergence of $\mathscr{H}^h$, note that for h small enough, $U_{(-R,R)} \subseteq \Omega^h$; this is clear from (27). It is readily verified that $\mathscr{H}^h(x,y) \to 1$ for $(x,y) \in U_{(0,R)}$, and $\mathscr{H}^h(x,y) \to 0$ for $(x,y) \in U_{(-R,0)}$, the key ingredients being Assumption 1, along with the fact that u is positive on the open set $U_{(0,R)}$ and negative on the open set $U_{(-R,0)}$. We can ignore any convergence questions on the boundary sets $U_{\{0\}}$, $U_{\{-R\}}$, and $U_{\{R\}}$ since they all have two-dimensional measure zero, and all of the relevant quantities remain uniformly bounded as $h \to 0$. With these facts in mind, along with the observation that both of the limiting quantities in (39) vanish identically for $(x,y) \notin U_{(-R,R)}$, we can finally apply the bounded convergence theorem, yielding

$$\mathscr{I}^h \to -\int\int_{U_{(-R,R)}} H(u(x,y)) \nabla \cdot \left(\tilde{f}(x,y) \frac{\nabla u(x,y)}{\|\nabla u(x,y)\|} \right) \mathrm{d}x\,\mathrm{d}y. \tag{40}$$

Since $u(x,y) < 0$ on $U_{(-R,0)}$, the integral on the right side of (40) is equal to

$$-\int\int_{U_{(0,R)}} \nabla \cdot \left(\tilde{f}(x,y) \frac{\nabla u(x,y)}{\|\nabla u(x,y)\|} \right) \mathrm{d}x\,\mathrm{d}y. \tag{41}$$

An application of the divergence theorem to this last integral yields

$$\mathscr{I}^h \to -\int_{\partial U_{(0,R)}} \tilde{f}(x,y) \frac{\nabla u(x,y)}{\|\nabla u(x,y)\|} \cdot \vec{n}(x,y)\,\mathrm{d}s, \tag{42}$$

where $\vec{n}(x,y)$ denotes the outward unit normal vector to the boundary of the domain $U_{(0,R)}$. Since $\partial U_{(0,R)} = U_{\{0\}} \cup U_{\{R\}}$, and $\tilde{f}$ vanishes on the level set $U_{\{R\}}$, the only contribution to the integral appearing in (42) comes from $\Gamma = U_{\{0\}}$. Moreover, $\tilde{f} = f$ when $\vec{x} \in \Gamma$. Finally, for $\vec{x} \in \Gamma$, $\vec{n} = -\nabla u / \|\nabla u\|$, and thus the limiting integral appearing in (42) is equal to $\int_\Gamma f\,\mathrm{d}s$, which completes the proof. □

A similar convergence theorem applies to Method 2.

Theorem 2.2. *Suppose that Assumption 2 holds, and assume that $\delta_2^h(\vec{x}_{\mathbf{k}};u)$ defined by (17) (i.e., Method 2) is used in (7) defining the approximation $\mathscr{I}^h$, and that the set $\mathscr{S}$ is defined by (24). Then $\mathscr{I}^h$ converges to the integral $\mathscr{I}$ in (1) as $h \to 0$.*

Proof. As in the proof of Theorem 2.1, we carry out the analysis in $\mathbf{R}^2$, but only to simplify the notation; how to generalize to $\mathbf{R}^n$ will be clear. The assertions (26)–(29) remain valid here with the exception that the first two are replaced by

$$\delta_2^h((x_j,y_k);u) = 0 \quad \text{for } |u_{j,k}| > \sigma h, \tag{43}$$

$$U_{[-\sigma h,\sigma h]} \subseteq U_{[-R/2,R/2]} \subseteq U_{[-R,R]} \subseteq (-\tilde{X}^h,\tilde{X}^h)\times(-\tilde{Y}^h,\tilde{Y}^h). \tag{44}$$

Using (17) (Method 2) for the quantity $\delta^h((x_j,y_k);u)$, the two-dimensional version of (7) becomes

$$\mathscr{I}^h = h^2\sum_{j=-J}^{J}\sum_{k=-K}^{K} f_{j,k}\left[\frac{\Delta^h I_{j,k}}{\|\nabla^h u_{j,k}\|} - \frac{\Delta^h u_{j,k}(\nabla^h I_{j,k}\cdot\nabla^h u_{j,k})}{\|\nabla^h u_{j,k}\|^3}\right]. \tag{45}$$

As in the proof of Theorem 2.1, for h sufficiently small, we can replace $f_{j,k}$ by $\tilde{f}_{j,k}$. With this substitution, and after breaking (45) into two separate sums, we get

$$\mathscr{I}^h = h^2\sum_{j=-J}^{J}\sum_{k=-K}^{K}\frac{\tilde{f}_{j,k}\Delta^h I_{j,k}}{\|\nabla^h u_{j,k}\|} - h^2\sum_{j=-J}^{J}\sum_{k=-K}^{K}\frac{\tilde{f}_{j,k}\Delta^h u_{j,k}(\nabla^h I_{j,k}\cdot\nabla^h u_{j,k})}{\|\nabla^h u_{j,k}\|^3} =: S_1^h - S_2^h. \tag{46}$$

We start by analyzing the sum S_1^h, which we can write as

$$S_1^h = \sum_{j=-J}^{J}\sum_{k=-K}^{K}\frac{\tilde{f}_{j,k}}{\|\nabla^h u_{j,k}\|}\left(D_+^x D_-^x I_{j,k} + D_+^y D_-^y I_{j,k}\right). \tag{47}$$

Here we are using the abbreviations

$$\begin{aligned} D_+^x I_{j,k} &= (I_{j+1,k} - I_{j,k})/h, \quad D_-^x I_{j,k} = (I_{j,k} - I_{j-1,k})/h,\\ D_+^y I_{j,k} &= (I_{j,k+1} - I_{j,k})/h, \quad D_-^y I_{j,k} = (I_{j,k} - I_{j,k-1})/h. \end{aligned} \tag{48}$$

As in the proof of Theorem 2.1, we can sum by parts without introducing any boundary contributions:

$$S_1^h = -\sum_{j=-J}^{J}\sum_{k=-K}^{K} D_+^x\left(\frac{\tilde{f}_{j,k}}{\|\nabla^h u_{j,k}\|}\right)D_+^x I_{j,k} - \sum_{j=-J}^{J}\sum_{k=-K}^{K} D_+^y\left(\frac{\tilde{f}_{j,k}}{\|\nabla^h u_{j,k}\|}\right)D_+^y I_{j,k}. \tag{49}$$

An application of the bounded convergence theorem yields $S_1^h \to S_1$ where

$$S_1 := -\int\int_{\Omega}\nabla\left(\frac{\tilde{f}}{\|\nabla u\|}\right)\cdot\nabla I(u)\,dx\,dy. \tag{50}$$

Another application of the bounded convergence theorem gives $S_2^h \to S_2$ where

$$S_2 := \int\int_{\Omega}\frac{\tilde{f}\Delta u(\nabla I(u)\cdot\nabla u)}{\|\nabla u\|^3}\,dx\,dy. \tag{51}$$

Thanks to the factor $\tilde{f}$, the integrands in (50) and (51) vanish identically if $(x,y)\notin U_{(-R,R)}$, and $\nabla I(u) = 0$ on the set $U_{(-R,0)}$. Thus $\mathscr{I}^h \to S_1 - S_2$, where

$$S_1 - S_2 = -\int\int_{U_{(0,R)}}\left(\nabla\left(\frac{\tilde{f}}{\|\nabla u\|}\right)\cdot\nabla I(u) + \frac{\tilde{f}\Delta u(\nabla I(u)\cdot\nabla u)}{\|\nabla u\|^3}\right)dx\,dy. \tag{52}$$

Since $u > 0$ on the set $U_{(0,R)}$, we can replace $\nabla I(u)$ by ∇u. With this observation, the integrand in (52) simplifies to

$$\nabla\left(\frac{\tilde{f}}{\|\nabla u\|}\right)\cdot\nabla u+\frac{\tilde{f}\Delta u}{\|\nabla u\|}=\nabla\cdot\left(\frac{\tilde{f}\nabla u}{\|\nabla u\|}\right). \tag{53}$$

The rest of the proof consists of an application of the divergence theorem, exactly as in the proof of Theorem 2.1. □

Remark 2.3. The smoothness conditions imposed by Assumption 2 can probably be weakened somewhat. In several of our numerical examples, it appears that we have convergence of the approximations using both methods even though u is only piecewise C^2, or even piecewise C^1 in one case.

Remark 2.4. From the proof of Theorem 2.1, it is clear that we could take $\mathscr{S}$ to be the much smaller set $\{\mathbf{k}\in\mathbf{Z}^n : |u(\vec{x}_{\mathbf{k}})|\leqslant(\alpha+\sigma)h\}$, thus reducing the amount of computation significantly. Similarly, from the proof of Theorem 2.2 we could take $\mathscr{S}$ to be $\{\mathbf{k}\in\mathbf{Z}^n : |u(\vec{x}_{\mathbf{k}})|\leqslant\sigma h\}$.

3. Analysis of the one-dimensional algorithms

Although our ultimate interest is in the multidimensional versions of the algorithms, some insight into the rate of convergence can be gained by analyzing their one-dimensional versions. In the one-dimensional case, computing the integral (1) is equivalent to an interpolation problem, making the analysis more manageable than the multidimensional case. In the case where $u(x)=x-\bar{x}$ (a one-dimensional signed distance function), Beyer and Leveque [1] and Tornberg and Engquist [10] showed that the error in approximating the integral (1) will be $O(h^q)$ if the following moment condition is satisfied for any $\bar{x}\in\mathbf{R}$:

$$h\sum_{j\in\mathbb{Z}}\delta^{\epsilon}(x_j-\bar{x})(x_j-\bar{x})^r=\begin{cases}1, & r=0,\\ 0, & 1\leqslant r<q.\end{cases} \tag{54}$$

Here $\delta^{\epsilon}(x)$ denotes an approximate delta function with compact support in $[-\epsilon,\epsilon]$ such that $\epsilon=O(h)$.

It is straightforward to extend the moment condition (54) to the situation where $u(x)$ is not necessarily a signed distance function. Suppose that u is strictly monotone, and that $u(\bar{x})=0$. Let $\delta^h(x_j;u)$ denote a one-dimensional approximation to the delta function. In order to approximate the integral (1) to order q using the one-dimensional version of (7), we must have

$$h\sum_{j\in\mathbb{Z}}f(x_j)\delta^h(x_j;u)\left|D_0u_j\right|=f(\bar{x})+O(h^q), \tag{55}$$

where $D_0u_j=(u(x_{j+1})-u(x_{j-1}))/2h$. Substituting the Taylor series

$$f(x_j)=f(\bar{x})+\sum_{r=1}^{q-1}\frac{f^{(r)}(\bar{x})}{r!}(x_j-\bar{x})^r+\frac{f^{(q)}(\xi)}{q!}(x_j-\bar{x})^q \tag{56}$$

into (55) yields

$$h\sum_{j\in\mathbb{Z}}(x_j-\bar{x})^r\delta^h(x_j;u)|D_0u_j|=\begin{cases}1+O(h^q), & r=0,\\ O(h^q), & 1\leqslant r<q,\end{cases} \tag{57}$$

as sufficient moment conditions for qth order accuracy when u is not necessarily a distance function. In deriving (57) we assume that $\delta^h(x_j;u)=O(1/h)$ and that $\delta^h(x_j;u)=0$ if $|x_j-\bar{x}|>O(h)$. These conditions are easily checked for both of the proposed discretizations δ_1^h and δ_2^h under the conditions of Theorem 3.1.

Theorem 3.1. *Assume that $f\in C^1(\mathbf{R})$, $u\in C^1(\mathbf{R})$, and that the level function satisfies $u(\bar{x})=0$, $\|u'(x)\|\geqslant\rho>0$ for all $x\in\mathbf{R}$. Then the one-dimensional version of the algorithm that results from using Method 1, with H^h satisfying Assumption 1, satisfies the moment condition (57) with $q=1$, implying at least $O(h)$ accuracy as $h\to0$. If we additionally assume that $f\in C^2(\mathbf{R})$, $u\in C^3(\mathbf{R})$, then the one-dimensional version of the algorithm that results from using Method 2 satisfies (57) with $q=2$, implying at least $O(h^2)$ accuracy.*

Proof. Assume that $u'(x) > 0$; the proof when $u'(x) < 0$ is similar. With this assumption, the one-dimensional version of the approximate delta function that results from using (12) (i.e., Method 1) is just

$$\delta_1^h(x_j;u) = \frac{H^h(u(x_{j+1})) - H^h(u(x_{j-1}))}{u(x_{j+1}) - u(x_{j-1})}. \tag{58}$$

Plugging this into the left side of (57) with $r = 0$ gives

$$\frac{1}{2}\sum_{j\in\mathbb{Z}}(H^h(u_{j+1}) - H^h(u_{j-1})). \tag{59}$$

Here we are using the abbreviation $u_j = u(x_j)$. Thanks to Assumption 1, along with the assumption that $\|u'\| \geqslant \rho$, there is an index J such that $H^h(u_j) = 0$ for $j \leqslant -J$, and $H^h(u_j) = 1$ for $j \geqslant J$. The telescoping series (59) is thus equal to one. This verifies (57) with $q = 1$, and which proves the portion of the theorem concerning Method 1.

To prove the assertion about Method 2, we must verify (57) with $q = 2$. We start by observing that the one-dimensional version of the delta function that results from using (17) is

$$\delta_2^h(x_j;u) = \frac{D_0u_j \cdot D_+D_-I_j - D_0I_j \cdot D_+D_-u_j}{\left(D_0u_j\right)^3}. \tag{60}$$

Here $I_j = I(u_j)$, and we are using the notation

$$D_+u_j = \frac{u_{j+1} - u_j}{h}, \quad D_-u_j = \frac{u_j - u_{j-1}}{h}. \tag{61}$$

In what follows, it will be convenient to work with the quantity $\gamma_2^h(x_j;u) := \delta_2^h(x_j;u)D_0u_j$. Inspection of (60) reveals that if $\bar{x} \in [x_{j_0}, x_{j_0+1})$, then only $\gamma_2^h(x_{j_0};u)$ and $\gamma_2^h(x_{j_0+1};u)$ are non-zero. It is easy to check that $\gamma_2^h(x_j;u) = \mathrm{O}(1/h)$. In addition, using the assumption that $u \in C^3(\mathbf{R})$, it is readily verified that $(D_0u_j)^2 = (D_+u_j)(D_-u_j) + \mathrm{O}(h^2)$. These two observations yield the approximation

$$\gamma_2^h(x_j;u) = \frac{D_0u_j \cdot D_+D_-I_j - D_0I_j \cdot D_+D_-u_j}{\left(D_+u_j\right)\left(D_-u_j\right)} + \mathrm{O}(h). \tag{62}$$

The first term on the right side of (62) is equal to $D_+(D_-I_j/D_-u_j)$, so we have

$$\gamma_2^h(x_j;u) = \tilde{\gamma}_2^h(x_j;u) + \mathrm{O}(h), \quad \tilde{\gamma}_2^h(x_j;u) := D_+\left(\frac{D_-I_j}{D_-u_j}\right). \tag{63}$$

To verify the $r = 0$ moment condition, we start by recalling that $\gamma_2^h(x_j;u)$ vanishes for all but at most two points. Thus multiplying the first equation in (63) by h and then summing over j gives

$$h\sum_{j\in\mathbb{Z}}\gamma_2^h(x_j;u) = h\sum_{j\in\mathbb{Z}}\tilde{\gamma}_2^h(x_j;u) + \mathrm{O}(h^2). \tag{64}$$

The sum on the right side of (64) is equal to $h\sum_{j\in\mathbb{Z}}D_+(D_-I_j/D_-u_j)$ which is telescoping. Recalling the definition of $I(\cdot)$, it is clear that this sum is equal to 1, which proves the $r = 0$ moment condition.

For the $r = 1$ moment condition, assume that $\bar{x} \in [x_{j_0}, x_{j_0+1})$. Like $\gamma_2^h(x_j;u)$, $\tilde{\gamma}_2^h(x_j;u)$ is only non-zero at the two grid points x_{j_0} and x_{j_0+1}. Thus, for the $r = 1$ moment condition, it suffices to show that

$$S := h\left(y_{j_0}\tilde{\gamma}_2^h(x_{j_0};u) + y_{j_0+1}\tilde{\gamma}_2^h(x_{j_0+1};u)\right) = \mathrm{O}(h^2). \tag{65}$$

Here we are using the abbreviation $y_j = x_j - \bar{x}$. From the definitions, it is not hard to check that

$$\tilde{\gamma}_2^h(x_{j_0};u) = \frac{u_{j_0+1}}{u_{j_0+1} - u_{j_0}}, \quad \tilde{\gamma}_2^h(x_{j_0+1};u) = \frac{-u_{j_0}}{u_{j_0+1} - u_{j_0}}, \tag{66}$$

and thus

$$S = \frac{h}{u_{j_0+1} - u_{j_0}}\left(y_{j_0}u_{j_0+1} - y_{j_0+1}u_{j_0}\right). \tag{67}$$

We next approximate u_{j_0} and u_{j_0+1} using Taylor polynomials:

$$u_{j_0} = u(\bar{x}) + u'(\bar{x})y_{j_0} + \mathrm{O}(h^2), \quad u_{j_0+1} = u(\bar{x}) + u'(\bar{x})y_{j_0+1} + \mathrm{O}(h^2). \tag{68}$$

Here we have used the fact that $x_{j_0} - \bar{x} = y_{j_0} = \mathrm{O}(h)$, and similarly $x_{j_0+1} - \bar{x} = y_{j_0+1} = \mathrm{O}(h)$. Plugging (68) into (67), we get some cancellation, leaving

$$S = \frac{h}{u_{j_0+1} - u_{j_0}}(y_{j_0}\mathrm{O}(h^2) - y_{j_0+1}\mathrm{O}(h^2)). \tag{69}$$

Recalling that y_{j_0} and y_{j_0+1} are $\mathrm{O}(h)$, and that $|u'(x)| \geqslant \rho > 0$, we have $S = \mathrm{O}(h^3)$, and the proof is complete. □

4. Analysis in two dimensions for linear u

In Section 2 we demonstrated that our two proposed methods give approximations $\mathscr{I}^h$ that converge to the integral $\mathscr{I}$ as $h \to 0$, and these results were valid in a fairly general multidimensional setting. These results help to justify the proposed methods, but do not address the rate of convergence. The numerical experiments described in Section 5 seem to indicate that these multidimensional approximations are at least $\mathrm{O}(h)$ for Method 1 and $\mathrm{O}(h^2)$ for Method 2, in agreement with the results specific to the one-dimensional setting of Section 3. We do not presently have a proof of these stronger modes of convergence for the multidimensional setup considered in Section 2. In this section, we take a modest step toward bridging this analytical gap. Specifically, we focus on $\mathbf{R}^2$, and assume that the level function u is linear:

$$u(x,y) = Ax + By, \quad A^2 + B^2 \neq 0. \tag{70}$$

Thus the zero level set Γ is the straight line through the origin defined by $Ax + By = 0$. We assume that f has compact support, so that the integral $\mathscr{I}$ appearing in (1) is finite.

Admittedly, this setup is greatly simplified, but the proofs of Theorems 4.1 and 4.2 below provide some insight into the mechanism by which the accuracy properties established in Section 3 for the one-dimensional setting are transferred to $\mathbf{R}^2$.

Theorem 4.1. *Suppose that u has the form given by (70), that $f \in C^1(\mathbf{R}^2)$, and that f is compactly supported. If H^h satisfies Assumption 1, then Method 1 gives an $\mathrm{O}(h)$ approximation to the integral $\mathscr{I}$ appearing in (1).*

Proof. Assume for now that $A \neq 0$, $B \neq 0$. From our assumptions about u, the integral $\mathscr{I}$ can be written in either of the equivalent forms

$$\sqrt{1 + A^2/B^2}\int_{-\infty}^{\infty} f(x, -Ax/B)\,\mathrm{d}x, \quad \sqrt{1 + B^2/A^2}\int_{-\infty}^{\infty} f(-By/A, y)\,\mathrm{d}y. \tag{71}$$

On the other hand, with $u(x,y) = Ax + By$, Method 1 yields the approximation

$$\mathscr{I}^h = \mathscr{A}h^2 \sum_{j\in\mathbb{Z}}\sum_{k\in\mathbb{Z}} f_{j,k} D_0^x H^h(u_{j,k}) + \mathscr{B}h^2 \sum_{j\in\mathbb{Z}}\sum_{k\in\mathbb{Z}} f_{j,k} D_0^y H^h(u_{j,k}), \tag{72}$$

where $\mathscr{A} = A/\sqrt{A^2 + B^2}$, $\mathscr{B} = B/\sqrt{A^2 + B^2}$.

By our one-dimensional accuracy result (Theorem 3.1) for Method 1,

$$h\sum_{j\in\mathbb{Z}} f_{j,k} D_0^x H^h(u_{j,k}) = \mathrm{sign}(A) f(-By_k/A, y_k) + \mathrm{O}(h). \tag{73}$$

Here $(-By_k/A, y_k)$ is the point where the line Γ intersects the horizontal mesh line $y = y_k$. By our assumptions about f, the $\mathrm{O}(h)$ bound in (73) is uniform in k, and so multiplying (73) by $\mathscr{A}h$ and summing over k yields

$$\mathscr{A}h^2 \sum_{j\in\mathbb{Z}}\sum_{k\in\mathbb{Z}} f_{j,k} D_0^x H^h(u_{j,k}) = |\mathscr{A}|h\sum_{k\in\mathbb{Z}} f(-By_k/A, y_k) + \mathrm{O}(h). \tag{74}$$

Since f has compact support, $|\mathscr{A}|h\sum_{k\in\mathbb{Z}} f(-By_k/A, y_k)$ is a trapezoidal rule approximation (with error $\mathrm{O}(h^2)$) to the integral $|\mathscr{A}|\int_{-\infty}^{\infty} f(-By/A, y)\,\mathrm{d}y$. Combining this observation with the identity $|\mathscr{A}| = \mathscr{A}^2\sqrt{1 + B^2/A^2}$ and

then referring to the second integral in (71), we see that the first sum on the right side of (72) is equal to $\mathscr{A}^2\mathscr{I} + \mathrm{O}(h)$.

Similarly

$$\mathscr{B}h^2 \sum_{j\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} f_{j,k} D_0^y H^h(u_{j,k}) = |\mathscr{B}| h \sum_{j\in\mathbb{Z}} f(x_j, -Ax_j/B) + \mathrm{O}(h), \tag{75}$$

where $(x_j, -Ax_j/B)$ is the point where Γ intersects the vertical line $x = x_j$. This time, we recognize $|\mathscr{B}|h\sum_{j\in\mathbb{Z}} f(x_j, -Ax_j/B)$ as a trapezoidal rule approximation to the integral $|\mathscr{B}| \int_{-\infty}^{\infty} f(x, -Ax/B)\,\mathrm{d}x$. We use the identity $|\mathscr{B}| = \mathscr{B}^2\sqrt{1 + A^2/B^2}$, and then refer to the first integral in (71) to conclude that the second sum on the right side of (72) is equal to $\mathscr{B}^2\mathscr{I} + \mathrm{O}(h)$. Combining this with the results of the previous paragraph, and finally noting that $\mathscr{A}^2 + \mathscr{B}^2 = 1$, the proof is complete under that assumption that $A \neq 0$, $B \neq 0$. To complete the proof, take the case where $B = 0$; the case where $A = 0$ is similar. In this situation, the second sum in (72) vanishes and examination of the argument above reveals that the first sum in (72) is an $\mathrm{O}(h)$ approximation to the second integral in (71). □

We have a similar theorem for Method 2.

Theorem 4.2. *Suppose that u has the form given by (70), that $f \in C^2(\mathbf{R})$, and that f is compactly supported. Then Method 2 gives an $\mathrm{O}(h^2)$ approximation to the integral $\mathscr{I}$ appearing in (1).*

Proof. With our assumptions about u, Method 2 simplifies to

$$\mathscr{I}^h = h^2 \sum_{j\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} \frac{f_{j,k} D_+^x D_-^x I(u_{j,k})}{\sqrt{A^2 + B^2}} + h^2 \sum_{j\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} \frac{f_{j,k} D_+^y D_-^y I(u_{j,k})}{\sqrt{A^2 + B^2}}. \tag{76}$$

As in the proof of Theorem 4.2, we first address the case where $A \neq 0$, $B \neq 0$. Let us focus for now on the first sum on the right side of (76). Our one-dimensional accuracy results (Theorem 3.1) for Method 2 imply that

$$h \sum_{j\in\mathbb{Z}} f_{j,k} \frac{D_+^x D_-^x I(u_{j,k})}{|A|} = f(-By_k/A, y_k) + \mathrm{O}(h^2). \tag{77}$$

Multiplying both sides of this equation by $|A|h$, then dividing by $\sqrt{A^2 + B^2}$, and finally summing over $k \in \mathbf{Z}$, we find that the first sum on the right side of (76) is equal to

$$|\mathscr{A}| h \sum_{k\in\mathbb{Z}} f(-By_k/A, y_k) + \mathrm{O}(h^2), \quad \mathscr{A} = A/\sqrt{A^2 + B^2}. \tag{78}$$

Similarly, we can apply our one-dimensional accuracy results to conclude that the second sum on the right side of (76) is equal to

$$|\mathscr{B}| h \sum_{j\in\mathbb{Z}} f(x_j, -Ax_j/B) + \mathrm{O}(h^2), \quad \mathscr{B} = B/\sqrt{A^2 + B^2}. \tag{79}$$

Recalling again that the error in the trapezoidal rule is $\mathrm{O}(h^2)$, the rest of the proof is virtually identical to the proof of Theorem 4.1. □

5. Numerical examples

In this section, we present the results of a number of numerical examples. When using Method 1, for the approximate Heaviside function H^h we always use $H^{C,\epsilon}$ with $\epsilon = 1.5h$ or $H^{L,\epsilon}$ with $\epsilon = 1.0h$.

To study the rate of convergence via mesh refinement, we average over small random grid shifts, following [2,8]. If the error $E(h)$ of our approximations was of the form $E(h) = C_0h^q + C_1h^{q+1} + \cdots$ for some constants $C_0, C_1, \ldots$, we could simply compute the error based on one calculation at each of the selected levels of mesh refinement. However, we only have that the quantity $E(h)/h^q$ is bounded as $h \to 0$. This makes it necessary to average over a number of small random grid shifts in order to observe the rate of convergence. The number of

grid shifts required depends on the problem and the method, and is determined in any particular case by trial and error. We have recorded the number of grid shifts used in each of the experiments that follow by placing them in parentheses in the headings of the tables.

Finally, all errors appearing in the tables below are relative errors unless the true solution is zero, in which case absolute errors are displayed.

Example 1. Our first example is taken from [2]. Tables 1 and 2 show the results when Γ is a capsule shaped curve of the type appearing in Figure 1 of [2]. The function f is identically equal to one for this example, so the integral $\mathscr{I}$ measures the length of Γ. This test case was designed by Tornberg and Engquist [11], specifically to demonstrate the O(1) errors that occur by simply using the cosine approximate delta function $\delta^{C,\epsilon}$ in a pointwise manner. Due to the 45° inclination of the capsule, there is very little error cancellation, making it difficult for an inconsistent method to give good results. The results from using Method 1 are shown in Table 1. Both variants of Method 1 seem to give second order rates of convergence. When using a signed distance function for the level function u, $H^{L,\epsilon}$ and $H^{C,\epsilon}$ give very similar results, but when using a non-distance function, $H^{L,\epsilon}$ is somewhat more accurate than $H^{C,\epsilon}$. From Table 2, it appears that Method 2 gives also $O(h^2)$ convergence for this example. In Table 2 we also show the result of using the pointwise approximate delta function $\delta^{C,\epsilon}$ with $\epsilon = 1.5h$, and u a signed distance function. As expected, the approximations using $\delta^{C,\epsilon}$ do not converge as $h \to 0$.

Example 2. In the example above, Method 1 gave second order accuracy. However, Method 1 is generally only first order accurate. To demonstrate this, let

$$\xi = (x-y)/\sqrt{2}, \quad \eta = (x+y)/\sqrt{2}.$$

We take $u(x,y) = \eta$, and

$$f(x,y) = \begin{cases} \eta\cos^2(\xi)\cos^2(\eta) & \text{if } |\xi| < \pi/2 \text{ and } |\eta| < \pi/2, \\ 0 & \text{otherwise.} \end{cases} \tag{80}$$

It is clear that $\mathscr{I} = 0$ for this example. Moreover, this provides an example of the situation analyzed in Section 4. The results are shown in Table 3. Both variants of Method 1 show approximately $O(h)$ accuracy, while for this particular example Method 2 seems to give $O(h^3)$ accuracy.

Table 1
Example 1 – Method 1

h	Using $H^{C,\epsilon}$ (8)				Using $H^{L,\epsilon}$ (32)			
	Dist. $u(\vec{x})$		Non-dist. $u(\vec{x})$		Dist. $u(\vec{x})$		Non-dist. $u(\vec{x})$	
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
.06	3.40e − 3		1.94e − 1		3.37e − 3		1.35e − 1	
.03	8.25e − 4	2.0	4.20e − 2	2.2	8.17e − 4	2.0	7.57e − 3	4.2
.015	2.05e − 4	2.0	2.46e − 3	4.1	2.06e − 4	2.0	1.44e − 3	2.4
.0075	5.13e − 5	2.0	5.84e − 4	2.1	5.20e − 5	2.0	3.52e − 4	2.0
.00375	1.29e − 5	2.0	1.45e − 4	2.0	1.30e − 5	2.0	8.73e − 5	2.0

Table 2
Example 1 – Method 2 and pointwise delta function $\delta^{C,\epsilon}$

h	Method 2 (8)				Using $\delta^{C,\epsilon}$ (512)	
	Dist. $u(\vec{x})$		Non-dist. $u(\vec{x})$			
	Error	Rate	Error	Rate	Error	Rate
.06	1.69e − 3		2.81e − 2		3.48e − 3	
.03	4.00e − 4	2.1	6.81e − 3	2.0	3.06e − 3	0.2
.015	1.01e − 4	2.0	1.70e − 3	2.0	3.06e − 3	0.0
.0075	2.53e − 5	2.0	4.24e − 4	2.0	3.09e − 3	0.0
.00375	6.38e − 6	2.0	1.06e − 4	2.0	3.15e − 3	0.0

Table 3
Example 2

h	Method 1 (128)				Method 2 (128)	
	Using $H^{C,\epsilon}$		Using $H^{L,\epsilon}$			
	Error	Rate	Error	Rate	Error	Rate
.06	4.20e − 5		6.42e − 4		7.33e − 6	
.03	2.12e − 5	1.0	2.96e − 4	1.1	9.03e − 7	3.0
.015	9.91e − 6	1.1	1.59e − 4	0.9	1.17e − 7	2.9
.0075	4.98e − 6	1.0	8.20e − 5	1.0	1.45e − 8	3.0

Example 3. In this example

$$\mathscr{I} = \int_{\Gamma} \frac{1}{2}(r - x)\,\mathrm{d}s = \pi r^2, \tag{81}$$

where Γ is a circle of radius $r = 0.35\sqrt{2}$ centered at the origin. Table 4 shows the results when u is a signed distance function. Both methods seem to give $O(h^2)$ convergence for this example. However, Method 2 is much more accurate than Method 1 over the range of h tested here. Table 4 also shows the result of using the pointwise approximate delta function $\delta^{C,\epsilon}$ with $\epsilon = 1.5h$. As the mesh is refined, it appears that the rate of convergence is slowing, indicating that perhaps these approximations do not converge to the correct solution.

Table 5 shows the results when for this same example when u is not a signed distance function. This time, Method 2 seems to be converging like $O(h^2)$, while Method 1 is converging at a rate somewhere between $O(h)$ and $O(h^2)$. For the range of h used in this experiment, Method 1 is more accurate. This example is a little unusual in that, at least for Method 1, the approximations are more accurate when using a level function u that is not a signed distance function. Finally, we again see the decreasing rate of convergence when using the pointwise approximate delta function $\delta^{C,\epsilon}$. For the $\delta^{C,\epsilon}$ approximation, we used $\epsilon = 1.5h$.

Example 4. In the next example, we let Γ be the ellipse $x^2/9 + y^2/4 = 1$, and $f(x,y) = \nabla \cdot (\nabla u(x,y)/\|\nabla u(x,y)\|)$ where $u(x,y) = x^2/9 + y^2/4 - 1$, so that

Table 4
Example 3 – $u(x,y)$ is a signed distance function

h	Method 1 (32)				Method 2 (32)		Using $\delta^{C,\epsilon}$ (64)	
	Using $H^{C,\epsilon}$		Using $H^{L,\epsilon}$					
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
.08	7.67e − 3		4.42e − 3		1.55e − 6		4.41e − 3	
.04	1.92e − 3	2.0	1.11e − 3	2.0	4.00e − 7	1.9	1.05e − 3	2.1
.02	4.80e − 4	2.0	2.74e − 4	2.0	1.03e − 7	2.0	3.67e − 4	1.5
.01	1.20e − 4	2.0	7.05e − 5	2.0	2.58e − 7	2.0	1.92e − 4	0.9
.005	3.00e − 5	2.0	1.73e − 5	2.0	6.40e − 7	2.0	1.21e − 4	0.7

Table 5
Example 3 – $u(x,y)$ is not a signed distance function

h	Method 1 (1024)				Method 2 (32)		Using $\delta^{C,\epsilon}$ (64)	
	Using $H^{C,\epsilon}$		Using $H^{L,\epsilon}$					
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
.08	1.42e − 4		3.29e − 4		1.31e − 2		2.40e − 3	
.04	3.00e − 5	2.2	1.04e − 4	1.7	3.26e − 3	2.0	1.24e − 3	1.0
.02	4.34e − 6	2.8	3.46e − 5	1.6	8.17e − 4	2.0	4.26e − 4	1.5
.01	1.26e − 6	1.8	1.20e − 5	1.5	2.04e − 4	2.0	2.03e − 4	1.1
.005	3.61e − 7	1.8	4.07e − 6	1.6	5.10e − 5	2.0	1.31e − 4	0.6

$$\mathscr{I} = \int_{\Gamma} \kappa(x,y)\,\mathrm{d}s, \tag{82}$$

where $f(x,y) = \kappa(x,y)$ is the curvature of Γ. By parameterizing the curve, we can approximate this integral by any standard quadrature technique:

$$\mathscr{I} = \int_0^{2\pi} \frac{1}{5\sin^2 t + 4}\,\mathrm{d}t \approx 6.28318530733266. \tag{83}$$

To mitigate possible error cancellation due to symmetry, we rotated the mesh by 45°. Although we could compute $\kappa(x_j,y_k)$ exactly, we used centered difference approximations. This was an attempt to simulate how the method would be used in applications, where κ would only be defined at the mesh points. Note that for this example, u is not a signed distance function. The results are shown in Table 6. From Table 6, it is clear that the convergence for Method 2 is $O(h^2)$, while for Method 1 the convergence is between $O(h)$ and $O(h^2)$.

Example 5. In this example, Γ is a square whose sides have length $\sqrt{2}$, and are oriented at a 45° angle to the coordinate axes. $f(x,y) \equiv 1$, so that $\int_\Gamma \mathrm{d}s$ is equal to the perimeter of the square. This is the example appearing in Table 1 of Smereka's paper [8]. We use the signed distance function u specified in [8]. This example is of interest because the level function u is only piecewise C^1. Also like the capsule example, this is another problem where using a pointwise defined delta function like $\delta^{C,\epsilon}$ or $\delta^{L,\epsilon}$ is known to fail to converge to the true solution. The results are shown in Table 7. We have convergence at a rate of $O(h)$ in all cases, no doubt due to the reduced smoothness of u. For this example, Method 2 is more accurate than Method 1.

Example 6. Table 8 shows the results from an experiment where Γ is the capsule shaped surface appearing in Fig. 12 of [2]. To be more specific, Γ is a cylinder that has hemispheres attached as caps at either end. It is rotated and shifted in space so that its axis is along the vector $(1,1,1)$. This is designed to minimize cancellation of errors. In this example, we took $f \equiv 1$, so the integral (1) simply gives the area of Γ. For Method 1, we used $H^{C,\epsilon}$. It appears that both methods have second order accuracy for this example, and again this is independent of whether u is a distance function.

Table 6
Example 4

h	Method 1 (128)				Method 2 (32)	
	Using $H^{C,\epsilon}$		Using $H^{L,\epsilon}$			
	Error	Rate	Error	Rate	Error	Rate
.32	4.57e − 3		4.04e − 3		7.78e − 3	
.16	1.03e − 3	2.1	1.00e − 3	2.0	1.94e − 3	2.0
.08	4.17e − 4	1.3	3.41e − 4	1.6	4.83e − 4	2.0
.04	9.62e − 5	2.1	9.70e − 5	1.8	1.21e − 4	2.0
.02	3.74e − 5	1.4	3.14e − 5	1.6	3.02e − 5	2.0

Table 7
Example 5

h	Method 1 (16)				Method 2 (128)	
	Using $H^{C,\epsilon}$		Using $H^{L,\epsilon}$			
	Error	Rate	Error	Rate	Error	Rate
.06	2.32e − 2		2.25e − 2		5.01e − 3	
.03	1.13e − 2	1.0	1.13e − 2	1.0	2.92e − 3	0.8
.015	5.81e − 3	1.0	5.78e − 3	1.0	1.51e − 3	1.0
.0075	2.92e − 3	1.0	2.89e − 3	1.0	7.24e − 4	1.1
.00375	1.43e − 3	1.0	1.43e − 3	1.0	3.73e − 4	1.0

Table 8
Example 6

h	Method 1 (1)				Method 2 (8)			
	Dist. $u(\vec{x})$		Non-dist. $u(\vec{x})$		Dist. $u(\vec{x})$		Non-dist. $u(\vec{x})$	
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
.075	7.16e − 3		8.23e − 2		8.69e − 3		6.48e − 2	
.05	2.98e − 3	2.2	6.35e − 2	0.6	3.52e − 3	2.2	2.85e − 2	2.0
.0375	1.64e − 3	2.1	3.85e − 2	1.7	1.94e − 3	2.1	1.60e − 2	2.0
.03	1.05e − 3	2.0	2.22e − 2	2.5	1.23e − 3	2.0	1.02e − 2	2.0
.025	7.16e − 4	2.1	1.44e − 2	2.4	8.55e − 4	2.0	7.09e − 3	2.0
.02	4.62e − 4	2.0	8.82e − 3	2.2	5.41e − 4	2.0	4.54e − 3	2.0

Example 7. In this example, Γ is the same capsule-shaped surface as in the previous example. Following [2], we took

$$f(x,y,z) = \operatorname{curl} \mathbf{F} \cdot \mathbf{n}_\Gamma, \quad \mathbf{F} = (x^2, y^2, z^2), \tag{84}$$

where $\mathbf{n}_\Gamma$ denotes the unit normal vector to the surface Γ. By Stokes' theorem, the integral (1) evaluates to zero with this choice of f. Table 9 shows the results of this experiment. It appears that both methods are converging at a rate of $O(h^2)$.

Example 8. Table 10 shows the results of using both methods to compute the surface integral

$$\mathscr{I} = \int_\Gamma (4 - 3x^2 + 2y^2 - z^2)\, dA, \tag{85}$$

where Γ is the sphere $x^2 + y^2 + z^2 = 1$. For the level function, we used $u(x,y,z) = x^2 + y^2 + z^2 - 1$, which is not a signed distance function. This is the example shown in Table 5 of Smereka's paper [8]. The rate of convergence appears to be $O(h^2)$ for each method.

Table 9
Example 7

h	Method 1 (1)				Method 2 (8)			
	Dist. $u(\vec{x})$		Non-dist. $u(\vec{x})$		Dist. $u(\vec{x})$		Non-dist. $u(\vec{x})$	
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
.075	2.34e − 3		3.24e − 3		2.47e − 4		1.59e − 2	
.05	1.07e − 3	1.9	1.62e − 3	1.7	4.56e − 4	−1.5	6.87e − 3	2.1
.0375	6.16e − 4	1.9	9.59e − 4	1.8	2.99e − 4	1.5	3.83e − 3	2.0
.03	3.97e − 4	2.0	6.29e − 4	1.9	2.13e − 4	1.5	2.43e − 3	2.0
.025	2.71e − 4	2.1	4.35e − 4	2.0	1.46e − 4	2.1	1.71e − 3	1.9
.02	1.76e − 4	1.9	2.80e − 4	2.0	9.63e − 5	1.9	1.09e − 3	2.0

Table 10
Example 8

h	Method 1 (64)				Method 2 (64)	
	Using $H^{C,\epsilon}$		Using $H^{L,\epsilon}$			
	Error	Rate	Error	Rate	Error	Rate
.2	2.93e − 2		2.06e − 2		3.69e − 2	
.1	3.80e − 3	2.9	3.60e − 3	2.5	8.30e − 3	2.2
.05	9.57e − 4	2.0	8.25e − 4	2.1	2.08e − 3	2.0
.025	2.38e − 4	2.0	2.26e − 4	1.9	5.19e − 4	2.0

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