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Second-Order Contingent Derivatives: Computation and Application

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Abstract It is known that second-order (Studniarski) contingent derivatives can be used to compute tangents to the solution set of a generalized equation when standard (first-order) regularity conditions are absent, but relaxed (second-order) regularity conditions are fulfilled. This fact, roughly speaking, is only relevant in practice as long as the computation of second-order contingent derivatives itself does not incur any additional cost, but by now the computation of these derivatives proved challenging. In this paper we explain how the second-order contingent derivative of the sum of a smooth single-valued and a generic set-valued mapping can be computed in terms of well-established first- and second-order objects from variational analysis. The key to these computations is a new verifiable condition that links first- and second-order information about the considered mappings. In addition, we study some tractable conditions guaranteeing relaxed regularity, and applications to generalized equations with polyhedral (set-valued) ingredients, including complementarity systems. Overall, our findings unify and improve a number of existing results on both the computation of second-order contingent derivatives and the computation of tangents to the solution set of a generalized equation under relaxed regularity conditions.

Keywords Second-Order Contingent Derivative · Studniarski Derivative · Generalized Equation · Tangent Cone · Second-Order Tangent Set · Hölder Metric Subregularity · 2-Regularity · Coderivative

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1 Introduction

Lipschitzian regularity conditions are central to modern variational analysis [12, 25]. Among their various applications, they enable the computation of tangents (and es-

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timation of normals) to the solution set of a generalized equation by means of well-established first-order generalized derivatives [36,44] of the underlying mapping. The computation of such tangents (and normals) is of interest in its own right, but it is of particular importance in constrained optimization for the formulation of tractable necessary optimality conditions in both primal and dual form [10,11]. The case where Lipschitzian regularity conditions are violated appears more involved, since this case opens the gates to a variety of relaxed (e.g., Hölderian or mixed-order) regularity conditions, all of which have already been successfully used in the context of constrained optimization to formulate tractable primal and dual necessary optimality conditions. Some works to be mentioned in this context are [9,20,21], dealing, among other things, with optimality conditions in the dual form, while [4,13,49] concern primal optimality conditions (and other things). This list of references is by no means complete – further works will be cited when credit is due.

In this paper, we content ourselves essentially to a first- and second-order analysis of the primal kind in a Euclidean setting. To be more specific, we introduce new calculus rules for the second-order (Studniarski) contingent derivative [13,39] (see also Section 2 for the definition) of a mapping defined as the sum of a smooth single-valued and a generic set-valued mapping. Such mappings are used to describe various problems considered in variational analysis and constrained optimization [10, 12,15,24,36,44], and for this reason alone, the study of their generalized derivatives is of interest. However, the usefulness of this study is further enhanced by the fact that the zeros of the second-order contingent derivative of a mapping coincide with the tangents to its (the mapping's) level-set under a square-root metric subregularity condition (see, e.g., [39] and also Section 4). Although there are several works that already address sum-rules mentioned above, we emphasize that the conclusions drawn so far in this context rely on assumptions that are too restrictive for broad classes of applications. For instance, the sum-rule [49, Theorem 3.2] (and its predecessors in [13,48]) relies on a smoothness condition that requires lower-order full-degeneracy of the smooth single-valued part (see discussions in Section 3.2), and along a similar line are the sum-rules in [30], which were developed without knowledge of [13,48, 49]. In contrast are the results in [39], which are tailored to special mappings only, but without degeneracy assumptions, and so too are constructions in [3,4], which, unlike the latter, cannot be made fully explicit in general. Thus, one goal of this paper is to formulate new sum-rules for second-order contingent derivatives without degeneracy assumptions that can be used for large classes of mappings and that can be made fully explicit. The key to achieving this goal is a new verifiable condition that links first- and second-order information about the considered mappings. It turns out that the new condition is always fulfilled when the set-valued part is polyhedral in the sense of [43] (but also beyond). With the new sum-rules at hand, tangents to the solution set of a generalized equation can be computed under a square-root metric subregularity condition. Sufficient conditions for square-root subregularity are also of interest, helping, in particular, to shed light on relations between existing (and new) results, which have not been seen before.

The organization of the paper is like this: In Section 2 we recall definitions, and formulate auxiliary results that will be needed in the further course of the paper. Section 3 contains our main results on the computation of second-order contingent derivatives. The obtained results are applied in Section 4 to compute tangents to the solution set of a generalized equation under relaxed regularity conditions. Relationships to existing results are elaborated in each of these sections as appropriate.

Finally, some words about our notation and terminology: All norms are Euclidean, dist stands for the Euclidean point-to-set distance (taking the value $+\infty$ when the set is empty), and $\mathscr{B}_r(a)$ is the closed Euclidean ball with radius $r > 0$ centered at a point a. *Convex polyhedral* sets are finite intersections of (closed) halfspaces, while *polyhedral* sets are finite unions of convex polyhedral sets. $\mathrm{gph}S, \mathrm{rge}S, \mathrm{dom}S$ stand for the graph, range, domain of a set-valued mapping S, while $\mathrm{im}L, \ker L$ are the range and the null-space of a linear operator L.

2 Preliminaries

This section contains the definitions and auxiliary results needed to prepare for the sections to come. As a first, we recall and briefly discuss some geometric objects known e.g. from [10,36,44,45]. After that, we will be concerned with concepts for the generalized differentiation of a generic set-valued mapping. We emphasize that the outcome of Lemma 1 will be important in Section 3.

Definition 1 Given a nonempty set $\Omega \subset \mathbb{R}^p$, and a point $\xi \in \Omega$.

(a) The *tangent (contingent) cone* to Ω at ξ is

$$T_\Omega(\xi) = \left\{ \omega \in \mathbb{R}^p \,\middle|\, \exists t_k \searrow 0, \exists \omega^k \to \omega : \ \xi + t_k\omega^k \in \Omega \ \forall k \right\}.$$

(b) The *second-order tangent set* to Ω at ξ for a direction $\omega \in T_\Omega(\xi)$ is

$$T^2_\Omega(\xi|\omega) = \left\{ \nu \in \mathbb{R}^p \,\middle|\, \exists t_k \searrow 0, \exists \nu^k \to \nu : \ \xi + t_k\omega + \frac{1}{2}t_k^2\nu^k \in \Omega \ \forall k \right\}.$$

(c) The *(limiting) normal cone* to Ω at ξ, when Ω is closed near ξ, is

$$N_\Omega(\xi) = \left\{ \nu \in \mathbb{R}^p \,\middle|\, \exists t_k \searrow 0, \exists \xi^k \to \xi, \exists \{\bar{\xi}^k\} \subset \Omega : \ \begin{array}{c} \mathrm{dist}[\xi^k, \Omega] = \|\xi^k - \bar{\xi}^k\| \, \forall k, \\ t_k^{-1}(\xi^k - \bar{\xi}^k) \to \nu \end{array} \right\}.$$

The next lemma is a key result for considerations yet to come. One of its statements uses the notion of *T–conicity* of a set Ω at a point $\xi \in \Omega$, a property that was coined in [17], which requires that the set Ω coincides with $\xi + T_\Omega(\xi)$ near ξ.

Lemma 1 *For a matrix $L \in \mathbb{R}^{q\times p}$, a nonempty set $\Omega \subset \mathbb{R}^p$, and a point $\xi \in \Omega$, the following statements are true for the set $Z := L(\Omega - \xi)$:*

(a) It always holds that $T^2_Z(0|0) = T_Z(0)$, and when Ω is closed convex, then

$$T_Z(0) = \mathrm{cl}\,(LT_\Omega(\xi)) = \mathrm{cl}\,\{L\nu \,|\, \nu \in T_\Omega(\xi)\}.$$

(b) Suppose $\omega \in \ker L \cap T_\Omega(\xi)$, and let any of the following conditions be in force:
 (i) Ω is a convex polyhedral set.
 (ii) It holds that $L = 0$ and $T^2_\Omega(\xi|\omega) \neq \varnothing$.

(iii) Ω is T–conical at ξ, and $\omega \in \operatorname{int}(T_\Omega(\xi))$.
Then, the following equality is fulfilled:

$$T_Z(0) = LT^2_\Omega(\xi|\omega). \tag{1}$$

Proof (a) : The equality $T^2_Z(0|0) = T_Z(0)$ is immediate from definitions. The representation of $T_Z(0)$, when Ω is closed convex, stems from [44, Theorem 6.43].

$(b),(i)$: Owing to [44, Proposition 13.12], and $\omega \in \ker L \cap T_\Omega(\xi)$, we have

$$LT^2_\Omega(\xi|\omega) = L(T_\Omega(\xi) + \mathbb{R}\omega) = L\{v + \gamma\omega \mid v \in T_\Omega(\xi), \gamma \in \mathbb{R}\} = LT_\Omega(\xi). \tag{2}$$

The cone $T_\Omega(\xi)$ is convex polyhedral, so [44, Proposition 3.55 (a)] particularly implies that $LT_\Omega(\xi)$ is closed. Thus, (1) follows from part (a) of the lemma, and (2).

(ii) : Here, we get (1) immediately, because $T_Z(0) = \{0\}$, and $LT^2_\Omega(\xi|\omega) = \{0\}$.

(iii) : For any $v \in \mathbb{R}^n$, we can find $t_k \searrow 0$, so that $\omega + t_k \frac{1}{2} v \in T_\Omega(\xi)$ holds for all k. Hence, thanks to T–conicity, we can assume that $\xi + t_k\omega + t_k^2 \frac{1}{2} v \in \Omega$ is satisfied for all k, which gives $T^2_\Omega(\xi|\omega) = \mathbb{R}^n$, because v was chosen arbitrarily. Thus, $LT^2_\Omega(\xi|\omega) = \operatorname{im} L$ follows, and so we observe:

$$Z = L(\Omega - \xi) \subset L\mathbb{R}^p = LT^2_\Omega(\xi|\omega).$$

From here, we get the inclusion $T_Z(0) \subset LT^2_\Omega(\xi|\omega)$. The converse inclusion, in turn, is always true, as follows by direct computations that rely on $\omega \in \ker L$ and the very first equality in part (a) of the lemma. □

The equality (1) will be relevant later. In the remainder of this section, we are concerned with first- and second-order contingent derivatives [39,45], and coderivatives [36].

Definition 2 Given a set-valued mapping $S : \mathbb{R}^p \rightrightarrows \mathbb{R}^q$, and a point $(\xi, \eta) \in \operatorname{gph} S$.

(a) The *contingent derivative* of S at (ξ, η) for $\omega \in \mathbb{R}^p$ is

$$CS(\xi|\eta)(\omega) := \left\{ \chi \in \mathbb{R}^q \,\middle|\, (\omega, \chi) \in T_{\operatorname{gph} S}(\xi, \eta) \right\}.$$

(b) The *second-order contingent derivative* of S at (ξ, η) for $\omega \in \mathbb{R}^p$ is

$$C^2S(\xi|\eta)(\omega) := \big\{ \chi \in \mathbb{R}^q \big|\ \exists t_k \searrow 0, \exists (\omega^k, \chi^k) \to (\omega, \chi) : \\ \eta + t_k^2 \chi^k \in S(\xi + t_k \omega^k)\, \forall k \big\}.$$

(c) The *coderivative* of S at (ξ, η) for $v \in \mathbb{R}^q$, when $\operatorname{gph} S$ is closed near (ξ, η), is

$$D^*S(\xi|\eta)(v) := \left\{ \zeta \in \mathbb{R}^p \,\middle|\, (\zeta, -v) \in N_{\operatorname{gph} S}(\xi, \eta) \right\}.$$

If S is single-valud at ξ, then we omit mentioning η.

The naming "second-order contingent derivative" was coined in [39], although these derivatives appeared earlier under the name *second-order Studniarski(-like) derivative*, giving credits to the author of [46], see [13] and references therein.

From the definitions, it is easily seen that the inclusion below always holds:

$$\operatorname{dom}\left(C^2S(\xi\,|\,\eta)\right) \subset CS(\xi\,|\,\eta)^{-1}(0) = \{\omega \in \mathbb{R}^p \,|\, 0 \in CS(\xi\,|\,\eta)(\omega)\}\,. \tag{3}$$

We will need coderivatives (and limiting normals) only in Section 4, but we would like to compute generalized derivatives of two important set-valued mappings here, one of which is the set-valued indicator, known e.g. from [36]. This mapping (the indicator) will be important in Section 3.

Lemma 2 *For a set $\Omega \subset \mathbb{R}^p$, the set-valued indicator $\Delta_\Omega : \mathbb{R}^p \rightrightarrows \mathbb{R}^q$ is*

$$\Delta_\Omega(\xi) := \begin{cases} \{0\} & \text{if } \xi \in \Omega, \\ \varnothing & \text{if } \xi \notin \Omega. \end{cases} \tag{4}$$

For a point $\xi \in \Omega$, around which Ω is closed, the following statements are in force:

(a) It holds that

$$C^2\Delta_\Omega(\xi) = C\Delta_\Omega(\xi) = \Delta_{T_\Omega(\xi)}, \quad D^*\Delta_\Omega(\xi) \equiv N_\Omega(\xi).$$

(b) For the mapping $\Sigma : \mathbb{R}^s \rightrightarrows \mathbb{R}^p$ with $\Sigma \equiv \Omega$, it holds for any $x \in \mathbb{R}^s$ that

$$C^2\Sigma(x|\xi) = C\Sigma(x|\xi) \equiv T_\Omega(\xi), \quad D^*\Sigma(x|\xi)(\nu) = \Delta_{N_\Omega(\xi)}(-\nu)\ \forall \nu \in \mathbb{R}^p.$$

Proof This follows directly from the definitions. □

Closedness of Ω in the lemma is needed only for the computation of coderivatives. To compute second-order contingent derivatives in the next sections, we want to use a smoothness property for single-valued mappings introduced in [30]:

Definition 3 A mapping $\Phi : \mathbb{R}^p \to \mathbb{R}^q$ has a *semi-quadratic expansion* at ξ for $\omega \neq 0$, if Φ is differentiable at ξ, and the limit below exists in $\mathbb{R}^q$:

$$E\Phi(\xi;\omega) := \lim_{\substack{t\searrow 0\\ \omega'\to\omega}} \frac{\Phi(\xi + t\omega') - \Phi(\xi) - t\Phi'(\xi)\omega'}{\frac{1}{2}t^2}.$$

The definition is inspired by concepts in [44, Definition 13.6], and we want to sensitize the reader to the fact that the limit in our definition appears to differ slightly from the limits in [49, Remark 3.1 (i)].

The case $\omega = 0$ is not of interest in Section 4, so we intend to exclude this case throughout. Next, we recall a criterion, and a sufficient condition for the existence of a semi-quadratic expansion.

Lemma 3 *Let a mapping $\Phi : \mathbb{R}^p \to \mathbb{R}^q$, and a point $\xi^* \in \mathbb{R}^p$ be given, at which Φ is differentiable. The following are equivalent for $\omega \neq 0$:*

(a) Φ has a semi-quadratic expansion at ξ^* for ω.

(b) *There is a continuous, 2-homogeneous mapping $\mathscr{E}:\mathbb{R}^p\to\mathbb{R}^q$ (the latter means $\mathscr{E}(\gamma\nu)=\gamma^2\mathscr{E}(\nu)\,\forall(\gamma,\nu)\in\mathbb{R}_+\times\mathbb{R}^p$), satisfying*

$$\left\|\Phi(\xi^*+t\omega')-\Phi(\xi^*)-t\Phi(x^*)\omega'-\frac{1}{2}t^2\mathscr{E}(\omega')\right\|=o(t^2)\quad\text{as } t\searrow 0,\omega'\to\omega.$$

In particular, the mapping $\mathscr{E}$ in (b), if it exists, satisfies $\mathscr{E}(\omega)=E\Phi(\xi^*;\omega)$. If Φ is differentiable near ξ^*, and Φ' is semidifferentiable at ξ^* for ω, i.e., the limit

$$\Phi''(\xi^*;\omega):=\lim_{\substack{t\searrow 0\\ \omega'\to\omega}}\frac{\Phi'(\xi^*+t\omega')-\Phi'(\xi^*)}{t}$$

exists in $\mathbb{R}^{q\times p}$, then Φ has a semi-quadratic expansion at ξ^* for ω, given by

$$E\Phi(\xi^*;\omega)=\Phi''(\xi^*;\omega)\omega.$$

Proof Apply [30, Lemma 6.12] with the unit direction $\nu=\omega/\|\omega\|$. □

The semidifferentiability of the derivative of Φ is necessary for the twice differentiability of Φ, but, in general, it is not sufficient. Examples confirming the latter can be found in [30, Section 6.3].

3 Computation of Second-Order Contingent Derivatives

It is known, e.g. from [13,30], that the computation of second-order contingent derivatives of mappings defined as a sum is subject to some complications. We introduce new calculus rules in this section: The main results are Theorems 1–2 on the computation of second-order contingent derivatives for mappings defined as the sum of a smooth single-valued and a set-valued mapping, the latter possibly consisting of a finite number of closed components (polyhedral mappings in the sense of [43] are well suited to that class). We will also explain that our findings complement and improve related results in [4,30,39,49].

3.1 The Case with the Indicator Mapping

In this subsection we deal with second-order contingent derivatives for mappings defined as the sum of a single-valued mapping and the indicator ((4) in Lemma 2) for a given set. The key to our main findings is as follows:

Lemma 4 *Let a mapping $\Phi:\mathbb{R}^p\to\mathbb{R}^q$, and a nonempty set $\Omega\subset\mathbb{R}^p$ be given. If Φ has a semi-quadratic expansion at $\xi^*\in\Omega$ for $\omega\neq 0$, then*

$$C^2\left(\Phi+\Delta_\Omega\right)(\xi^*)(\omega)\subset\begin{cases}\frac{1}{2}E\Phi(\xi^*;\omega)+T_Z(0) & \text{if } \omega\in\ker\Phi'(\xi^*)\cap T_\Omega(\xi^*),\\ \varnothing & \text{if } \omega\notin\ker\Phi'(\xi^*)\cap T_\Omega(\xi^*),\end{cases}\tag{5}$$

where $Z:=\Phi'(\xi^*)(\Omega-\xi^*)$. Furthermore, for $\omega\in\ker\Phi'(\xi^*)\cap T_\Omega(\xi^*)$, the inclusion in (5) *holds with equality, if*

$$T_Z(0)=\begin{cases}\Phi'(\xi^*)T^2_\Omega(\xi^*|\omega) & \text{if } T^2_\Omega(\xi^*|\omega)\neq\varnothing,\\ \{0\} & \text{if } T^2_\Omega(\xi^*|\omega)=\varnothing.\end{cases}\tag{6}$$

Proof " $\subset$ " : Pick $\chi \in C^2(\Phi+\Delta_\Omega)(\xi^*)(\omega)$, and find $t_k \searrow 0$, $\omega^k \to \omega$, $\chi^k \to \chi$ with

$$\Phi(\xi^*)+t_k^2\chi^k = \Phi(\xi^*+t_k\omega^k), \qquad \xi^*+t_k\omega^k \in \Omega \qquad \forall k. \tag{7}$$

The second of the two conditions already implies

$$\omega \in T_\Omega(\xi^*). \tag{8}$$

Using Lemma 3, then the first condition in (7) can be written as

$$t_k^2\chi^k = t_k\Phi'(\xi^*)\omega^k + \frac{1}{2}t_k^2\mathscr{E}(\omega^k)+R^k \qquad \forall k \tag{9}$$

for a continuous, 2-homogeneous mapping $\mathscr{E}:\mathbb{R}^p \to \mathbb{R}^q$ with $\mathscr{E}(\omega) = E\Phi(\xi^*;\omega)$, and where $\|R^k\| = o(t_k^2)$. Multiplying both sides of (9) by t_k^{-2} yields

$$t_k^{-1}\Phi'(\xi^*)\omega^k \to \chi - \frac{1}{2}E\Phi(\xi^*;\omega). \tag{10}$$

Multiplying the latter again with t_k entails $\omega \in \ker\Phi'(\xi^*)$. So, together with (8), the inclusion $\omega \in \ker\Phi'(\xi^*)\cap T_\Omega(\xi^*)$ follows, and it remains to show:

$$\chi - \frac{1}{2}E\Phi(\xi^*;\omega) \in T_Z(0). \tag{11}$$

To this end, recall from (7) that $t_k\omega^k \in \Omega - \xi^*$ holds for all k. From the latter, we get

$$t_k^{-1}\Phi'(\xi^*)\omega^k \in t_k^{-2}\Phi'(\xi^*)\,(\Omega-\xi^*) \quad \forall k.$$

Combining this with (10) leads to $\chi - \frac{1}{2}E\Phi(\xi^*;\omega) \in T_Z^2(0|0)$. Therefore, Lemma 1 (a) implies (11) and with this, the inclusion in (5) follows.

" $\supset$ " : Suppose $\omega \in \ker\Phi'(\xi^*)\cap T_\Omega(\xi^*)$, and assume that (6) is in force. Pick $\chi \in \frac{1}{2}E\Phi(\xi^*;\omega)+T_Z(0)$ arbitrarily. First, we assume $T_\Omega^2(\xi^*|\omega) = \varnothing$. Then, (6) yields $T_Z(0) = \{0\}$, i.e., 0 is isolated in Z, and

$$\chi = \frac{1}{2}E\Phi(\xi^*;\omega). \tag{12}$$

Since $\omega \in T_\Omega(\xi^*)$, we can find $t_k \searrow 0$, $\omega^k \to \omega$, so that

$$\xi^*+t_k\omega^k \in \Omega \qquad \forall k. \tag{13}$$

Combing this fact with Lemma 3, and isolatedness of 0 in Z, then we get:

$$\begin{aligned}(\Phi+\Delta_\Omega)(\xi^*+t_k\omega^k) &= \Phi\left(\xi^*+t_k\omega^k\right)\\ &= \Phi(\xi^*)+\Phi'(\xi^*)\left(\xi^*+t_k\omega^k-\xi^*\right)+t_k^2\frac{1}{2}\mathscr{E}(\omega^k)+R^k\\ &= \Phi(\xi^*)+t_k^2\frac{1}{2}\mathscr{E}(\omega^k)+R^k,\end{aligned}$$

where $\mathscr{E}:\mathbb{R}^p\to\mathbb{R}^q$ is continuous, 2-homogeneous, with $\mathscr{E}(\omega) = E\Phi(\xi^*;\omega)$, and $\|R^k\| = o(t_k^2)$ holds true. Hence, the equality in (12) entails $\chi \in C^2(\Phi+\Delta_\Omega)(\xi^*)(\omega)$.

From now on, we assume $T^2_\Omega(\xi^*|\omega) \neq \varnothing$. Then, (6) gives $\zeta \in T^2_\Omega(\xi^*|\omega)$ with

$$\chi - \frac{1}{2}E\Phi(\xi^*;\omega) = \frac{1}{2}\Phi'(\xi^*)\zeta. \tag{14}$$

There are sequences $t_k \searrow 0$, $\zeta^k \to \zeta$, so that (13) holds with $\{\omega^k\}$ being defined by

$$\omega^k := \omega + \frac{1}{2}t_k\zeta^k.$$

Yet again, Lemma 3, $\omega \in \ker\Phi'(\xi^*)$, and (13), yield

$$\begin{aligned}(\Phi+\Delta_\Omega)(\xi^*+t_k\omega^k) &= \Phi\left(\xi^*+t_k\omega+\frac{1}{2}t_k^2\zeta^k\right)\\ &= \Phi(\xi^*)+t_k^2\frac{1}{2}\left(\Phi'(\xi^*)\zeta^k+\mathscr{E}(\omega^k)+\frac{R^k}{t_k^2}\right),\end{aligned}$$

where $\mathscr{E}:\mathbb{R}^p\to\mathbb{R}^q$ and $\{R^k\}$ have the usual properties. Therefore, $\zeta^k \to \zeta$, and (14), imply $\chi \in C^2(\Phi+\Delta_\Omega)(\xi^*)(\omega)$. □

The lemma says that directions $\omega \notin \ker\Phi'(\xi^*)\cap T_\Omega(\xi^*)$ are not worth further consideration when dealing with second-order contingent derivatives of $\Phi+\Delta_\Omega$.

The condition (6) is used here for the first time to compute second-order contingent derivatives, and Lemma 1 equips us with sufficient conditions. Observe that (6) implies that the set $\Phi'(\xi^*)T^2_\Omega(\xi^*|\omega)$ is closed (which is of course not for free). Let us demonstrate that the inclusion (5) can be strict in the absence of (6):

Example 1 Let $\Omega := \{(\xi_1,\xi_2)\in\mathbb{R}^2 \mid \xi_1=\xi_2^2\}$, and $\Phi(\xi) := \xi_1$ for $\xi=(\xi_1,\xi_2)\in\mathbb{R}^2$. For the point $\xi^* := (0,0)$, we have $\Phi'(\xi^*)=(1,0)$ and $T_\Omega(\xi^*)=\{0\}\times\mathbb{R}$. So, the direction $\omega := (0,1)$ belongs to $\ker\Phi'(\xi^*)\cap T_\Omega(\xi^*)$. Short computations show

$$Z = \Phi'(\xi^*)(\Omega-\xi^*) = \mathbb{R}_+, \qquad T^2_\Omega(\xi^*|\omega) = \{2\}\times\mathbb{R},$$

hence, we get $T_Z(0)=\mathbb{R}_+$ and $\Phi'(\xi^*)T^2_\Omega(\xi^*|\omega)=\{2\}$, which implies that (6) can not hold. We have $E\Phi(\xi^*;\omega)=0$, so the set on the right-hand-side of (5) is $\mathbb{R}_+$. Let us compute elements of $C^2(\Phi+\Delta_\Omega)(\xi^*)(\omega)$ from the definitions. Suppose χ is an arbitrary element of the second-order contingent derivative. Then, there are sequences $t_k \searrow 0$, $\omega^k=(\omega_1^k,\omega_2^k)\to\omega=(0,1)$, and $\chi^k\to\chi$, such that $\xi^*+t_k\omega^k\in\Omega$ and $t_k^2\chi^k=\Phi(\xi^*+t_k\omega^k)$ hold for all k. Using the definition of Ω and Φ, we can write the latter as:

$$t_k\omega_1^k = (t_k\omega_2^k)^2, \qquad t_k^2\chi^k = t_k\omega_1^k \qquad \forall k,$$

implying that $\chi^k=(\omega_2^k)^2$ holds for all k. Since χ was arbitrarily chosen, we get $C^2(\Phi+\Delta_\Omega)(\xi^*)(\omega)=\{1\}$, which means that the inclusion in (5) now is strict. □

We want to compute second-order contingent derivatives of $\Phi+\Delta_\Omega$, when Ω is the union of closed sets, and for this we need another auxiliary result.

Lemma 5 *Let mappings $S, S_1, \dots, S_r : \mathbb{R}^p \rightrightarrows \mathbb{R}^q$ with the property*

$$\mathrm{gph} S = \bigcup_{i=1}^{r} \mathrm{gph} S_i \tag{15}$$

be given. Let $(\xi,\eta) \in \mathrm{gph} S$ be such that $\mathrm{gph} S, \mathrm{gph} S_i$ are closed near (ξ,η) for all $i = 1,\dots,r$, i.e., for some $\varepsilon > 0$, the sets $\mathrm{gph} S \cap \mathscr{B}_\varepsilon(\xi,\eta), \mathrm{gph} S_1 \cap \mathscr{B}_\varepsilon(\xi,\eta), \dots, \mathrm{gph} S_r \cap \mathscr{B}_\varepsilon(\xi,\eta)$ are closed. Then, for any $\omega \in \mathbb{R}^p$, it holds that

$$C^2 S(\xi|\eta)(\omega) = \bigcup_{i \in I} C^2 S_i(\xi|\eta)(\omega),$$

where $I := \{i \mid (\xi,\eta) \in \mathrm{gph} S_i\}$.

Proof " $\subset$ " : Pick $\omega \in \mathbb{R}^p$ arbitrarily. Nothing needs to be proved when $C^2 S(\xi|\eta)(\omega)$ is empty. So take $\chi \in C^2 S(\xi|\eta)(\omega)$ arbitrarily, and find sequences $t_k \searrow 0$, $\omega^k \to \omega$, and $\chi^k \to \chi$, such that $(\xi + t_k\omega^k, \eta + t_k^2\chi^k) \in \mathrm{gph} S$ holds for all k. According to (15), we can find an index $j \in \{1,\dots,r\}$, so that $(\xi + t_k\omega^k, \eta + t_k^2\chi^k) \in \mathrm{gph} S_j$ is satisfied, without loss of generality, for all k. Because $\mathrm{gph} S_j$ is closed near (ξ,η), we get $j \in I$ and therefore, $\chi \in C^2 S_j(\xi|\eta)(\omega)$ follows.

" $\supset$ " : This inclusion is a direct consequence of (15), and the definitions. □

Let us introduce the first main result of the section. There and below, we call mappings $S_1,\dots,S_r$ *components* of a mapping S, whenever (15) is satisfied. Likewise, sets $\Omega_1,\dots,\Omega_r$ are *components* of a set Ω, if the latter is union of the former.

Theorem 1 *In the setting of Lemma 4, suppose Φ is continuous, Ω is a union of closed (component-)sets $\Omega_1,\dots,\Omega_r$, and $\omega \in \ker \Phi'(\xi^*) \cap T_\Omega(\xi^*)$. Define the sets $I_0 := \{i \mid \xi^* \in \Omega_i,\ \omega \in \ker \Phi'(\xi^*) \cap T_{\Omega_i}(\xi^*)\}$ and $Z_i := \Phi'(\xi^*)(\Omega_i - \xi^*)$ for $i \in I_0$, and assume*

$$T_{Z_i}(0) = \begin{cases} \Phi'(\xi^*) T^2_{\Omega_i}(\xi^*|\omega) & \text{if } T^2_{\Omega_i}(\xi^*|\omega) \neq \varnothing, \\ \{0\} & \text{if } T^2_{\Omega_i}(\xi^*|\omega) = \varnothing \end{cases} \qquad \forall i \in I_0. \tag{16}$$

Then, it holds that

$$C^2(\Phi + \Delta_\Omega)(\xi^*)(\omega) = \bigcup_{i \in I_0} \left(\frac{1}{2} E\Phi(\xi^*;\omega) + T_{Z_i}(0) \right).$$

Proof Because Ω is the union of the components $\Omega_1,\dots,\Omega_r$, we get $\mathrm{gph}(\Delta_\Omega) = \bigcup_{i=1}^r \mathrm{gph}(\Delta_{\Omega_i})$. Since Φ is continuous, and each Ω_i is closed, we can apply Lemma 5 with $S = \Phi + \Delta_\Omega$ and $S_i = \Phi + \Delta_{\Omega_i}$ for $i = 1,\dots r$, giving

$$C^2(\Phi + \Delta_\Omega)(\xi^*) = \bigcup_{i \in I} C^2\left(\Phi + \Delta_{\Omega_i}\right)(\xi^*),$$

where $I = \{i \mid (\xi^*,0) \in \mathrm{gph}(\Delta_{\Omega_i})\} = \{i \mid \xi^* \in \Omega_i\}$. From here, the claim becomes a direct consequence of Lemma 4. □

The outcome of the theorem is new, and we will soon discuss relations to existing results in Remarks 1–2 (and 4, 6) below. Before doing so, we introduce a specialization of the theorem useful for applications in Section 4:

Corollary 1 *In the setting of Theorem 1, suppose Ω is polyhedral, i.e., it is the union of convex polyhedral (component-)sets $\Omega_1,\dots,\Omega_r$. Then, it holds that*

$$C^2(\Phi+\Delta_\Omega)(\xi^*)(\omega) = \bigcup_{i\in I_0}\left(\frac{1}{2}E\Phi(\xi^*;\omega)+\Phi'(\xi^*)T_{\Omega_i}(\xi^*)\right)$$
$$= \bigcup_{i\in I_0}\left(\frac{1}{2}E\Phi(\xi^*;\omega)+\Phi'(\xi^*)T^2_{\Omega_i}(\xi^*|\omega)\right),$$

where $I_0=\{i \mid \xi^*\in\Omega_i, \omega\in\ker\Phi'(\xi^*)\cap T_{\Omega_i}(\xi^*)\}$.

Proof Thanks to polyhedrality of Ω, and Lemma 1 (b), we know that (16) holds with $T^2_{\Omega_i}(\xi^*|\omega)$ being nonempty for all $i\in I_0$. The equalities in (2) also yield $T_{Z_i}(0)=\Phi'(\xi^*)T_{\Omega_i}(\xi^*)$ for $i\in I_0$. Therefore, the claim follows by Theorem 1. □

Remark 1 The observations made so far generalize a number of existing results on the computation of second-order contingent derivatives. For example, a combination of Lemmas 1,3 and Theorem 1 allows the recovery, e.g., of [30, Example 6.15] and [39, Proposition 35].

Remark 2 Several papers appeared in recent years, dealing, among other things, with calculus rules for generalized higher-order derivatives. We pay attention to the sum-rule [49, Theorem 3.2]: According to Lemma 2, [47, Remark 2.1 (iii)–(iv)], and [49, Remark 3.1 (i)], it asserts under a novel smoothness assumption on a mapping Φ at a point $\xi^*\in\Omega$ (with Ω closed) that for $\omega\in\ker\Phi'(\xi^*)\cap T_\Omega(\xi^*)$, the equality

$$C^2(\Phi+\Delta_\Omega)(\xi^*)(\omega) = d_1^h\Phi(\xi^*)(\omega) \tag{17}$$

holds, where $d_1^h\Phi(u^*)(\omega)$ is a novel derivative, which, when Φ is twice differentiable, is claimed to satisfy $d_1^h\Phi(u^*)(\omega)\subset\{\frac{1}{2}\Phi''(u^*;\omega)\omega\}$. Note that the equality in (17) fails to hold in Example 1 for the (arbitrarily smooth) mapping Φ therein. An explanation for this is outlined in Remark 3.

3.2 The General Case

In this subsection we deal with second-order contingent derivatives for mappings defined as the sum of a single-valued and a set-valued mapping. Our key to proceeding is as follows:

Lemma 6 *For a mapping $F:\mathbb{R}^n\to\mathbb{R}^m$, and a mapping $\Gamma:\mathbb{R}^n\rightrightarrows\mathbb{R}^m$, define*

$$\Phi(u,y):=F(u)+y \qquad \forall(u,y)\in\mathbb{R}^n\times\mathbb{R}^m, \qquad \Omega:=\operatorname{gph}\Gamma. \tag{18}$$

Suppose $u^* \in \mathbb{R}^n$ *is a solution to the generalized equation*

$$0 \in F(u) + \Gamma(u), \tag{19}$$

and put $y^* := -F(u^*)$. *If* F *is differentiable at* u^*, *then, for any* $(w,\lambda) \in \mathbb{R}^n \times \mathbb{R}^m$,

$$x \in C^2(\Phi + \Delta_\Omega)(u^*, y^*)(w,\lambda) \quad \Longleftrightarrow \quad \begin{cases} \lambda = -F'(u^*)w \in C\Gamma(u^*|y^*)(w), \\ \quad x \in C^2(F+\Gamma)(u^*|0)(w). \end{cases} \tag{20}$$

.

Proof " $\Longrightarrow$ " : Pick $(w,\lambda) \in \mathbb{R}^n \times \mathbb{R}^m$, and $x \in C^2(\Phi + \Delta_\Omega)(u^*, y^*)(w,\lambda)$ arbitrarily. Then, there are sequences $t_k \searrow 0$, $w^k \to w$, $\lambda^k \to \lambda$, and $x^k \to x$, so that

$$t_k^2 x^k = \Phi(u^* + t_k w^k, y^* + t_k \lambda^k) = F(u^* + t_k w^k) + (y^* + t_k \lambda^k) \qquad \forall k, \tag{21}$$

and also

$$(u^* + t_k w^k, y^* + t_k \lambda^k) \in \Omega = \text{gph}\Gamma \qquad \forall k. \tag{22}$$

The two conditions readily imply

$$t_k^2 x^k \in F(u^* + t_k w^k) + \Gamma(u^* + t_k w^k) \quad \forall k,$$

which precisely means $x \in C^2(F+\Gamma)(u^*|0)(w)$. Combining (21)–(22), then we get:

$$t_k^2 x^k - F(u^* + t_k w^k) = y^* + t_k \lambda^k \in \Gamma(u^* + t_k w^k) \qquad \forall k. \tag{23}$$

Differentiability of F at u^*, and $y^* = -F(u^*)$, allows to write the equality in (23) as

$$-F(u^*) + t_k \left(-F'(u^*) w^k + t_k^{-1} R^k + t_k x^k \right) = -F(u^*) + t_k \lambda^k \qquad \forall k, \tag{24}$$

where $\|R^k\| = o(t_k)$. So, together with (23), and $\lambda^k \to \lambda$, we come to the conclusion that $\lambda = -F'(u^*)w \in C\Gamma(u^*|y^*)(w)$.

" $\Longleftarrow$ " : Pick $x \in C^2(F+\Gamma)(u^*|0)(w)$ arbitrarily, and find $t_k \searrow 0$, $w^k \to w$, $x^k \to x$, $\{\eta^k\}$, with

$$\eta^k = -F(u^* + t_k w^k) + t_k^2 x^k, \qquad \eta^k \in \Gamma(u^* + t_k w^k) \qquad \forall k. \tag{25}$$

Thanks to differentiability of F, and $y^* = -F(u^*)$, we can write

$$\eta^k = y^* + t_k \lambda^k \qquad \forall k, \tag{26}$$

where the sequence $\{\lambda^k\}$ is determined by

$$\lambda^k := -F'(u^*) w^k + t_k^{-1} R^k + t_k x^k,$$

with some $\{R^k\}$ satisfying $\|R^k\| = o(t_k)$. By assumption, and constructions, we get

$$\lambda^k \to -F'(u^*) w = \lambda. \tag{27}$$

At the same time, (25)–(26) entail

$$\begin{aligned} t_k^2 x^k &= F(u^* + t_k w^k) + \left(y^* + t_k \lambda^k \right) \\ &= \Phi\left(u^* + t_k w^k, y^* + t_k \lambda^k \right) + \Delta_\Omega \left(u^* + t_k w^k, y^* + t_k \lambda^k \right) \qquad \forall k. \end{aligned}$$

Therefore, with (27) in mind, we conclude $x \in C^2(\Phi + \Delta_\Omega)(u^*, y^*)(w,\lambda)$. □

The lemma builds a bridge to the results from Section 3.1. Furthermore, with the comment below Lemma 4 in mind, Lemma 6 says that directions w with $-F'(u^*)w \notin C\Gamma(u^*|y^*)(w)$ are not worth further consideration for our purposes.

Theorem 2 *In the setting of Lemma 6, suppose F is continuous, and Γ has closed components $\Gamma_1,\ldots,\Gamma_r : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$, i.e., $\mathrm{gph}\Gamma_i$ is closed for each $i \in \{1,\ldots,r\}$, and*

$$\mathrm{gph}\Gamma = \bigcup_{i=1}^{r} \mathrm{gph}\Gamma_i. \tag{28}$$

Suppose F has a semi-quadratic expansion for a direction $w \neq 0$ with $-F'(u^*)w \in C\Gamma(u^*|y^*)(w)$. Define the sets $I_0 := \{i \mid y^* \in \Gamma_i(u^*), -F'(u^*)w \in C\Gamma_i(u^*|y^*)(w)\}$ and $Z_i := \{F'(u^*)(u-u^*) + (y-y^*) \mid (u,y) \in \mathrm{gph}\Gamma_i\}$ for $i \in I_0$. If the condition

$$T_{Z_i}(0) = \begin{cases} \left\{F'(u^*)v + z \,\middle|\, (v,z) \in T_i^2\right\} & \text{if } T_i^2 \neq \varnothing, \\ \{0\} & \text{if } T_i^2 = \varnothing \end{cases} \qquad \forall i \in I_0$$

is satisfied with $T_i^2 := T^2_{\mathrm{gph}\Gamma_i}((u^*,y^*)\,|(w,-F'(u^*)w))$ $(i \in I_0)$, then

$$C^2(F+\Gamma)(u^*|0)(w) = \bigcup_{i\in I_0} \left(\frac{1}{2}EF(u^*;w) + T_{Z_i}(0)\right).$$

Proof Let the mapping Φ and the set Ω be defined according to (18), and put $\Omega_i = \mathrm{gph}\Gamma_i$ for $i = 1,\ldots,r$. For this particular choice, we observe that

$$\begin{aligned} E\Phi((u^*,y^*);(w,\nu)) &= EF(u^*;w) \quad \forall \nu \in \mathbb{R}^m, \\ \Phi'(u^*,y^*) &= (F'(u^*),\mathscr{I}), \\ T_{\Omega_i}(u^*,y^*) &= \{(v,z) \mid z \in C\Gamma_i(u^*|y^*)(v)\} \qquad (i \in I_0), \end{aligned}$$

where $\mathscr{I}$ denotes the $m \times m$ unit matrix. The claim is now a direct consequence of Theorem 1 and Lemma 6. □

Lemma 2 and Theorem 2 combined lead to the conclusion of Theorem 1. At the same time, we used the latter theorem to prove the former, so the two theorems are equivalent. Let us discuss relations to some existing results:

Remark 3 With Lemma 1 (b) in mind, Theorem 2 can be used to reestablish [30, Theorem 6.13 (b)]. However, it cannot be used to recover [30, Theorem 6.13 (a)] – a result developed specifically for the fully degenerate case where $F'(u^*) = 0$. Note that (a specialization, suitable for our purposes, of) [49, Theorem 3.2], mentioned in Remark 2, must be of a similar nature, as follows by [49, Remark 3.1 (i)]. Thus, we will refrain from further comparisons with results in [49] (and [31,47,48]).

Remark 4 In the setting of Lemma 6, suppose F is continuous, and $\Gamma \equiv -\Gamma_0$ holds for a closed set $\Gamma_0 \subset \mathbb{R}^m$. For a direction $w \neq 0$, consider the following set, introduced in [4, formula (55)]:

$$\mathscr{T}^2(w) = \left\{ z \in \mathbb{R}^m \,\middle|\, \exists t_k \searrow 0, \exists w^k \to w\colon \mathrm{dist}[F(u^*) + t_k F'(u^*)w^k + \frac{1}{2}t_k^2 z, \Gamma_0] = o(t_k^2) \right\}.$$

Direct computations, relying on an application of Lemma 3, when F has a semi-quadratic expansion at u^* for w, imply

$$C^2(F+\Gamma)(u^*|0)(w) = \frac{1}{2}\left(EF(u^*;w) - \mathscr{T}^2(w)\right). \tag{29}$$

This observation appears new, and apart of [4, formula (54)] (the case where Γ_0 is convex polyhedral), no other formula on the explicit computation of $\mathscr{T}^2(w)$ is known to the author by now. Thanks to (29), the outcome of Theorem 2 can be used to make some statements in [4] more explicit. Finally, note that [4] addresses the case where Γ_0 is closed convex only.

New conclusions can be drawn for the case where Γ is polyhedral in the sense of [43]:

Corollary 2 *In the setting of Theorem 2, suppose Γ is polyhedral, i.e., there are (component-)mappings $\Gamma_1,\dots,\Gamma_r : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$, so that each* $\mathrm{gph}\Gamma_i$ *($i \in \{1,\dots,r\}$) is a convex polyhedral set, and* (28) *is fulfilled. Then, it holds that*

$$\begin{aligned} C^2(F+\Gamma)(u^*|0)(w) &= \bigcup_{i\in I_0}\left(\frac{1}{2}EF(u^*;w) + \bigcup_{v\in\mathbb{R}^n}\ \bigcup_{z\in C\Gamma_i(u^*|y^*)(v)}\left(F'(u^*)v+z\right)\right) \\ &= \bigcup_{i\in I_0}\left(\frac{1}{2}EF(u^*;w) + \bigcup_{(v,z)\in T_i^2}\left(F'(u^*)v+z\right)\right), \end{aligned}$$

where $T_i^2 := T^2_{\mathrm{gph}\Gamma_i}\left((u^*,y^*)\,|(w,-F'(u^*)w)\right)$ for $i \in I_0$.

Proof Use ideas from the proof of Corollary 1, and apply Theorem 2. □

We close this section with further remarks, the first concerning the computation of second-order contingent derivatives of generic polyhedral mappings, the second is about relations to a result in [39].

Remark 5 Corollary 2 particularly implies for a polyhedral mapping Γ with components $\Gamma_1,\dots,\Gamma_r$ that, for any $(u^*,y^*) \in \mathrm{gph}\Gamma$, and any $w \neq 0$,

$$\begin{aligned} C^2\Gamma(u^*|y^*)(w) &= \bigcup_{i\in I_0(w)} \mathrm{rge}C\Gamma_i(u^*|y^*) \\ &= \bigcup_{i\in I_0(w)} \left\{z\,\middle|\,\exists v\in\mathbb{R}^n:\ (v,z)\in T^2_{\mathrm{gph}\Gamma_i}\left((u^*,y^*)\,|(w,0)\right)\right\} \end{aligned}$$

holds true, where $I_0(w) := \{i \mid y^* \in \Gamma_i(u^*),\, 0 \in C\Gamma_i(u^*|y^*)(w)\}$. This fact is new and allows, for the first time, a direct computation of second-order contingent derivatives of a generic polyhedral mapping.

Remark 6 Another result on the computation of $C^2(F+\Gamma)$ is [39, Lemma 38] on the case where $F=(G,H)$ is twice differentiable, and $\Gamma \equiv \mathbb{R}^l_+ \times \{0\}$. For this special choice, one gets (from the cited lemma or our observations):

$$C^2(F+\Gamma)(u^*|0)(w) = \begin{cases} \frac{1}{2}F''(u^*;w)w + \mathrm{im}F'(u^*) + T_0 & \text{if } -F'(u^*)w \in T_0, \\ \varnothing & \text{if } -F'(u^*)w \notin T_0, \end{cases} \tag{30}$$

where $T_0 = T_{\mathbb{R}^l_+}(-G(u^*)) \times \{0\}$. At the same time, Corollary 2, and calculus rules for second-order tangents on [10, p. 168] lead to a new insight, namely that the *equality* in (30) also holds with $T^2_{\mathbb{R}^l_+}(-G(u^*)|-G'(u^*)w) \times \ \{0\}$ in place of T_0.

4 Application: Computation of Tangents under Relaxed Regularity Conditions

The goal of the section is to illustrate how second-order contingent derivatives can be used to compute tangents to the solution set of a generalized equation

$$0 \in S(\xi), \tag{31}$$

for some specific set-valued mapping $S:\mathbb{R}^p \rightrightarrows \mathbb{R}^q$, under relaxed regularity conditions. This topic is of interest in its own right, but it is of particular importance in constrained optimization, where constraints are determined by (31). Under standard Lipschitzian regularity conditions (e.g., *metric subregularity* of the mapping S [12]), it is known [14] that tangents (and second-order tangents) to the solution set of (31) can be computed by means of contingent derivatives of S, while the corresponding normals necessarily belong to the range of the coderivative of S, cf. [25]. These conclusions lead not only to tractable optimality conditions for *mathematical programs with equilibrium constraints* [11,15,35,36,41], they also set the stage for the design of Newton-type methods for solving (19), see [12,15,16,29] among others. At the same time, if the above conclusions are violated, then standard Lipschitzian regularity conditions inevitably cannot apply, and so relaxed regularity conditions come into play. Among them is the following condition, which we want to use in the rest of the paper.

Definition 4 A set-valued mapping $S:\mathbb{R}^p \rightrightarrows \mathbb{R}^q$ is $\sqrt{}$*–metrically subregular* at a solution $\xi^* \in \mathbb{R}^p$ of the generalized equation (31), if there are $\varepsilon, c > 0$, such that

$$\operatorname{dist}\left[\xi, S^{-1}(0)\right] \le c \cdot \sqrt{\operatorname{dist}[0, S(\xi)]} \qquad \forall \xi \in \mathscr{B}_\varepsilon(\xi^*). \tag{32}$$

Checking whether a mapping is $\sqrt{}$–metrically subregular can be difficult from the definition. Hence, sufficient conditions for that property are subject of interest, too.

Theorem 3 *For a mapping $S:\mathbb{R}^p \rightrightarrows \mathbb{R}^q$, with* gph$S$ *closed, and a point $(\xi^*,0) \in$* gph$S$*, the following implies $\sqrt{}$–metric subregularity of S at ξ^*:*

$$\left.\begin{array}{l} 0 \neq \omega, \\ 0 \in CS^2(\xi^*|0)(\omega), \\ 0 = \ell_S(\xi^*,0) \end{array}\right\} \qquad \Longrightarrow \qquad 0 < \liminf_{\substack{t \searrow 0 \\ \omega' \to \omega \\ v' \to 0}} \left(\frac{\ell_S(\xi^* + t\omega', tv')}{t} \right), \tag{33}$$

where

$$\ell_S(\xi,\eta) := \begin{cases} \inf\limits_{\|v\|=1} \operatorname{dist}[0, D^*S(\xi|\eta)(v)] & \text{if } (\xi,\eta) \in \operatorname{gph} S, \\ +\infty & \text{if } (\xi,\eta) \notin \operatorname{gph} S \end{cases} \qquad ((\xi,\eta) \in \mathbb{R}^p \times \mathbb{R}^q).$$

Proof For $\omega \in C^2(\xi^*|0)^{-1}(0) \setminus \{0\}$, we get $0 \in CS(\xi^*|0)(\omega)$ from (3). So, a combination of [30, Theorem 6.2 and Theorem 6.7] implies for such ω that the estimate in (32) holds for some $c = c(\omega) > 0$, and all ξ in a directional neighborhood of ξ^* relative to ω. For $\omega \notin C^2(\xi^*|0)^{-1}(0)$, in turn, such a conclusion is guaranteed by [39, Proposition 17] without further assumptions. Hence, we get directional $\surd$–metric subregularity for any $\omega \neq 0$, giving $\surd$–metric subregularity of S at ξ^*. □

The function ℓ_S in the theorem was introduced and studied in [30], where it was called *least-singular-value function* for the coderivative of S. Although the condition in (33) is technical, its validity can be easily guaranteed in several cases, some of which are addressed in subsections below. For completeness, we would like to mention [9,20,21,32,33,34,37,38,40,50], containing further (possibly sharper) sufficient conditions for $\surd$–metric subregularity.

Now, we recall how second-order contingent derivatives can be used to compute tangents to the solution set of the generalized equation (31).

Theorem 4 *In the setting of Theorem 3, if S is $\surd$–metrically subregular at ξ^*, then*

$$T_{S^{-1}(0)}(\xi^*) = C^2S(\xi^*|0)^{-1}(0) = \left\{ \omega \in \mathbb{R}^p \,\middle|\, 0 \in C^2S(\xi^*|0)(\omega) \right\}.$$

Proof This is a consequence, e.g., of [39, Proposition 34]. □

Apart from its use in computing tangents, $\surd$–metric subregularity and other (possibly stronger) relaxed regularity conditions have been successfully applied, e.g., in [8,18,19,27,34], in the design and convergence analysis of Newton-type and other numerical methods for solving some instances of (31).

Theorems 3–4 will be specialized in the following subsections.

4.1 Equations with Polyhedral Constraints

Let us consider the constrained equation

$$\Phi(\xi) = 0, \qquad \xi \in \Omega, \tag{34}$$

where $\Phi : \mathbb{R}^p \to \mathbb{R}^q$ is continuous, and $\Omega \subset \mathbb{R}^p$ is polyhedral with components $\Omega_1, \ldots, \Omega_r$. We denote the solution set of (34) by SOL, i.e., $\mathrm{SOL} = \Phi^{-1}(0) \cap \Omega$.

A specialization of Theorems 3–4 combined reads as follows:

Theorem 5 *In the setting of this subsection, suppose Φ has a semi-quadratic expansion at $\xi^* \in$ SOL for all $v \neq 0$. Then, under the error bound condition*

$$\exists \varepsilon, c > 0 : \qquad \operatorname{dist}[\xi, \mathrm{SOL}] \leq c \cdot \sqrt{\|\Phi(\xi)\|} \qquad \forall \xi \in \mathscr{B}_\varepsilon(\xi^*) \cap \Omega, \tag{35}$$

it holds that

$$T_{\mathrm{SOL}}(\xi^*) = \{0\} \cup \mathscr{T}, \tag{36}$$

in which

$$\begin{aligned}\mathscr{T} &= \left\{\omega \neq 0 \,\middle|\, \exists i \in I : \omega \in \ker \Phi'(\xi^*) \cap T_{\Omega_i}(\xi^*), -E\Phi(\xi^*;\omega) \in \Phi'(\xi^*) T_{\Omega_i}(\xi^*) \right\} \\ &= \left\{\omega \neq 0 \,\middle|\, \exists i \in I : \omega \in \ker \Phi'(\xi^*) \cap T_{\Omega_i}(\xi^*), -E\Phi(\xi^*;\omega) \in \Phi'(\xi^*) T^2_{\Omega_i}(\xi^*|\omega) \right\},\end{aligned}$$

where $I := \{i \mid \xi^* \in \Omega_i\}$. *If* Φ *is differentiable near* ξ^* *with* Φ' *being semidifferentiable at* ξ^* *for all* $\nu \in \mathscr{T}$*, then the following implies the error bound* (35)*:*

$$\left.\begin{aligned} \omega &\in \mathscr{T}, \\ \Phi'(\xi^*)^\top \zeta &\in N_\Omega(\xi^*), \\ \Phi''(\xi^*;\omega)^\top \zeta &\in \operatorname{im}\Phi'(\xi^*)^\top + N_\Omega(\xi^*) \end{aligned}\right\} \quad \Longrightarrow \quad \zeta = 0. \tag{37}$$

Proof Put $S := \Phi + \Delta_\Omega$, and observe that $\sqrt{}$–metric subregularity of this S at ξ^* is nothing else than the error bound condition (35). Theorem 4 is applicable, and it yields $T_{\mathrm{SOL}}(\xi^*) = C^2(\Phi+\Delta)(\xi^*)^{-1}(0)$. Hence, (36) (with the two formulas for $\mathscr{T}$) follows by Corollary 1, and the evident fact $0 \in T_{\mathrm{SOL}}(\xi^*)$. Considerations on [30, p. 74] combined with [30, Theorem 4.18] imply sufficiency of (37) for (33). Thus, the final claim of this theorem is due to Theorem 3. □

The theorem can be used to develop formulas for computing normals to SOL:

Remark 7 Under the assumptions of Theorem 5, if Ω is convex polyhedral, we get

$$T_{\mathrm{SOL}}(\xi^*) = \ker \Phi'(\xi^*) \cap T_\Omega(\xi^*) \cap \mathscr{Q}^{-1}\left(\Phi'(\xi^*) T_\Omega(\xi^*)\right),$$

with $\mathscr{Q} : \mathbb{R}^p \to \mathbb{R}^q$ being defined by $\mathscr{Q}(0) := 0$, and $\mathscr{Q}(\nu) := -E\Phi(\xi^*;\nu)$ for $\nu \neq 0$. Assuming that the cone $\mathscr{Q}^{-1}(\Phi'(\xi^*) T_\Omega(\xi^*))$ is a finite union of closed convex cones $Q_1, \ldots, Q_r$, then

$$(T_{\mathrm{SOL}}(\xi^*))^\circ = \bigcap_{i=1}^{r} \operatorname{cl}\left(\operatorname{im}\Phi'(\xi^*)^\top + N_\Omega(\xi^*) + Q_i^\circ\right), \tag{38}$$

where K° denotes the polar of a cone K. Since the error bound (35) is preserved for all points $\xi \in \mathrm{SOL}$ sufficiently close to ξ^*, a representation for $N_{\mathrm{SOL}}(\xi^*)$ can be derived on the basis of (38) from an equivalent definition of (limiting) normals [36]. These arguments can even be extended to the case where Ω itself is polyhedral. As an example of the former, consider $\Phi(\xi) := \xi_1\xi_2$ for $\xi = (\xi_1, \xi_2) \in \mathbb{R}^2$, the set $\Omega := \mathbb{R}^2$, and the point $\xi^* := (0,0)$. We have $\mathscr{T} = ((\mathbb{R} \times \{0\}) \cup (\{0\} \times \mathbb{R})) \setminus \{0\}$, (37) is in force, and considerations above entail $N_{\mathrm{SOL}}(\xi^*) = T_{\mathrm{SOL}}(\xi^*) = \{0\} \cup \mathscr{T}$.

We want to compare the outcome of Theorem 5 with some existing results:

Remark 8 Suppose $\Omega = \mathbb{R}^p$, and Φ is differentiable with Φ' Lipschitz continuous, and semidifferentiable at ξ^* for all $v \in \mathscr{T}$ (with $\mathscr{T}$ determined as in the theorem). Then, [30, Example 6.4] says that the condition (37) corresponds to the *2-regularity* condition in [28, Definition 2]. Sufficiency of the latter for the error bound (35) is mentioned in [28, Remark 7], and the formula in (36) corresponds to the one established in [28, Theorem 5]. A similar result on the representation of tangents is given in [5,7] under smoothness assumptions stronger than those imposed in this remark.

Remark 9 Suppose Ω is convex polyhedral, and Φ is twice differentiable. It is explained in [30, Remark 4.25] that the condition (37) is stronger than a *2-regularity* condition in [2] (which is also used in [6]). An application of [2, Theorem 3] confirms that the latter 2-regularity condition can be used to ensure the error bound (35). The formula in (36) (with the first representation of $\mathscr{T}$, i.e., the one with $\Phi'(\xi)T_\Omega(\xi^*)$) is established in [2, Theorem 6] under 2-regularity.

The remarks indicate that Theorem 5 is closely related to existing results. It complements some of them and, at least in parts, goes beyond their scope.

4.2 Generalized Equations with Polyhedrality

Let us consider the generalized equation (19) with a continuous mapping $F : \mathbb{R}^n \to \mathbb{R}^m$, and a polyhedral mapping $\Gamma : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$ with components $\Gamma_1, \ldots, \Gamma_r$. We denote its solution set again by SOL, i.e., $\mathrm{SOL} = \{u \mid 0 \in F(u) + \Gamma(u)\}$.

A specialization of Theorems 3–4 combined is:

Theorem 6 *In the setting of this subsection, suppose F has a semi-quadratic expansion at $u^* \in \mathrm{SOL}$ for all $v \neq 0$. If $F + \Gamma$ is $\sqrt{}$–metrically subregular at u^*, then*

$$T_{\mathrm{SOL}}(u^*) = \{0\} \cup \mathscr{T} \tag{39}$$

holds true, where

$$\begin{aligned}\mathscr{T} &= \left\{ w \neq 0 \,\middle|\, \exists i \in I, \exists \mu \in \mathbb{R}^n : \begin{array}{l} 0 \in EF(u^*;w) + F'(u^*)\mu + C\Gamma_i(u^*|y^*)(\mu), \\ 0 \in F'(u^*)w + C\Gamma_i(u^*|y^*)(w) \end{array} \right\} \\ &= \bigcup_{i \in I} \left\{ w \neq 0 \,\middle|\, \exists (\mu, z) \in T_i^2(w) : \ 0 \in EF(u^*;w) + F'(u^*)\mu + z \right\},\end{aligned}$$

in which $y^* := -F(u^*)$, $I := \{i \mid y^* \in \Gamma_i(u^*)\}$, and, for $v \neq 0$ and $i \in I$,

$$T_i^2(v) := \begin{cases} T^2_{\mathrm{gph}\Gamma_i}((u^*,y^*)|(v,-F'(u^*)v)) & \text{if } -F'(u^*)v \in C\Gamma_i(u^*|y^*)(v), \\ \varnothing & \text{if } -F'(u^*)v \notin C\Gamma_i(u^*|y^*)(v). \end{cases}$$

If F is differentiable near u^* with F' being semidifferentiable at u^* for all $v \in \mathscr{T}$, then the following implies $\sqrt{}$–metric subregularity of $F + \Gamma$ at u^*:

$$\left. \begin{array}{l} w \in \mathscr{T}, \\ 0 \in F'(u^*)^\top z + D^*\Gamma(u^*|y^*)(z), \\ 0 \in F''(u^*;w)^\top z + \bigcup\limits_{\lambda \in \mathbb{R}^m} \left(F'(u^*)^\top \lambda + D^*\Gamma(u^*|y^*)(\lambda)\right) \end{array} \right\} \implies z = 0. \tag{40}$$

Proof The formula in (39) is due to Theorem 4 applied with $S = F + \Gamma$ and $\xi^* = u^*$, and Corollary 2. From [30, Example 4.23 and Theorem 4.18], we get sufficiency of (40) for (33), so the remaining claim follows by Theorem 3. $\square$

Remark 10 It is well-known [12,43] that the mapping associated with the normal cone to a convex polyhedral set Ω_0 is polyhedral. From the two references, it is also known that this (normal cone) mapping coincides with the *subgradient* [12] of the indicator function for Ω_0. Identifying Γ in Theorem 6 with that subgradient, then the formulas in our theorem can be rewritten by means of results in [36, Section 3.3] and [44, Section 13].

Remark 11 We know from [30, Theorem 6.2] that the condition in (33) characterizes a property that originated in [20], called *metric pseudo-regularity of order 2* of S at $(\xi^*, 0)$ for the directions in $\mathscr{T} \times \{0\}$. With this observation at hand, the results in [20] lead to the conclusion of Theorem 3. In the setting of Theorem 6, assuming that F is twice differentiable, a sufficient condition for metric pseudo-regularity of $F + \Gamma$ is stated in [20, Theorem 2]. That condition is weaker than (40), but we find it too technical to present here. Results on the computation of tangents (in terms of second-order contingent derivatives) have not been developed in [20]. Instead, the considerations in [20, Section 6] refer, among other things, to applications in optimization on the existence of multipliers. Further works to be mentioned in this context are [9,22,23,31,47], see also Remark 13 below.

To discuss some other existing results, we specialize our theorem to inclusions:

Corollary 3 *In the setting of Theorem 6, suppose $\Gamma \equiv \Gamma_0$ for a polyhedral set Γ_0 with components $\Gamma_1, \ldots, \Gamma_r$. If $F + \Gamma$ is $\sqrt{}$–metrically subregular at u^*, then* (39) *holds with*

$$\begin{aligned} \mathscr{T} &= \left\{ w \neq 0 \,\middle|\, \exists i \in I \colon\ 0 \in F'(u^*)w + T_{\Gamma_i}(y^*),\, 0 \in EF(u^*;w) + \operatorname{im} F'(u^*) + T_{\Gamma_i}(y^*) \right\} \\ &= \left\{ w \neq 0 \,\middle|\, \exists i \in I \colon\ 0 \in EF(u^*;w) + \operatorname{im} F'(u^*) + T_i^2(w) \right\}, \end{aligned}$$

in which $y^* := -F(u^*)$, $I := \{ i \mid y^* \in \Gamma_i \}$, and, for $v \neq 0$ and $i \in I$,

$$T_i^2(v) := \begin{cases} T_{\Gamma_i}^2(u^* | -F'(u^*)v) & \text{if } -F'(u^*)v \in T_{\Gamma_i}(y^*), \\ \varnothing & \text{if } -F'(u^*)v \notin T_{\Gamma_i}(y^*). \end{cases}$$

If F is differentiable near u^* with F' being semidifferentiable at u^* for all $v \in \mathscr{T}$, then the following implies $\sqrt{}$–metric subregularity of $F + \Gamma$ at u^*:

$$w \in \mathscr{T},\, z \in (-N_{\Gamma_0}(y^*)) \cap \ker F'(u^*)^\top,\, F''(u^*;w)^\top z \in F'(u^*)^\top N_{\Gamma_0}(y^*) \implies z = 0. \tag{41}$$

Proof This follows by Theorem 6, Lemma 2, and calculus rules for second-order tangents, cited in Remark 6. $\square$

Remark 12 Suppose Γ_0 is convex polyhedral, and F is twice differentiable. Then, it is explained in [30, Remark 4.22] (and more recently in [9, Section 3.2]) that (41) is equivalent to a *2-regularity* condition in [1,3,4]. Hence, with Remark 4 in mind, results on the computation of tangents in the latter papers established under 2-regularity are recovered by our analysis (provided Γ_0 is convex polyhedral).

Remark 13 In the setting of Corollary 3, suppose F is twice differentiable. Then, conditions weaker than (41), but stronger than $\sqrt{}$–metric subregularity of $F+\Gamma$, are developed in [9, Section 3.1]. Results on the computation of tangents have not been developed in that paper, but the considerations therein refer, among other things, to the existence of multipliers in optimization under relaxed regularity conditions.

4.3 Complementarity Systems

In this last subsection, we consider the complementarity system

$$G(u) \geq 0, \quad H(u) \geq 0, \quad G(u)^\top H(u) = 0, \tag{42}$$

where $G, H : \mathbb{R}^n \to \mathbb{R}^l$ are at least locally Lipschitz continuous. Again, we denote the solution set of (42) by SOL, and aim to specialize Theorems 3–4. Before, we give an auxiliary result that is useful to replace the $\sqrt{}$–metric subregularity by a simpler error bound condition.

Lemma 7 *Let a polyhedral mapping $\mathscr{P} : \mathbb{R}^p \to \mathbb{R}^q$, a point $\xi^* \in \mathscr{P}^{-1}(0)$, a locally Lipschitz continuous mapping $\mathscr{L} : \mathbb{R}^s \to \mathbb{R}^p$, and a point $x^* \in \mathscr{L}^{-1}(\xi^*)$ be given. Then, there are constants $\varepsilon, c_1, c_2 > 0$, such that for any $x \in \mathscr{B}_\varepsilon(x^*)$,*

$$c_1 \operatorname{dist}\left[\mathscr{L}(x), \mathscr{P}^{-1}(0)\right] \leq \|\mathscr{P}(\mathscr{L}(x))\| \leq c_2 \operatorname{dist}\left[\mathscr{L}(x), \mathscr{P}^{-1}(0)\right].$$

Proof The first estimate follows by Lipschitz continuity of $\mathscr{L}$, and [12, Theorem 3D.1 and Theorem 3H.3], the second is simply due to Lipschitz continuity of $\mathscr{L}, \mathscr{P}$. □

Theorem 7 *In the setting of this subsection, suppose G, H have a semi-quadratic expansion at $u^* \in \mathrm{SOL}$ for all $v \neq 0$. Then, under the error bound condition*

$$\exists \varepsilon, c > 0: \qquad \operatorname{dist}[u, \mathrm{SOL}] \leq c \cdot \sqrt{\|\min\{G(u), H(u)\}\|} \qquad \forall u \in \mathscr{B}_\varepsilon(u^*) \tag{43}$$

(with min *being applied componentwise), the equality in* (39) *holds with*

$$\mathscr{T} = \left\{ w \neq 0 \;\middle|\; \exists \mu \in \mathbb{R}^n : \begin{array}{r} (G'(u^*)w, H'(u^*)w) \in T_0, \\ (EG(u^*; w) + G'(u^*)\mu, EH(u^*; w) + H'(u^*)\mu) \in T_1(w) \end{array} \right\},$$

where

$$T_0 := \left\{ (a,b) \in \mathbb{R}^l \times \mathbb{R}^l \;\middle|\; \min\{a_i, b_i\} = 0 \forall i \in I_0,\, a_i = 0 \forall i \in I_1,\, b_i = 0 \forall i \in I_2 \right\},$$

$$T_1(v) := \left\{ (a,b) \in \mathbb{R}^l \times \mathbb{R}^l \;\middle|\; \begin{array}{r} \min\{a_i, b_i\} = 0 \forall i \in I_{00}(v), \\ a_i = 0 \forall i \in I_{01}(v) \cup I_1, \\ b_i = 0 \forall i \in I_{02}(v) \cup I_2 \end{array} \right\} \qquad (v \in \mathbb{R}^n),$$

in which $I_0 := \{i \mid G_i(u^*) = H_i(u^*) = 0\}$, $I_1 := \{i \mid H_i(u^*) > 0\}$, $I_2 := \{i \mid G_i(u^*) > 0\}$,

$$\begin{aligned} I_{00}(v) &:= \{i \in I_0 \mid G_i'(u^*)v = H_i'(u^*)v = 0\}, \\ I_{01}(v) &:= \{i \in I_0 \mid H_i'(u^*)v > 0\}, \\ I_{02}(v) &:= \{i \in I_0 \mid G_i'(u^*)v > 0\}. \end{aligned}$$

If G,H are differentiable near u^* with G',H' being semidifferentiable at u^* for all $v \in \mathscr{T}$, then the following implies (43)*:*

$$\left.\begin{array}{l} w \in \mathscr{T},\ (\kappa,\lambda),(\alpha,\beta) \in N_0, \\ 0 = G'(u^*)^\top \kappa + H'(u^*)^\top \lambda, \\ 0 = G''(u^*;w)^\top \kappa + G'(u^*)^\top \alpha + H''(u^*;w)^\top \lambda + H'(u^*)^\top \beta \end{array}\right\} \implies \kappa = \lambda = 0, \tag{44}$$

where

$$N_0 := \left\{ (a,b) \in \mathbb{R}^l \times \mathbb{R}^l \;\middle|\; (a_i,b_i) \in \left\{ \begin{array}{cl} \mathbb{R}^2_- \cup (\mathbb{R}\times\{0\}) \cup (\{0\}\times\mathbb{R}) & \text{if } i \in I_0, \\ \mathbb{R}\times\{0\} & \text{if } i \in I_1, \\ \{0\}\times\mathbb{R} & \text{if } i \in I_2 \end{array} \right\} \right\}.$$

Proof Define the polyhedral set $\Gamma_0 := \bigotimes_{i=1}^l (\mathbb{R}_+ \times \{0\}) \cup (\{0\} \times \mathbb{R}_+)$, and the mappings $F := (-G,-H)$ and $\Gamma \equiv \Gamma_0$. We know from [42] that $u \in \mathrm{SOL}$ holds if and only if $0 \in F(u) + \Gamma(u) = F(u) + \Gamma_0$. For $\mathscr{P}(x,y) := \min\{x,y\}$, we have $\mathscr{P}^{-1}(0) = \Gamma_0$. So, applying Lemma 7 with this $\mathscr{P}$, and $\mathscr{L} := -F$, yields an equivalence between (43) and $\sqrt{}$–metric subregularity of $F+\Gamma$ at u^*. The assertions of this theorem follow by Corollary 3 and direct computations. □

Remark 14 The outcome of the theorem is close to observations in [30, Remark 6.26] and [26]. Relations to [9, Section 4.4.2] are those mentioned in Remark 13.

Conclusion

We have established several new calculus rules for second-order contingent derivatives. Our key to achieving them is the use of the property in (1), which says that tangents to a linearly transformed set coincide with the transformation of the second-order tangent set for directions from the null-space of the transformation. This property could be guaranteed, e.g., when the set (to be transformed) is convex polyhedral, and with this knowledge we were particularly able to compute second-order contingent derivatives for mappings defined as the sum of a smooth single-valued and a polyhedral set-valued mapping in Section 3. We explained relations to results in [4, 30, 39, 49] among others. Under a weak error bound condition, second-order contingent derivatives can be used to compute tangents to the solution set of a generalized equation in absence of standard Lipschitzian regularity conditions. We used this fact in Section 4 to compute such tangents with respect to relevant classes of generalized equations. A number of previously unknown relations could be established with existing results in this direction. Sufficient conditions for the needed error bound are studied, too.

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