On Sum-Rules for Second-Order Contingent Derivatives

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Abstract. We are concerned with contingent derivatives and their second-order counterparts (introduced by Ngai et al.) of set-valued mappings. Special attention is given to the development of new sum-rules for second-order contingent derivatives. To be precise, we want to find conditions under which the second-order contingent derivative of the sum of a smooth and a set-valued mapping coincides with the sum of the derivatives. An application to the computation of tangents to the solution set of a generalized equation is also included.

Keywords: Second-Order Contingent Derivative · Generalized Equation · Error Bound · Tangent Cone

1 Introduction

For a single-valued mapping $F : \mathbb{R}^n \to \mathbb{R}^m$, and a set-valued mapping $\Gamma : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$, we consider the generalized equation,

$$0 \in F(u) + \Gamma(u), \tag{1}$$

and denote its solution set by Σ, i.e., $\Sigma = \{u \in \mathbb{R}^n \mid 0 \in F(u) + \Gamma(u)\}$. Numerous problems can be modeled by a generalized equation (1), including constrained systems of equations, as well as more concrete problems in engineering and economics, see for example [1,6,7,9,10] among others.

Two issues related to the generalized equation (1) are addressed in this note. In Sects. 2–3 we deal with first- and second-order contingent derivatives of the set-valued mapping $F+\Gamma$. The former contingent (or *graphical*) derivative is well studied [9,11], but second-order contingent derivatives (which have their origin in [8]) have not received much attention so far. We formulate new sum-rules in Sect. 3 for this derivative. To be specific, we prove under some assumptions that the second-order contingent derivative of $F+\Gamma$ can be written as the sum of the second-order contingent derivatives of F and Γ. Besides sufficient smoothness of F, other additional assumptions, such as full degeneracy of the first derivative of F, are used to establish the sum-rule, and we will explain that these additional assumptions cannot generally be dropped without destroying the sum-rule. At the end of this note, in Sect. 4, we use both a Lipschitzian and a square-root error bound condition to express the *(Bouligand) tangent cone* to Σ as the zeros of the derivatives of $F+\Gamma$. Recall in this respect from [1,9] that for some $u^* \in \Sigma$, the aforementioned tangent cone is given as

$$T_\Sigma(u^*) = \left\{ w \in \mathbb{R}^n \,\middle|\, \exists t_k \searrow 0, \exists w^k \to w : \; u^* + t_k w^k \in \Sigma \forall k \in \mathbb{N} \right\}.$$

Formulas that allow a simplified computation of the tangent cone are relevant in their own right, but they are particularly important in mathematical optimization for the purpose of detecting stationary points of a constrained optimization problem, cf. [1,5,10,11].

Notation: Throughout, $u^* \in \Sigma$ is an arbitrary but fixed solution of (1); $\|\cdot\|$ is the Euclidean norm, and dist the Euclidean point-to-set distance; $\mathscr{B}_\varepsilon(a)$ stands for the Euclidean ball centered at a with radius ε; gph$S$, rge$S$, dom$S$ are the graph, range, and domain of a set-valued mapping S; int(A) is the (topological) interior of a set A; ker$L$ is the nullspace of a linear operator L, and im$L$ is its range; $t_k \searrow 0$ means that the sequence $\{t_k\}$ converges to 0 with all its elements being positive.

2 Preliminaries

In this section we recall the definition of first- and second-order contingent derivatives of a mapping from [8,11]. We will also discuss basic relations between these derivatives and show how they are computed for some examples that will be of interest later.

Definition 1. *Given a set-valued mapping $S : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$, and a point $(u,y) \in \text{gph}S$.*

(a) The contingent derivative of S at (u,y) is defined for $w \in \mathbb{R}^n$ as

$$CS(u|y)(w) := \left\{ x \in \mathbb{R}^m \,\middle|\, \exists t_k \searrow 0, \exists (w^k, x^k) \to (w,x) : \; y + t_k x^k \in S(u + t_k w^k)\, \forall k \right\}.$$

(b) The second-order contingent derivative of S at (u,y) is defined for $w \in \mathbb{R}^n$ as

$$C^2S(u|y)(w) := \left\{ x \in \mathbb{R}^m \,\middle|\, \exists t_k \searrow 0, \exists (w^k, x^k) \to (w,x) : \; y + t_k^2 x^k \in S(u + t_k w^k)\, \forall k \right\}.$$

The following states a relation between the domain of the second-order contingent derivative, and the zero set of the contingent derivative.

Lemma 1. *For a set-valued mapping $S : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$, it holds for any $(u,y) \in \text{gph}S$ that*

$$\text{dom}\left(C^2S(u|y)\right) \subset \{ w \in \mathbb{R}^n \mid 0 \in CS(u|y)(w) \}.$$

Proof. Pick $w \in \text{dom}\left(C^2S(u|y)\right)$ arbitrarily, and find $x \in \mathbb{R}^m$, and $t_k \searrow 0$, $w^k \to w$, $x^k \to x$, so that $y + t_k^2 x^k \in S(u + t_k w^k)$ holds for all $k \in \mathbb{N}$. We have $v^k := t_k x^k \to 0$, thus, together with previous considerations, $0 \in CS(u|y)(w)$ follows. □

Now, we compute generalized derivatives of the set-valued indicator for a set $\Gamma_0 \subset \mathbb{R}^n$,

$$\Delta_{\Gamma_0}(u) := \begin{cases} \{0\} & \text{if } u \in \Gamma_0, \\ \varnothing & \text{if } u \notin \Gamma_0. \end{cases} \tag{2}$$

This mapping is known, e.g., from [7], and it can be used in particular for reformulating generalized equations as constrained systems of equations (and vice versa), cf. [6].

Proposition 1. *For a set $\Gamma_0 \subset \mathbb{R}^n$, it holds for any $(u,w) \in \Gamma_0 \times \mathbb{R}^n$ that*

$$C^2\Delta_{\Gamma_0}(u|0)(w) = C\Delta_{\Gamma_0}(u|0)(w) = \Delta_{T_{\Gamma_0}(u)}(w).$$

Proof. This follows from the definitions of the derivatives, the tangent cone, and the indicator. □

To compute the second-order contingent derivative of the single-valued mapping F, we want to use a smoothness property introduced in [6], namely:

Definition 2. *The mapping F has a semi-quadratic expansion at u^* for a direction $w \neq 0$, if F is differentiable at u^*, and the limit below exists in $\mathbb{R}^m$:*

$$E(u^*;w) := \lim_{\substack{t \searrow 0 \\ v \to w}} \frac{F(u^*+tv) - F(u^*) - tF'(u^*)v}{0.5t^2}.$$

A sufficient condition for the existence of a semi-quadratic expansion is as follows:

Lemma 2 (Lem. 6.12, [6]). *If F is differentiable near u^*, and F' is semidifferentiable at u^* for $w \neq 0$, i.e., the following limit exists in $\mathbb{R}^{m \times n}$*

$$F''(u^*;w) := \lim_{\substack{t \searrow 0 \\ w' \to w}} \frac{F'(u^*+tw') - F'(u^*)}{t},$$

then F has a semi-quadratic expansion at u^* for w, satisfying $E(u^*;w) = F''(u^*;w)w$.

Note that semidifferentiability of F' is necessary for twice differentiability of F, but it is not sufficient in general, as we will now illustrate.

Example 1. Let $F(u) := \max\{0,u\}^2$ and $u^* := 0$. This F is continuously differentiable with $F'(u) = 2\max\{0,u\}$ for any $u \in \mathbb{R}$. Since F' is not differentiable at u^*, we find that F can not be twice differentiable at u^*. At the same time, F' is semidifferentiable at u^* with $F''(u^*;w) = 2\max\{0,w\}$ for any $w \in \mathbb{R}$. In particular, by Lem. 2 we know that F has a semi-quadratic expansion at u^*, given by $E(u^*;w) = 2\max\{0,w\}w$ for $w \neq 0$. □

Finally, we want to compute the (second-order) contingent derivative of F.

Proposition 2. *If F is differentiable at u^*, then*

$$CF(u^*|F(u^*))(w) = F'(u^*)w \qquad \forall w \in \mathbb{R}^n. \tag{3}$$

If F has a semi-quadratic expansion at u^* for a direction $w \neq 0$, then

$$C^2F(u^*|F(u^*))(w) = \begin{cases} 0.5E(u^*;w) + \operatorname{im} F'(u^*) & \text{if } w \in \ker F'(u^*), \\ \varnothing & \text{if } w \notin \ker F'(u^*). \end{cases} \tag{4}$$

Proof. The formula in (3) can be extracted from [9, Exerc. 9.25 (b)], while the one in (4) follows from an application of [6, Ex. 6.15] with $C_0 = \mathbb{R}^n$. □

The formula in (4) is a slight generalization of [8, Prop. 35], where a similar observation was made under the assumption that F is twice differentiable at u^*.

3 Sum-Rules for (Second-Order) Contingent Derivatives

We present sum-rules for the two derivatives from Sect. 2. The one concerning contingent derivatives (Prop. 3) is well known and serves as a prototype result. For illustration purposes, we also specialize sum-rules to the case where the indicator (2) is involved.

Proposition 3 (Exerc. 10.43, [9]). *If F is differentiable at u^*, then, for all $w \in \mathbb{R}^n$,*

$$\begin{aligned} C(F+\Gamma)(u^*|0)(w) &= CF(u^*|F(u^*))(w) + C\Gamma(u^*|-F(u^*))(w) \\ &= F'(u^*)w + C\Gamma(u^*|-F(u^*))(w). \end{aligned}$$

Corollary 1. *For a nonempty closed set $\Gamma_0 \subset \mathbb{R}^n$, suppose $\Gamma = \Delta_{\Gamma_0}$ holds, where the mapping Δ_{Γ_0} is defined according to (2). If F is differentiable at u^*, then*

$$C(F+\Delta_{\Gamma_0})(u^*|0)(w) = CF(u^*|0)(w) + C\Delta_{\Gamma_0}(u^*|0)(w) = \begin{cases} F'(u^*)w & \text{if } w \in T_{\Gamma_0}(u^*), \\ \varnothing & \text{if } w \notin T_{\Gamma_0}(u^*). \end{cases}$$

Proof. Here, we have $\Sigma = F^{-1}(0) \cap \Gamma_0$, so the claim is due to Props. 1,3. □

We give a counterpart to Prop. 3 with respect to second-order contingent derivatives next. Unlike Prop. 3, additional assumptions (not only concerning smoothness of F) come into play. One of these is the *T–conicity* of a set $\Gamma_0 \subset \mathbb{R}^n$ at $u^* \in \Gamma_0$, a property coined in [2], which requires that Γ_0 and $u^* + T_{\Gamma_0}(u^*)$ coincide in a neighborhood of u^*.

Proposition 4. *Suppose F has a semi-quadratic expansion at u^* for $w \neq 0$, and one of the following conditions is true:*

(a) $F'(u^*) = 0$.
(b) $F(u^*)$ *is isolated in* $\mathrm{rge}(-\Gamma)$, $\mathrm{dom}\Gamma$ *is T–conical at u^*, and* $w \in \mathrm{int}(T_{\mathrm{dom}\Gamma}(u^*))$.

Then, it holds that

$$C^2(F+\Gamma)(u^*|0)(w) = C^2F(u^*|F(u^*))(w) + C^2\Gamma(u^*|-F(u^*))(w). \tag{5}$$

Proof. Put $y^* := -F(u^*)$. Suppose (a) holds. Then, [6, Thm. 6.13 (a)] yields

$$C^2(F+\Gamma)(u^*|0)(w) = \begin{cases} 0.5E(u^*;w) + C^2\Gamma(u^*|y^*)(w) & \text{if } 0 \in C\Gamma(u^*|y^*)(w), \\ \varnothing & \text{if } 0 \notin C\Gamma(u^*|y^*)(w). \end{cases} \tag{6}$$

From Lem. 1, we know $C^2\Gamma(u^*|y^*)(w) \neq \varnothing$ necessitates $0 \in C\Gamma(u^*|y^*)(w)$, so (6) can be written as $C^2(F+\Gamma)(u^*|0)(w) = 0.5E(u^*;w) + C^2\Gamma(u^*|y^*)(w)$. Therefore, and because $\mathrm{im}F'(u^*) = \{0\}$ and $\ker F'(u^*) = \mathbb{R}^n$ are valid, the formula in (5) follows by Prop. 2. Under conditions in (b), in turn, we can apply [6, Thm. 6.13 (b)], which gives us $C^2(F+\Gamma)(u^*|0)(w) = 0.5E(u^*;w) + \mathrm{im}F'(u^*)$ for $w \in \ker F'(u^*) \cap C\Gamma(u^*|y^*)^{-1}(0)$, and $C^2(F+\Gamma)(u^*|0)(w) = \varnothing$ otherwise. The imposed assumptions also imply $\{0\} = C\Gamma(u^*|y^*)(w) = C^2\Gamma(u^*|y^*)(w)$, so (5) follows from considerations above, and Prop. 2. (Note that although used in the proof, the T–conicity of Γ_0 at u^* was not mentioned in the list of assumptions of [6, Thm. 6.13 (b)].) □

Corollary 2. *In the setting of Cor. 1, suppose F has a semi-quadratic expansion at u^* for $w \neq 0$, and one of the following conditions is true:*

(a) $F'(u^*) = 0$.
(b) Γ_0 *is T–conical at u^*, and* $w \in \mathrm{int}(T_{\Gamma_0}(u^*))$.

Then, it holds that

$$C^2(F+\Delta_{\Gamma_0})(u^*|0)(w) = C^2F(u^*|0)(w) + C^2\Delta_{\Gamma_0}(u^*|0)(w)$$
$$= \begin{cases} 0.5E(u^*;w)+\mathrm{im}F'(u^*) & \text{if } w \in \ker F'(u^*)\cap T_{\Gamma_0}(u^*), \\ \varnothing & \text{if } w \notin \ker F'(u^*)\cap T_{\Gamma_0}(u^*). \end{cases}$$

Proof. Here, we have $\mathrm{rge}\Gamma = \{0\}$ and $\mathrm{dom}\Gamma = \Gamma_0$, so condition (b) of this corollary is a specialization of condition (b) in Prop. 4 with $\Gamma = \Delta_{\Gamma_0}$. Thus, (a)–(b) are sufficient for $C^2(F+\Delta_{\Gamma_0})(u^*|0)(w) = C^2F(u^*|0)(w) + C^2\Delta_{\Gamma_0}(u^*|0)(w)$ to hold. (Note here that $u^* \in \Sigma$ and $\Gamma = \Delta_{\Gamma_0}$ together imply $F(u^*) = 0$.) Combining the latter equality with Props. 1–2, and the definition of the indicator (2), then we get

$$C^2(F+\Delta_{\Gamma_0})(u^*|0)(w) = \begin{cases} 0.5E(u^*;w)+\mathrm{im}F'(u^*) & \text{if } w \in \ker F'(u^*), \\ \varnothing & \text{if } w \notin \ker F'(u^*) \end{cases}$$
$$+ \begin{cases} \{0\} & \text{if } w \in T_{\Gamma_0}(u^*), \\ \varnothing & \text{if } w \notin T_{\Gamma_0}(u^*) \end{cases}$$
$$= \begin{cases} 0.5E(u^*;w)+\mathrm{im}F'(u^*) & \text{if } w \in \ker F'(u^*)\cap T_{\Gamma_0}(u^*), \\ \varnothing & \text{if } w \notin \ker F'(u^*)\cap T_{\Gamma_0}(u^*). \end{cases}$$

The proof of this corollary is complete. □

The next example shows that the conclusion of the corollary does not necessarily hold without the additional assumptions it makes, implying that a sum-rule for second-order contingent derivatives (Prop. 4) cannot generally hold without such assumptions.

Example 2. Take $F(u_1,u_2) = u_1 + u_2^2$ and $\Gamma_0 = \{0\} \times \mathbb{R}$. For $u^* = (0,0)$, we have $F'(u^*) = (1,0) \neq (0,0)$ and $\mathrm{int}(T_{\Gamma_0}(u^*)) = \varnothing$. So, e.g., for $w = (0,1)$, conditions (a)–(b) in Cor. 2 do not hold. We have $w \in \ker F'(u^*)\cap T_{\Gamma_0}(u^*)$, and $0.5E(u^*;w)+\mathrm{im}F'(u^*) = \mathbb{R}$, while for any small $t > 0$, and $v = (0,\mu)$ near w, we see that $t^2x = (t\mu)^2$ can only hold for $x = \mu^2$, which implies $C^2(F+\Delta_{\Gamma_0})(u^*|0)(w) \subset \mathbb{R}_+$. Thus, the conclusion of Cor. 2 may not hold when conditions (a) and (b) are both violated. □

4 Error Bounds and the Computation of Tangents to Σ

The derivatives from Sect. 2 can be used to compute tangents to the solution set Σ of the generalized equation (1) under appropriate error bound conditions:

Proposition 5 (Prop. 34, [8]). *The following hold, if* $\mathrm{gph}(F+\Gamma)$ *is closed near* $(u^*,0)$*:*

(a) The Lipschitzian error bound condition,

$$\exists \varepsilon, c > 0: \quad \mathrm{dist}[u,\Sigma] \leq c \cdot \mathrm{dist}[0, F(u)+\Gamma(u)] \quad \forall u \in \mathscr{B}_\varepsilon(u^*), \tag{7}$$

is sufficient for $T_\Sigma(u^*) = \{w \in \mathbb{R}^n \,|\, 0 \in C(F+\Gamma)(u^*|0)(w)\}$.

(b) The square-root error bound condition,

$$\exists \varepsilon, c > 0: \quad \mathrm{dist}[u,\Sigma] \leq c \cdot \sqrt{\mathrm{dist}[0, F(u)+\Gamma(u)]} \quad \forall u \in \mathscr{B}_\varepsilon(u^*), \tag{8}$$

is sufficient for $T_\Sigma(u^*) = \left\{w \in \mathbb{R}^n \,\middle|\, 0 \in C^2(F+\Gamma)(u^*|0)(w)\right\}$.

Conditions guaranteeing error bound properties are not our concern in this note. The reader interested in these things is referred to [1,2,5,6,8] and the works cited therein.

Specializations of the proposition for the case where Γ is the indicator can be easily derived from the results in Sect. 3 – we omit details here for brevity. Instead, improving on the outcome of [5, Rem. 3], we present a necessary condition for the error bound (7).

Corollary 3. *In the setting of Prop. 5 with $\Gamma \equiv \{0\}$, suppose the error bound condition* (7) *holds. If F has a semi-quadratic expansion at u^* for all $v \in \ker F'(u^*) \setminus \{0\}$, then*

$$F'(u^*)w = 0, \quad w \neq 0 \qquad \Longrightarrow \qquad E(u^*;w) \in \mathrm{im}F'(u^*). \tag{9}$$

Proof. Clearly, error bound (7) implies (8). Thus, Prop. 5 applied with $\Gamma \equiv \{0\}$ gives

$$T_{F^{-1}(0)}(u^*) = \{w \in \mathbb{R}^n \mid 0 \in CF(u^*|0)(w)\} = \left\{w \in \mathbb{R}^n \;\middle|\; 0 \in C^2F(u^*|0)(w)\right\}.$$

With regard to Prop. 2, we now find that $0 \in 0.5E(u^*;w) + \mathrm{im}F'(u^*)$ is satisfied for all $w \in \ker F'(u^*) = T_{F^{-1}(0)}(u^*)$. In other words, the condition in (9) holds true. □

It is not true, in general, that (9) implies (7) when $\Gamma \equiv \{0\}$, just consider $F(u) = u^3$. Without (7), the conclusion of Cor. 3 does not necessarily hold, as can be illustrated by Ex. 1. At the same time, we emphasize that the violation of (9) necessitates the absence of the Lipschitzian error bound (7), and this is of interest for the considerations in [3,4].

Conclusion. We formulated new sum-rules for second-order contingent derivatives. These derivatives were introduced in [8] without formulating important calculus rules for them. Under an error bound condition, second-order contingent derivatives can help to compute tangents to the level set of a mapping. We used this fact to get a new necessary condition for Lipschitzian error bounds.

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