

A convergence rate theorem for finite difference approximations to delta functions

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Abstract

We prove a rate of convergence theorem for approximations to certain integrals over codimension one manifolds in \mathbb{R}^n . The type of manifold involved here is defined by the zero level set of a smooth mapping $u : \mathbb{R}^n \mapsto \mathbb{R}$. Our approximations are based on the two finite difference methods for discretizing delta functions presented in [16]. We included a convergence proof in that paper, but only proved rates of convergence in some greatly simplified situations. Numerical experiments indicated that our two methods were at least first and second order accurate, respectively. In this note we prove those empirical convergence rates for the two algorithms under fairly general hypotheses.

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1. Introduction

Like [16], this note concerns the problem of approximating the integral

$$\mathcal{I} := \int_{\Gamma} f(\vec{x}) ds, \quad (1)$$

where $\vec{x} = (x^1, \dots, x^n) \in \mathbf{R}^n$, and Γ is a compact manifold of codimension one defined by the zero level set of a function $u(\vec{x})$. The data f and u are only defined at the discrete set of mesh points of a regular grid. It is natural in this situation to replace the integral on the right side of (1) by the integral

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

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where $\delta(\cdot)$ denotes the Dirac delta function. Ref. [3] contains a proof that the integrals appearing in (1) and (2) are equal. The problem of approximating the integral \mathcal{I} thus amounts to producing a discrete version of the delta function $\delta(u(\vec{x}))$.

In level set applications [8], f and u are often only defined in a narrow band containing Γ . Even if u is defined more globally, it will often be a signed distance function, and will be smooth near Γ , but may have cusps at some finite distance away.

We assume that for some $\alpha > 0$, u is defined and smooth on a band of the form $B_\alpha = \{\vec{x} : |u(\vec{x})| < \alpha\}$ surrounding Γ . We further assume that f is also defined and smooth on B_α , and that for some $\sigma > 0$, $\|\nabla u\| > \sigma$ for $\vec{x} \in B_\alpha$.

Finally, we assume that one component of $\mathbb{R}^n \setminus \Gamma$ is a bounded domain Ω . See Fig. 1. Without loss of generality, we take $u > 0$ in $\Omega \cap B_\alpha$, i.e., u is positive (wherever defined) in the region enclosed by Γ . With this convention, the unit outward (from Ω) normal vector \vec{n} satisfies $\vec{n} = -\nabla u / \|\nabla u\|$.

For our analysis (but not for our algorithms), we will require an extended version \tilde{f} of the function f . To construct \tilde{f} , we start with a C^∞ function $\mu : \mathbf{R} \mapsto [0, 1]$ such that $\mu(r) = 1$ for $|r| \leq \alpha/2$ and $\mu(r) = 0$ for $|r| \geq \alpha$. Let $\rho(\vec{x}) = \mu(u(\vec{x}))$, and define

$$\tilde{f}(\vec{x}) = \begin{cases} \rho(\vec{x})f(\vec{x}) & \vec{x} \in B_\alpha \\ 0 & \vec{x} \notin B_\alpha. \end{cases} \tag{3}$$

The extension \tilde{f} is as smooth as f , it is defined on all of \mathbb{R}^n , and it has compact support. It is clear that quantities like $\tilde{f}u/\|\nabla u\|$ can also be understood to be smooth (and compactly supported) on all of \mathbb{R}^n .

Let $\{\vec{x}_{\mathbf{k}} = (x_{k_1}^i, \dots, x_{k_n}^i) : \mathbf{k} := (k_1, \dots, k_n) \in \mathbf{Z}^n\}$ denote the set of mesh points of the regular grid. We assume that the mesh spacing h is the same in all directions, $x_{k_i}^i = k_i h, k_i \in \mathbf{Z}$. Let $\{\vec{e}_1, \dots, \vec{e}_n\}$ be the standard basis for \mathbb{R}^n . If $v_{\mathbf{k}} = v(\vec{x}_{\mathbf{k}})$ is a function defined at each grid point $\vec{x}_{\mathbf{k}}$, we define the second order accurate discrete gradient operator ∇^h via

$$\nabla^h v_{\mathbf{k}} = \sum_{m=1}^n \left(\frac{v(\vec{x}_{\mathbf{k}} + h\vec{e}_m) - v(\vec{x}_{\mathbf{k}} - h\vec{e}_m)}{2h} \right) \vec{e}_m. \tag{4}$$

It is easy to see that if $\vec{w}_{\mathbf{k}}$ vanishes for $\max\{|k_1|, \dots, |k_n|\}$ sufficiently large, then the following summation by parts formula holds:

$$\sum_{\mathbf{k} \in \mathbf{Z}^n} \nabla^h v_{\mathbf{k}} \cdot \vec{w}_{\mathbf{k}} = - \sum_{\mathbf{k} \in \mathbf{Z}^n} v_{\mathbf{k}} \nabla^h \cdot \vec{w}_{\mathbf{k}}. \tag{5}$$

Let $H(\cdot)$ denote the Heaviside function

$$H(z) = \begin{cases} 0, & z < 0, \\ 1, & z > 0, \end{cases} \tag{6}$$

and define $I(z) = \int_0^z H(\zeta) d\zeta$. Note that

$$\begin{aligned} \nabla I(u(\vec{x})) &= H(u(\vec{x})) \nabla u(\vec{x}), \\ \nabla H(u(\vec{x})) &= \delta(u(\vec{x})) \nabla u(\vec{x}). \end{aligned} \tag{7}$$

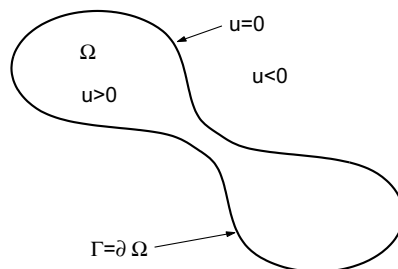


Fig. 1. A level set $\Gamma \subseteq \mathbb{R}^2$ defined by $u(\vec{x}) = 0$.

The second of these relationships is purely formal; it relies on the fact that $H'(z) = \delta(z)$ in the sense of distributions. By taking the inner product with ∇u , we get the relationships

$$\begin{aligned} H(u) &= \nabla I(u) \cdot \nabla u / \|\nabla u\|^2, \\ \delta(u) &= \nabla H(u) \cdot \nabla u / \|\nabla u\|^2. \end{aligned} \tag{8}$$

Before continuing, we emphasize that our convergence proof does not rely on the formal calculations that yield (8); they are included solely for motivation. Our finite difference approximations are simply discretizations of (8).

FDM₁ :

$$\delta_k^{1,h} = \nabla^h H(u_k) \cdot \nabla^h u_k / \|\nabla^h u_k\|^2. \tag{9}$$

FDM₂ :

$$\begin{aligned} H_k^{1,h} &= \nabla^h I(u_k) \cdot \nabla^h u_k / \|\nabla^h u_k\|^2, \\ \delta_k^{2,h} &= \nabla^h H_k^{1,h} \cdot \nabla^h u_k / \|\nabla^h u_k\|^2. \end{aligned} \tag{10}$$

Both of these approximate delta functions vanish outside of a narrow band surrounding Γ . Specifically, $\delta_k^{q,h} = 0$ if $d(\vec{x}_k, \Gamma) > qh$. This narrow support is a desirable property in practical applications.

Remark 1.1. It is possible to build more accurate algorithms (FDM_q, $q > 2$) by starting with higher order primitives of $H(\cdot)$, and then differencing as many times as necessary. The second order ∇^h must be replaced by a more accurate discrete gradient, but this is straightforward. Unfortunately, for $q > 2$ the support of the discrete delta function constructed in this way expands to fill up all of Ω . Since we are interested in keeping the support of our delta functions narrow, we only consider $q = 1, 2$ here.

Once we have computed the approximate delta function $\delta_k^{q,h}$, we approximate the integral (2) via

$$\mathcal{I}^{q,h} = h^n \sum_{k \in \mathbb{Z}^n} \delta_k^{q,h} f(\vec{x}_k) \|\nabla^h u_k\|, \quad q = 1, 2. \tag{11}$$

FDM₁ and FDM₂ are the algorithms that we referred to as Method 1 and Method 2 in [16]. In that paper, we found by numerical experiments that FDM₁ was generally first order accurate, and if we smoothed $H(z)$ by a small amount, it gave second order accuracy on certain problems. Our numerical experiments showed that FDM₂ was second order accurate in general. Note that in the previous paper, we combined the two stages of FDM₂ into a single formula. The performance of the two-stage algorithm of this note turns out to be similar to the one-step version in [16]. The two-stage version is somewhat easier to implement and analyze.

The problem of discretizing a codimension one delta function on a regular mesh occurs naturally in applications of the level set method [8,9,12]. This topic has attracted some attention recently due to the results of Engquist, Tornberg, and Tsai. Tornberg and Engquist showed in [14,15] that seemingly reasonable discretizations may not converge to the correct value of the integral \mathcal{I} . Following this, Engquist et al. [4] constructed first and second order accurate approximate delta functions that overcome this difficulty. Next, Smereka [13] devised first and second order discrete delta functions. His approximations are based on a technique due to Mayo [6] for solving elliptic equations on irregular regions. Let us also mention that Wen [19] has constructed very accurate discrete one-dimensional delta functions.

Gibou and Min [7] have also proposed a method for approximating $\int_{\Gamma} f(\vec{x}) ds$. Their approach is more geometric in nature, and does not require any discretization of delta functions.

In the special case where $n = 2$, and $f(\vec{x}) \equiv 1$, Candela and Marquina [2] have proposed a parameter to measure the complexity of Γ , which relates to the accuracy of approximating the integral \mathcal{I} .

There has also been some work related to approximating integrals involving delta functions supported on sets of higher codimension [5,17,18]. The case of full codimension (where the delta function is supported on a discrete set of points in \mathbb{R}^n) is important in level set methods for modeling high frequency wave propagation [5,11].

Although there is substantial numerical evidence that the second order algorithms of [4,13,16] all converge at a rate of $O(h^2)$, until recently there was no proof of this. Very recently Beale [1] provided a simple proof that Smereka's algorithm converges at a rate of $O(h^2)$.

In this note, we prove that the algorithm FDM_1 converges at a rate of $O(h)$, and that FDM_2 converges at a rate of $O(h^2)$.

2. Convergence

We start by defining

$$\begin{aligned}\mathcal{F}^1(\vec{x}) &= -\nabla \cdot (\tilde{f}(\vec{x})\nabla u / \|\nabla u\|), \\ \mathcal{F}^2(\vec{x}) &= -\nabla \cdot (\mathcal{F}^1(\vec{x})\nabla u / \|\nabla u\|^2).\end{aligned}\tag{12}$$

Lemma 2.1. *If $f \in C^1(B_x)$, $u \in C^2(B_x)$, then*

$$\int_{\mathbb{R}^n} H(u)\mathcal{F}^1(\vec{x})d\vec{x} = \int_{\Gamma} f(\vec{x})ds.\tag{13}$$

If $f \in C^2(B_x)$, $u \in C^3(B_x)$, then

$$\int_{\mathbb{R}^n} I(u)\mathcal{F}^2(\vec{x})d\vec{x} = \int_{\Gamma} f(\vec{x})ds.\tag{14}$$

Proof. For (14), we integrate by parts:

$$\begin{aligned}\int_{\mathbb{R}^n} I(u)\mathcal{F}^2(\vec{x})d\vec{x} &= -\int_{\mathbb{R}^n} I(u)\nabla \cdot (\mathcal{F}^1(\vec{x})\nabla u / \|\nabla u\|^2)d\vec{x} \\ &= -\int_{\mathbb{R}^n} \nabla \cdot (I(u)\mathcal{F}^1(\vec{x})\nabla u / \|\nabla u\|^2)d\vec{x} + \int_{\mathbb{R}^n} \nabla I(u) \cdot (\mathcal{F}^1(\vec{x})\nabla u / \|\nabla u\|^2)d\vec{x} \\ &= \int_{\mathbb{R}^n} H(u)\nabla u \cdot (\mathcal{F}^1(\vec{x})\nabla u / \|\nabla u\|^2)d\vec{x} = \int_{\mathbb{R}^n} H(u)\mathcal{F}^1(\vec{x})d\vec{x}.\end{aligned}\tag{15}$$

Here, we have used the fact that the first integral on the second line vanishes; this results from the fact that the quantity in parentheses is compactly supported.

Both (13) and (14) will be established as soon as we verify (13). For this we use the divergence theorem:

$$\begin{aligned}\int_{\mathbb{R}^n} H(u)\mathcal{F}^1(\vec{x})d\vec{x} &= -\int_{\mathbb{R}^n} H(u)\nabla \cdot (\tilde{f}(\vec{x})\nabla u / \|\nabla u\|)d\vec{x} = -\int_{\Omega} \nabla \cdot (\tilde{f}(\vec{x})\nabla u / \|\nabla u\|)d\vec{x} \\ &= -\int_{\Gamma} (\tilde{f}(\vec{x})\nabla u / \|\nabla u\|) \cdot \vec{n}ds = \int_{\Gamma} f(\vec{x})ds,\end{aligned}\tag{16}$$

and the proof is complete. \square

We can now state our convergence rate theorem.

Theorem 2.1. *If $f \in C^3(B_x)$, $u \in C^4(B_x)$, then $\mathcal{I}^{1,h} \rightarrow \int_{\Gamma} f(\vec{x})ds$ as $h \rightarrow 0$, and*

$$\mathcal{I}^{1,h} = \int_{\Gamma} f(\vec{x})ds + O(h).\tag{17}$$

If $f \in C^4(B_x)$, $u \in C^5(B_x)$, then $\mathcal{I}^{2,h} \rightarrow \int_{\Gamma} f(\vec{x})ds$ as $h \rightarrow 0$, and

$$\mathcal{I}^{2,h} = \int_{\Gamma} f(\vec{x})ds + O(h^2).\tag{18}$$

Proof. We first prove the assertion concerning $\mathcal{I}^{2,h}$. Define

$$\begin{aligned} \mathcal{F}_k^{1,h} &= -\nabla^h \cdot (\tilde{f}(\vec{x}_k) \nabla^h u_k / \|\nabla^h u_k\|), \\ \mathcal{F}_k^{2,h} &= -\nabla^h \cdot (\mathcal{F}_k^{1,h} \nabla^h u_k / \|\nabla^h u_k\|^2). \end{aligned} \tag{19}$$

Starting from the definitions,

$$\mathcal{I}^{2,h} = h^n \sum_{k \in \mathbb{Z}^n} \delta_k^{2,h} \tilde{f}(\vec{x}_k) \|\nabla^h u_k\| = h^n \sum_{k \in \mathbb{Z}^n} (\nabla^h H_k^{1,h} \cdot \nabla^h u_k / \|\nabla^h u_k\|^2) \tilde{f}(\vec{x}_k) \|\nabla^h u_k\|. \tag{20}$$

Here we have replaced f by \tilde{f} . This replacement is valid for sufficiently small h due to the fact that $\delta_k^{2,h}$ is zero if \vec{x}_k is more than an $O(h)$ distance from Γ . Summing this last quantity by parts using (5), and then recalling (19) yields

$$\mathcal{I}^{2,h} = h^n \sum_{k \in \mathbb{Z}^n} H_k^{1,h} \mathcal{F}_k^{1,h}. \tag{21}$$

We sum by parts again, arriving at

$$\mathcal{I}^{2,h} = h^n \sum_{k \in \mathbb{Z}^n} I(u_k) \mathcal{F}_k^{2,h}. \tag{22}$$

Due to the regularity assumptions about f and u , $\mathcal{F}_k^{2,h} = \mathcal{F}^2(\vec{x}_k) + O(h^2)$. Also, note that the number of indices k where either $\mathcal{F}_k^{2,h}$ or $\mathcal{F}^2(\vec{x}_k)$ is nonzero is $O(h^{-n})$. With these observations in mind, we have

$$\mathcal{I}^{2,h} = h^n \sum_{k \in \mathbb{Z}^n} I(u_k) \mathcal{F}^2(\vec{x}_k) + O(h^2). \tag{23}$$

Let R_k denote the grid cube centered at \vec{x}_k whose edges all have length h . Let K denote the set of indices k where $I(u) \mathcal{F}^2(\vec{x})$ is not identically zero on R_k . In view of (23), Lemma 2.1, and the fact that

$$\int_{\mathbb{R}^n} I(u) \mathcal{F}^2(\vec{x}) d\vec{x} = \sum_{k \in K} \int_{R_k} I(u) \mathcal{F}^2(\vec{x}) d\vec{x}, \tag{24}$$

the proof of (18) will be complete if we can show that

$$h^n \sum_{k \in K} I(u_k) \mathcal{F}^2(\vec{x}_k) = \sum_{k \in K} \int_{R_k} I(u) \mathcal{F}^2(\vec{x}) d\vec{x} + O(h^2). \tag{25}$$

Let K_1 denote the set of indices $k \in K$ where R_k does not intersect Γ , and let $K_2 = K \setminus K_1$. For $k \in K_1$, $I(u) \mathcal{F}^2(\vec{x}) \in C^2(R_k)$. The multi-dimensional version of the midpoint rule yields

$$h^n I(u_k) \mathcal{F}^2(\vec{x}_k) = \int_{R_k} I(u) \mathcal{F}^2(\vec{x}) d\vec{x} + O(h^{n+2}), \quad k \in K_1. \tag{26}$$

For $k \in K_2$, the regularity is lower: $I(u) \mathcal{F}^2(\vec{x}) \in \text{Lip}(R_k)$. Thus,

$$h^n I(u_k) \mathcal{F}^2(\vec{x}_k) = \int_{R_k} I(u) \mathcal{F}^2(\vec{x}) d\vec{x} + O(h^{n+1}), \quad k \in K_2. \tag{27}$$

Since $\mathcal{F}^2(\vec{x})$ has compact support, the number of indices $k \in K_1$ is $O(h^{-n})$. The number of indices $k \in K_2$ is $O(h^{1-n})$; this is due to the fact that Γ is a compact $n - 1$ -dimensional manifold. Combining these observations with (26) and (27), we have (25), and the proof of (18) is complete.

The proof of (17) is similar. After a single summation by parts, and then replacing $\mathcal{F}_k^{1,h}$ by $\mathcal{F}^1(\vec{x}_k)$, the proof reduces to showing that

$$h^n \sum_{k \in K} H(u_k) \mathcal{F}^1(\vec{x}_k) = \sum_{k \in K} \int_{R_k} H(u) \mathcal{F}^1(\vec{x}) d\vec{x} + O(h). \tag{28}$$

This time K is defined in terms of $H(u) \mathcal{F}^1(\vec{x})$. The analysis for $k \in K_1$ is basically the same as in the proof of (18), but for $k \in K_2$, we can only guarantee that $H(u) \mathcal{F}^1(\vec{x})$ is bounded, and so

Table 1
Numerical example—integral of curvature of ellipse in \mathbb{R}^2

h	FDM ₁ (256)		FDM ₂ (16)	
	Error	Rate	Error	Rate
.32	3.30e−3		3.30e−3	
.16	1.07e−3	1.6	7.91e−4	2.1
.08	3.77e−4	1.5	1.96e−4	2.0
.04	9.63e−5	2.0	4.86e−5	2.0
.02	3.47e−5	1.5	1.22e−5	2.0
.01	1.61e−5	1.1	3.04e−6	2.0
.005	5.09e−6	1.7	7.56e−7	2.0

$$h^n H(u_{\mathbf{k}}) \mathcal{F}^1(\vec{x}_{\mathbf{k}}) = \int_{R_{\mathbf{k}}} H(u) \mathcal{F}^1(\vec{x}) d\vec{x} + O(h^n), \quad \mathbf{k} \in K_2. \quad (29)$$

The remainder of the proof of (17) is essentially the same as that of (18), the main ingredients being Lemma 2.1 and the fact that the sizes of the sets K_1 and K_2 are $O(h^{-n})$ and $O(h^{1-n})$ respectively. \square

3. A numerical example

The previous paper [16] contains a number of computational experiments, which we need not repeat here. However, since we worked with a slightly different version of FDM₂ in that paper, we provide one numerical example by way of indicating that the two versions give similar results. For this purpose we use Example 4 of [16]. Γ is the ellipse $x^2/9 + y^2/4 = 1$, and $f(x, y) = \nabla \cdot (\nabla u(x, y) / \|\nabla u(x, y)\|)$ where $u(x, y) = 1 - (x^2/9 + y^2/4)$, so that

$$\mathcal{I} = \int_{\Gamma} \kappa(x, y) ds = 2\pi, \quad (30)$$

where $f(x, y) = \kappa(x, y)$ is the curvature of Γ . Integrals of curvature like (30) arise in level set applications [10]. We use centered differences to approximate $\kappa(x_j, y_k)$ using the grid-defined values of u , the idea being to simulate how the method would be used in applications. Also, we rotate the mesh by 45° to reduce possible error cancellation due to symmetry. Table 1 demonstrates results that are similar to those obtained for this example in [16]. As expected, FDM₂ is converging at a rate of $O(h^2)$. FDM₁ seems to be converging at a rate of at least $O(h)$. For FDM₁ we averaged the absolute values of the relative errors over 256 small random grid shifts, while for FDM₂, we averaged over only 16. This is a reflection of the fact that FDM₂ is much more stable under small grid shifts. FDM₁ can be stabilized somewhat by smoothing the Heaviside function a small amount, as we did in [16]. We did not apply any smoothing here.

Acknowledgments

In the proof of Theorem 2.1, the idea of analyzing separately the regular grid points (those $\vec{x}_{\mathbf{k}}$ with $\mathbf{k} \in K_1$) and the irregular grid points (those $\vec{x}_{\mathbf{k}}$ with $\mathbf{k} \in K_2$) is borrowed from Beale [1].

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