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RECONSTRUCTION OF DISCONTINUITIES OF FUNCTIONS GIVEN NOISY DATA

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ABSTRACT. Suppose one is given noisy data of a discontinuous piecewise-smooth function along with a bound on its second derivative. The locations of the points of discontinuity of f and their jump sizes are not assumed known, but are instead retrieved stably from the noisy data. The novelty of this paper is a numerical method that allows one to locate some of these points of discontinuity with an accuracy that can be made arbitrarily small.

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1. INTRODUCTION

Real life applications sometimes require one to compute approximations f' of the derivative of f , when f is acquired experimentally (with some noise). The differentiation of noisy data is an ill-posed problem: small perturbations in $L^\infty(0, 1)$ – norm of the function may lead to large errors in its derivative in $L^\infty(0, 1)$ – norm. In [5] and [6], different regularization algorithms for stable differentiation of f , given $f_\delta, \|f_\delta - f\|_\infty = \delta$, were analyzed; namely, the regularized difference method, the method by spline approximation, and the method of variational regularization. Before computing an approximation to f' , one has to first locate the discontinuity points of f . In this paper, we propose and justify a method for finding jump discontinuities of the function f defined on $[a, b]$, given the set $\{f_\delta, \delta\}$ and M_2 ($M_2 := \sup_{x \in [a, b]} |f^{(2)}(x)|$ where $f \in C^2([a, b])$).

2. DISCONTINUITIES OF PIECEWISE-SMOOTH DISCONTINUOUS FUNCTIONS

Let f be a piecewise- $C^2([a, b])$ function, and $a < x_1 < x_2 < \dots < x_J < b, 1 \leq j \leq J$ be the points of discontinuity of f . We do not have any information about their number J and their location. We assume that their limits $f(x_j \pm 0)$ exist, and

$$(2.1) \quad \sup_{x \neq x_j, 1 \leq j \leq J} |f^{(m)}(x)| \leq M_m, \quad m = 0, 1, 2.$$

Suppose that f_δ is given, $\|f_\delta - f\|_\infty \leq \delta$, where $f_\delta \in L^\infty(0, 1)$ represents the noisy samples of f that are known at points on a uniform grid

$$(2.2) \quad \Delta := \{a < a + h < a + 2h < \dots < b\}.$$

The problem is: given the set $\{f_\delta, \delta\}$ and M_2 , where $\delta \in (0, \delta_0)$ and $\delta_0 > 0$ is small, find the locations of discontinuity points x_j of f , their number J , and estimate the jumps $P_j := f(x_j + 0) - f(x_j - 0)$ of f across $x_j, 1 \leq j \leq J$.

The method discussed in this paper, unlike the methods in [3] and [8], looks for these points x_j at which the gradient of the first derivative is greater than M_2 . The points x_j corresponding to jump sizes of a specific order of magnitude can be located with an accuracy h , where the parameter h can be made arbitrarily small.

Lemma 2.1. *Suppose $f : D \subset \mathbb{R}^n \rightarrow \mathbb{R}$ is twice continuously differentiable. Then for all $x \in D$ such that $B_{\|h\|_p}(x) := \{y : \|y - x\|_p \leq \|h\|_p\} \subset D$, the inequality*

$$(2.3) \quad \frac{|f(x+h) - 2f(x) + f(x-h)|}{\|h\|_p \|h\|_q} \leq \zeta$$

holds. Here $h \in \mathbb{R}^n$ with $\|h\|_p < h_0$ and $\zeta := \sup_{x \in D} \|\nabla^2 f(x)\|_p, 1 \leq p < \infty, \frac{1}{p} + \frac{1}{q} = 1$ and $\|\cdot\|_p$ denotes the p -norm for a vector ($\|h\|_p := (\sum_{j=1}^n |h_j|^p)^{1/p}$) or the induced p -norm for a matrix ($\|A\|_p := \sup_{x \neq 0} \frac{\|Ax\|_p}{\|x\|_p}$).

Proof. Since f is $C^2(D)$, the hessian is continuous for all $x \in D$. Using Taylor's theorem and Hölder's inequality, we obtain

$$\begin{aligned} |f(x+h) - 2f(x) + f(x-h)| &= \left| \frac{1}{2} h^T \nabla^2 f(x+th)h + \frac{1}{2} h^T \nabla^2 f(x-sh)h \right| \\ &\leq \frac{1}{2} |h^T \nabla^2 f(x+th)h| + \frac{1}{2} |h^T \nabla^2 f(x-sh)h| \\ &\leq \frac{1}{2} \|h\|_p \|h\|_q (\|\nabla^2 f(x+th)\|_p + \|\nabla^2 f(x-sh)\|_p) \end{aligned}$$

$$\leq \|h\|_p \|h\|_q \zeta,$$

for some t and s in $(0,1)$. ■

Theorem 2.2. *Let f be a piecewise- $C^2([a, b])$ function with $J \geq 1$ points of discontinuity $\{x_j\}_{j=1}^J$ which are unknown a priori. Suppose the set $\{f_\delta, \delta\}$ and M_2 are given, where f_δ is known on the uniform grid Δ as defined in (2.2), and M_2 is as defined in (2.1). For a given δ one can locate the discontinuity points of f having jump sizes $|P_j| > 8\delta$, with an accuracy h and their number $k, k \leq J$. The intervals $[x - h, x + h]$ where the inequality:*

$$(2.4) \quad |f_\delta(x + h) - 2f_\delta(x) + f_\delta(x - h)| > M_2 h^2 + 4\delta$$

holds contain discontinuity points of f . For h small enough ($h \ll 1$), the jump sizes can be estimated by the formula

$$P_j \approx f_\delta(x + h) - f_\delta(x - h),$$

with an error estimate

$$(2.5) \quad |P_j - (f_\delta(x + h) - f_\delta(x - h))| \approx 2\delta.$$

If f' also has points of discontinuity, then the points x for which inequality (2.4) holds are either in the h -neighborhood of points of discontinuity of f or in the h -neighborhood of points of discontinuity of f' . They are in the h -neighborhood of points of discontinuity of f' if

$$(2.6) \quad |f_\delta(x + h) - f_\delta(x - h)| < 4\delta.$$

Let f_j be defined as follows:

$$f_j := \frac{f_\delta(a + jh + h(\delta)) - f_\delta(a + jh - h(\delta))}{2h(\delta)}.$$

To locate the points of discontinuity of f' , one can compute the quantities f_j and $|f_{j+1} - f_j|$, $n \leq j \leq k$. Here $n = \frac{h(\delta)}{h}$ and $k = \frac{b-h(\delta)}{h}$. The discontinuity points of f' are located on the intervals $(jh, jh + h)$, where the inequality:

$$(2.7) \quad |f_{j+1} - f_j| > 2\varepsilon(\delta) + M_2 h$$

holds. Here $h(\delta) := \sqrt{\frac{2\delta}{M_2}}$ and $\varepsilon(\delta) := \sqrt{2M_2\delta}$ represent respectively the discretization parameter and the approximation error as defined in [7].

Remark 2.1. In (2.7), h represents the mesh size of the grid Δ , which can be made arbitrarily small. In Theorem 2.2, we only consider the case when h is a constant; however, proceeding along the same lines one only needs to make some minor modifications to derive Theorem 2.2 for the most general case (h varies on each subinterval of the grid Δ).

Proof. Suppose f is a piecewise- $C^2([a, b])$ function. Then, $\forall x \in S_\delta := [a, b] \setminus \bigcup_{j=1}^J (x_j - h, x_j + h)$ such that $B_h(x) := \{y : |y - x| \leq h\} \subset S_\delta$, we have:

$$\frac{|f_\delta(x + h) - 2f_\delta(x) + f_\delta(x - h)|}{h^2} \leq \frac{|f(x + h) - 2f(x) + f(x - h)|}{h^2} + \frac{4\delta}{h^2}.$$

Since $f \in C^2(S_\delta)$, by Lemma 2.1 we obtain:

$$\frac{|f_\delta(x + h) - 2f_\delta(x) + f_\delta(x - h)|}{h^2} \leq M_2 + \frac{4\delta}{h^2}.$$

Therefore, given that a point in $[a, b]$ is either a point where f is twice differentiable or a point where f has a discontinuity, it follows that if inequality (2.4) holds, f has a discontinuity somewhere on the interval $(x - h, x + h)$.

Estimate (2.5) can be obtained as follows. Suppose $x_j \in (x - h, x + h)$. One has:

$$\begin{aligned} |P_j - f_\delta(x + h) + f_\delta(x - h)| &= |f(x_j + 0) - f(x_j - 0) - f_\delta(x + h) + f_\delta(x - h)| \\ &\leq 2\delta + |f(x_j + 0) - f(x + h)| + |f(x_j - 0) - f(x - h)| \\ &\leq 2\delta + 2hM_1. \end{aligned}$$

For $h \ll 1$, $\gamma = 2hM_1 + 2\delta \approx 2\delta$ and we have:

$$|P_j - (f_\delta(x + h) - f_\delta(x - h))| \leq \gamma \approx 2\delta.$$

To obtain inequality (2.7), let us now assume that $\xi \in S_\delta := [a + h(\delta), b - h(\delta)] \setminus \bigcup_{j=1}^J (x_j + h(\delta), x_j - h(\delta))$, is a point at which f is continuous but f' is not. For all $x \in S_\delta$ such that $(x - h(\delta), x + h + h(\delta)) \subset S_\delta$, one has:

$$|f_{j+1} - f_j| \leq C + \frac{2\delta}{h(\delta)},$$

where $C = \left| \frac{f(x+h+h(\delta)) - f(x+h-h(\delta)) - f(x+h(\delta)) + f(x-h(\delta))}{2h(\delta)} \right|$ and $\frac{2\delta}{h(\delta)} = \varepsilon(\delta)$. Using Taylor's expansion formula one can derive the estimate:

$$C \leq \varepsilon(\delta) + hM_2.$$

So,

$$|f_{j+1} - f_j| \leq 2\varepsilon(\delta) + hM_2.$$

Therefore, if inequality (2.7) holds, there is a point $\xi \in (x - h(\delta), x + h + h(\delta))$ where f is not twice continuously differentiable. Since ξ is not a point of discontinuity of f , it is a point of discontinuity of f' . ■

3. DISCONTINUITIES OF PIECEWISE-SMOOTH DISCONTINUOUS FUNCTIONS IN \mathbb{R}^n

The numerical method described in the previous section is computationally efficient when f is a function of one variable. The whole computation only takes $O(k)$ operations, where k is the number of data points on the grid Δ . The same idea can be used to locate points of discontinuity of functions of n variables. One will have to repeat the process described above on each axis using different values of M_2 along each axis; however, such a method is not computationally efficient as it takes $O(k^n)$ operations which can become very large as n gets large. Instead, when n is large ($n \geq 3$) one can consider a different approach that only takes $O(k)$ operations.

Theorem 3.1. *Suppose $f : A \subset \mathbb{R}^n \longrightarrow B \subset \mathbb{R}$ is a piecewise- $C^2(A)$ function. Let $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ represent the canonical orthonormal basis in \mathbb{R}^n . Assume that the noisy samples f_δ ($\|f_\delta - f\|_\infty \leq \delta$) are known at points on a uniform n -dimensional grid Δ_n on which consecutive points along lines parallel to the coordinate axis are equidistant. That is $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{h}_j$, if the line through the points x_{k+1} and x_k on Δ_n is parallel to \mathbf{e}_j . Here $\mathbf{h}_j = h_0 \mathbf{e}_j$, $1 \leq j \leq n$ and $h_0 > 0$. Denote by R the set of all points in A where f is discontinuous and by S the set of all points $\{y_l\}_{l=1}^K$ on Δ_n where f has a discontinuity. Let $\Sigma_\delta(\mathbf{x})$ be defined as $\Sigma_\delta(\mathbf{x}) := \max_{1 \leq j \leq n} \Sigma_\delta^j(\mathbf{x})$, where*

$$\Sigma_\delta^j(\mathbf{x}) = |f_\delta(\mathbf{x} + \mathbf{h}_j) - 2f_\delta(\mathbf{x}) + f_\delta(\mathbf{x} - \mathbf{h}_j)|.$$

For a given δ one can locate the discontinuity points of f having jump sizes

$|P_j| > 8\delta$, with an accuracy h . These points are located in the h -neighborhood of points x on Δ_n where the inequality

$$(3.1) \quad \Sigma_\delta(\mathbf{x}) > 4\delta + h_0^2 \|\nabla^2 f\|_{p,A}$$

holds; $1 \leq p < \infty$. Here $\|\nabla^2 f\|_{p,A}$ denotes $\sup_{x \in A \setminus R} \|\nabla^2 f(x)\|_p$. In particular, when $p = 2$ we obtain

$$(3.2) \quad \Sigma(\mathbf{x}) > 4\delta + h_0^2 \lambda$$

where $\lambda := \sup_{x \in A \setminus R} \max\{\sqrt{\lambda_j^2(x)}\}_{j=1}^n$ and $\lambda_j(x)$ represent the eigenvalues of the hessian of f at a point x in A .

Proof. Let us first note that as $x \in A \setminus R$ and f is $C^2(A \setminus R)$, $\nabla^2 f(x)$ is well defined and symmetric. Suppose $x \in A \setminus R$ is such that $B_{h_0}(x) \subset A \setminus R$. We then have:

$$(3.3) \quad \Sigma_\delta(x) \leq \Sigma(x) + 4\delta.$$

From Lemma 2.1 we obtain

$$(3.4) \quad \Sigma(x) \leq \|h\|_p \|h\|_q \|\nabla^2 f\|_{p,A} = h_0^2 \|\nabla^2 f\|_{p,A}.$$

Therefore,

$$\Sigma_\delta(x) \leq h_0^2 \|\nabla^2 f\|_{p,A} + 4\delta.$$

This result holds for all p ($1 \leq p \leq \infty$) and thus certainly holds for $p = 2$. As $\nabla^2 f(x)$ is symmetric for all $x \in A \setminus R$, we have

$$(3.5) \quad \|\nabla^2 f(x)\|_2 = \max_{1 \leq j \leq n} \sqrt{\lambda_j^2(x)}.$$

Let $\lambda := \sup_{x \in A \setminus R} \|\nabla^2 f(x)\|_2$, we obtain

$$(3.6) \quad \Sigma_\delta(x) \leq 4\delta + h_0^2 \lambda.$$

We thus conclude that if inequality (3.1) or (3.2) holds at a point x , then x does not belong to $A \setminus R$. Therefore x belongs to R or is in the h -neighborhood of a discontinuity point of f . ■

4. DEPENDENCE OF THE METHOD ON M_2

Let f, f_δ, R, S and Δ_n be defined as in the statement of Theorem 3.1. Suppose f is discontinuous at $\xi \in \mathbb{R}^n$ in the direction of \mathbf{v} . Let P_ξ be defined as:

$$P_\xi := |f(\xi + 0) - f(\xi - 0)|,$$

where $f(\xi + 0) = \lim_{\epsilon \rightarrow 0} f(\xi + \epsilon \mathbf{v})$ and $f(\xi - 0) = \lim_{\epsilon \rightarrow 0} f(\xi - \epsilon \mathbf{v})$. Suppose that one does not know the values of $\|\nabla f\|_{p,A}$ and $\|\nabla^2 f\|_{p,A}$, but instead knows them to be bounded by β ,

$$\|\nabla f\|_{p,A} + \|\nabla^2 f\|_{p,A} \leq \beta.$$

Here $\|\nabla f\|_{p,A} := \sup_{x \in A \setminus R} \|\nabla f(x)\|_p$, $\|\nabla^2 f\|_{p,A} := \sup_{x \in A \setminus R} \|\nabla^2 f(x)\|_p$, and $p \geq 1$. The problem is: given the set $\{f_\delta, \delta, \varrho, \beta\}$, what values of the parameter h can one use to locate all the discontinuity points x_j of f on Δ_n having jump size

$$(4.1) \quad P_{x_j} > 8\delta + \varrho,$$

$\varrho \in (0, 1)$.

Theorem 4.1. *Suppose one is given the set $\{f_\delta, \delta, \varrho, \beta\}$. Then $\forall h \in (0, H)$, inequality 3.1 holds at every point $x \in \Delta_n$ located in the proximity of a point of discontinuity x_j of f having jump size $P_{x_j} > 8\delta + \varrho$, given that $\min_j |x_{j+1} - x_j| > 2h$. Here*

$$(4.2) \quad H := \frac{\varrho}{4\beta}.$$

Proof. Let $\xi \in B_{h_0}(\mathbf{x})$ be a discontinuity points of f where (4.1) holds. Here \mathbf{x} , $\mathbf{x} + \mathbf{h}_j$, $\mathbf{x} - \mathbf{h}_j \in \Delta_n$ are points where f is twice continuously differentiable and $B_{h_0}(\mathbf{x}) := \{y \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{y}\|_1 \leq h_0\}$. Let us assume that ξ is the only discontinuity point of f that belongs to B_{h_0} . Let $\Sigma_\delta(\mathbf{x})$ be defined as in Theorem 3.1. One has:

$$\begin{aligned} \Sigma_\delta(\mathbf{x}) &= |f_\delta(\mathbf{x} + \mathbf{h}_j) - 2f_\delta(\mathbf{x}) + f_\delta(\mathbf{x} - \mathbf{h}_j)| \\ &= |f_\delta(\mathbf{x} + \mathbf{h}_j) - f(\boldsymbol{\xi} + 0) + f(\boldsymbol{\xi} + 0) + f(\boldsymbol{\xi} - 0) - f(\boldsymbol{\xi} - 0) \\ &\quad - 2f_\delta(\mathbf{x}) + f_\delta(\mathbf{x} - \mathbf{h}_j)| \\ &\geq |f(\boldsymbol{\xi} + 0) - f(\boldsymbol{\xi} - 0)| - |f_\delta(\mathbf{x} + \mathbf{h}_j) - f(\boldsymbol{\xi} + 0)| \\ &\quad - |f(\boldsymbol{\xi} - 0) - f_\delta(\mathbf{x})| - |f_\delta(\mathbf{x}) - f_\delta(\mathbf{x} - \mathbf{h}_j)| \end{aligned}$$

for some j , $1 \leq j \leq n$. From Taylor's formula, we get:

$$\begin{aligned} \Sigma_\delta(\mathbf{x}) &\geq P_\xi - 4\delta \\ &\quad - |(\boldsymbol{\xi} - \mathbf{x} - \mathbf{h}_j)^T \nabla f(\mathbf{x} + \mathbf{h}_j + t_1(\boldsymbol{\xi} - \mathbf{x} - \mathbf{h}_j))| \\ &\quad - |(\boldsymbol{\xi} - \mathbf{x})^T \nabla f(\mathbf{x} + t_2(\boldsymbol{\xi} - \mathbf{x}))| \\ &\quad - |\mathbf{h}_j^T \nabla f(\mathbf{x} - (1 - t_3)\mathbf{h}_j)|, \end{aligned}$$

where $t_1, t_2, t_3 \in (0, 1)$. Using Hölder's and Minkowski's inequality we obtain

$$\begin{aligned} \Sigma_\delta(\mathbf{x}) &\geq P_\xi - 4\delta \\ &\quad - \|(\boldsymbol{\xi} - \mathbf{x} - \mathbf{h}_j)\|_q \|\nabla f(\mathbf{x} + \mathbf{h}_j + t_1(\boldsymbol{\xi} - \mathbf{x} - \mathbf{h}_j))\|_p \\ &\quad - \|(\boldsymbol{\xi} - \mathbf{x})\|_q \|\nabla f(\mathbf{x} + t_2(\boldsymbol{\xi} - \mathbf{x}))\|_p \\ &\quad - \|\mathbf{h}_j\|_q \|\nabla f(\mathbf{x} - (1 - t_3)\mathbf{h}_j)\|_p \\ &\geq P_\xi - 4(\delta + h_0 \|\nabla f\|_{p,A}), \quad \frac{1}{p} + \frac{1}{q} = 1. \end{aligned}$$

Note that

$$\|\boldsymbol{\xi} - \mathbf{x} - \mathbf{h}_j\|_q \leq \|\mathbf{h}_j\|_q + \|\mathbf{x} - \boldsymbol{\xi}\|_q \leq 2h_0,$$

since $\|\mathbf{h}_j\|_q = h_0$ and

$$\|\boldsymbol{\xi} - \mathbf{x}\|_q \leq \|\boldsymbol{\xi} - \mathbf{x}\|_1 \leq h_0.$$

Let us assume that

$$P_\xi - 4(\delta + h_0 \|\nabla f\|_{p,A}) \geq 4\delta + h_0^2 \|\nabla^2 f\|_{p,A}.$$

Using the fact that P_ξ satisfies (4.1), we obtain

$$(4.3) \quad \varrho > h_0^2 \|\nabla^2 f\|_{p,A} + 4h_0 \|\nabla f\|_{p,A}.$$

For small values of h_0 ($h_0 < 1$), if

$$(4.4) \quad \varrho > 4h_0 \|\nabla^2 f\|_{p,A} + 4h_0 \|\nabla f\|_{p,A}$$

holds, inequality (4.3) follows. From (4.4), we obtain:

$$h_0 < \frac{\varrho}{4\beta}.$$

Note that the assumption $h_0 < 1$ still holds, since $0 < \varrho < 1$ and $\beta \geq \frac{1}{4}$. ■

5. COMPARISON OF SOME METHODS OF NUMERICAL DIFFERENTIATION

Over the course of years different methods have been developed for numerical differentiation. In this section we analyze and discuss two well known methods: Ramm's method and the method of approximation by cubic splines.

Let $\|\cdot\|$ denote the L^2 -norm of square integrable functions over $(0, 1)$, and let f_δ be the noisy samples of f , $\|f_\delta - f\| \leq \delta$. For the purpose of this paper we will only consider the case when $f \in H^2[0, 1]$, where $H^2[0, 1]$ denotes the Sobolev space of functions $f \in C^1[0, 1]$ whose 2nd derivative belongs to $L^2(0, 1)$.

The method of approximation by cubic splines for stable numerical differentiation was discussed in [2] and recently in [1]. The general approach to the method of approximation by cubic splines is presented in [1]. Given the noisy samples f_δ of a smooth function f over a uniform grid $\Delta = \{0 = x_0 < x_1 < \dots < x_n = 1\}$, and the boundary data which are assumed to be known exactly ($f_\delta(0) = f(0)$, $f_\delta(1) = f(1)$), one computes a smooth approximation g'_* of f' defined for all $x \in (0, 1)$. The function g_* is obtained by minimizing the functional

$$(5.1) \quad \Phi(g) := \frac{1}{n-1} \sum_{i=1}^{n-1} (f_\delta(x_i) - g(x_i))^2 + \alpha \|g''\|^2$$

over the class of all smooth functions g satisfying the boundary conditions $g(0) = f(0)$, $g(1) = f(1)$, where The regularization parameter α is chosen such that the minimizing function g_* satisfies:

$$(5.2) \quad \frac{1}{n-1} \sum_{i=1}^{n-1} (f_\delta(x_i) - g_*(x_i))^2 = \delta^2.$$

It was shown by Schoenberg [11] and Reinsch [10] that the minimizer of (5.1) is a natural cubic spline over Δ . Using the properties of natural cubic splines, it was shown in [1] that the error bound in this particular method of numerical differentiation is:

$$(5.3) \quad \|g'_*(x) - f'(x)\| \leq \sqrt{8}(hM_2 + \sqrt{\delta M_2}) := \xi(\delta, h),$$

where $M_2 := \|f^{(2)}\|$.

The general approach to Ramm's algorithm using a finite difference formula depending on δ was first given in [9]. Given the set $\{f_\delta, \delta\}$, one obtains an approximation of f' defined as follows:

$$(5.4) \quad R_h f_\delta(x) := \begin{cases} \frac{f_\delta(x+h) - f_\delta(x)}{h} & 0 < x < h \\ \frac{f_\delta(x+h) - f_\delta(x-h)}{2h} & h \leq x \leq 1-h \\ \frac{f_\delta(x) - f_\delta(x-h)}{h} & 1-h < x < 1, h > 0. \end{cases}$$

Here h is a discretization parameter. Using Taylor's expansion, the error estimate obtained by this approximation is then:

$$(5.5) \quad \|R_h f_\delta - f'\| \leq \begin{cases} \frac{2\delta}{h} + \frac{hM_2}{2} & 0 < x < h \\ \frac{\delta}{h} + \frac{hM_2}{2} & h \leq x \leq 1-h \\ \frac{2\delta}{h} + \frac{hM_2}{2} & 1-h < x < 1, h > 0. \end{cases}$$

To minimize the approximation error, we then choose $h = h(\delta)$ defined as follows:

$$(5.6) \quad h(\delta) := \begin{cases} 2\sqrt{\frac{\delta}{M_2}} & 0 < x < h(\delta) \\ \sqrt{\frac{2\delta}{M_2}} & h(\delta) < x < 1 - h(\delta) \\ 2\sqrt{\frac{\delta}{M_2}} & 1 - h(\delta) < x < 1, h > 0. \end{cases}$$

The minimal error bound obtained using $h(\delta)$ is then:

$$(5.7) \quad \varepsilon(\delta) := \begin{cases} 2\sqrt{\delta M_2} & 0 < x < h(\delta) \\ \sqrt{2\delta M_2} & h(\delta) < x < 1 - h(\delta) \\ 2\sqrt{\delta M_2} & 1 - h(\delta) < x < 1, h > 0. \end{cases}$$

While using Ramm's method, one is only interested in the datum at a uniform spacing $h(\delta)$; however, if one is given datum at a uniform spacing $t = \frac{h(\delta)}{n}$ where $n > 1$ is an integer, by using all the data one can obtain a better (over smaller subintervals) piecewise-linear approximation of f' on the interval $h(\delta) \leq x \leq 1 - h(\delta)$, where the error bound defined in (5.7) still holds. The new approximation of f' , for all $x \in S$, $S = \{nt, (n+1)t, (n+2)t, \dots, kt\}$, $k = \frac{1-h(\delta)}{t}$, is then:

$$(5.8) \quad R_{h(\delta)}f_\delta(jt) := \frac{f_\delta(jt + h(\delta)) - f_\delta(jt - h(\delta))}{2h(\delta)}, \quad n \leq j \leq k.$$

The complete algorithm for the Ramm's method takes $O(m) \approx 4m$ operations, while the computation of the method of approximation by cubic splines, excluding the determination of the lagrangian multipliers takes $O(n) \approx 12n$ operations ($m = \frac{1}{h(\delta)}$, $n = \frac{1}{h}$). Here $h(\delta)$ and h represent respectively the discretization parameter of Ramm's method and the mesh size of the grid Δ . For a given value of δ , both methods have error bounds of the same order ($O(\sqrt{\delta})$); however, $\forall M_2$ such that $M_2 \neq 0$, we have:

$$\xi(\delta, h) = 2\varepsilon(\delta) + hM_2\sqrt{8}.$$

The optimal error bound that one can attain using the method of approximation by cubic splines is:

$$(5.9) \quad \xi_{opt}(\delta, h) = \sqrt{8\delta M_2}.$$

This error bound is twice that of Ramm's method over the interval ($h(\delta) < x < 1 - h(\delta)$) for the same value of δ and is obtained by taking $\lim_{x \rightarrow 0} \xi(\delta, h)$ which requires $O(n)$ operations, $n \mapsto \infty$.

So far we have only defined Ramm's method for values of $h = \frac{h(\delta)}{n}$, $n \in \mathbb{N}$ (5.8); however, it might occur in practice that $h = \frac{h(\delta)}{r}$, $r \in \mathbb{R}^+$. In this case we extend Ramm's method, and we examine how its error bound compares to the method of approximation by cubic splines.

Let $\sigma(h)$ be defined as:

$$(5.10) \quad \sigma(h) = \|T(h, x) - f'(x)\|$$

where $T(h, x) := \frac{f(x+h) - f(x-h)}{2h}$. We assume that f is smooth over the interval $(0, 1)$.

Lemma 5.1. *Suppose the observation points are given at a spacing $ch(\delta)$ on a uniform grid Δ , where $c > 0$. For all $c \in I$, $I := (2 - \sqrt{3}, 2 + \sqrt{3})$,*

$$(5.11) \quad \sigma(ch(\delta)) < \xi_{opt}(\delta, h),$$

$\forall M_2 \neq 0$ and $\forall \delta > 0$ on the interval $(ch(\delta), 1 - ch(\delta))$.

Proof. suppose $x \in (ch(\delta), 1 - ch(\delta))$. If one computes $\sigma(ch(\delta))$, after a Taylor's expansion and a short manipulation, one gets:

$$(5.12) \quad \begin{aligned} \sigma(ch(\delta)) &\leq \left(\frac{1}{c} + c\right) \sqrt{\frac{\delta M_2}{2}} \\ &\leq \frac{1}{2} \varepsilon(\delta) \left(\frac{1}{c} + c\right). \end{aligned}$$

If

$$(5.13) \quad \frac{1}{2} \left(\frac{1}{c} + c\right) < 2$$

holds, then by (5.9), we have:

$$(5.14) \quad \sigma(ch(\delta)) < \xi_{opt}(\delta, h).$$

Assuming (5.13) and solving for c , we obtain:

$$(5.15) \quad 2 - \sqrt{3} < c < 2 + \sqrt{3}.$$

■

Lemma 5.2. *Suppose the observation points are given at a spacing $h \geq \frac{1}{4}h(\delta)$ on a uniform grid Δ . Then $\forall M_2 \neq 0$, and $\forall \delta > 0$, we have:*

$$(5.16) \quad \sigma(h) < \xi(\delta, h),$$

for all $x \in (h, 1 - h)$.

Proof. Suppose $x \in (h, 1 - h)$. If we bound and then perform a Taylor expansion on $\sigma(h)$, we obtain:

$$(5.17) \quad \sigma(h) = \|T(h, x) - f'(x)\| \leq \frac{\delta}{h} + \frac{hM_2}{2}.$$

From (5.3) and (5.17) if:

$$(5.18) \quad \sqrt{8M_2\delta} \geq \frac{\delta}{h},$$

then inequality (5.16) holds. Assuming (5.18) and solving for h we get:

$$(5.19) \quad h \geq \sqrt{\frac{\delta}{8M_2}} \geq \frac{1}{4}h(\delta)$$

■

Theorem 5.3. *Let h be the spacing between consecutive data points on a uniform grid Δ . $\forall h > 0$, $\exists h_0(\delta) > 0$ defined on Δ such that:*

$$(5.20) \quad \sigma(h_0(\delta)) < \xi(\delta, h).$$

Proof. Given a mesh size h , there are two cases to consider:

Let us first assume that

$$h \geq \frac{1}{4}h(\delta).$$

By Lemma 5.2, $\forall h_0(\delta) \geq h$, inequality (5.20) holds, thus proving Theorem 5.3 for the first case.

Let us now assume that

$$h < \frac{1}{4}h(\delta).$$

Let ϵ be defined as

$$(5.21) \quad \epsilon = \inf_{n \in \mathbb{N}} |h(\delta) - nh|,$$

where \mathbb{N} denotes the set of positive integers. We have

$$(5.22) \quad \epsilon \leq \frac{1}{8}h(\delta).$$

Let $h_0(\delta)$ satisfy (5.21), so

$$(5.23) \quad h_0(\delta) = nh.$$

Combining inequalities (5.21), (5.22), and (5.23), we obtain:

$$(5.24) \quad h(\delta) - \frac{1}{8}h(\delta) \leq h_0(\delta) \leq h(\delta) + \frac{1}{8}h(\delta).$$

If we let c be defined as

$$(5.25) \quad c = \frac{h_0(\delta)}{h(\delta)},$$

we then obtain

$$(5.26) \quad \frac{7}{8} \leq c \leq \frac{9}{8}.$$

Since $h_0(\delta) = ch(\delta)$, with $c \in [\frac{7}{8}, \frac{9}{8}] \subset I$, where $I := (2 - \sqrt{3}, 2 + \sqrt{3})$, by Lemma 5.1 we have:

$$(5.27) \quad \sigma(ch(\delta)) < \xi_{opt}(\delta, h).$$

■

Ramm's method therefore has a better error bound than the method of approximation by cubic splines for all possible choices of the parameters δ , M_2 , and h . Though in Ramm's method h depends on M_2 , in many practical problems the value of M_2 is an a priori knowledge; however, even if one mistakenly takes M_2 10 times its actual value the resulting error is still $O(\sqrt{\delta})$.

Let us now assume that f is a piecewise- $C^2([0, 1])$ function with a discontinuity located at the point $x_j \in (0, 1)$ having a jump size of P_j . If one uses either method to approximate f' without excluding the discontinuity, there is an additional error $\varphi(P_j)$ that is added to the original error bound, due to the jump discontinuity at the point x_j . A topic of interest is that of the effect of $\varphi(P_j)$ on the approximation of f' in general. One would especially want to know how far $\varphi(P_j)$ propagates from the discontinuity x_j . If one uses Ramm's method, $\varphi(P_j) = 0$ on $(0, 1) \setminus (x_j - h(\delta), x_j + h(\delta))$, and it reaches its maximum somewhere on the interval $(x_j - h(\delta), x_j + h(\delta))$. If one uses the method of approximation by cubic splines instead, because of the smoothness condition on g_* , $\varphi(p_j)$ will propagate over the entire interval $(0, 1)$, and the error bound will grow as h becomes small. Therefore, Ramm's method is better if the function f is a piecewise- $C^2([0, 1])$ function.

In general, Ramm's method is superior given that it uses far fewer operations, it has a better error bound, and it localizes additional error introduced by discontinuities over finite subintervals.

6. EXPERIMENTAL RESULTS

We used a series of experiments to test the performance of the newly developed method. The remainder of this section is divided into three parts. In part 6.1, we test the method on functions of one variable; noisy data from discontinuous piecewise-smooth functions are constructed and the method is used to locate the discontinuities. In part 6.2, the method is tested on multi-variable functions; gray scale image files are generated and the method is used to find discontinuities in the color intensity of the image. In part 6.3, we give some results of our comparison on methods of stable numerical differentiation.

6.1. Reconstruction of discontinuities of functions of one variable. In this section we used a computer program to generate noisy data from discontinuous piecewise-smooth functions. The method of section 2 was then used in to locate the points of discontinuity. The method was tested for large, medium, and small values of the parameters h , M_2 , and δ . The functions used in this experiment were:

$$(6.1) \quad f_1(x) := \begin{cases} x^2 & -1 \leq x < -.5, \\ x & -.5 \leq x < 0, \\ \cos(x^2) & 0 \leq x < .5, \\ x^3 & .5 \leq x \leq 1. \end{cases}$$

$$(6.2) \quad f_2(x) := \begin{cases} \sin(25x) & -1 \leq x < 0, \\ \cos(65x) & 0 \leq x < 1. \end{cases}$$

And

$$(6.3) \quad f_3(x) := \begin{cases} e^{5x^3} - .5 & 0 \leq x < .5, \\ e^{5x^3} & .5 \leq x < 1. \end{cases}$$

The noise function used in this experiment was $\psi(x) = (-1)^{\lfloor \frac{x-a}{h} \rfloor} \delta \cos(x)$, for all $x \in [a, b]$. The values of the parameters δ , h , and M_2 used and the results are given in the following table.

Functions	$f_1(x)$	$f_2(x)$	$f_3(x)$
M_2	6	4225	39700
Noise level	.1	.2	.1
Step size	.1	.01	.001
discontinuities found	x=-.5, 0, .49	x=0	x=.499
Run time(second)	.04	.09	.06

Table 6.1: Results

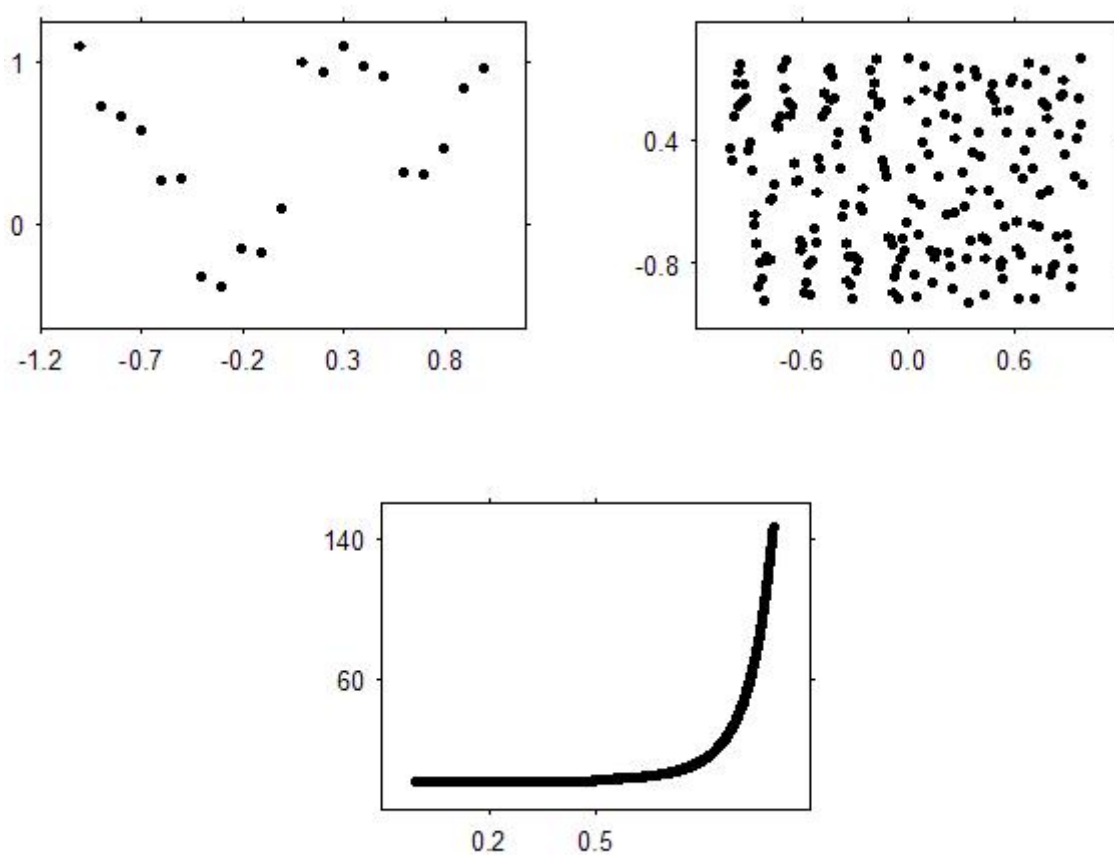


Figure 1: Noisy data obtained from $f_1(x)$ upper left-hand corner, $f_2(x)$ upper right-hand corner, and $f_3(x)$ bottom.

6.2. An application to edge detection. In this experiment we tested the method on image files. Image files can be considered as functions of two variables where each pixel represents a point in the xy plane and the grayscale value represents the color intensity evaluated at that point. We converted image files into 8-bit grayscale pgm files and then used Theorem 3.1 integrated in a Matlab program to detect the edges of the image. We tested inequality (2.4) at each pixel in the x and y direction separately. The discontinuities obtained in both directions were then combined to produce the final output. The pixels corresponding to discontinuities in the color intensity were assigned the grayscale value of 255 (white). Those corresponding to points of continuity were assigned the grayscale value of 0 (black). The method was tested on four different images (Lena, Gull, Bridge, Baboon) for different values of the parameter M_2 . No noise was added to the image files and the distance between two consecutive pixels was set equal to one ($h = 1$). The difficulty encountered while processing the images was that of defining an optimal value for the parameter M_2 . We do not offer a definite algorithm that allows one to determine the right value of the parameter M_2 for a given image file. For large values of M_2 we lost some minor details in the image, and for small values of M_2 we detected additional unwanted discontinuities. The computer time (RT) for each experiment was fairly low. The results of the experiments are presented below.

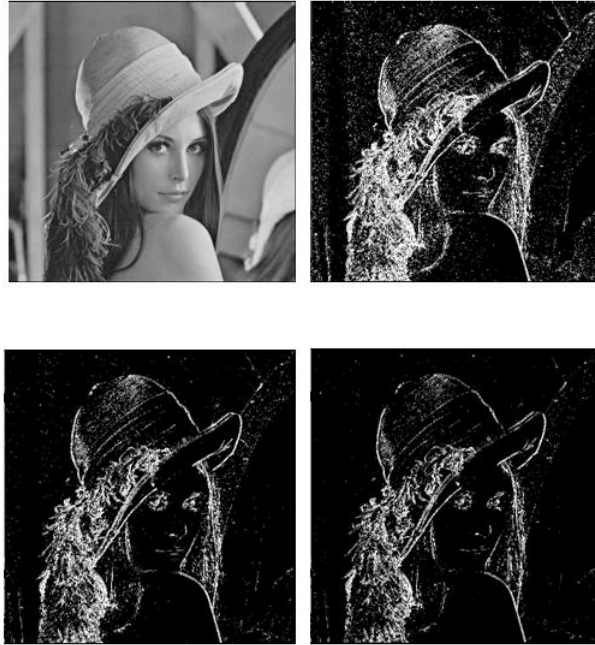


Figure 2: Lena: Original image Top left. Top right, processed image with $M_2 = 7$. Bottom left processed image with $M_2 = 10$. Bottom right, processed image with $M_2 = 13$. RT=.109s.

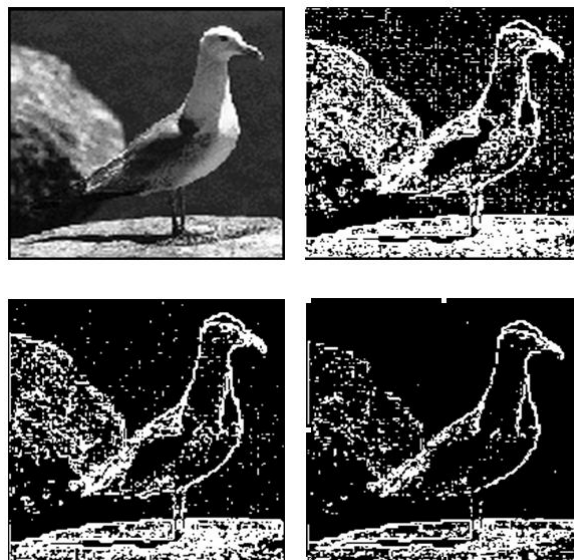


Figure 3: Gull: Original image Top left. Top right, processed image with $M_2 = 10$. Bottom left processed image with $M_2 = 15$. Bottom right, processed image with $M_2 = 20$. RT=.075s.

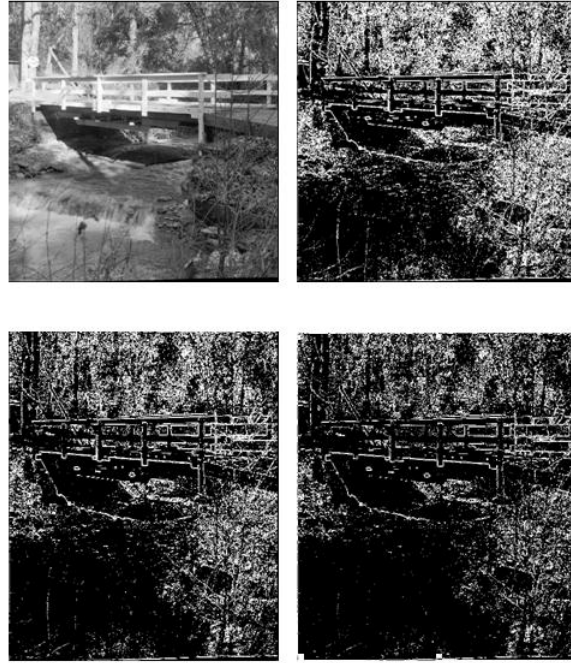


Figure 4: Bridge: Original image Top left. Top right, processed image with $M_2 = 15$. Bottom left processed image with $M_2 = 20$. Bottom right, processed image with $M_2 = 25$. RT=.110s.

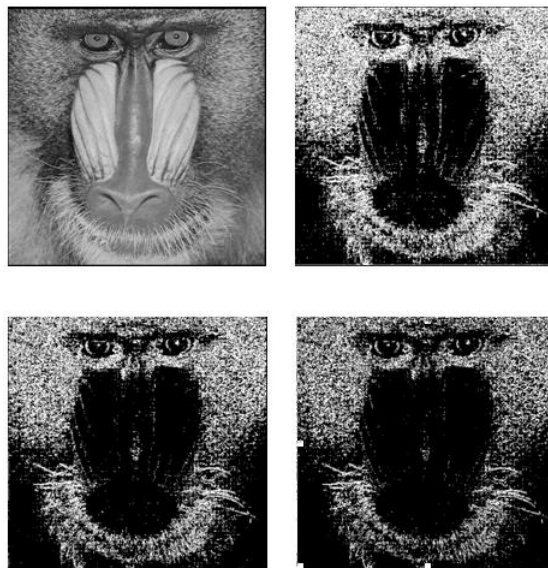


Figure 5: Baboon: Original image Top left. Top right, processed image with $M_2 = 15$. Bottom left processed image with $M_2 = 20$. Bottom right, processed image with $M_2 = 25$. RT=.081s.

6.3. Ramm's method compared to the method of approximation by cubic splines. Our main goal was to compare Ramm's method to the method of approximation by cubic splines. The comparison was based on the computational speed (RT) and on the relative error (RE). Here $RE = \frac{CE}{M_1}$, where $CE = \sup_{x \in [a,b]} |f'_\delta - f'|$ (f'_δ is the approximation of f' obtained by either

method) which was less than the theoretical error for both methods, and M_1 is defined as in (2.1). The detailed results are given in Figure 6, 7, and 8. It is clear from these plots that Ramm's method outperforms the method of approximation by cubic splines both in relative error and in computational speed, even though the underlying model is the same in both cases. The relative error obtained from the method of approximation by cubic splines (*MCS*) was far larger than that of Ramm's method (*RM*) in the first experiment (Figure 6). The superiority of *RM* is also apparent in the third experiment as shown in Figure 8. The computational speed of the *RM* was much greater than that of the *MCS* (by a factor of one hundred) for all experiments. Furthermore, the *MCS* had a relatively poor performance in the second experiment. The fundamental reason for this poor performance is the discontinuity in the derivative of f at $x = 0$. Note however that the additional error caused by this discontinuity affected the error bound of the *RM* only on the interval $(-.1, .1)$. On the other hand, that additional error propagated outside of the interval $(-.1, .1)$ in the case of the *MCS* and increased the error bound of approximation over the entire interval $(-\pi, \pi)$. These results are consistent with the theory developed in Section 5.

The functions used in each experiment are given in the following table along with the values of the parameters δ , h , M_2 , and RE . The noise function used was $\psi(x) = \delta \sin^2(x)$.

Functions	$f(x) = \sin(50x)$	$f(x) = \sin(x) $	$f(x) = e^{-x^2}$
M_2	2500	1	2
Noise level	.1	.005	.25
Step size	.001	.1	.5
RE from the <i>MCS</i> (%)	30	40	75
RE from the <i>RM</i> (%)	3	10	40
Interval	$[-1, 1]$	$[-\pi, \pi]$	$[-5, 5]$

Table 6.2: Results

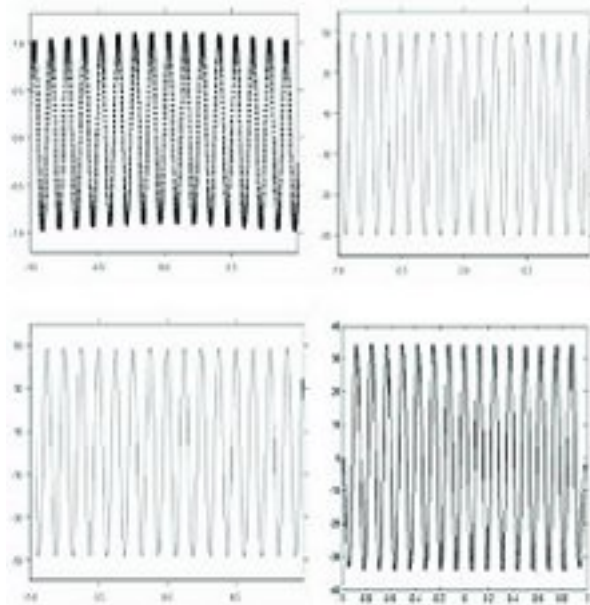


Figure 6: Noisy data Top left. Top right, derivative of the original function. Bottom left, numerical approximation using RM, RT= .062s. Bottom right, numerical approximation using MCS, RT=5.547s.

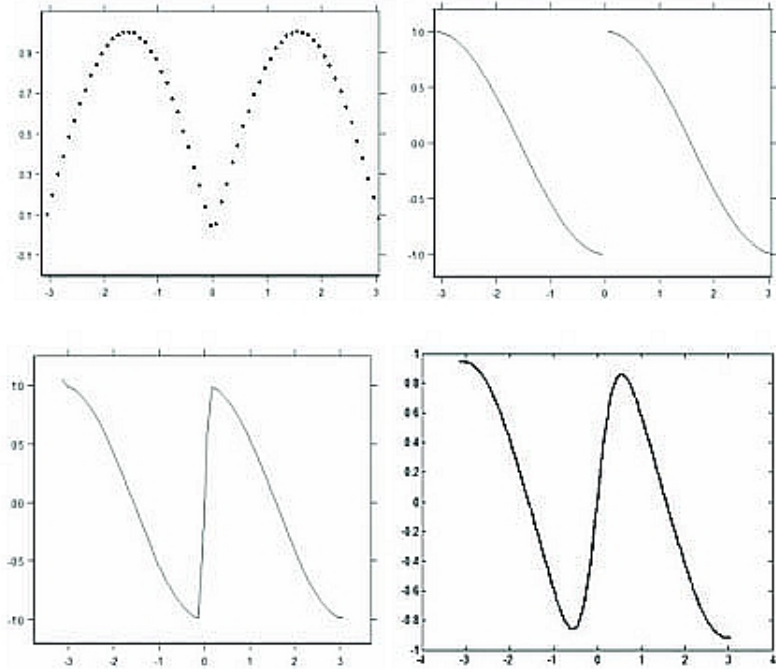


Figure 7: Noisy data Top left. Top right, derivative of the original function. Bottom left, numerical approximation using RM, RT= .032s. Bottom right, numerical approximation using MCS, RT=4.45s.

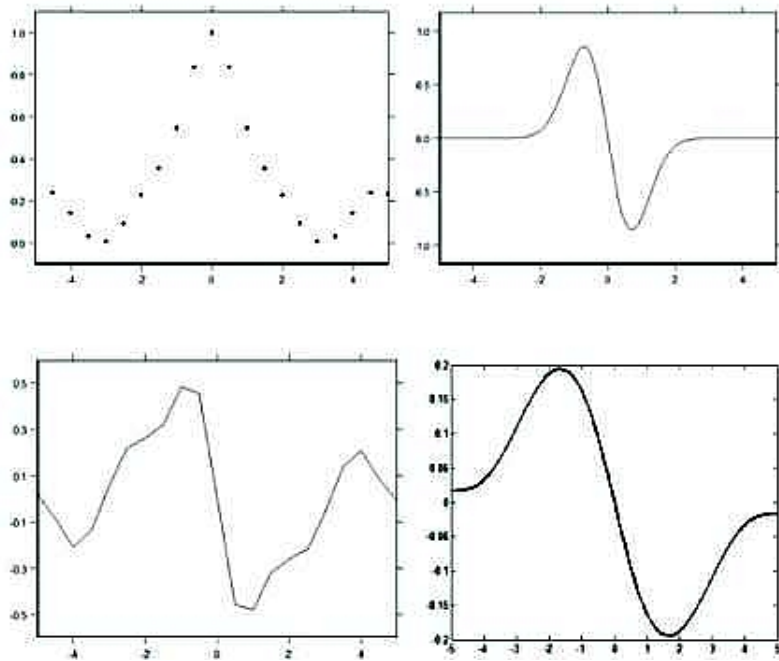


Figure 8: Noisy data Top left. Top right, derivative of the original function. Bottom left, numerical approximation using RM, RT= 0.001s. Bottom right, numerical approximation using MCS, RT=6.59s.

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