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A New Approach for the Generalized First Derivative and Extension It to the Generalized Second Derivative of Nonsmooth Functions

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Abstract— In this paper, first derivative of smooth function is defined by the optimal solution of a special optimization problem. In the next step, by using this optimization problem for nonsmooth function, we obtain an approximation for first derivative of nonsmooth function which it is called generalized first derivative. We then extend it to define generalized second derivative for nonsmooth function. Finally, we show the efficiency of our approach by evaluating derivative and generalized first and second derivative of some smooth and nonsmooth functions, respectively.

Index Terms— Generalized Derivative, Smooth and Nonsmooth Functions, Linear Programming, Optimization

I. Introduction

One of the most important concepts of nonsmooth analysis is the study of the generalized derivative (GD). In various fields such as optimization, control theory, differential equations, mechanics and economic when studying problems for different classes of nonsmooth functions, GD successfully has been applied. For instance, GDs use in solving of problems which mechanical engineers survey the evolution of rigid bodies that is subject to velocity jumps and force discontinuities as a result of friction and impacts. In addition, GDs use in solving of many areas problems such as diodes and transistors in electrical circuits or in problems of switching systems that arise in air traffic management, scheduling of automated railway systems and economic models of markets. In general, all systems contain switching systems that treat in nonsmooth systems (for more details see [1] and references therein).

There are some of well known generalized first derivative (GFD) especially Clarke GD [2], Ioffe

prederivative [3] and Mordukhovich coderivative [4,5] (for more details see [6]). On the other hand, generalized second derivative (GSD) has developed because of its application importance in many of problems of applied mathematics and engineering including variational inequalities, semi-infinite programming, penalty functions, optimization problems and especially sensitivity analysis of optimal solutions involve nonsmooth functions. Many authors have defined GSD in different ways, for instance Lemarechal and Nurminski [7], Hiriart-Urruty [8], Aubin [9], Auslender [10] and Chaney [11], Ben-Tal and Zowe [12-14], Rockafellar [15], Cominetti and Correa[16] (for more details see [17]).

In spite of the existence of different methods for GD, we see some restrictions and difficults in all of existing works in definitions of GFD and GSD, which it has been caused these GDs cannot use in applied problems. For example in these works, the nonsmooth function f(.) must be locally Lipschitz or convex and the points of nonsmoothness of nonsmooth function f(.) must be known. Moreover, the concepts limsup and liminf are applied to obtain the GD in which calculation of these is usually hard and complicated, and in general, deriving the GFD and GSD are very difficult and complex. It is therefore natural that we achieve a useful and practical approach for defining GD. This paper is basically an extended version of the results presented in [18]. Our intention here is to propose a useful and practical definition for GFD and in what follows, we will extend it to a new GSD (see [1] for application of practical new GFD in order to solve nonsmooth ordinary differential equations).

The structure of this paper is as follows. Section 2 defines GFD of nonsmooth functions which is based on functional optimization. Section 3 introduces a new definition for GSD based on last section. Some numerical examples and conclusions of this paper will be stated in Sections 4 and 5, respectively.

II. GFD of Nonsmooth Functions

We mainly utilize the new GD of Kamyad et al. ([18]) for nonsmooth functions. This kind of GD is particularly helpful and practical when dealing with nonsmooth continuous and discontinuous functions and it can be easily computed. In deriving our approach; first we introduce a functional optimization problem that its optimal solution is the derivative of smooth function on interval [0,1]. For solving this problem, we consider a linear programming problem and by solving it for nonsmooth functions, we obtain an approximate derivative for these functions on interval [0,1] which is GFD. In what follows, let us now devote just a short section to the generalized derivative of Kamyad et al. ([18]).

Let
$$V = v_k(.) : v_k(x) = \sin(k\pi x) : x \in [0,1], \ k = 1,2,\dots$$
 .

For given function f(x) on [0,1], define the following functional optimization problem:

$$\begin{aligned} & \text{Minimize} \quad J(g(.)) = \sum_{k=1}^{\infty} \left| \int_{0}^{1} v_{k}(x) g(x) \, dx - \lambda_{k} \right| \\ & \text{subject to} \\ & \int_{s_{i}-\delta}^{s_{i}+\delta} \left| f(x) - f(s_{i}) - (x-s_{i}) g(s_{i}) \right| dx \leq \varepsilon \delta^{2}, \\ & g(.) \in C[0,1], \, s_{i} \in (\frac{i-1}{m}, \frac{i}{m}), \, i = 1, 2, \ldots, m \end{aligned} \tag{1}$$

where $v_k(.)\in V$, $\lambda_k=-\int_0^1 v_k'(x)f(x)\,dx,\ k=1,2,3,...$ and ε , δ are positive sufficiently small numbers.

Theorem II.1 (see [18]): Let $f(.) \in C^1[0,1]$ and $g^*(.) \in C[0,1]$ be the optimal solution of the functional optimization problem (1). Then $f'(.) = g^*(.)$.

Definition II.2 (see [18]): Let f(.) be a nonsmooth continuous function on the interval [0,1] and $g^*(.)$ be the optimal solution of the functional optimization problem (1). We denote the generalized first derivative (GFD) of f(.) by $GF_df(.)$ and define as $GF_df(.)=g^*(.)$.

Remark II.3: Note that if f(.) is a smooth function on [0,1] then the $GF_df(.)$ in definition II.2 is f'(.). Further, if f(.) is a nonsmooth integrable function on [0,1] then GFD of f(.) is an approximation for first derivative of f(.).

In what follows, the problem (1) is approximated as the following finite dimensional problem ([18]):

$$\begin{aligned} & \text{Minimize} \quad J(g(.)) = \sum_{k=1}^{N} \left| \int_{0}^{1} v_{k}(x) g(x) \, dx - \lambda_{k} \right| \\ & \text{subject to} \\ & \int_{s_{i}-\delta}^{s_{i}+\delta} \left| f(x) - f(s_{i}) - (x - s_{i}) g(s_{i}) \right| dx \leq \varepsilon \delta^{2}, \\ & g(.) \in C[0,1], \, s_{i} \in (\frac{i-1}{m}, \frac{i}{m}), \, i = 1, 2, \dots, m \end{aligned} \tag{2}$$

where N is a given large number. We assume that $g_i=g(s_i), f_{i1}=f(s_i-\delta), f_{i2}=f(s_i+\delta)$ and $f_i=f(s_i)$ for all i=1,2,...,m. In addition, we choose the arbitrary points $s_i\in(\frac{i-1}{m},\frac{i}{m}),\ i=1,2,...,m$. By trapezoidal and midpoint integration rules, problem (2) can be written as the following problem which $g_1,g_2,...,g_m$ are its unknown variables:

$$\begin{split} & \text{Minimize} & \sum_{k=1}^{N} \left| \delta \sum_{i=1}^{m} v_{ki} g_{i} - \lambda_{k} \right| \\ & \text{subject to} \\ & \left| f_{i1} - f_{i} + \delta g_{i} \right| + \left| f_{i2} - f_{i} - \delta g_{i} \right| \leq \varepsilon \delta, \\ & i = 1, 2, \dots, m. \end{split} \tag{3}$$

Lemma II.4: Let pairs $(v_i^*, u_i^*), i = 1, 2, ..., m$ be the optimal solutions of the following LP problem:

$$\begin{split} & \text{Minimize} & & \sum_{i=1}^m v_i \\ & \text{subject to} & & v_i \geq u_i, \ v_i \geq -u_i, \ v_i \geq 0, u_i \in I. \end{split}$$

Then $u_i^*, i = 1, 2, ..., m$ are the optimal solutions of the following nonlinear programming problem (NLP):

$$\underset{u \in I}{\operatorname{Minimize}} \quad \sum_{i=1}^{m} \left| u_i \right|$$

where *I* is a compact set.

Proof: Since $(v_i^*, u_i^*), i = 1, 2, ..., m$ are the optimal solutions of the LP problem, so they satisfy the constraints. Thus we have $v_i^* \geq u_i^*$ and $v_i^* \geq -u_i^*$ for i = 1, 2, ..., m. Hence, $\left|u_i^*\right| \leq v_i^*$, i = 1, 2, ..., m and so $\sum_{i=1}^m \left|u_i^*\right| \leq \sum_{i=1}^m v_i^*$. Now, let there

exist $\overline{u}_i^* \in I$, i=1,2,...,m such that $\sum_{i=1}^m \left| \overline{u}_i^* \right| < \sum_{i=1}^m \left| u_i^* \right|$. Define, $\overline{v}_i^* = \left| \overline{u}_i^* \right|$ for i=1,2,...,m. Then $\overline{v}_i^* \geq \overline{u}_i^*$ and $\overline{v}_i^* \geq -\overline{u}_i^*$. Moreover, $\sum_{i=1}^m \overline{v}_i^* = \sum_{i=1}^m \left| \overline{u}_i^* \right|$ and hence $\sum_{i=1}^m \overline{v}_i^* = \sum_{i=1}^m \left| \overline{u}_i^* \right| < \sum_{i=1}^m \left| u_i^* \right| < \sum_{i=1}^m \left| v_i^* \right|$.

So
$$\sum_{i=1}^{m} \overline{v}_{i}^{*} < \sum_{i=1}^{m} v_{i}^{*}$$
 ,this is a contradiction.

Now, by Lemma II.4 and techniques of mathematical programming, problem (3) can be converted to the following equivalent linear programming problem which $g_i, i=1,...,m$, $\mu_k, k=1,2,...,N$ and ω_i, z_i, u_i, v_i for i=1,2,...,m are decision variables of the problem:

$$\begin{split} \text{Minimize} & & \sum_{k=1}^{N} \mu_{k} \\ \text{subject to} & & -\mu_{k} + \delta \sum_{i=0}^{m} v_{ki} g_{i} \leq \lambda_{k} \,, \\ & & -\mu_{k} - \delta \sum_{i=0}^{m} v_{ki} g_{i} \leq -\lambda_{k} \,, \\ & & (u_{i} + v_{i}) + (\omega_{i} + z_{i}) \leq \varepsilon \delta, \\ & & u_{i} - v_{i} - \delta g_{i} = f_{i1} - f_{i}, \\ & & \omega_{i} - z_{i} + \delta g_{i} = f_{i2} - f_{i}, \\ & & \omega_{i}, z_{i}, u_{i}, v_{i}, \mu_{k} \geq 0, \\ & & k = 1, 2, \dots, N; \quad i = 1, 2, \dots, m \end{split}$$

where λ_k for k = 1, 2, 3, ..., N satisfies in relation.

$$\lambda_k = -\int_0^1 v_k'(x)f(x) dx, \ k = 1, 2, 3, \dots$$

Remark II.5: Note that ε and δ are sufficiently small numbers and points $s_i \in (\frac{i-1}{m}, \frac{i}{m}),$ i=1,2,...,m can be chosen as arbitrary numbers.

Remark II.6: Note that if g_i^* , i=1,...,m are the optimal solutions of problem (4), then $GF_df(s_i)=g_i^*$, i=1,2,...,m.

III. GSD of Nonsmooth Functions

In this section, based on Section 2, we introduce an optimization problem similar to the problem (1) whose the optimal solution is the second order derivative of

smooth functions on an interval. By using this problem for nonsmooth functions, we approximate the second order derivative of these functions on an interval which is GSD. Firstly, we consider again Lemma II.1 in [18] and state the following theorem and prove it where $C^2[0,1]$ is the space of twice differentiable functions with the continuous derivative on [0,1].

Theorem III.1: Let $f(.) \in C^2[0,1], g(.) \in C[0,1]$ and $\int_0^1 v(x)g(x) - v''(x)f(x) \ dx = 0 \qquad \text{for} \qquad \text{any}$ $v(.) \in C^2[0,1] \quad \text{where} \quad v(0) = v(1) = v'(0) = v'(1) = 0$. Then we have f''(.) = g(.).

Proof: We use integration by parts twice and conditions v(0) = v(1) = v'(0) = v'(1) = 0:

$$\int_{0}^{1} v''(x)f(x) dx = \left[v'(1)f(1) - v'(0)f(0) - \int_{0}^{1} v'(x)f'(x) dx \right]$$

$$= -\int_{0}^{1} v'(x)f'(x) dx$$

$$= -\left[v(1)f'(1) - v(0)f'(0) - \int_{0}^{1} v(x)f''(x) dx \right]$$

$$= \int_{0}^{1} v(x)f''(x) dx.$$

Here

$$\int_{0}^{1} v''(x)f(x) dx = \int_{0}^{1} v(x)f''(x) dx.$$
 (5)

On the other hand, by assumptions of theorem, we have:

$$\int_0^1 v''(x)f(x) dx = \int_0^1 v(x)g(x)dx.$$
 (6)

Therefore, by (5) and (6)

$$\int_0^1 v(x) \ f''(x) - g(x) \ dx = 0. \tag{7}$$

So using equation (7) and by Lemma II.1 we have v(.) f''(.)-g(.) = 0 or f''(.)=g(.). \Box

Let the set

$$\begin{split} V &= \ v_k(.) : v_k(x) = 1 - \cos(2k\pi x) \colon x \in [0,1], \, k = 1,2,\dots \ . \end{split}$$
 Then $v(0) = v(1) = 0$ and $v'(0) = v'(1) = 0$ for all $v_k(.) \in V$. We note that V is a total set in
$$U = \ v(.) \in C^2[0,1] \colon v(0) = v(1) = v'(0) = v'(1) = 0 \ . \end{split}$$

So for any $v(.) \in U$ there exist coefficients a_0, a_1, \ldots in $\mathbb R$ such that

$$v(x) = \sum_{k} a_k v_k(x), \quad x \in [0, 1], v_k(.) \in V.$$
 (8)

Theorem III.2: Let $f(.),g(.)\in C^2[0,1]$ and $\int_0^1 v_k(x)g(x)-v_k''(x)f(x)\ dx=0\ \text{for any}\ v_k(.)\in V$ where v(0)=v(1)=v'(0)=v'(1)=0 . Then we have f''(.)=g(.) .

Proof: By attention to the relation (8) and the proof of Theorem III.1, we can conclude the proof of this theorem.

Theorem III.3: Let $\varepsilon>0$ be a given small number, $f(.)\in C^2[0,1]$ and $m\in\mathbb{N}$. Then there exist $\delta>0$ such that for all

$$\int_{s_i-\delta}^{s_i+\delta} \left| f'(x) - f'(s_i) - (x - s_i)f''(s_i) \right| dx \le \varepsilon \delta^2. \tag{9}$$

Proof: We have $f''(s_i)=\lim_{x\to s_i}\frac{f'(x)-f'(s_i)}{x-s_i}\,,$ $i=1,2,\ldots,m$. Then there exist $\delta_i>0$ such that for all $x\in(s_i-\delta_i,s_i+\delta_i)$

$$\left| \frac{f'(x) - f'(s_i)}{x - s_i} - f''(s_i) \right| \le \frac{\varepsilon}{2}, \quad i = 1, 2, ..., m.$$
 (10)

Now assume that $\delta=\min$ $\delta_i, i=1,2,...,m$. So for $s_i\in(\frac{i-1}{m},\frac{i}{m})$ and $x\in(s_i-\delta_i,s_i+\delta_i)$, i=1,2,...,m the inequality (10) is held. On the other hand, $(s_i-\delta,s_i+\delta)\subseteq(s_i-\delta_{s_i},s_i+\delta_{s_i})$. Thus by inequality (10) we obtain for all i=1,2,...,m

$$\left|f'(x) - f'(s_i) - (x - s_i)f''(s_i)\right| \le \frac{\varepsilon}{2} \left|x - s_i\right| \le \frac{\varepsilon}{2} \delta. \tag{11}$$

Thus by integrating both sides of inequality (11) on interval $(s_i-\delta,s_i+\delta)$, i=1,2,...,m we can obtain inequality (9). \square

Suppose $\varepsilon>0$ and $\delta>0$ are two sufficiently small given number and $m\in\mathbb{N}$. For given continuous function f(x) on [0,1], we define the following functional optimization problem

$$\begin{aligned} & \underset{g(.) \in C[0,1]}{\operatorname{Minimize}} \quad I(g(.)) = \sum_{k=1}^{\infty} \left| \int_{0}^{1} v_{k}(x) g(x) \, dx - \lambda_{k} \right| \\ & \text{subject to} \\ & \int_{s_{i} - \delta}^{s_{i} + \delta} \left| h(x) - h(s_{i}) - (x - s_{i}) g(s_{i}) \right| dx \leq \varepsilon \delta^{2}, \\ & g(.) \in C[0,1], \, s_{i} \in (\frac{i-1}{m}, \frac{i}{m}), \, i = 1, 2, \ldots, m \end{aligned} \tag{12}$$

where $v_k(.) \in V$ for all k = 1, 2, 3, ... and

$$\lambda_k = \int_0^1 v_k(x) f''(x) dx,\tag{13}$$

and if $f(.) \in C^1[0,1]$, then h(.) = f'(.) and otherwise $h(.) = GF_df(.)$ which the function $GF_df(.)$ is the GFD of f(x) (see [18]).

Theorem III.4: Let $f(.) \in C^2[0,1]$ be given and $g^*(.) \in C[0,1]$ is the optimal solution of functional optimization problem (12). Then, we have $g^*(.) = f''(.)$.

Proof: It is trivial that $\sum_{k=1}^{\infty} \left| \int_0^1 v_k(x) g(x) \, dx - \lambda_k \right| \geq 0 \ \text{ for all } g(.) \in C[0,1] \ . \ \text{ By }$

Theorem III.1, we have $\left|\int_0^1 v_k(x)g(x)\,dx - \lambda_k\right| = 0 \ \text{ for}$ all $v_k(.) \in V \quad \text{ where } \quad g(.) = f''(.)$ on [0,1]. So $\sum_{k=0}^{\infty} \left|\int_0^1 v_k(x)f''(x)\,dx - \lambda_k\right| = 0 \ \text{, hence}$

$$\sum_{k=1}^{\infty}\left|\int_{0}^{1}\,v(x)f''(x)\,dx-\lambda_{k}\right|\leq \sum_{k=1}^{\infty}\left|\int_{0}^{1}\,v(x)g(x)\,dx-\lambda_{k}\right|.$$

On the other hand, $f''(.) \in C^2[0,1]$ which by Theorem III.2 satisfies in constraints of problem (12). Thus, f''(.) is optimal solution of functional optimization (12).

By Theorem III.2 and solving problem (12), we will obtain the approximate second order derivative of nonsmooth functions. Thus, the GSD of nonsmooth functions will be defined as follows:

Definition III.5: Let f(.) be a continuous nonsmooth function on interval [0,1] and $g^*(.)$ is the optimal solution of the functional optimization problem (12). We denote the GSD of f(.) by $GS_df(.)$ and define as

$$GS_d f(.) = g^*(.)$$
.

Remark III.6: Note that if f(.) is a smooth function then the $GS_df(.)$ is f''(.). Also if f(.) is a nonsmooth function then GSD of f(.) is an approximation for second order derivative of f(.).

However, the functional optimization problem (12) is an infinite dimensional problem. Thus we will convert this problem to the corresponding finite dimensional problem. For this goal, suppose functions $v_k(.) \in V$ for k=1,2,3,...,N as follows:

$$v_k(x) = 1 - \cos(2k\pi x), \quad k = 1, 2, 3, ..., N$$
 (14)

where N is a given big number. Thus, the objective function of problem (12) is approximated as the following function:

$$I(g(.)) \approx \sum_{k=1}^{N} \left| \int_{0}^{1} v_{k}(x)g(x) dx - \lambda_{k} \right|.$$
 (15)

Thus, the objective function of problem (12) can be written as the following which g_0,g_1,\ldots,g_M are the decision variables:

$$\underset{a_0, a_1, \dots a_M}{\text{Minimize}} \quad \sum_{k=1}^{N} \left| \delta \sum_{i=0}^{m} v_{ki} \ g_i - \lambda_k \right| \tag{16}$$

where $v_{ki}=v_k(x_i)$ and $g_i=g(x_i)$ for $k=1,2,3,...,N,\ j=0,1,...,m$. Moreover, we approxi- mate the constraints of the problem (12) using simple trapezoidal rule as follows:

$$\left|h_{i1} - h_i - \delta g_i\right| + \left|h_{i2} - h_i - \delta g_i\right| \le \varepsilon\delta \tag{17}$$

where $g_i=g(s_i), h_{i1}=h(s_i-\delta), h_{i2}=h(s_i+\delta)$ and $h_i=h(s_i)$ for all i=1,2,...,m.

Thus, according to the above-mention relations (16) and (17), problem (12) is converted to the following equivalent linear programming problem which $\mu_1,\mu_2,...,\mu_N$ and ω_i,z_i,u_i,v_i for i=1,2,...,m are unknown variables of the problem:

$$Minimize \sum_{k=1}^{N} \mu_k 18$$

subject to
$$\begin{split} &-\mu_k + \delta \sum_{i=0}^m v_{ki} g_i \leq \lambda_k \,, \quad k=1,2,...,N \\ &-\mu_k - \delta \sum_{i=0}^m v_{ki} g_i \leq -\lambda_k \,, \quad k=1,2,...,N \\ &(u_i+v_i) + (\omega_i+z_i) \leq \varepsilon \delta, \quad i=1,2,...,m \end{split}$$

$$\begin{split} &u_i - v_i - \delta g_i = h_{i1} - h_i, & i = 1, 2, ..., m\\ &\omega_i - z_i + \delta g_i = h_{i2} - h_i, & i = 1, 2, ..., m\\ &\omega_i, z_i, u_i, v_i, \mu_k \geq 0, & k = 1, 2, ..., N; & i = 1, 2, ..., m \end{split}$$

where λ_k for k = 1, 2, 3, ..., N are known parameters by relations (13).

Then by solving problem (18), we will obtain the optimal solutions $g_0^*, g_1^*, \dots, g_m^*$ and so by definition III.5 we have $GS_df(x_i) = g_i^*$ for all $x \in [0,1]$.

IV. Numerical examples

In this stage, we find the GSD of smooth and nonsmooth functions in several examples using problem (18). Here we assume $\varepsilon = \delta = 0.01$, N = 20, m = 99 and $s_i = 0.01i$ for all $i = 1, \ldots, 99$. The problem (18) is solved for functions in these examples using Simplex method in MATLAB software. Attend that in our approach points in [0,1] are selected arbitrarily, and with selection very of these points, we can cover this interval. Thus this is a global approach, while the previous approaches and methods act as locally on a fixed given point in [0,1].

Example IV.1: Consider the smooth function $f(x) = e^x \sin^2(x)$ on interval [0,1]. The function f(x) is illustrated in Fig.1. The exact second derivative of f(x) is shown in Fig.2 and Fig.3 shows the GSD of f(x) which has been obtained by using the problem (18). The absolute error of GSD is presented in Fig.4.

Example IV.2: Consider the nonsmooth function f(x) = |2x - 1| on [0,1]. This function is not differentiable in x = 0.5 (see Fig.5) and according to the problem (18), GSD of f(x) has been shown in Fig.6.

Example IV.3: Consider the function $f(x) = e^{0.5(x-0.5)^2 \operatorname{sgn}(x-0.5)}$ on [0,1]. According to Fig.7 (the graph of f(x)) and Fig.8 (the graph of exact first derivative (FD) of f(x)), see that $f(x) \in C^1[0,1]$, but $f(x) \not\in C^2[0,1]$. Using problem (18), we calculate the GSD of f(x) which it has been shown in Fig. 9.

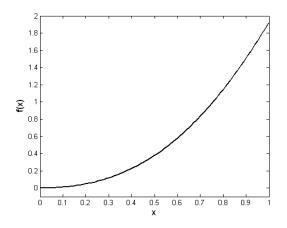


Fig. 1: The graph of $f(x) = e^x \sin^2(x)$

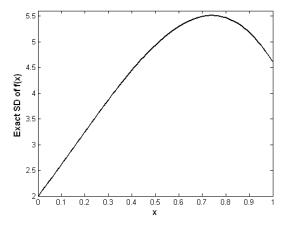


Fig. 2: The graph of exact second derivative of $\,f(x)\,$

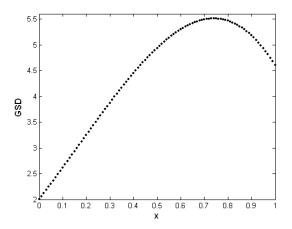


Fig. 3: The graph of GSD of f(x)

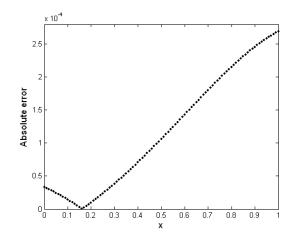


Fig. 4: The absolute error of GSD of f(x)

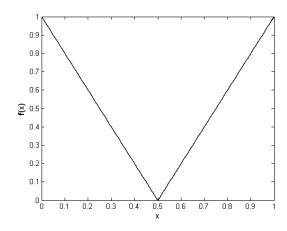


Fig. 5: The graph of $f(x) = \left| 2x - 1 \right|$

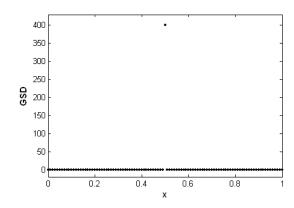


Fig. 6: The graph of GSD of f(x)

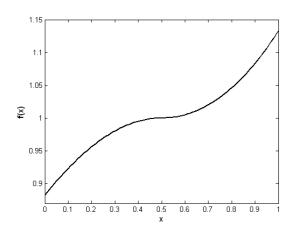


Fig. 7: The graph of $f(x)=e^{0.5(x-0.5)^2\operatorname{sgn}(x-0.5)}$

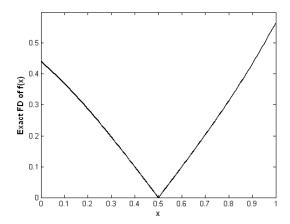


Fig. 8: The graph of first derivative of f(x)

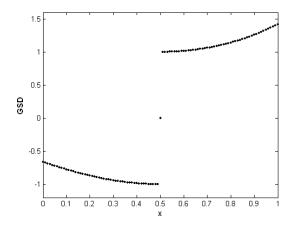


Fig. 9: The graph of GSD of f(x)

V. Conclusions

In this paper, we have proposed a GSD for nonsmooth functions. This approach can be applied to all of nonsmo- oth optimization problems including problems with nonsmooth objective functions and constraints.

We have tested the new approach on some smooth and nonsmooth functions. Preliminary results of numerical experiments show that GSD outperforms other methods considered in this paper. We can conclude that GSD is a good alternative to defining generalized second order derivative. Moreover, in other approaches were defined usually for special functions such as Lipschitz or convex functions while we defined GSD for nonsmooth integrable functions.

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