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Surface Fitting and Numerical Gradient Computations by Discrete Mollification

S. ZHAN* AND D. A. MURIO†
Department of Mathematical Sciences
University of Cincinnati
Cincinnati, OH 45221-0025, U.S.A.
zhans@math.uc.edu diego@dmurio.csm.uc.edu

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Abstract—We review the δ-mollification procedure for automatic fitting of surfaces defined from discrete noisy data functions in $\mathbf{R}^2$. As a further application, the stable numerical computation of gradient fields from discrete noisy data is also investigated. The main features of the algorithm are:

1. information about the noise is needed;
2. the mollification parameters are chosen automatically by means of the Generalized Cross Validation (GCV) procedure.

A complete error analysis of the method is provided together with several numerical examples of interest.

Keywords—Ill-posed problems, Discrete mollification, Automatic filtering.

1. INTRODUCTION

It is well known that appropriate regularization techniques are crucial for solving ill-posed problems. In this paper, we analyze an automatic δ-mollification procedure to approximately solve two related identification problems: given a discrete noisy data function defined on a bounded domain in $\mathbf{R}^2$, recover an underlying smooth fitting surface (well-posed problem) and the corresponding gradient field (ill-posed problem).

2. MOLLIFICATION

The mollification method is a filtering procedure that has been proven to be effective for the regularization of a variety of ill-posed problems [1]. In this section, we introduce the mollification method in $\mathbf{R}^2$ and prove the main results.

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2.1. Abstract Setting

Recall that for a function f which is integrable on $[0,1] \subset \mathbf{R}^1$, the δ-mollification with parameters $\delta_1 > 0$, $p_1 > 0$ is defined, for every $t \in [p_1\delta_1, 1 - p_1\delta_1]$, by

$$J_\delta f(t) = \int_0^1 \rho_{\delta_1,p_1}(t-s) f(s)\, ds,$$

where the δ-mollifier $\rho_{\delta_1,p_1}(t)$ is given by

$$\rho_{\delta_1,p_1}(t) = \begin{cases} A_{p_1}\delta_1^{-1} \exp\left(-\dfrac{t^2}{\delta_1^2}\right), & |t| \le p_1\delta_1, \\ 0, & \text{otherwise,} \end{cases}$$

with $A_{p_1} = (\int_{-p_1}^{p_1} \exp(-s^2)\, ds)^{-1}$.

We now consider the δ-mollification for functions with two independent variables. Let $x = (x_1, x_2)$, $p = (p_1, p_2)$, and $\delta = (\delta_1, \delta_2)$, $p_i > 0$, $\delta_i > 0$, $x_i \in \mathbf{R}^1$ $(i = 1, 2)$. We use the following notations for simplicity:

$$\begin{aligned} I &= [0,1] \times [0,1], \\ |\delta|_\infty &= \max(\delta_1, \delta_2), \\ |\delta|_{-\infty} &= \min(\delta_1, \delta_2), \\ I_p &= [-p_1, p_1] \times [-p_2, p_2], \\ I_{p\delta} &= [-p_1\delta_1, p_1\delta_1] \times [-p_2\delta_2, p_2\delta_2], \\ I_\delta &= [p_1\delta_1, 1 - p_1\delta_1] \times [p_2\delta_2, 1 - p_2\delta_2]. \end{aligned}$$

It should be noticed that the set I_δ is nonempty whenever $p_i < (1/2\delta_i)$ $(i = 1, 2)$.

For a function which is integrable on $\mathbf{R}^2$, the δ-mollification with parameters δ, p is based on the convolution with the kernel

$$\varphi_{\delta,p}(x) = \rho_{\delta_1,p_1}(x_1)\rho_{\delta_2,p_2}(x_2) \equiv \begin{cases} A_p\delta_1^{-1}\delta_2^{-1} \exp\left(-\left(\dfrac{x_1^2}{\delta_1^2} + \dfrac{x_2^2}{\delta_2^2}\right)\right), & x \in I_{p\delta}, \\ 0, & \text{otherwise,} \end{cases}$$

where $A_p = (\int_{I_p} \exp(-\|x\|^2)\, dx)^{-1}$, $\|x\|^2 = x_1^2 + x_2^2$.

The δ-mollifier $\varphi_{\delta,p}$ is a nonnegative $C^\infty(I_{p\delta})$ function vanishing outside $I_{p\delta}$ and satisfying $\int_{I_{p\delta}} \varphi_{\delta,p}(x)\, dx = 1$.

If $f(x)$ is integrable on I, we define its δ-mollification on I_δ by the convolution

$$J_\delta f(x) = \int_I \varphi_\delta(x-s) f(s)\, ds,$$

where the p-dependency on the kernel has been dropped for simplicity.

Notice that $J_\delta f(x) = J_{\delta_1}(J_{\delta_2} f(x_1, x_2)) = J_{\delta_2}(J_{\delta_1} f(x_1, x_2))$ where $J_{\delta_i} f(x_1, x_2)$ $(i = 1, 2)$ denotes the δ-mollification of f with parameters δ_i, p_i with respect to the variable x_i.

The δ-mollification of an integrable function satisfies well-known consistency and stability estimates. In what follows, C will represent a generic constant independent of δ.

THEOREM 2.1. L^2 NORM CONVERGENCE. *If $f(x) \in L^2(I)$, then*

$$\lim_{\delta \to (0,0)} \|J_\delta f - f\|_{L^2(I_\delta)} = 0.$$

PROOF. For any $x \in I_\delta$,

$$\begin{aligned} J_\delta f(x) - f(x) &= \int_I \varphi_\delta(x-s) f(s)\, ds - f(x) \\ &= \int_I \varphi_\delta(x-s)(f(s) - f(x))\, ds \\ &= \int_{I_{p\delta}} \varphi_\delta(-y)(f(x+y) - f(x))\, dy, \end{aligned}$$

after the change of variables $y = s - x$. Consequently, by Hölder inequality,

$$\begin{aligned} |J_\delta f(x) - f(x)|^2 &\le \int_{I_{p\delta}} (\varphi_\delta(-y))^2\, dy \int_{I_{p\delta}} |f(x+y) - f(x)|^2\, dy \\ &\le \frac{A_p}{\delta_1 \delta_2} \int_{I_{p\delta}} (f(x+y) - f(x))^2\, dy. \end{aligned}$$

Therefore,

$$\begin{aligned} \|J_\delta f - f\|^2_{L^2(I_\delta)} &\le \frac{A_p}{\delta_1\delta_2} \int_{I_\delta} \int_{I_{p\delta}} |f(x+y) - f(x)|^2\, dy\, dx \\ &= \frac{A_p}{\delta_1\delta_2} \int_{I_{p\delta}} \int_{I_\delta} |f(x+y) - f(x)|^2\, dx\, dy. \end{aligned}$$

By the continuity of L^2 functions with respect to their norm, $\forall \varepsilon > 0$, $\exists\, \beta > 0$, such that whenever $\|y\| < \beta$,

$$\int_I |f(x+y) - f(x)|^2\, dx < \varepsilon^2.$$

This implies that for $0 < \delta_i < (\beta/4p_i)$ $(i = 1, 2)$,

$$\|J_\delta f - f\|^2_{L^2(I_\delta)} \le \frac{A_p}{\delta_1\delta_2} 4p_1\delta_1 p_2 \delta_2 \varepsilon^2 = 4p_1p_2A_p\varepsilon^2$$

and the theorem follows.

COROLLARY 2.2. *If $\nabla f(x) \in L^2(I) \times L^2(I)$, then*

$$\lim_{\delta \to (0,0)} \|\nabla(J_\delta f) - \nabla f\|_{L^2(I_\delta)\times L^2(I_\delta)} = 0,$$

where the norm $\|(f_1, f_2)\|_{L^2 \times L^2} = \sqrt{\|f_1\|^2_{L^2} + \|f_2\|^2_{L^2}}$ is defined for $(f_1, f_2) \in L^2 \times L^2$.

REMARK. This result shows that the gradient of the mollified function approximates the gradient of the function in L^2. Consequently, we shall concentrate on developing an approximation to the smooth function $\nabla(J_\delta f)$.

LEMMA 2.3. MAXIMUM NORM CONSISTENCY. *If $f(x)$ is uniformly Lipschitz on I, with Lipschitz constant L, then there exists a constant C such that*

$$\|J_\delta f - f\|_{\infty, I_\delta} \le C\, |\delta|_\infty.$$

PROOF. For any $x \in I_\delta$,

$$\begin{aligned}|J_\delta f(x) - f(x)| &= \left|\int_I \varphi_\delta(x-s)f(s)\,ds - f(x)\right| \\ &\le \int_I |\varphi_\delta(x-s)(f(s)-f(x))|\,ds \\ &= \int_{I_{p\delta}} \varphi_\delta(-y)|f(x+y)-f(x)|\,dy \\ &\le L\int_{I_{p\delta}} \varphi_\delta(-y)\|y\|\,dy \\ &= \frac{4LA_p}{\delta_1\delta_2}\int_0^{p_1\delta_1}\int_0^{p_2\delta_2} \exp\left(-\left(\frac{y_1^2}{\delta_1^2}+\frac{y_2^2}{\delta_2^2}\right)\right)\|y\|\,dy_1\,dy_2 \\ &\le 4LA_p\int_0^{p_1}\int_0^{p_2}\exp\left(-\left(y_1^2+y_2^2\right)\right)(\delta_1 y_1+\delta_2 y_2)\,dy_1\,dy_2 \\ &\le 4LA_p\left[\frac{\sqrt{\pi}}{2}\delta_1\int_0^{p_1}\exp\left(-y_1^2\right)\ y_1\,dy_1 + \frac{\sqrt{\pi}}{2}\delta_2\int_0^{p_2}\exp\left(-y_2^2\right)\ y_2\,dy_2\right] \\ &\le \sqrt{\pi}LA_p(\delta_1+\delta_2) \\ &\le 2\sqrt{\pi}LA_p|\delta|_\infty.\end{aligned}$$

COROLLARY 2.4. *If $\frac{\partial}{\partial x_1}f(x)$ and $\frac{\partial}{\partial x_2}f(x)$ are uniformly Lipschitz on I, then*

$$\|\nabla(J_\delta f) - \nabla f\|_{\infty,I_\delta} \le C|\delta|_\infty,$$

where for $(f_1,f_2)\in C(I)\times C(I)$, the norm is defined by $\|(f_1,f_2)\|_{\infty,I} = \max\left(\|f_1\|_{\infty,I},\|f_2\|_{\infty,I}\right)$.

LEMMA 2.5. MAXIMUM NORM STABILITY. *If $f(x)$, $f^\epsilon(x)$ are integrable on I and $\operatorname{Sup}_{x\in I}|f(x)-f^\epsilon(x)|\le\epsilon$, then there exists a constant C such that*

$$\|J_\delta f - J_\delta f^\epsilon\|_{\infty,I_\delta}\le\epsilon \quad \text{and} \quad \|\nabla(J_\delta f)-\nabla(J_\delta f^\epsilon)\|_{\infty,I_\delta}\le C\frac{\epsilon}{|\delta|_{-\infty}}.$$

PROOF. The first estimate follows immediately from $\int_{I_{p\delta}}\varphi_{\delta,p}(x)\,dx = 1$. We prove the second inequality. For $x\in I_\delta$,

$$\begin{aligned}&\left|\frac{\partial(J_\delta f)}{\partial x_1}(x) - \frac{\partial(J_\delta f^\epsilon)}{\partial x_1}(x)\right| \\ &= \left|\frac{\partial}{\partial x_1}\left(\int_I \varphi_\delta(x-s)[f(s)-f^\epsilon(s)]\,ds\right)\right| \\ &= \left|\frac{\partial}{\partial x_1}\left(\int_{x_1-p_1\delta_1}^{x_1+p_1\delta_1}\int_{x_2-p_2\delta_2}^{x_2+p_2\delta_2}\varphi_\delta(x-s)[f(s)-f^\epsilon(s)]\,ds_2\,ds_1\right)\right| \\ &= \left|\int_{x_2-p_2\delta_2}^{x_2+p_2\delta_2}\varphi_\delta(-p_1\delta_1,x_2-s_2)[f(x_1+p_1\delta_1,s_2)-f^\epsilon(x_1+p_1\delta_1,s_2)]\,ds_2\right. \\ &\quad -\int_{x_2-p_2\delta_2}^{x_2+p_2\delta_2}\varphi_\delta(p_1\delta_1,x_2-s_2)[f(x_1-p_1\delta_1,s_2)-f^\epsilon(x_1-p_1\delta_1,s_2)]\,ds_2 \\ &\quad \left.+\int_{x_1-p_1\delta_1}^{x_1+p_1\delta_1}\int_{x_2-p_2\delta_2}^{x_2+p_2\delta_2}\frac{\partial}{\partial x_1}\varphi_\delta(x-s)[f(s)-f^\epsilon(s)]\,ds_2\,ds_1\right| \\ &\le \sqrt{\pi}A_p\frac{\epsilon}{\delta_1}+\sqrt{\pi}A_p\frac{\epsilon}{\delta_1}+\epsilon\int_{I_{p\delta}}\left|\frac{\partial}{\partial x_1}\varphi_\delta(-y)\right|\,dy \\ &= 2\sqrt{\pi}A_p\frac{\epsilon}{\delta_1}+A_p\frac{\epsilon}{\delta_2}\left(\int_{-p_2\delta_2}^{p_2\delta_2}\exp\left(-\frac{y_2^2}{\delta_2^2}\right)\,dy_2\right)\frac{2}{\delta_1^3}\left(\int_{-p_1\delta_1}^{p_1\delta_1}\exp\left(-\frac{y_1^2}{\delta_1^2}\right)|y_1|\,dy_1\right) \\ &\le 4\sqrt{\pi}A_p\frac{\epsilon}{\delta_1}.\end{aligned}$$

Similarly,

$$\left|\frac{\partial(J_\delta f)}{\partial x_2}(x) - \frac{\partial(J_\delta f^\epsilon)}{\partial x_2}(x)\right| \le 4\sqrt{\pi} A_p \frac{\epsilon}{\delta_2}.$$

By the previous two lemmas, we have proved the following convergence theorem.

THEOREM 2.6. MAXIMUM NORM CONVERGENCE. *If $\frac{\partial f}{\partial x_1}(x)$ and $\frac{\partial f}{\partial x_2}(x)$ are uniformly Lipschitz on I, and f^ϵ is integrable satisfying* $\mathrm{Sup}_{x\in I}|f(x) - f^\epsilon(x)| \le \epsilon$, *then*

$$\|J_\delta f^\epsilon - f\|_{\infty, I_\delta} \le C|\delta|_\infty + \epsilon \quad \text{and} \quad \|\nabla(J_\delta f^\epsilon) - \nabla f\|_{\infty, I_\delta} \le C\left(|\delta|_\infty + \frac{\epsilon}{|\delta|_{-\infty}}\right).$$

We observe that in order to obtain convergence as $\epsilon \to 0$, in the first case it suffices to consider $|\delta|_\infty \to 0$, but in the second case we need to relate both parameters (ϵ and δ). For example, we can choose $\delta_i = O(\sqrt{\epsilon})$, $i = 1, 2$. This is a consequence of the ill-posedness of differentiation of noisy data.

From the proof of Lemma 2.5, if $f(x)$ is bounded and integrable on I, then we have

$$\|\nabla(J_\delta f)\|_{\infty, I_\delta} \le \frac{4\sqrt{\pi} A_p}{|\delta|_{-\infty}} \|f\|_{\infty, I}.$$

This implies that ∇J_δ is a bounded operator with

$$\|\nabla J_\delta\| \le \frac{4\sqrt{\pi} A_p}{|\delta|_{-\infty}}.$$

The boundedness of ∇J_δ explains the restoration of continuity with respect to perturbations in the data for differentiation by mollification.

3. DISCRETE MOLLIFICATION

In this section, we consider the δ-mollification of a discrete function defined on the discrete set $K = \{(x_1^{(i)}, x_2^{(j)}) : 1 \le i \le m, 1 \le j \le n\} \subset I$, with

$$0 \le x_1^{(1)} < x_1^{(2)} < \cdots < x_1^{(m)} \le 1, \qquad 0 \le x_2^{(1)} < x_2^{(2)} < \cdots < x_2^{(n)} \le 1.$$

Set

$$\begin{aligned} s_1^{(0)} &= 0, \qquad s_1^{(m)} = 1, \qquad s_2^{(0)} = 0, \qquad s_2^{(n)} = 1, \\ s_1^{(i)} &= \frac{1}{2}\left(x_1^{(i)} + x_1^{(i+1)}\right), \qquad (i = 1, 2, \dots, m-1), \\ s_2^{(j)} &= \frac{1}{2}\left(x_2^{(j)} + x_2^{(j+1)}\right), \qquad (j = 1, 2, \dots, n-1), \\ \Delta x &= \max_{1\le i\le m-1,\ 1\le j\le n-1} \sqrt{\left|x_1^{(i+1)} - x_1^{(i)}\right|^2 + \left|x_2^{(j+1)} - x_2^{(j)}\right|^2}. \end{aligned}$$

Let $G = \{g_{ij} : 1 \le i \le m,\ 1 \le j \le n\}$ be a discrete function defined on K. The discrete δ-mollification of G is defined as follows.

For $x \in I_\delta$,

$$J_\delta G(x) = \sum_{i=1}^{m} \sum_{j=1}^{n} \left(\int_{s_1^{(i-1)}}^{s_1^{(i)}} \int_{s_2^{(j-1)}}^{s_2^{(j)}} \varphi_\delta(x - s)\, ds_1\, ds_2 \right) g_{ij}.$$

Notice that $\sum_{i=1}^{m} \sum_{j=1}^{n} (\int_{s_1^{(i-1)}}^{s_1^{(i)}} \int_{s_2^{(j-1)}}^{s_2^{(j)}} \varphi_\delta(x - s)\, ds_1\, ds_2) = \int_{I_{p\delta}} \varphi_\delta(-s)\, ds = 1$.

The consistency estimates for the discrete δ-mollification are presented in the following lemma.

LEMMA 3.1. MAXIMUM NORM CONSISTENCY OF DISCRETE MOLLIFICATION. *Let $g(x)$ be defined on I, $G = \{g_{ij} : 1 \le i \le m,\ 1 \le j \le n\}$ be the discrete version of g with $g_{ij} = g(x_1^{(i)}, x_2^{(j)})$.*

(1) *If g is uniformly Lipschitz on I with Lipschitz constant L, then there exists a constant C such that*

$$\|J_\delta G - g\|_{\infty, I_\delta} \le C(|\delta|_\infty + \Delta x).$$

(2) *If $\frac{\partial g}{\partial x_1}$ and $\frac{\partial g}{\partial x_1}$ are uniformly Lipschitz on I with Lipschitz constant L, then there exists a constant C such that*

$$\|\nabla(J_\delta G) - \nabla g\|_{\infty, I_\delta} \le C\left(|\delta|_\infty + \frac{\Delta x}{|\delta|_{-\infty}}\right).$$

PROOF. For $x \in I_\delta$,

$$|J_\delta G(x) - J_\delta g(x)| \le \sum_{i=1}^{m}\sum_{j=1}^{n}\int_{s_1^{(i-1)}}^{s_1^{(i)}}\int_{s_2^{(j-1)}}^{s_2^{(j)}} \varphi_\delta(x-s)|g_{ij} - g(s)|\,ds_1\,ds_2 \le L\Delta x.$$

By Lemma 2.3 and the triangle inequality, Part (1) follows.

To prove Part (2), observe that

$$\begin{aligned}
&\left|\frac{\partial}{\partial x_1}(J_\delta G(x) - J_\delta g(x))\right| \\
&\le \sum_{i=1}^{m}\sum_{j=1}^{n}\int_{s_1^{(i-1)}}^{s_1^{(i)}}\int_{s_2^{(j-1)}}^{s_2^{(j)}} \left|\frac{\partial}{\partial x_1}\varphi_\delta(x-s)\right| |g_{ij} - g(s)|\,ds_1\,ds_2 \\
&\le L\Delta x \int_{I_{p\delta}} \left|\frac{\partial}{\partial x_1}\varphi_\delta(-y)\right| dy \\
&= L\Delta x \frac{A_p}{\delta_2}\left(\int_{-p_2\delta_2}^{p_2\delta_2} \exp\left(-\frac{y_2^2}{\delta_2^2}\right) dy_2\right)\frac{2}{\delta_1^3}\left(\int_{-p_1\delta_1}^{p_1\delta_1} \exp\left(-\frac{y_1^2}{\delta_1^2}\right)|y_1|\,dy_1\right) \\
&\le 2LA_p\sqrt{\pi}\frac{\Delta x}{\delta_1}.
\end{aligned}$$

Similarly,

$$\left|\frac{\partial}{\partial x_1}(J_\delta G(x) - J_\delta g(x))\right| \le 2LA_p\sqrt{\pi}\frac{\Delta x}{\delta_2}.$$

Hence, Part (2) follows from the triangle inequality and Corollary 2.4.

In most applications, the only available data is a perturbed discrete version of g, denoted $G^\epsilon = \{g_{ij}^\epsilon : 1 \le i \le m,\ 1 \le j \le n\}$, satisfying $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, where $G = \{g_{ij} : 1 \le i \le m,\ 1 \le j \le n\}$ with $g_{ij} = g(x_1^{(i)}, x_2^{(j)})$. The stability of the discrete δ-mollification is proved in the following lemma.

LEMMA 3.2. MAXIMUM NORM STABILITY OF DISCRETE MOLLIFICATION. *If the discrete functions G and G^ϵ satisfy $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, then*

$$\|J_\delta G^\epsilon - J_\delta G\|_{\infty, I_\delta} \le \epsilon, \quad \text{and} \quad \|\nabla(J_\delta G^\epsilon) - \nabla(J_\delta G)\|_{\infty, I_\delta} \le C\frac{\epsilon}{|\delta|_{-\infty}}.$$

PROOF. We prove the second inequality. For $x \in I_\delta$, $i = 1, 2$,

$$\begin{aligned}
&\left|\frac{\partial(J_\delta G^\epsilon)}{\partial x_i}(x) - \frac{\partial(J_\delta G)}{\partial x_i}(x)\right| \\
&= \left|\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\int_{s_1^{(i-1)}}^{s_1^{(i)}}\int_{s_2^{(j-1)}}^{s_2^{(j)}} \frac{\partial}{\partial x_i}\varphi_\delta(x-s)\,ds_1\,ds_2\right)\left(g_{ij}-g_{ij}^\epsilon\right)\right| \\
&\le \epsilon \int_I \left|\frac{\partial}{\partial x_i}\varphi_\delta(x-s)\right| ds \\
&\le 2A_p\sqrt{\pi}\frac{\epsilon}{\delta_i}.
\end{aligned}$$

The next theorem indicates that the discrete δ-mollification of G^ϵ is a reasonable approximation of the function g.

THEOREM 3.3. MAXIMUM NORM CONVERGENCE OF DISCRETE MOLLIFICATION. *Let g be uniformly Lipschitz on I, with Lipschitz constant L. If G is its discrete version on K and G^ϵ is a discrete function on K satisfying $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, then there exists a constant C such that*

$$\|J_\delta G^\epsilon - g\|_{\infty,I_\delta} \le C(\epsilon + |\delta|_\infty + \Delta x).$$

PROOF. The result is obtained immediately from Lemmas 3.1, 3.2, and the triangle inequality.

NOTE. The corresponding abstract convergence statement readily follows: $\|J_\delta G^\epsilon - g\|_{\infty,I_\delta} \to 0$, as $\epsilon, \Delta x \to 0$, and $\delta \to (0,0)$. The numerical convergence result establishes that the computed mollified function $J_\delta G^\epsilon$ converges to the mollified function $J_\delta g$. More precisely, we have the following.

THEOREM 3.4. MAXIMUM NORM NUMERICAL CONVERGENCE OF DISCRETE MOLLIFICATION. *Under the conditions of Theorem 3.3, there exists a constant C, such that*

$$\|J_\delta G^\epsilon - J_\delta g\|_{\infty,I_\delta} \le C(\epsilon + \Delta x).$$

PROOF. By Lemma 3.2 and

$$|J_\delta G(x) - J_\delta g(x)| \le L\Delta x, \qquad \text{for } x \in I_\delta,$$

the result follows from the triangle inequality.

3.1. Computation of the Gradient

This subsection discusses the main results on stable computation of numerical gradients by the mollification method.

THEOREM 3.5. MAXIMUM NORM CONVERGENCE OF THE GRADIENT COMPUTED BY DISCRETE MOLLIFICATION. *If $\frac{\partial g}{\partial x_i}$ $(i = 1, 2)$ are uniformly Lipschitz on I with Lipschitz constant L, G, G^ϵ as described in Theorem 3.3, then there exists a constant C such that*

$$\|\nabla(J_\delta G^\epsilon) - \nabla g\|_{\infty,I_\delta} \le C\left(|\delta|_\infty + \frac{\epsilon}{|\delta|_{-\infty}} + \frac{\Delta x}{|\delta|_{-\infty}}\right).$$

PROOF. The theorem follows immediately from Lemmas 3.1, 3.2, and the triangle inequality.

NOTE. The corresponding abstract convergence statement should prescribe a link between the parameters δ, ϵ, and Δx as $\epsilon \to 0$. We could establish convergence of $\nabla(J_\delta G^\epsilon)$ to ∇g by prescribing a rule as $\Delta x = \epsilon$ and $\delta_i = \sqrt{\epsilon}$ $(i = 1, 2)$.

A numerical convergence statement should relate $\nabla(J_\delta G^\epsilon)$ with $\nabla(J_\delta g)$, that is, the computed gradient and the gradient of the mollified version of g. This is presented in the following theorem which states that, for fixed δ, $\|\nabla(J_\delta G^\epsilon) - \nabla(J_\delta g)\|_{\infty,I_\delta} \to 0$, as ϵ, $\Delta x \to 0$.

THEOREM 3.6. MAXIMUM NORM NUMERICAL CONVERGENCE OF THE GRADIENT COMPUTED BY DISCRETE MOLLIFICATION. *Under the conditions of Theorem 3.3, there exists a constant C such that*

$$\|\nabla(J_\delta G^\epsilon) - \nabla(J_\delta g)\|_{\infty,I_\delta} \le C\left(\frac{\epsilon}{|\delta|_{-\infty}} + \frac{\Delta x}{|\delta|_{-\infty}}\right).$$

PROOF. By Lemma 3.2 and for $x \in I_\delta$, $i = 1, 2$,

$$\left|\frac{\partial(J_\delta G)}{\partial x_i}(x) - \frac{\partial(J_\delta g)}{\partial x_i}(x)\right| \le 2LA_p\sqrt{\pi}\frac{\Delta x}{\delta_i},$$

(see the proof of Lemma 3.1), the triangle inequality then yields the result.

Assuming from now on that

$$x_1^{(i)} - x_1^{(i-1)} = x_1^{(i+1)} - x_1^{(i)} \equiv \Delta x_1, \quad i = 2, \dots, m-1,$$
$$x_2^{(j)} - x_2^{(j-1)} = x_2^{(j+1)} - x_2^{(j)} \equiv \Delta x_2, \quad j = 2, \dots, n-1,$$

given G^ϵ, a perturbed discrete version of g, in order to approximate ∇g, instead of utilizing $\frac{\partial}{\partial x_i}\varphi_\delta$ and convolution with the noisy data G^ϵ, computations are carried out by using the centered differences of $J_\delta G^\epsilon$. That is, we use $\nabla_0(J_\delta G^\epsilon)$ to approximate $\nabla(J_\delta G^\epsilon)$ in $\widetilde{I}_\delta$. Here $\nabla_0 = (D_0^{(1)}, D_0^{(2)})$, $D_0^{(i)}$ $(i = 1, 2)$ denotes the centered difference operator with respect to the variable x_i, and

$$\widetilde{I}_\delta = [p_1\delta_1 + \Delta x_1, 1 - p_1\delta_1 - \Delta x_1] \times [p_2\delta_2 + \Delta x_2, 1 - p_2\delta_2 - \Delta x_2].$$

LEMMA 3.7. *Under the conditions of Theorem 3.5, there exist a constant C and a constant C_δ, depending on δ, such that*

$$\|\nabla_0(J_\delta G^\epsilon) - \nabla g\|_{\infty,\widetilde{I}_\delta} \le C\left(|\delta|_\infty + \frac{\epsilon}{|\delta|_{-\infty}} + \frac{\Delta x}{|\delta|_{-\infty}}\right) + C_\delta(\Delta x)^2.$$

PROOF. The result is a consequence of Theorem 3.5 and the estimate

$$|\nabla_0(J_\delta G^\epsilon)(x) - \nabla(J_\delta G^\epsilon)(x)| \le C_\delta(\Delta x)^2, \tag{$*$}$$

for $x \in \widetilde{I}_\delta$.

For fixed δ, as a direct consequence of $(*)$ and Theorem 3.6, a numerical convergence statement establishing convergence of $\|\nabla_0(J_\delta G^\epsilon) - \nabla J_\delta g\|_{\infty,\widetilde{I}_\delta}$ to zero as ϵ, $\Delta x \to 0$ is given by the following.

LEMMA 3.8. *Under the conditions of Theorem 3.3, there exist a constant C and a constant C_δ, depending on δ, such that*

$$\|\nabla_0\,(J_\delta G^\epsilon) - \nabla\,(J_\delta g)\|_{\infty,\widetilde{I}_\delta} \le C\left(\frac{\epsilon}{|\delta|_{-\infty}} + \frac{\Delta x}{|\delta|_{-\infty}}\right) + C_\delta(\Delta x)^2.$$

Let G be a discrete function on K and $\nabla_0^\delta G \equiv \nabla_0(J_\delta G)$. The next theorem states that ∇_0^δ is a bounded operator.

THEOREM 3.9. *There exists a constant C such that*

$$\left\|\nabla_0^\delta G\right\|_{\infty,\widetilde{I}_\delta} \le \frac{C}{|\delta|_{-\infty}}\|G\|_{\infty,K}.$$

PROOF. For $x \in \widetilde{I}_\delta$,

$$
\begin{aligned}
&\left|D_0^{(1)}(J_\delta G)(x)\right| \\
&= \left|\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\int_{s_1^{(i-1)}}^{s_1^{(i)}}\int_{s_2^{(j-1)}}^{s_2^{(j)}} D_0^{(1)}\varphi_\delta(x-s)\,ds_1\,ds_2\right) g_{ij}\right| \\
&\le \|G\|_{\infty,K}\int_I \left|D_0^{(1)}\varphi_\delta(x-s)\right| ds \\
&= \|G\|_{\infty,K}\int_I \frac{1}{2\Delta x_1}\left|\varphi_\delta(x_1+\Delta x_1-s_1,x_2-s_2)-\varphi_\delta(x_1-\Delta x_1-s_1,x_2-s_2)\right| ds \\
&= \|G\|_{\infty,K}\frac{1}{2\Delta x_1}\int_{-p_2\delta_2}^{p_2\delta_2}\int_{-p_1\delta_1-\Delta x_1}^{p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1-\Delta x_1,y_2)-\varphi_\delta(y_1+\Delta x_1,y_2)\right| dy_1\,dy_2.
\end{aligned}
$$

First, we consider the case $p_1\delta_1 \le \Delta x_1$. In such case, we have

$$
\begin{aligned}
&\int_{-p_1\delta_1-\Delta x_1}^{p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1-\Delta x_1,y_2)-\varphi_\delta(y_1+\Delta x_1,y_2)\right| dy_1 \\
&\quad= \int_{-p_1\delta_1-\Delta x_1}^{p_1\delta_1-\Delta x_1}\left|\varphi_\delta(y_1+\Delta x_1,y_2)\right| dy_1 + \int_{-p_1\delta_1+\Delta x_1}^{p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1-\Delta x_1,y_2)\right| dy_1 \\
&\quad= 2\int_{-p_1\delta_1}^{p_1\delta_1}\varphi_\delta(y_1,y_2)\,dy_1.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\left|D_0^{(1)}(J_\delta G)(x)\right| &\le \|G\|_{\infty,K}\frac{1}{\Delta x_1}\int_{I_{p\delta}}\varphi_\delta(y)\,dy \\
&= \|G\|_{\infty,K}\frac{1}{\Delta x_1} \\
&\le \frac{p_1^{-1}}{\delta_1}\|G\|_{\infty,K}.
\end{aligned}
$$

Now assuming $p_1\delta_1 > \Delta x_1$,

$$
\begin{aligned}
&\int_{-p_1\delta_1-\Delta x_1}^{p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1-\Delta x_1,y_2)-\varphi_\delta(y_1+\Delta x_1,y_2)\right| dy_1 \\
&\quad= \int_{-p_1\delta_1-\Delta x_1}^{-p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1+\Delta x_1,y_2)\right| dy_1 \qquad (**)
\end{aligned}
$$

$$
\begin{aligned}
&+\int_{-p_1\delta_1+\Delta x_1}^{p_1\delta_1-\Delta x_1}\left|\varphi_\delta(y_1-\Delta x_1,y_2)-\varphi_\delta(y_1+\Delta x_1,y_2)\right| dy_1 \qquad (**)(\text{cont.}) \\
&+\int_{p_1\delta_1-\Delta x_1}^{p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1-\Delta x_1,y_2)\right| dy_1.
\end{aligned}
$$

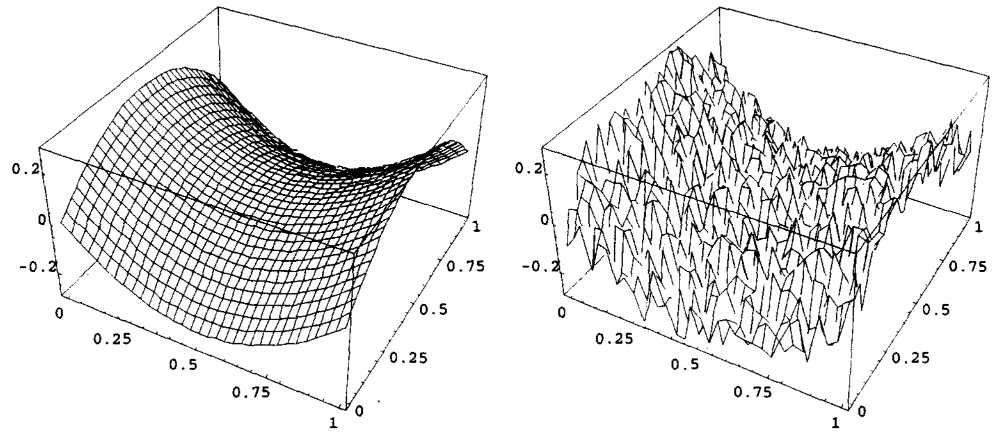
For the first and third terms in $(**)$, we have

$$
\begin{aligned}
&\int_{-p_1\delta_1-\Delta x_1}^{-p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1+\Delta x_1,y_2)\right| dy_1 \le 2\Delta x_1\varphi_\delta(0,y_2), \\
&\int_{p_1\delta_1-\Delta x_1}^{p_1\delta_1+\Delta x_1}\left|\varphi_\delta(y_1-\Delta x_1,y_2)\right| dy_1 \le 2\Delta x_1\varphi_\delta(0,y_2).
\end{aligned}
$$

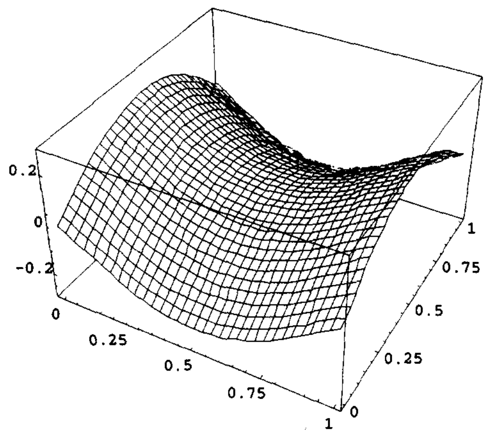
Using the fact that $\varphi_\delta(y_1-\Delta x_1,y_2) \ge \varphi_\delta(y_1+\Delta x_1,y_2)$ for $y_1 \in [0,p_1\delta_1-\Delta x_1]$, and a mean value theorem in the following form: if $f \in C[a-h,b+h]$, then there exist constants θ_i, with $|\theta_i| \le 1$ $(i=1,2)$ such that

$$
\int_a^b (f(x-h)-f(x+h))\,dx = 2h(f(a+\theta_1 h)-f(b+\theta_2 h)),
$$

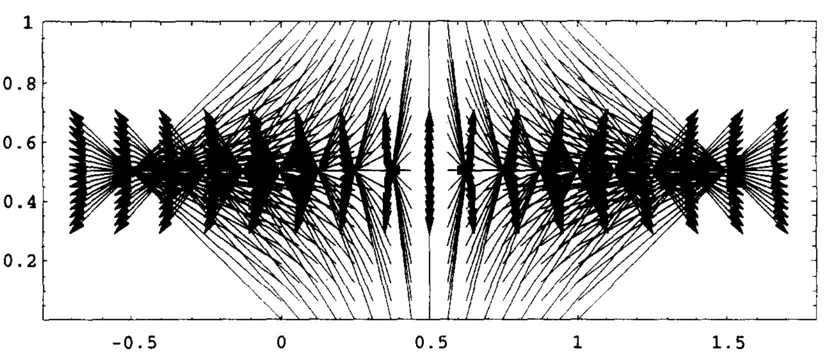
we obtain the following estimate for the second term in $(**)$:



(a) Exact and noisy surfaces, $\epsilon = 0.1$.



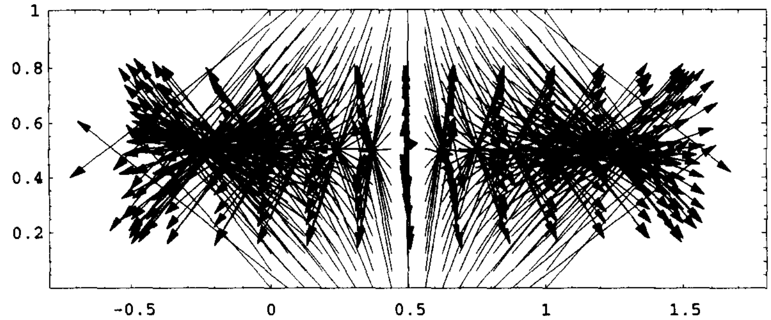
(b) Reconstructed surface.



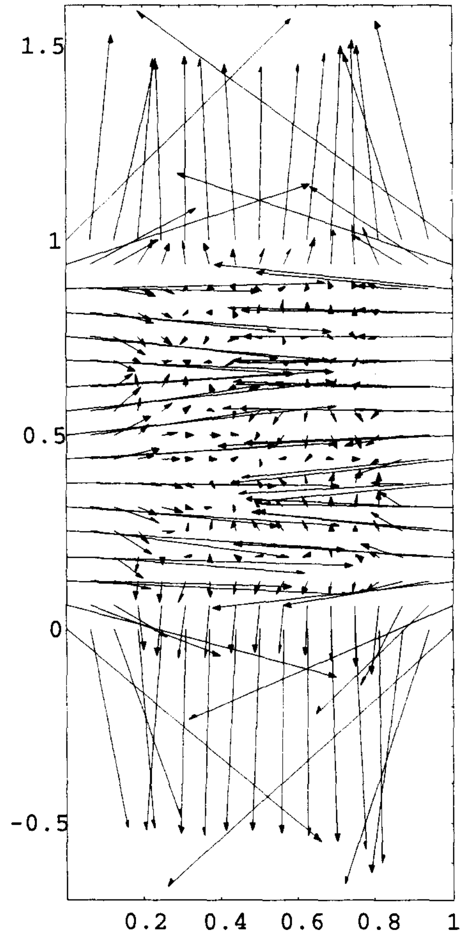
(c) Exact gradient field.

Figure 1.

$$\begin{aligned}
&\int_{-p_1\delta_1+\Delta x_1}^{p_1\delta_1-\Delta x_1} \left|\varphi_\delta(y_1-\Delta x_1, y_2) - \varphi_\delta(y_1+\Delta x_1, y_2)\right| dy_1 \\
&= 2\int_0^{p_1\delta_1-\Delta x_1} \left|\varphi_\delta(y_1-\Delta x_1, y_2) - \varphi_\delta(y_1+\Delta x_1, y_2)\right| dy_1 \\
&= 2\int_0^{p_1\delta_1-\Delta x_1} \left(\varphi_\delta(y_1-\Delta x_1, y_2) - \varphi_\delta(y_1+\Delta x_1, y_2)\right) dy_1 \\
&= 4\Delta x_1 (\varphi_\delta(\theta_1 \Delta x_1, y_2) - \varphi_\delta(p_1\delta_1 - \Delta x_1 + \theta_2\Delta x_1, y_2)) \\
&\le 4\Delta x_1 \varphi_\delta(0, y_2).
\end{aligned}$$



(d) Reconstructed gradient field.

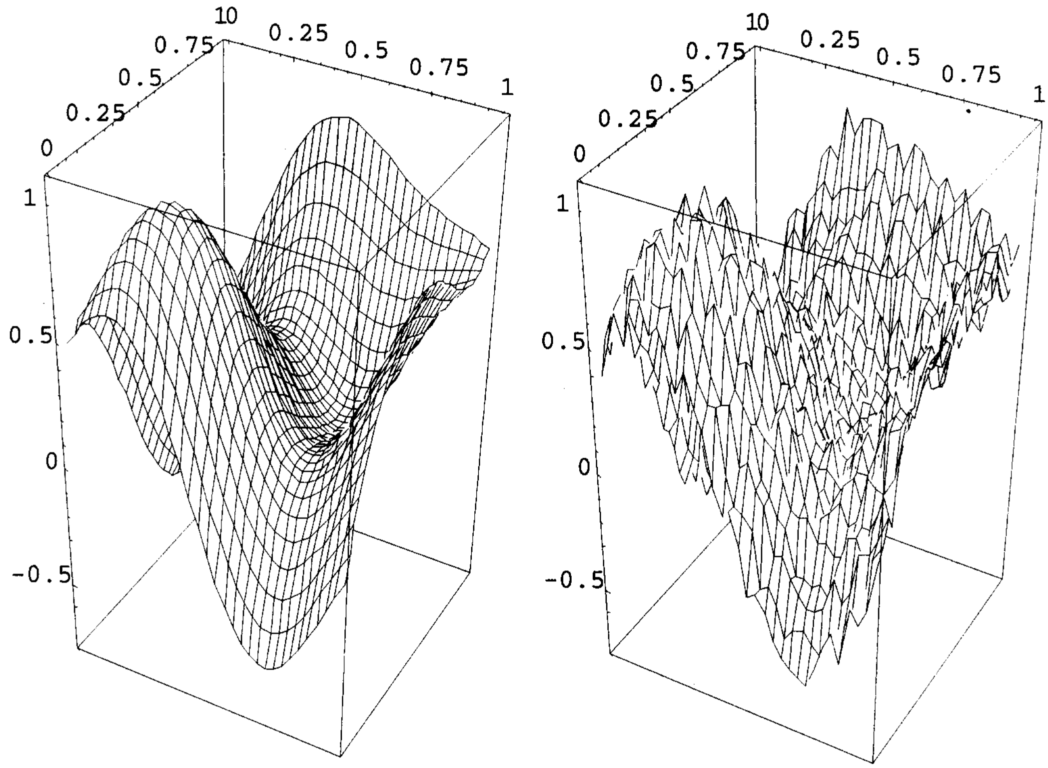


(e) Error gradient field: exact-computed.

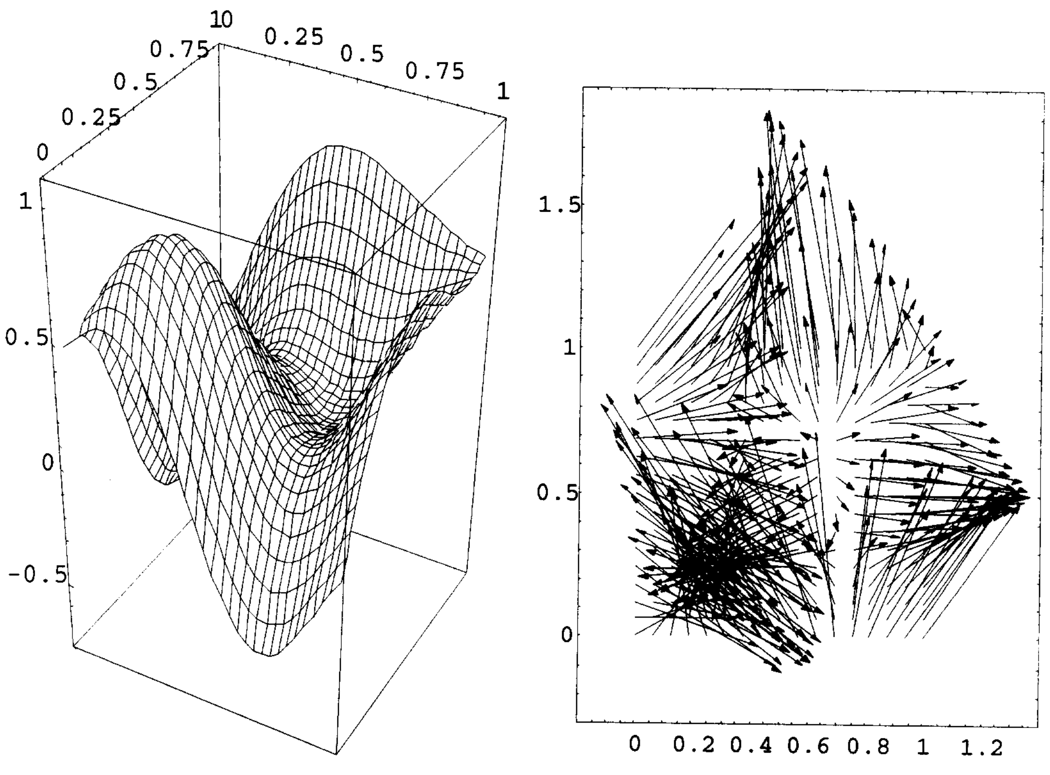
Figure 1. (cont.)

Consequently, for $p_1\delta_1 > \Delta x_1$,

$$
\begin{aligned}
\left|D_0^{(1)}(J_\delta G)(x)\right| &\le 4\|G\|_{\infty,K}\int_{-p_2\delta_2}^{p_2\delta_2}\varphi_\delta(0,y_2)\,dy_2\\
&= 4\|G\|_{\infty,K}\frac{A_p}{\delta_1}\int_{-p_2}^{p_2}\exp\left(-y_2^2\right)\,dy_2\\
&\le \frac{4\sqrt{\pi}A_p}{\delta_1}\|G\|_{\infty,K}.
\end{aligned}
$$

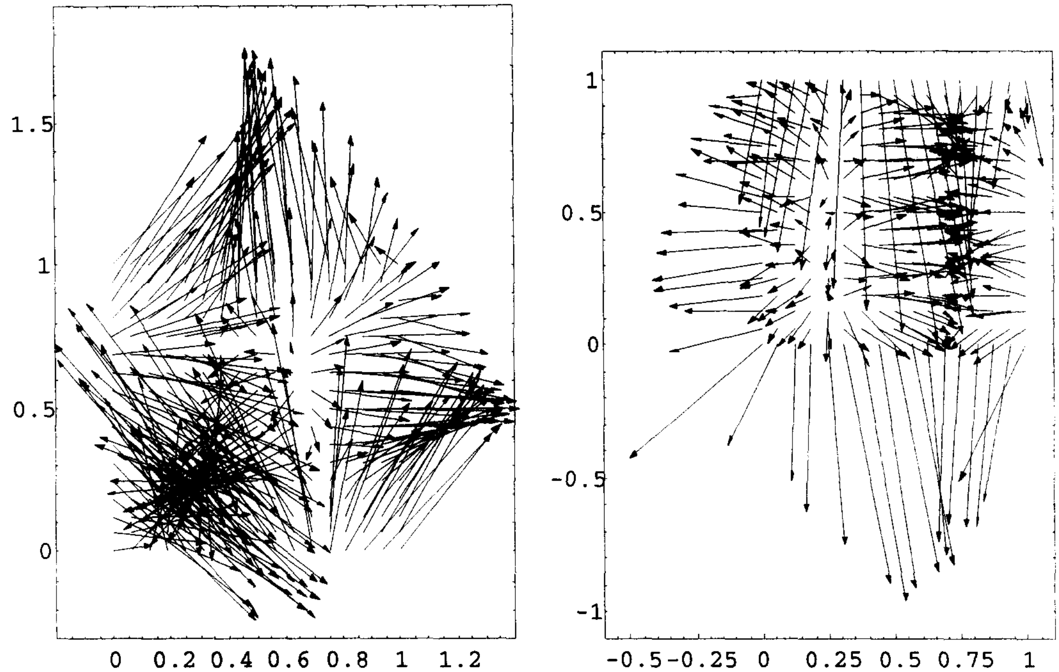


(a) Exact and noisy surfaces, $\epsilon = 0.1$.



(b) Reconstructed surface and exact gradient field.

Figure 2.



(c) Computed and error gradient fields.

Figure 2. (cont.)

Finally, with $C \equiv \max(p_1^{-1}, p_2^{-1}, 4\sqrt{\pi}A_p)$, we have

$$\left\| D_0^{(1)}(J_\delta G) \right\|_{\infty, \widetilde{I_\delta}} \le \frac{C}{|\delta|_{-\infty}} \|G\|_{\infty,K}.$$

Table 1. Error norms for $\varepsilon = 0.1$, $M = N = 1/128$.

Relative l^2-Error Norms on [0.1] × [0, 1]					
	Example 1	Example 2	Example 3	Example 4	Example 5
Surface	0.095311	0.076833	0.203602	0.006517	0.128756
Gradient	0.207191	0.132708	0.458221	0.072133	0.212290

Similarly,

$$\left\| D_0^{(2)}(J_\delta G) \right\|_{\infty, \widetilde{I_\delta}} \le \frac{C}{|\delta|_{-\infty}} \|G\|_{\infty,K}.$$

4. IMPLEMENTATION

4.1. Extension of Data

Computation of $J_\delta f$ throughout the domain $I = [0,1] \times [0,1]$, requires the extension of f to a slightly larger rectangle $I'_\delta = [-p_1\delta_1, 1 + p_1\delta_1] \times [-p_2\delta_2, 1 + p_2\delta_2]$. Since $J_\delta f = J_{\delta_2}(J_{\delta_1} f(x_1, x_2))$, we only need to consider the extension in the one-dimensional case.

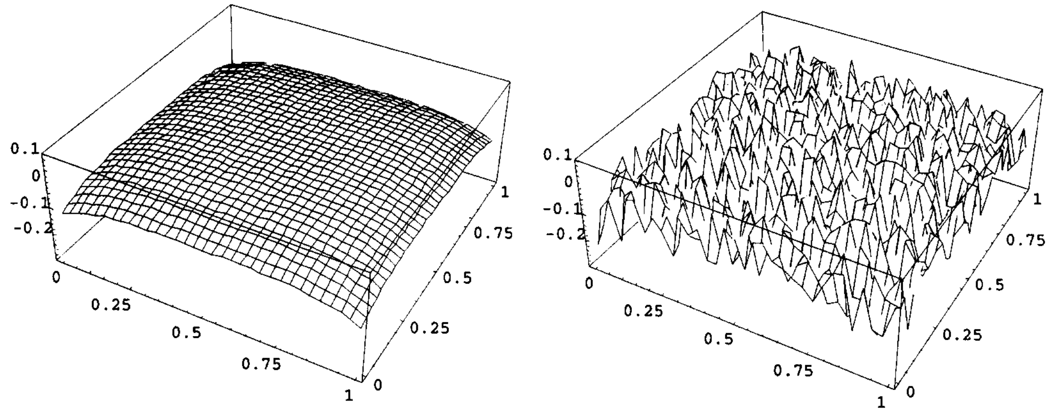
For each fixed $x_2 \in [0,1]$, we seek constant extensions f^* of $f(\cdot, x_2)$ to the intervals $[-p_1\delta_1, 0]$ and $[1, 1 + p_1\delta_1]$, satisfying the conditions

$$\|J_{\delta_1}(f^*) - f(\cdot, x_2)\|_{L^2[0, p_1\delta_1]} \text{ is minimum}$$

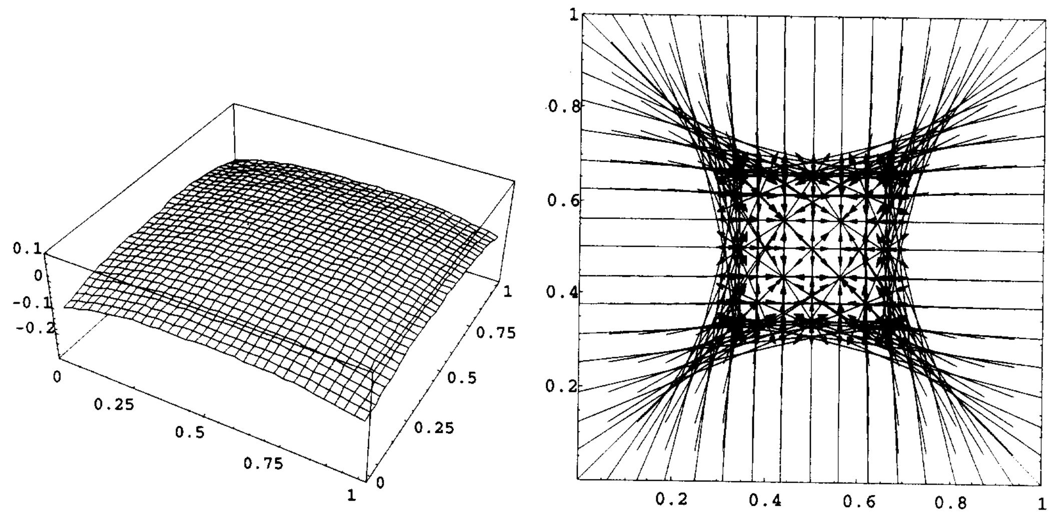
and

$$\|J_{\delta_1}(f^*) - f(\cdot, x_2)\|_{L^2[1 - p_1\delta_1, 1]} \text{ is minimum.}$$

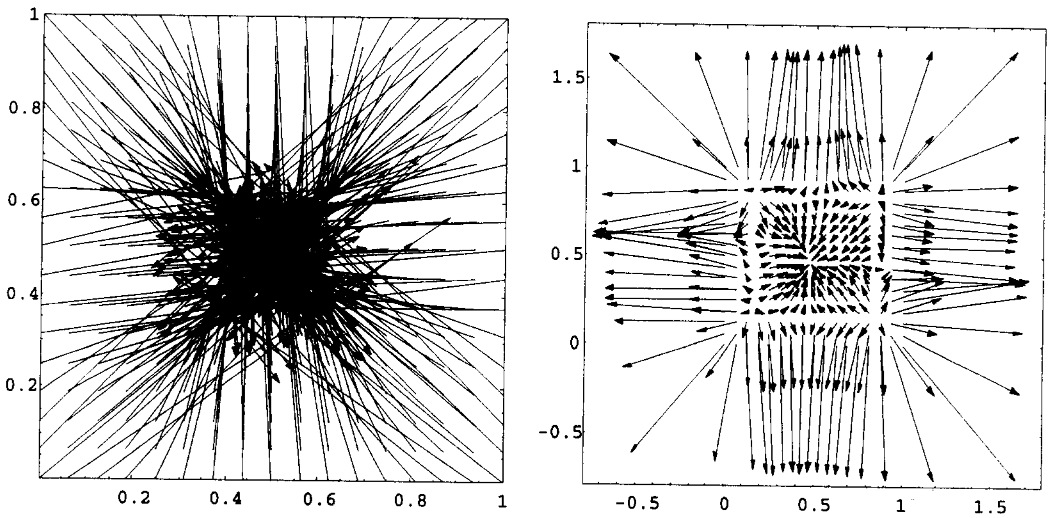
A closed formula for the constants can be found in [2].



(a) Exact and noisy surfaces, $\epsilon = 0.1$.

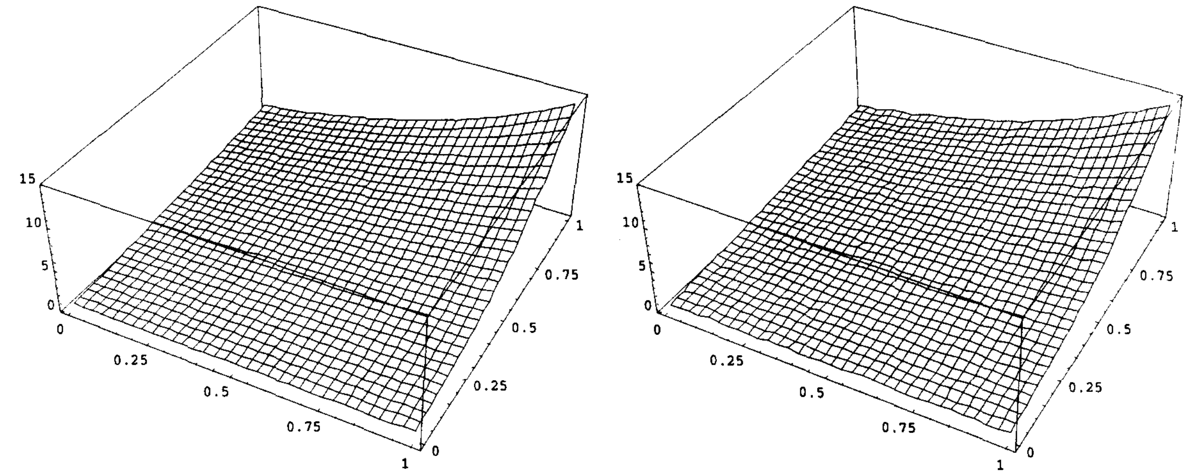


(b) Reconstructed surface and exact gradient field.

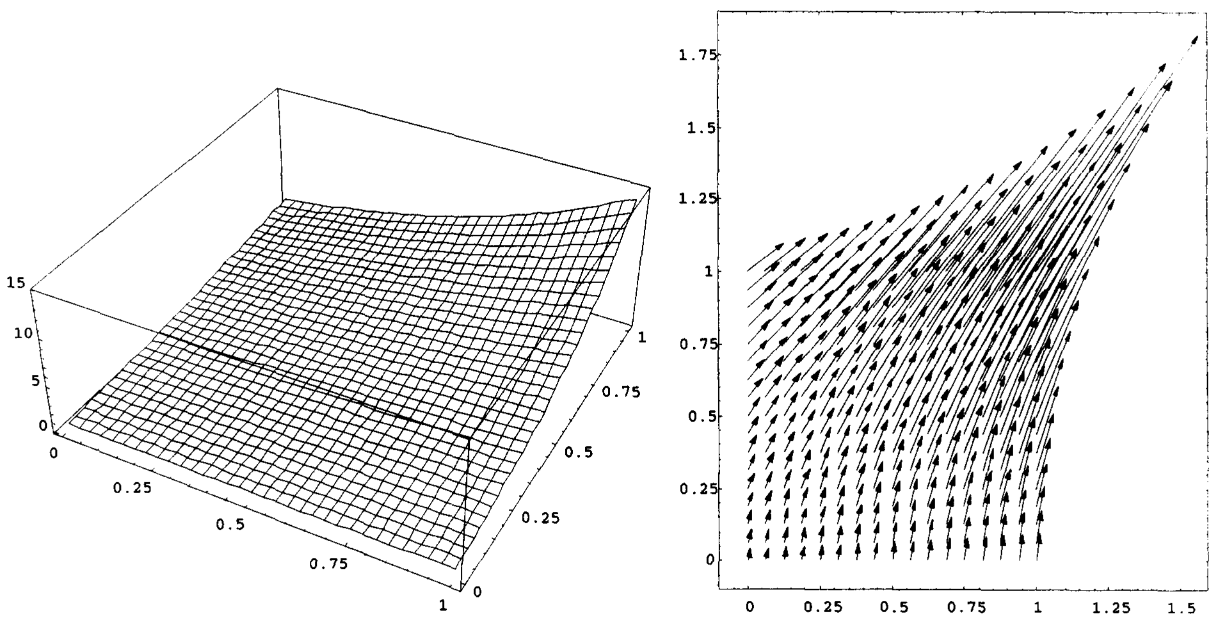


(c) Computed and error gradient fields.

Figure 3.



(a) Exact and noisy surfaces, $\epsilon = 0.1$.



(b) Reconstructed surface and exact gradient field.

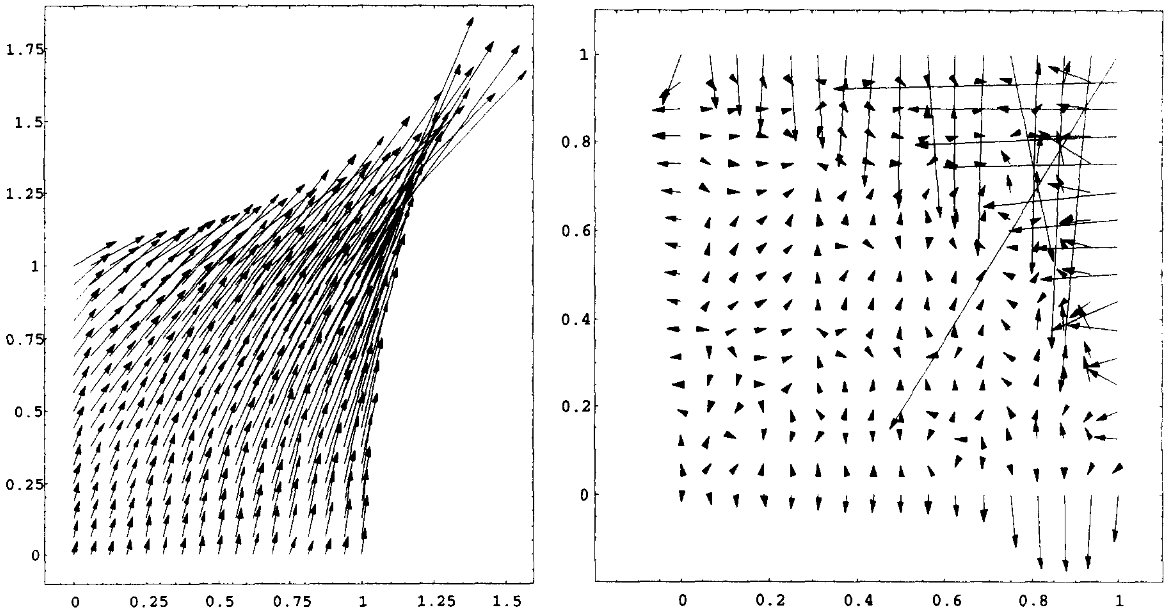
Figure 4.

4.2. Selection of Mollification Parameters

As indicated in previous sections, the parameter $\delta = (\delta_1, \delta_2)$ plays a crucial role in the regularization procedure. The discrete δ-mollification of $G = \{g_{ij} : 1 \le i \le m, 1 \le j \le n\}$,

$$J_\delta G(x) = \sum_{j=1}^{n} \int_{s_2^{(j-1)}}^{s_2^{(j)}} \rho_{\delta_2,x_2}(x_2 - s_2) \left(\sum_{i=1}^{m} \int_{s_1^{(i-1)}}^{s_1^{(i)}} \rho_{\delta_1,x_1}(x_1 - s_1) g_{ij}\, ds_1 \right) ds_2$$

is reduced to a double "mollification sweep" of several one-dimensional functions. First, for each fixed j, the discrete δ-mollification of the one-dimensional data set $\{g_{ij} : 1 \le i \le m\}$ is evaluated and then, for each fixed x_1, another discrete δ-mollification with respect to x_2 of the previously mollified data (the one-dimensional data set $\{\sum_{i=1}^{m} \int_{s_1^{(i-1)}}^{s_1^{(i)}} \rho_{\delta_1,x_1}(x_1 - s_1) g_{ij}\, ds_1 : 1 \le j \le n\}$) is computed. Hence, the problem of parameter selection is reduced to that of one-dimensional δ-mollification. This problem can then be solved effectively using the method of Generalized Cross



(c) Computed and error gradient fields.

Figure 4. (cont.)

Validation, without information on the noise in the data. See [3] for the first implementation of GCV in the context of mollification and, more recently, consult [4] for numerical differentiation problems.

4.3. Numerical Examples

In this section, to illustrate the effectiveness of the discrete δ-mollification, we present several numerical examples. In all cases, $\triangle x_1 = 1/M$, $\triangle x_2 = 1/N$, and the discrete data set $G = \{g_{ij} : 0 \le i \le M, 0 \le j \le N\}$ is generated as follows:

$$g_{ij} = f\left(x_1^{(i)}, x_2^{(j)}\right) + \epsilon_{ij}, \qquad i = 0, \dots, M, \quad j = 0, \dots, N,$$

where $x_1^{(i)} = i\triangle x_1$, $x_2^{(j)} = j\triangle x_2$, and the $\epsilon_{ij}'s$ are uniformly distributed random variables on $[-\epsilon, \epsilon]$. The maximum noise level ϵ is used only for the simulation of the noisy data. Without loss of generality, we set $p = (3, 3)$.

The errors between the mollified and exact data are measured by the weighted l^2-norms

$$\left(\frac{1}{MN}\sum_{i=0}^{M}\sum_{j=0}^{N}\left|J_\delta G\left(x_1^{(i)}, x_2^{(j)}\right) - f\left(x_1^{(i)}, x_2^{(j)}\right)\right|^2\right)^{1/2}.$$

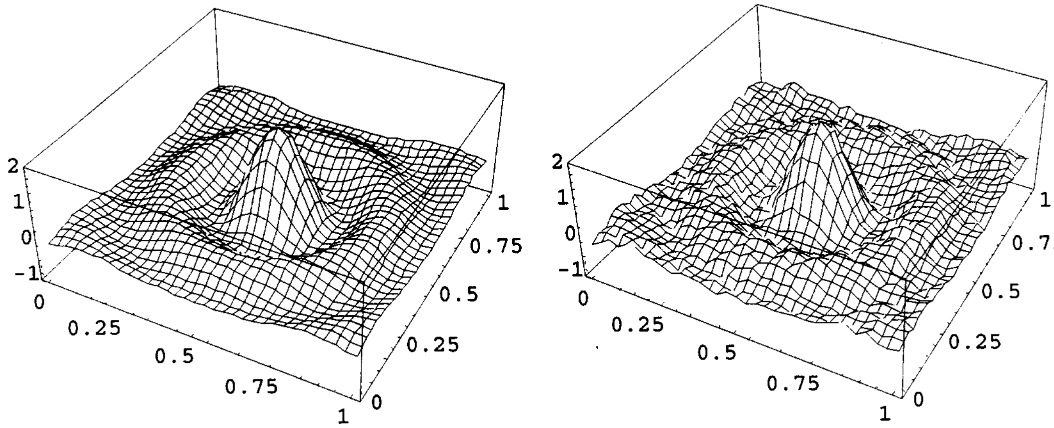
The errors between the computed and exact gradients are also measured by the weighted l^2-norms

$$\left(\frac{1}{MN}\sum_{i=0}^{M}\sum_{j=0}^{N}\left\|\nabla\left(J_\delta G\right)\left(x_1^{(i)}, x_2^{(j)}\right) - \nabla f\left(x_1^{(i)}, x_2^{(j)}\right)\right\|^2\right)^{1/2}.$$

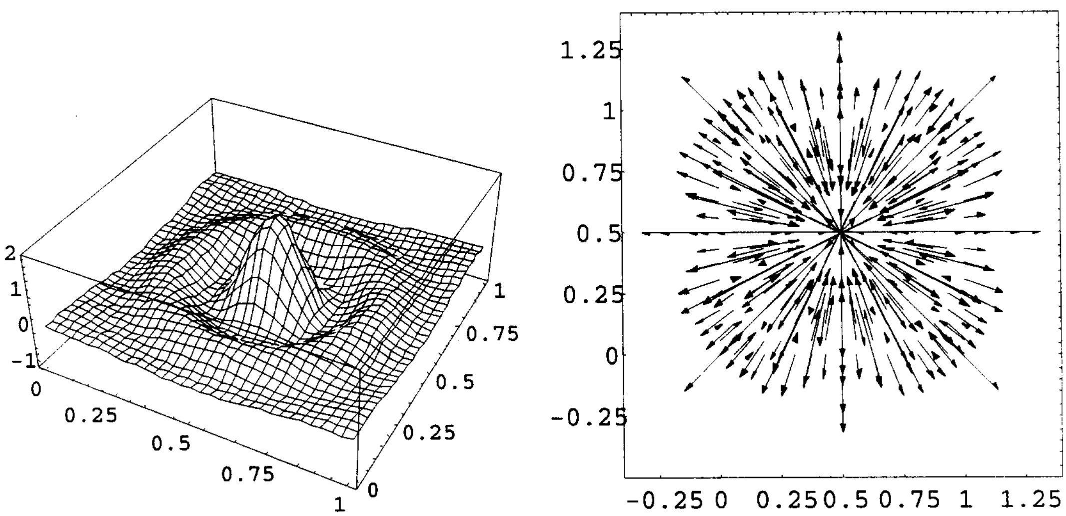
In all the examples, the maximum level of noise in the data is $\epsilon = 0.1$. Numerical results are summarized in Table 1 and the qualitative behaviors of the approximate solutions can be observed in Figures 1–5.

EXAMPLE 1.

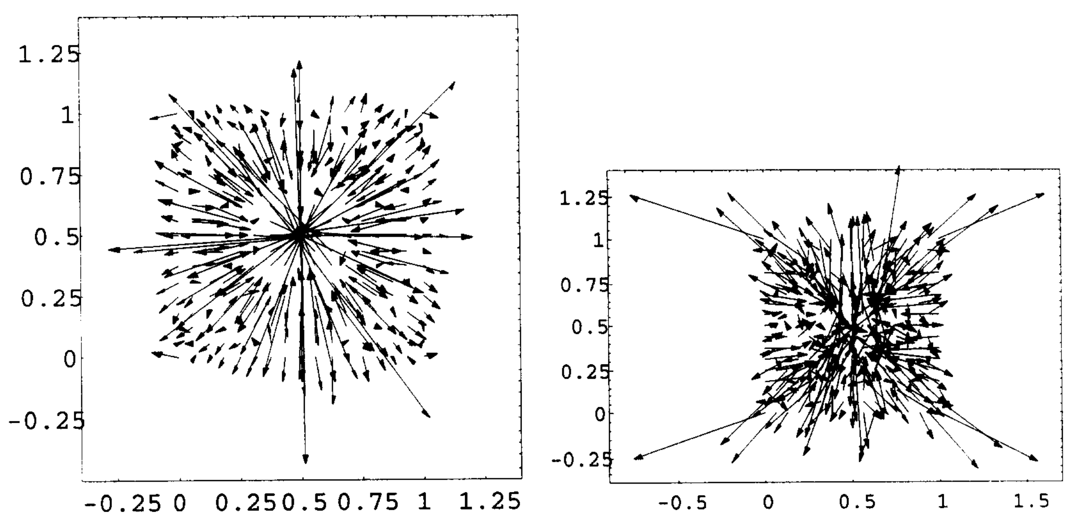
$$f(x_1, x_2) = (x_1 - 0.5)^2 - (x_2 - 0.5)^2.$$



(a) Exact and noisy surfaces, $\epsilon = 0.1$.



(b) Reconstructed surface and exact gradient field.



(c) Computed and error gradient fields.

Figure 5.

EXAMPLE 2.

$$f(x_1,x_2) = \frac{1}{4}\left[3(1-a)^2\exp\left(-a^2-(b+1)^2\right) - 10\left(\frac{a}{5}-a^3-b^5\right)\exp\left(-a^2-b^2\right) - \frac{1}{3}\exp\left(-(a+1)^2-b^2\right)\right],$$

where $a = 2(x_1 - 0.5)$ and $b = 2(x_2 - 0.5)$.

EXAMPLE 3.

$$f(x_1,x_2) = -(x_1-0.5)^4 - (x_2-0.5)^4.$$

EXAMPLE 4.

$$f(x_1,x_2) = (0.5+x_1)\exp((0.5+x_1)(0.5+x_2)).$$

EXAMPLE 5.

$$f(x_1,x_2) = \frac{\sin(2r)}{r},$$

where $r = 8\sqrt{2[(x_1-0.5)^2+(x_2-0.5)^2}$.

Examination of the pictures shows that the computed surfaces and gradient fields behave as predicted by the theory in I_δ. The errors associated with the reconstructed gradient fields deteriorate substantially near the boundaries.

REFERENCES

1. D.A. Murio, *The Mollification Method and the Numerical Solution of Ill-Posed Problems*, John Wiley, New York, (1993).
2. C.E. Mejía and D.A. Murio, Mollified hyperbolic method for coefficient identification problems, *Computers Math. Applic.* **26** (5), 1–12, (1993).
3. C.E. Mejía and D.A. Murio, Numerical solution of generalized IHCP by discrete mollification, *Computers Math. Applic.* **32** (2), 33–50, (1996).
4. D.A. Murio, C.E. Mejía and S. Zhan, Discrete mollification and automatic numerical differentiation, *Computers Math. Applic.* **35** (5), 1–16, (1998).