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On stable piecewise linearization and generalized algorithmic differentiation

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On stable piecewise linearization† and generalized algorithmic differentiation

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It is shown how functions that are defined by evaluation programs involving the absolute value function **abs**() (besides smooth elementals) can be approximated locally by piecewise-linear models in the style of algorithmic or automatic differentiation (AD). The model can be generated by a minor modification of standard AD tools and it is Lipschitz continuous with respect to the base point at which it is developed. The discrepancy between the original function, which is *piecewise differentiable*, and the piecewise linear model is of second order in the distance to the base point. Consequently, successive piecewise linearization yields bundle type methods for unconstrained minimization and Newton-type equation solvers. As a third fundamental numerical task we consider the integration of ordinary differential equations, for which we examine generalizations of the midpoint and the trapezoidal rule for the case of Lipschitz continuous right hand sides (RHSs). As a by-product of piecewise linearization, we show how to compute at any base point some generalized Jacobians of the original function, namely those that are *conically active* as defined by Khan and Barton. This subset of the Clarke Jacobian is never empty, independent of the particular function representation in terms of elementals, and also invariant with respect to linear transformations on domain and range. However, like all generalized derivatives the conically active Jacobians reduce almost everywhere to the singleton formed by the proper Jacobian, which may approximate the original function only in a minuscule neighbourhood. Since the piecewise linearization always reflects kinks in the vicinity, we illustrate how it can be used to approximate generalized Jacobians at nearby points along a user specified preferred direction.

Keywords: piecewise differentiability; Lipschitz continuity; directional derivative; automatic differentiation; computational graph; ADOL-C; bundle methods; midpoint method; trapezoidal rule; piecewise Newton; coherent orientation; generalized gradients and Jacobians; conical activity; Bouligand derivative

1. Introduction and motivation

Most algorithms in nonlinear scientific computing rely on successive local linearizations of the problem functions at hand to solve certain computational tasks. In particular, we have in mind the solution of nonlinear equations, scalar or vector optimization with or without constraints, and the integration of ODEs and other evolutionary systems. Frequently, statements about domains of attraction and asymptotic convergence rates of iterative solvers or adaptive discretizations rely implicitly or explicitly on sufficient differentiability properties.

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†Our notion of linearity includes nonhomogeneous functions, where the adjective *affine* or perhaps *polyhedral* would be more precise. However, such mathematical terminology might be less appealing to computational practitioners and to the best of our knowledge there are no good nouns corresponding to *linearity* and *linearization* for the adjectives affine and polyhedral.

1.1 *Realistic scenarios for nonsmoothness*

On the other hand, many or most realistic computer models are nondifferentiable in that the functional relation between input and output variables is not everywhere smooth. We are particularly interested in Lipschitz continuous models that arise for example in aerodynamics as well as in meteorology and oceanography through the discretization of PDEs using upwinding, slope limiters and other stabilization strategies. In optimization, we may have gradients of objective functions and constraints that are pieced together from local models or approximations in a C^1 fashion. While in one spatial dimension it is quite easy to interpolate scattered data or even solve differential equations by cubic splines with continuous second order derivatives, just making gradients continuous requires considerable computational effort in multivariate interpolation [3] or PDE solving [7]. Then the corresponding Karush–Kuhn–Tucker (KKT) equations will also be $C^{0,1}$ but generally not smoother. Another class of $C^{1,1}$ models are convex envelopes of smooth functions, which have in general (only) Lipschitz continuous gradients [18].

In some other applications, the nonsmoothness arises through the incorporation of sign and complementarity conditions for optimality. Finally, many exact penalty functions are only Lipschitz continuous. If they are based on the l^1 or l^∞ norm function their piecewise linearization is obvious. These norms may also occur in intermediate scalings and unscalings for numerical purposes, with the end result not necessarily being nonsmooth at all. Whenever the Euclidean norm occurs, we do not have piecewise differentiability, which is also the case for problems where the modulus of complex numbers occurs in the objective of constraint functions. Besides the handling of the Euclidean norm, another subject of ongoing research is the handling of if-statements and general gotos in the given function evaluation procedure. From a mathematical point of view, more interesting are multi-level problems, where the solution operators of lower levels are typically Lipschitz continuous. However, they are naturally only implicitly defined and require inner iterations with variable step numbers to be accurately evaluated.

1.2 *Practical predicament of generalized differentiation*

Assuming that a finite, deterministic program is evaluated in (exact) real arithmetic, it follows immediately [19] that the functional relation between input and output variables is almost everywhere differentiable and even real analytic. Hence, the probability of chancing upon a point of nondifferentiability in a numerical simulation or optimization calculation is practically zero. Consequently, the provisions for exact one-sided differentiation made in ADOL-C, ADIFOR and some other automatic differentiation (AD) tools are of rather limited use. The same applies to the coding of generalized derivatives by hand as the result reduces almost everywhere to the conventional derivative. This is a familiar experience for implementers of generalized Newton methods, which reduce to the standard Newton iteration, possibly with modified step size control [6].

Nevertheless, it is at least of theoretical interest that even at points right on a kink or jump, computer evaluated functions have convergent one-sided Taylor expansions [19]. In other words, directional derivatives can be unambiguously propagated in the forward mode of AD. The key practical question for nonsmooth analysis is what can be done in the situation where the current argument is not right on but merely close to a kink or jump. Then the function has local linear and even higher order approximations by the appropriate Taylor polynomial, but that model's very limited range renders it useless for optimization and other numerical purposes. For example, it is easy to construct an objective function in two variables with a slanted V-shaped valley, where gradient-based optimization methods will zig–zag across the bottom using ever smaller steps and making very little progress along the valley. Moreover, the sloped valley can be modified to piecewise linear functions, such that even in combination with an exact line-search this zig-zagging leads to convergence to a nonstationary point [4]. In the theory of bundle methods for unconstrained optimization, singleton gradients are enlarged to so-called ε-gradients, which may be interpreted as generalized gradients at nearby points.

1.3 *Purposes and concepts of differentiation*

There is by now a very rich literature on nonsmooth analysis (see, e.g. [8,11,13,14,24,25,28,30,35,37], to name just a few), which for the most part means developing some kind of derivative concept and utilizing it for the following purposes:

Estimation of function variations by mean value theorems.
Characterization of special points via necessary or sufficient conditions.
Implicit stability under suitable regularity assumption on derivative.
Modelling by local approximations for use in iterative algorithms.

One might rate derivative concepts and the resulting models by the following criteria:

Local fit that reflects the essential features of the underlying function.
Stability of the derivative object w.r.t. the *development or base* point(s).
Homogeniety with respect to (positive) scaling of the domain and range.
Invariance with respect to linear transformations on domain and/or range.
Efficiency and accuracy of derivative evaluation by differentiation rules.
Solvability of corresponding model problems as inner loop calculation.
Simplicity of data structures and significance of values to practitioners.

In the smooth case, rectangular arrays of first and second derivatives serve these purposes quite well and also fulfill the additional criteria by and large. Many derivative matrices are sparse and otherwise structured, so that they must be stored and manipulated with some care. It is apparently in the nature of generalized derivatives that their complexity may vary drastically from point to point, both in terms of computational effort and data representation. The desirable property of stability usually holds only in the sense that the set valued derivative mappings are outer semi-continuous. Mordukhovich interprets this property as *robustness*.

Overall, the usual nonsmooth concepts, which will be discussed in some more detail in Section 6, fall short of most of the requirements, even for the example pair $f_\pm(x) \equiv \pm|x|$. On those archetypical embodiments of nonsmoothness, the set of limiting Jacobians and their convex hull, the Clarke differential make at the crucial point $x = 0$ no difference at all between f_+ and f_-. This elementary observation alone suggests that their modelling ability is somewhat limited. In contrast the *co-derivative* of Mordukhovich [30] makes a big distinction between f_+ and f_-, yielding in the first case the same interval $[-1, 1]$ as Clarke and in the second the two limiting slopes $\{-1, 1\}$. Of course, this means that we can have only positive homogeneity on the range, which makes a lot of sense for objective functions and Lagrangians in optimization, but much less for nonsmooth systems of equations. In this paper, we will consider only primal derivative concepts for vector functions and require that they be fully invariant with respect to linear range space transformations and thus also the chosen norm.

1.4 *The piecewise linearization idea*

The approach discussed here ensures continuity and a good local fit in that the discrepancy between model and underlying function will be uniform of second order in the distance to the base point. It is debatable to what extent the requirements efficiency and simplicity are satisfied. One can certainly obtain piecewise linear model problems that are NP hard to solve.

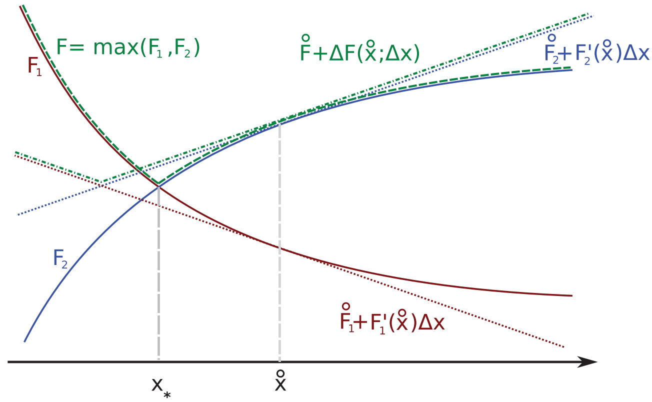

Figure 1. Piecewise linearization of univariate F via tangents.

To illustrate what we have in mind let us consider a univariate function of the form $F(x) = \max(F_1(x), F_2(x))$ as depicted in Figure 1. Since F_1 and F_2 are assumed smooth, the function F is everywhere differentiable except at the kink point x_* where the two values tie. There the generalized gradient $\nabla^C F(x_*) = [F_1'(x_*), F_2'(x_*)]$ in the sense of Clarke is the interval spanned by the negative slope $F_1'(x_*)$ of the red branch and the positive slope $F_2'(x_*)$ of the blue branch. This reflects the fact that the set-valued Clarke derivative is just the convex and outer semicontinuous hull of the classical derivative $F'(x)$, which is undefined at $x = x_*$ itself.

At any $x \neq x_*$ Clarke's and all other derivative concepts reduce simply to the slope, which gives no indication of the nearby kink whatsoever. If the F is repeatedly evaluated as part of a larger interactive computation in floating point arithmetic, the kink will almost certainly never be hit exactly, and modelling F by the tangent line of either F_1 or F_2 may of course yield rather poor results. All we are suggesting is to model F by the dashed green function $F(\mathring{x}) + \Delta F(\mathring{x}; \Delta x)$. As we will see later this piecewise linear function is obtained by approximating $F_1(x)$ as well as $F_2(x)$ by their tangent line at the base point $\mathring{x}$ and then taking the maximum afterwards. It is intuitively clear that this approximating function varies continuously with $\mathring{x}$ and yields a rather good approximation to the original function F on both sides of its kink.

In Figure 2 we see a similar piecewise linear approximation that is based on two interpolation points $\check{x}$ and $\hat{x}$. This secant-based piecewise linearization will be described and analysed in

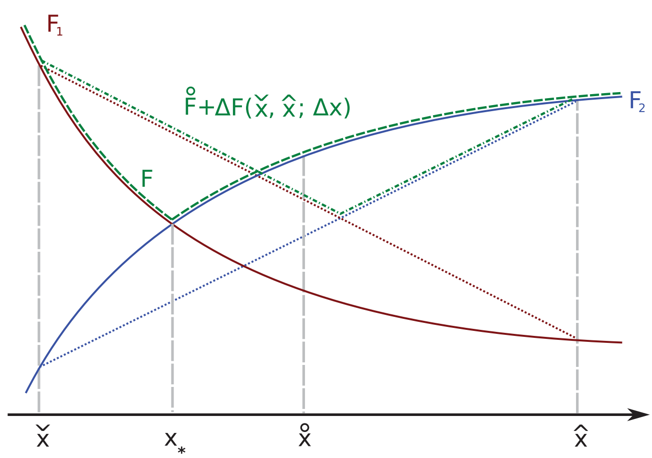

Figure 2. Piecewise linearization of univariate F via secants.

Section 7. It seems particularly promising in the context of ODE solving, where one can show that a generalization of the trapezoidal method to piecewise smooth RHSs still achieves a global error of order 2. Nevertheless, our main focus is on the tangent-based piecewise linearization, which is in fact the limiting case of the secant model when $\check{x}$ and $\hat{x}$ coalesce at $\mathring{x}$. If the secant mode is not explicitly mentioned piecewise linearization is always based on tangents.

1.5 *Results and applications for piecewise linear models*

There exists a very substantial literature on continuous piecewise linear functions [36]. The book [29] discusses piecewise linear modelling of electronic circuits, and many models of that nature are used in economics, visualization and other applications. KKT systems for quadratic programs and other linear complementarity problems (LCPs) [9] can be naturally written as a system of piecewise linear equations $F(x) = 0$. Conversely, any such system can be rewritten as an LCP, albeit with an increased number of variables [12]. There has been considerable debate about the most convenient way of representing a piecewise linear system. That question is answered in a natural way by our algorithmic piecewise linearization, since in effect we are always dealing with piecewise linear straight line programs. Finally, we note that much of what is currently known about nonsmooth dynamical systems [2] has been observed or established for piecewise linear RHSs.

In contrast to higher order models, the class of piecewise linear functions and the subclass of corresponding straight line programs are closed with respect to composition and linear combination. There is always the danger of combinatorial explosion regarding the number of linear pieces, but in terms of the program length the complexity growth is quite moderate. Even conditional assignments maintain piecewise linearity and the code structure, though they are quite likely to destroy continuity, unless special precautions are taken. On an analytical level, piecewise linear models maintain two interesting implications from the linear case. First, continuity implies Lipschitz continuity, and second, local homeomorphy at all points implies global homeomorphy.

2. Straightline representation and general assumptions

The weird and wonderful world of generalized differentiation becomes a lot more manageable (but certainly much less interesting to some) if we impose finite dimensionality and consider ‘only’ piecewise differentiable functions of the following kind. Throughout, we assume that the given mapping $y = F(x)$ from $x \in \mathbb{R}^n$ to $y \in \mathbb{R}^m$ is defined by an evaluation procedure consisting of a sequence of elemental functions

$$v_i = \varphi_i(v_j)_{j \prec i} \quad \text{for} \quad i = 1 \cdots l.$$

In other words, we assume that we have a straight line program without any variations in the control flow. The situation where there are branches in the form of conditional gotos remains to be investigated. The data dependence relation $\prec$ generates a partial ordering, which can be visualized as a directed acyclic graph. Also, we will assume that there is no overwriting so that we have a so-called single assignment code, which simplifies the presentation a little without affecting the key observations at all.

2.1 *Composite piecewise differentiability*

Piecewise differentiability must arise if there are no program branches but some calls to **abs**() and min() or max(). The latter can be simply expressed as

$$\max(u, w) = (u + w + \mathbf{abs}(u - w))/2, \quad \min(u, w) = (u + w - \mathbf{abs}(u - w))/2,$$

so that we can describe the situation exclusively in terms of **abs**(). There is a slight implicit restriction, namely we assume that whenever min or max is evaluated both their arguments have well defined finite values so that the same is true for their sum and difference. On the other hand, the expression $\min(1, 1/\mathbf{abs}(u))$ makes perfect sense in IEEE arithmetic, but rewriting it as above leads to a *NaN* at $u = 0$. While this restriction may appear quite technical it imposes the requirement that all relevant quantities are well defined at least in some open neighbourhood, which is exactly in the nature of piecewise differentiability.

We will call procedures containing only $C^{1,1}$ functions φ_i and the absolute value **abs**() *composite piecewise differentiable*. Obviously, any one of them may still be properly composite differentiable if the programmer has used **abs**() wisely, for example only to first scale and later unscale variables to improve numerical stability. Then these operations will not affect the theoretical function values and their differentiability properties. Moreover, we will see that our piecewise linearization approach will in fact yield the correct derivatives of such composite differentiable functions. We consider this a very important achievement for AD tools.

In the terminology of Khan and Barton [26,27] our concept *composite piecewise differentiability* is called **abs**-factorable, and in the notation of Scholtes and others our functions belong to the class $PC^{1,1}$. They are locally characterized as continuous selections from a finite number of continuously differentiable functions. There is a large body of literature (see, e.g. [36]) concerning the properties of such piecewise smooth functions $F(x) \in PC^{1,1}$ and the corresponding Bouligand derivatives $F'(x; \Delta x)$ and limiting Jacobians $\nabla^L F(x)$. We can apply many of these results constructively and will also derive additional properties using the straightline code structure, which apparently has so far only been considered for this purpose in [17,26,27]. The composite piecewise differentiable functions are also a very small subset of the class of lexicographically differentiable functions introduced by Nesterov [32], which includes amongst others all convex functions.

Apparently, the process by which the various candidate functions are selected has hitherto been viewed as external and somewhat arbitrary, except for the requirement that the result turns out to be continuous. In contrast, we can analyse the selection as a hierarchical process that is part of the evaluation procedure.

2.2 *Ruling out the Euclidean norm*

Piecewise linearization does not yield second order approximations for all Lipschitzian functions. In particular it is well known that the Euclidean norm

$$\|x\|_2 = [x_1^2 + \cdots + x_i^2 + \cdots + x_n^2]^{1/2} \quad \text{for } x \in \mathbb{R}^n \quad \text{with } n > 1$$

is Lipschitz continuous with constant 1. However, it is not piecewise differentiable in the sense of Scholtes, because near the origin it cannot be interpreted as a selection from a finite set of functions that are locally differentiable.

Nevertheless, things are not that bad. Because, if the square root of a scalar value z is interpreted as $\sqrt{\mathbf{abs}(z)}$ and piecewise-linearized accordingly, then the resulting approximation to the Euclidean norm $\|x\|_2$ is quite reasonable. Namely, it represents exactly the V-shaped valley, whose bottom runs perpendicular to $x \neq 0$ with minimal value zero. Where the argument $\|x\|^2$ of the square root vanishes exactly, so will its piecewise linearization and treating the root as an even function it makes sense to set its linearization at a constant zero argument to zero too.

In general, we can expect that nondifferentiability of the Euclidean norm only occurs at manifolds of dimension less than or equal to $n-2$ in the domain $\mathbb{R}^n$. Hence, the iteration sequences generated by numerical algorithms have the chance to 'go around' them. This optimistic assessment regarding the nondifferentiability of the Euclidean norm may not apply when it occurs as part of the Fischer–Burmeister complementarity function [16] and the solution in question lacks strict complementarity. Then piecewise linearization as suggested above must certainly lack the second order approximation property which will be established in Proposition 2 for the piecewise differentiable case.

Note also that the modulus of complex numbers is the Euclidean norm of its real and imaginary part so that especially the approximation of the Euclidean norm in $\mathbb{R}^2$ deserves some future investigation. Finally, the Euclidean norm frequently occurs as a distance function between points and sets. Then its argument is quite likely to be defined implicitly by solutions to systems of equations and inequalities. In this paper we will consider only the case of explicitly defined functions, rather than a hierarchy of partly implicit mathematical relations.

2.3 *Possible extension to conditional assignments*

Even without program branching, discontinuities may arise through conditional assignments. In C syntax, one codes

$$v = u > 0\,?\,w1 : w2,$$

so that v gets the value of $w1$ if $u > 0$ and otherwise that of $w2$. The conditional assignment can be rewritten as

$$v = (w1 + w2) + \text{sign\_}(u)(w1 - w2)/2 \quad \text{with } \text{sign\_}(0) \equiv -1.$$

Therefore, basically we only have to worry about a conditional sign switch of the form

$$v \equiv \mathbf{copysign}(u, w) \equiv \mathbf{sign}(u) * w.$$

Everything else in the conditional assignment represents smooth operations. In expressing the conditional assignment in terms of the **copysign** we have implicitly imposed a similar condition to that we used when we rewrote max and min in terms of **abs**. Namely, we assume that both values $w1$ and $w2$ are well defined when v is to be computed so that their sum and difference are also well defined real numbers. Therefore the expression $v = u > 0\,?\,1/u : 1$ cannot be rewritten in the desired way and would have to be treated as general branching.

In contrast to proper branching **copysign** can still be viewed as a purely arithmetic binary instruction. It maintains the evaluation procedure as a straight-line code and allows one to update the Jacobians by rank-one corrections. Of course, continuity is lost, unless the programmer ascertains it for the composite function. It is not yet clear what the software can do with such an expression of good faith. Then $u = 0$ must always imply $w = 0$ where both intermediate variables depend on the base point x. Possibly, the AD software could check this implication with a suitable tolerance and give corresponding warnings otherwise.

In this paper, we will assume throughout that all piecewise smooth or piecewise linear functions are continuous, at least in the interior of their domain of definition. As stated in [36], all continuous piecewise linear functions can be expressed in terms of one level of minima and one level of maxima, so that conditional assignments and gotos can be eliminated in the theory. However from a practical point of view, this rewriting is entirely unrealistic and will not even be attempted.

2.3.1 *Paper organization*

The paper is organized as follows. In the following Section 3 we consider the process of piecewise linearization in the composite piecewise differentiable case. Its homogeneous part at the origin corresponds to the so-called Bouligand derivative, whose characteristics are briefly reviewed. We also establish the main mathematical properties of our approximation. In Section 4 we show how the piecewise linear model can be generated, stored and manipulated. In Section 5 we show how successive piecewise linearization can be used for unconstrained nonsmooth optimization, the numerical integration of Lipschitzian dynamical systems and the solution of piecewise smooth nonlinear equations. In the subsequent Section 6 we will show how selected Jacobians of the piecewise linearization can be computed, and that they are indeed limiting Jacobians of the underlying vector function and thus elements of the generalized Jacobian in the sense of Clarke. In Section 7 we generalize the piecewise linearization approach to secant-based approximations and use it for a version of the trapezoidal rule. In the final Section 8 we summarize our observations and discuss various extensions.

As pointed out by one of the referees the new material is largely confined to the Sections 3.4, 5.1, 5.2, 4, 6 and 7. Moreover, the other parts do not give a full account of the rich, previous contributions to the literature. Instead we have striven to provide a self-contained and readable description of the chances and opportunities of piecewise linearization. It will hopefully be appreciated by practitioners since it is probably fair to state that classical nonsmooth analysis requires a considerable level of analytical background.

3. Piecewise linearization and directional differentiation

Let the vector function $F : \mathcal{D} \subset \mathbb{R}^n \mapsto \mathbb{R}^m$ in question be evaluated by a sequence of assignments

$$v_i = v_j \circ v_k \quad \text{or} \quad v_i = \varphi_i(v_j) \quad \text{for} \quad i = 1 \cdots l.$$

Here $\circ \in \{+, -, *\}$ is a polynomial arithmetic operation and

$$\varphi_i \in \Phi \equiv \{\text{rec}, \text{sqrt}, \sin, \cos, \exp, \log, \ldots, \textbf{abs}, \ldots\}$$

a univariate function. To simplify the notation we interpret the division as a reciprocal $\text{rec}(u) \equiv 1/u$, followed by a multiplication, although that would mean an unnecessary loss of efficiency and numerical stability in an actual AD tool. Also, a possible extension to the approach discussed in this paper would be to approximate all intermediates by quotients of two piecewise linear functions, which would lead to a completely different treatment of the division operation.

The user or reader may extend the library by other locally Lipschitz-continuously differentiable functions like the analysis favourites

$$\varphi(u) \equiv |u| > 0\, ?\, u^p \sin(u^1) : 0 \quad \text{for} \quad p \geq 3.$$

But then he or she is responsible for supplying an evaluation procedure for both, the elemental function φ and its derivative φ', which cannot be based mechanically on the chain rule in this case.

Following the notation from [19] we partition the sequence of scalar variables v_i into the vector triple

$$(x, z, y) = (v_{1-n}, \ldots, v_{-1}, v_0, \ldots, v_{l-m}, v_{l-m+1}, \ldots, v_l) \in \mathbb{R}^{n+l},$$

such that $x \in \mathbb{R}^n$ is the vector of independent, $y \in \mathbb{R}^m$ the vector of dependent variables and $z \in \mathbb{R}^{l-m}$ the (internal) vector of intermediates.

Some of the elemental functions like the reciprocal, the square root and the logarithm are not globally defined. Hence, we will assume throughout this paper that all elementals are evaluated in the interior of their domain of definition. In other words we will assume that the input variables x are restricted to an open domain $\mathcal{D} \subset \mathbb{R}^n$ such that all resulting intermediate values $v_i = v_i(x)$ are well defined.

Throughout, we will assume that the evaluation procedure for F involves exactly $s \geq 0$ calls to **abs**(), including min and max rewritten or at least reinterpreted as discussed above. Starting from $\mathring{x}$ and an increment $\Delta x = x - \mathring{x}$, we will now construct for each intermediate v_i with the reference value $\mathring{v}_i = v_i(\mathring{x})$ an approximation

$$v_i(\mathring{x} + \Delta x) - \mathring{v}_i \approx \Delta v_i \equiv \Delta v_i(\Delta x).$$

The incremental function $\Delta v_i(\Delta x)$ will be contained continuous and piecewise linear with respect to Δx for $\mathring{x}$ considered constant. Hence, we will often list Δx, but only rarely in proofs $\mathring{x}$ as arguments of the Δv_i.

3.1 *Defining relations for tangent approximation*

We assume that all φ_i other than the absolute value function are differentiable within the domain of interest, we may use the tangent linearizations

$$\Delta v_i = \Delta v_j \pm \Delta v_k \quad \text{for } v_i = v_j \pm v_k, \tag{1}$$

$$\Delta v_i = \mathring{v}_j * \Delta v_k + \Delta v_j * \mathring{v}_k \quad \text{for } v_i = v_j * v_k, \tag{2}$$

$$\Delta v_i = \mathring{c}_{ij} * \Delta v_j \quad \text{for } v_i = \varphi_i(v_j) \not\equiv \mathbf{abs}(v_j), \tag{3}$$

where $\mathring{c}_{ij} \equiv \varphi_i'(\mathring{v}_j)$ is the local partial derivative.

If no absolute value or other nonsmooth elemental occurs, the function $y = F(x)$ is at the current point $\mathring{x}$ differentiable and by the chain rule we have the relation

$$\Delta y = \Delta F(\mathring{x}; \Delta x) \equiv \nabla F(\mathring{x})\Delta x,$$

where $\nabla F(x) \in \mathbb{R}^{m\times n}$ is the Jacobian matrix. Thus we observe the obvious fact that smooth differentiation is equivalent to linearizing all elemental functions.

Now, let us move to the piecewise differentiable scenario, where the absolute value function does occur $s > 0$ times. We then may obtain a piecewise linearization of the vector function $F(\mathring{x} + \Delta x) - F(\mathring{x})$ by incrementing

$$\Delta v_i = \mathbf{abs}(\mathring{v}_j + \Delta v_j) - \mathring{v}_i, \quad \text{when } v_i = \mathbf{abs}(v_j). \tag{4}$$

In other words, we keep the piecewise linear function **abs**() unchanged so that the resulting Δy represents for each fixed $x \in \mathcal{D}$ the piecewise linear and continuous *increment function*

$$\Delta y = \Delta y(\Delta x) = \Delta F(\mathring{x}; \Delta x) : \mathbb{R}^n \mapsto \mathbb{R}^m.$$

As observed by one of the referees, our global nonhomogeneous approximation may also lead to curious effects. For example, the simple function $f(x) = \min(\exp(x), 0)$ will be approximated from some point $\mathring{x}$ according to

$$0 = \min(\exp(x), 0) \approx f(\mathring{x}) + \Delta f(\mathring{x}; \Delta x) = \min(\exp(\mathring{x})(1 + \Delta x), 0).$$

Hence, the RHS will go negative when $\Delta x < -1$.

There are two ripostes to this observation. First, one may blame the user for coding something as silly as $y = \min(\exp(x), 0)$ rather than setting $y = 0$ right away. Second, a more constructive suggestion would be to not approximate the smooth elementals $\exp(x)$ and $\sin(x)$ simply by their tangents but cutting those affine functions off at the natural lower and upper bounds. In some sense that would acerbate the combinatorial aspect of the problem, but there is reason to believe that these extra switches would not be active except in the very early stages of an iterative computation. Thus we could set

$$\exp(\mathring{x} + \Delta x) \approx f(\mathring{x}) + \Delta f(\mathring{x}; \Delta x) \equiv \max(0, \exp(\mathring{x})(1 + \Delta x))$$

and

$$\sin(\mathring{x} + \Delta x) \approx f(\mathring{x}) + \Delta f(\mathring{x}; \Delta x) \equiv \max(-1, \min(1, \sin(\mathring{x}) + \cos(\mathring{x})\Delta x)).$$

Actually, the double cut-off for the sin is better implemented in the form

$$f(\mathring{x}) + \Delta f(\mathring{x}; \Delta x) \equiv \tfrac{1}{2}[\mathbf{abs}(\sin(\mathring{x}) + \cos(\mathring{x})\Delta x + 1) - \mathbf{abs}(\sin(\mathring{x}) + \cos(\mathring{x})\Delta x - 1)].$$

The advantage here is that the kinks represented by min, max and abs are not nested or superimposed. Generally, it is a good idea to keep the switching depth, i.e. the maximal number of nonsmooth elements along any path in the computational graph as small as possible.

3.2 *Relationship to Bouligand differentiability*

Obviously the more general function $\Delta F(\mathring{x}; \Delta x)$ can no longer be expressed as a matrix–vector product, which may seem a little off-putting to computational practitioners. However, the same objection already applies to the directional derivative

$$\Delta y = F'(\mathring{x}; \Delta x) \equiv \lim_{t \searrow 0} \frac{1}{t}[F(\mathring{x} + t\Delta x) - F(\mathring{x})] \in \mathbb{R}^m, \tag{5}$$

which may depend in a rather complicated way on the direction Δx.

We will refer to $F'(\mathring{x}; \Delta x)$ viewed as a mapping from $\Delta x \in \mathbb{R}^n$ to $\Delta y \in \mathbb{R}^m$ as the *Bouligand derivative* of F at $\mathring{x} \in \mathbb{R}^n$. On piecewise differentiable functions $F'(\mathring{x}; \Delta x)$ is also piecewise linear, but in contrast to $\Delta F(\mathring{x}; \Delta x)$, it is positively homogeneous. Clearly, especially in higher dimensions that does not reduce the difficulty of representing and manipulation these piecewise linear functions by much. We will always deal with $\Delta F(\mathring{x}; \Delta x)$ as a piecewise linear evaluation procedure, whose temporal and spatial complexity is much the same as that of the given nonlinear function F.

In order to evaluate the Bouligand derivative itself we simply have to replace (4) by the conditional assignment

$$\Delta v_i = (\mathring{v}_j \neq 0)?\mathbf{sign}(\mathring{v}_j)\Delta v_j : \mathbf{abs}(\Delta v_j), \quad \text{when} \quad v_i = \mathbf{abs}(v_j). \tag{6}$$

In other words, unless its argument $\mathring{v}_j$ is exactly zero the absolute value function is replaced by its tangent line, like the smooth elementals. Only when the argument vanishes we set $\Delta v_i = \mathbf{abs}(\Delta v_j)$. This makes the Bouligand derivative discontinuous with respect to the base point $\mathring{x}$ for fixed Δx. In contrast we will see that the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$ is jointly continuous in its two arguments. It is well known [35] that if this was also true for the Bouligand derivative $F'(\mathring{x}; \Delta x)$ the function would in fact be Fréchet differentiable at $\mathring{x}$.

One can easily check that for fixed $\mathring{x}$ and thus $\mathring{v}_j$ the relation (4) reduces to (6) when Δx and thus Δv_j become sufficiently small. Hence there exists a bound ρ depending on $\mathring{x}$ such that

$$\Delta F(\mathring{x}; \Delta x) = F'(\mathring{x}; \Delta x) \quad \text{if} \quad \|\Delta x\| \leq \rho(\mathring{x}). \tag{7}$$

As for the function $F(x) = \mathbf{abs}(x)$ itself, the bound $\rho = \rho(\mathring{x})$ tends to zero as the base point $\mathring{x}$ approaches a nondifferentiability. The main advantage of the piecewise linearization is that we obtain a much more uniform approximation to $F(x)$ as we will see later.

Of course under our assumptions on the underlying evaluation procedure we get

$$F(\mathring{x} + \Delta x) - F(\mathring{x}) = F'(\mathring{x}; \Delta x) + \mathcal{O}(\|\Delta x\|)^2,$$

where the order term is again strongly dependent on $\mathring{x}$. In other words we have Bouligand differentiability as defined in [34].

However, in general we do not have *strong Bouligand differentiability* in the sense that the discrepancy function $F(\mathring{x} + \Delta x) - F(\mathring{x}) - F'(\mathring{x}; \Delta x)$ has local Lipschitz constants that are arbitrarily small in the vicinity of the origin $\Delta x = 0$. This can be seen from the scalar values example

$$f(x, y) = (y^2 - x_+)_+ \quad \text{with} \quad z_+ \equiv \max(0, z), \tag{8}$$

whose graph is depicted in Figure 3. At the origin $(x, y) = 0 \in \mathbb{R}^2$ we have $\Delta f(0; \Delta x) \equiv 0$ and also $f'(0; \Delta x) \equiv 0$ so that $f(x, y)$ itself is the discrepancy in question. In the subdomain where $y^2 > x_+ > 0$ the selection function is $y^2 - x$, whose Lipschitz constant is bounded below by 1 everywhere. The example is also quite instructive in the following sense. The kink-lines of the original function $f(x, y)$ are represented by the red lines underneath, which form a pitchfork.

The corresponding piecewise linearization at $(\mathring{x} = 0.125, \mathring{y} = 0.5)$ is given by

$$\Delta f((\mathring{x}, \mathring{y})^\top; (\Delta x, \Delta y)^\top) = [\mathring{y}^2 + 2\mathring{y}\Delta y - (\mathring{x} + \Delta x)_+]_+ - \mathring{y}^2 + \mathring{x}. \tag{9}$$

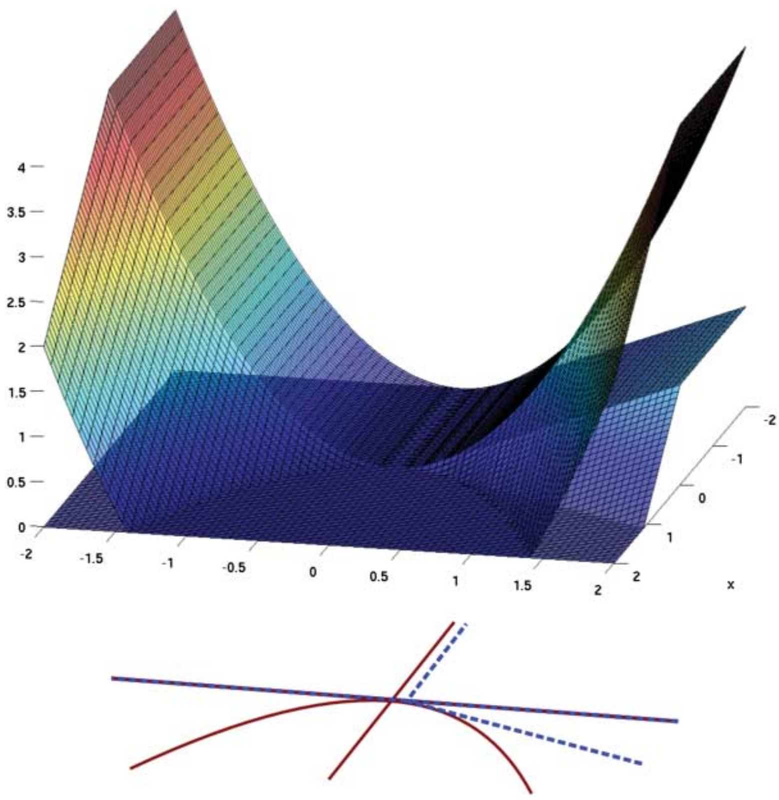

Figure 3. Example that is not strongly Bouligand differentiable at the origin.

It is only nontrivial in the far right corner where the outer positive part function $[\cdots]_+$ has a positive argument. It is important to note that only the blue line created by the inner positive part function $(\cdots)_+$ along the y-axis runs straight through, whereas the second line caused by the outer positive part function $[\cdots]_+$ is refracted at the first line. This is quite typical when nonsmooth elementals are superimposed on each other rather than occurring at the same evaluation level and thus being in some sense mutually independent.

That special situation arises for example in KKT conditions or other complementarity systems, where the components of a smooth vector functions are combined in a piecewise linear fashion at the top level. Whereas it is then quite easy to write down generalized Jacobians, computing them is quite a difficult task in the general case where some nonsmooth elementals are super imposed.

The general lack of strong Bouligand differentiability means for the square case $m = n$, that the inverse function theorem of Scholtes (Corollary 3.2.1 in [36]) does not apply. Moreover, there can be no implicit function theorem based on invertibility of the Bouligand derivative at $\mathring{x}$ as demonstrated by Scholtes piecewise smooth example 3.2.2.

3.3 *Exemplary observations on solvability and stability*

We can construct an even simpler counter example based on (8), namely the system

$$F(x, y) = \begin{bmatrix} x/2 + (y^2 - x_+)_+ \\ y \end{bmatrix} = \begin{bmatrix} \delta \\ \varepsilon \end{bmatrix}. \tag{10}$$

It has for $x \le 0$, $0 < x < y^2$ and $y^2 < x$, respectively, the Fréchet derivatives

$$\nabla F(x, y) = \begin{bmatrix} \frac{1}{2} & 2y \\ 0 & 1 \end{bmatrix}, \quad \nabla F(x, y) = \begin{bmatrix} -\frac{1}{2} & 2y \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \nabla F(x, y) = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{bmatrix}.$$

Due to homogeniety, its piecewise linearization and Bouligand derivative coincide at the origin where $F(0) = 0$ and

$$F'\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}; \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix}\right) = \begin{bmatrix} \Delta x/2 \\ \Delta y \end{bmatrix} = \Delta F\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}; \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix}\right).$$

This means that the Fréchet derivative of F is nonsingular at the root 0. However as one can easily see that$F$ is not even locally invertible.

The second equation in (10) requires $y_* = \varepsilon$, which substituted into the first yields the univariate equation depicted in Figure 4. Hence we see that any desired RHS value for $\delta \in \mathbb{R}$ can be reached

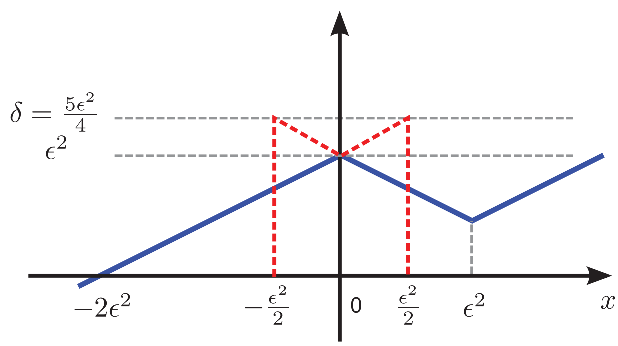

Figure 4. Surjective but noninvertible example.

but for $\delta \in (\varepsilon^2/2, \varepsilon^2)$ we have three inverse images and for the special values $\delta \in \{\varepsilon^2/2, \varepsilon^2\}$ we have exactly two. For $\delta \notin [\varepsilon^2/2, \varepsilon^2]$ there is exactly one solution, but it is not evident how that can be computed by an iterative algorithm if one starts in the zone where the slope is $-1/2$. In fact this is exactly where the Jacobian has a negative determinant, whereas outside it is positive. This violates the condition of coherent orientation, which is equivalent to openness in case of piecewise linear functions as we will discuss in Section 5 on equation solving.

Hence, coherent orientation which holds for the piecewise linearization $\Delta F(0; \Delta x)$ is not inherited by all neighbouring $\Delta F(\mathring{x}; \Delta x)$ for $\mathring{x} \approx 0$, a regrettable lack of stability. Moreover, the same is true for the recession function

$$\Delta F^{\infty}(\mathring{x}; \Delta x) \equiv \lim_{t\to\infty} \frac{\Delta F(\mathring{x}; t\Delta x)}{t},$$

which represents the homogeneous part of $\Delta F(\mathring{x}; \Delta x)$ at infinity. In case of the linearized scalar example (9) the recession function takes the form

$$\Delta f^{\infty}((\mathring{x}, \mathring{y})^{\top}; (\Delta x, \Delta y)^{\top}) = [2\mathring{y}\Delta y - (\Delta x)_+]_+.$$

Here one sees that on the cone $0 < \Delta x < 2\mathring{y}\Delta y$ the gradient is $(-1, 2\mathring{y})$. This means that the corresponding recession function of $\Delta F^{\infty}((\mathring{x}, \mathring{y})^{\top}; (\Delta x, \Delta y)^{\top})$ is also lacking the coherent orientation that $\Delta F((0, 0)^{\top}; (\Delta x, \Delta y)^{\top})$ has. The latter is homogeneous and thus its own recession function, which buries any hope that the latter's coherent orientation might be a stable property of our piecewise linearization.

We can also highlight a characteristic property of the semi-smooth Newton method on the above example. Our assumptions on the composite piecewise differentiable functions immediately imply that they are semi-smooth. And since for our specific example all limiting Jacobians are nonsingular, the local and superlinear convergence result applies at all points $(\mathring{x}, \mathring{y})$ with the corresponding RHS $(\delta, \varepsilon)^{\top} = F(\mathring{x}, \mathring{y})$. However, from Figure 4 one can see that when $\delta = 1.25\varepsilon^2$ then starting at any point (x_0, ε) with $x_0 \in (0, \varepsilon^2)$ will lead to the oscillating sequence $(x_k, \varepsilon) = ((-1)^k\varepsilon^2/2, \varepsilon)$, which of course does not converge to the unique root $(x_*, y_*) = (2\delta, \varepsilon)$. In other words, the radius of contraction for Newton's method applied to the perturbed systems $F(x, y) = (\delta, \varepsilon)$ becomes arbitrarily small for suitable perturbations (δ, ε) that also tend to zero. It was found in [10] that the same effect can occur for functions, like the Rosette examples displayed in Figure 6, that are piecewise linear and coherently oriented on all of $\mathbb{R}^n$. Thus we conclude that the semi-smooth local convergence result is indeed extremely local, much more so than the usual theorem for smooth Newton.

3.3.1 *Section summary*

For functions defined by straight-line evaluation procedures involving **abs**, min and max besides smooth elementals, we obtain an incremental piecewise linearization $\Delta F(\mathring{x}; \Delta x) \approx F(\mathring{x} + \Delta x) - F(\mathring{x})$. Its homogeneous part near the origin coincides with the Bouligand derivative $F'(x; \Delta x)$. The functions F are $PC^{1,1}$ and thus Bouligand differentiable, but in general not strongly Bouligand differentiable. When $m = 1$ a point $\mathring{x}$ can only be a local unconstrained minimizer of f if $\Delta x = 0$ is a local minimizer of $\Delta f(\mathring{x}; \Delta x)$ and equivalently $f'(\mathring{x}; \Delta x)$, i.e. we need $f'(\mathring{x}; \Delta x) \geq 0$ for all $\Delta x \in \mathbb{R}^n$. We will call such points *first order minimal*.

3.4 *Approximation, stability and composition*

In this section we first establish the main analytical properties of our model.

PROPOSITION 1 Quadratic approximation and Lipschitz continuity *Suppose F is composite Lipschitz continuously differentiable on some open neighbourhood $\mathcal{D}$ of a closed convex domain $\mathcal{K} \subset \mathbb{R}^n$. Then there exists a constant γ such that for all pairs $\mathring{x}, x \in \mathcal{K}$*

$$\|F(x) - F(\mathring{x}) - \Delta F(\mathring{x}; x - \mathring{x})\| \leq \gamma \|x - \mathring{x}\|^2.$$

Moreover, we have for any pair $\tilde{x}, \mathring{x} \in \mathcal{K}$ and $\Delta x \in \mathbb{R}^n$ and a constant $\tilde{\gamma}$

$$\frac{\|\Delta F(\tilde{x}; \Delta x) - \Delta F(\mathring{x}; \Delta x)\|}{1 + \|\Delta x\|} \leq \tilde{\gamma} \|\tilde{x} - \mathring{x}\|.$$

Proof The first assertion follows by induction on i, i.e. we show that for all intermediates

$$v_i(\mathring{x} + \Delta x) - v_i(\mathring{x}) = \Delta v_i(\mathring{x}; \Delta x) + \mathcal{O}(\|\Delta x\|^2).$$

For the first n intermediates, namely the v_{i-n}, this holds trivially since we set $\Delta v_{i-n} = \Delta x_i$. For the arithmetic operations and the smooth univariate functions $v_i = \varphi_i(v_j)$ the classical rules of differentiation (1), (2) and (3) make sure that the resulting Δv_i have the asserted approximation property.

Thus we only have to consider the case $v_i = \mathbf{abs}(v_j)$; where according to (4)

$$\begin{aligned} & v_i(\mathring{x}) + \Delta v_i(\mathring{x}; \Delta x) - v_i(\mathring{x} + \Delta x) \\ &\quad = \mathbf{abs}(v_j(\mathring{x})) + [\mathbf{abs}(v_j(\mathring{x}) + \Delta v_j(\mathring{x}; \Delta x)) - \mathbf{abs}(v_j(\mathring{x}))] - \mathbf{abs}(v_j(\mathring{x} + \Delta x)) \\ &\quad = \mathbf{abs}(v_j(\mathring{x}) + \Delta v_j(\mathring{x}; \Delta x)) - \mathbf{abs}(v_j(\mathring{x} + \Delta x)) = \mathcal{O}(\|\Delta x\|^2). \end{aligned}$$

Here the last relation follows from the induction hypothesis and Lipschitz continuity of all quantities in question.

To prove the second assertion we first note that again by induction for all i

$$v_i(\mathring{x}) - v_i(\tilde{x}) = \mathcal{O}(\|\tilde{x} - \mathring{x}\|) \quad \text{and} \quad \|\Delta v_i(\mathring{x}; \Delta x)\| \leq c_i \|\Delta x\|,$$

where c_i is a suitable constant. The first property implies for all smooth elementals by assumption of Lipschitz continuous differentiability that also

$$c_{ij}(\tilde{x}) - c_{ij}(\mathring{x}) = \mathcal{O}(\|\tilde{x} - \mathring{x}\|) \quad \text{for } j \prec i.$$

Now we can derive the actual assertion by showing that for all i

$$\frac{|\Delta v_i(\tilde{x}; \Delta x) - \Delta v_i(\mathring{x}; \Delta x)|}{1 + \|\Delta x\|} = \mathcal{O}(\|\tilde{x} - \mathring{x}\|).$$

It is obviously true for the independent values v_i for $i = 1 - n \cdots 0$ whose increments $\Delta v_i = \Delta x_{i+n}$ are chosen independently of x. Then it follows by induction for smooth elementals $v_i = \varphi_i(v_j)_{j \prec i}$ that

$$\begin{aligned} & \frac{|\Delta v_i(\tilde{x}; \Delta x) - \Delta v_i(\mathring{x}; \Delta x)|}{1 + \|\Delta x\|} \\ &\quad \leq \frac{|\sum_{j \prec i}(c_{ij}(\tilde{x}) - c_{ij}(\mathring{x}))\Delta v_j(\tilde{x}; \Delta x) + \sum_{j \prec i} c_{ij}(\mathring{x})(\Delta v_j(\tilde{x}; \Delta x) - \Delta v_j(\mathring{x}; \Delta x))|}{1 + \|\Delta x\|} \end{aligned}$$

$$\leq \frac{\sum_{j\prec i}\mathcal{O}(\|\tilde{x}-\mathring{x}\|)c_j\|\Delta x\| + \sum_{j\prec i}|c_{ij}(\mathring{x})||\Delta v_j(\tilde{x};\Delta x) - \Delta v_j(\mathring{x};\Delta x)|}{1+\|\Delta x\|}$$

$$\leq \mathcal{O}(\|\tilde{x}-x\|) + \sum_{j\prec i}|c_{ij}(\mathring{x})|\,\mathcal{O}(\|\tilde{x}-x\|) = \mathcal{O}(\|\tilde{x}-x\|).$$

Here the c_j are the Lipschitz constants, whose existence has been asserted at the beginning of the second part of the proof.

Hence we only have to prove the assertion for the absolute value where

$$\begin{aligned}
&|\Delta v_i(\tilde{x};\Delta x) - \Delta v_i(\mathring{x};\Delta x)| \\
&\quad = |\mathbf{abs}(v_j(\tilde{x}) + \Delta v_j(\tilde{x};\Delta x)) - \mathbf{abs}(v_j(\tilde{x})) - [\mathbf{abs}(v_j(\mathring{x}) + \Delta v_j(\mathring{x};\Delta x)) - \mathbf{abs}(v_j(\mathring{x}))]| \\
&\quad \leq |v_j(\tilde{x}) + \Delta v_j(\tilde{x};\Delta x) - [v_j(\mathring{x}) + \Delta v_j(\mathring{x};\Delta x)]| + |v_j(\tilde{x}) - v_j(\mathring{x})| \\
&\quad \leq |v_j(\tilde{x}) - v_j(\mathring{x})| + |\Delta v_j(\tilde{x};\Delta x) - \Delta v_j(\mathring{x};\Delta x)| + |v_j(\tilde{x}) - v_j(\mathring{x})| \\
&\quad = (1+\|\Delta x\|)\mathcal{O}(\|\tilde{x}-\mathring{x}\|) + 2\mathcal{O}(\|\tilde{x}-\mathring{x}\|) = (1+\|\Delta x\|)\mathcal{O}(\|\tilde{x}-\mathring{x}\|),
\end{aligned}$$

which completes the proof of the second assertion. ■

The proposition shows that our model $F(\mathring{x}) + \Delta F(\mathring{x};\Delta x)$ yields indeed a second order approximation to the underlying function $F(\mathring{x}+\Delta x)$. Thus we can expect quadratic convergence of a Newton-like procedure based on successive local piecewise linear models in the case $m = n$. The second property is crucial for the convergence proof of bundle type optimization methods in the unconstrained case $m = 1$. It can be interpreted as local Lipschitz continuity on the space of piecewise linear functions $G : \mathbb{R}^n \mapsto \mathbb{R}^m$ endowed with the norm

$$\|G\| \equiv \sup_{x\in\mathbb{R}^n}\left\{\frac{\|G(x)\|}{1+\|x\|}\right\} = \left\|\frac{G(x)}{1+\|x\|}\right\|_\infty.$$

This norm is finite for all piecewise linear G with finitely many pieces, which form a linear subspace of the Banach space of all mappings for which this norm is bounded. Any Cauchy sequence of piecewise linear functions with a uniform bound on the number of pieces has a piecewise linear limit. Without such a bound limits need not be piecewise linear of course. Here, we have such an a priori bound, namely 3^s, where s is the number of calls to the nonsmooth elementals **abs**, min and max in our evaluation procedure. However, the resulting piecewise linear functions are not closed with respect to linear combinations and thus do not form a subspace of the Banach space mentioned above.

3.5 *Piecewise linearization of combinations and composites*

There are a few other conclusions that can be drawn from Proposition 1. First, suppose that a function is coded in two different ways but according to the rules defined above. We will denote them as F and G. Then their piecewise linearizations $\Delta F(\mathring{x};\Delta x)$ and $\Delta G(\mathring{x};\Delta x)$ may differ globally, but because of the second order contact property their homogeneous parts at the origin, namely the Bouligand derivatives $F'(\mathring{x};\Delta x)$ and $G'(\mathring{x};\Delta x)$ must be identical. Of course this implies that also their limiting Jacobians at $\mathring{x}$ agree, so that $\nabla^L F(\mathring{x}) = \nabla^L G(\mathring{x})$. These relations will be analysed more closely in Section 6.

Globally we have some other nice properties, namely for $F, G : \mathcal{D} \subset \mathbb{R}^n \mapsto \mathbb{R}^m$ and $\alpha \in \mathbb{R}$ we have the piecewise linearization rules

$$\Delta[F + \alpha G](x; \Delta x) = \Delta F(x; \Delta x) + \alpha \Delta G(x; \Delta x),$$
$$\Delta[F^\top G](x; \Delta x) = G(x)^\top \Delta F(x; \Delta x) + F(x)^\top \Delta G(x; \Delta x).$$

Moreover, when $F : \mathcal{D} \subset \mathbb{R}^n \mapsto \mathbb{R}^m$ and $G : E \subset \mathbb{R}^m \mapsto \mathbb{R}^p$ with $F(\mathcal{D}) \subset E$ then we have the chain rule

$$\Delta[G \circ F](x; \Delta x) = \Delta G(F(x); \Delta F(x; \Delta x)).$$

The last identity holds in particular if F or G is linear which means that piecewise linearization is of course linearly invariant. For the corresponding generalized Jacobians one only obtains set inclusions rather than identities, since there explicit dependence on Δx is lost.

4. Model generation and polyhedral structure

In the previous section we have defined our piecewise linearization $\Delta F(\mathring{x}; \Delta x)$ and foreshadowed its usefulness in terms of characterizing special points. In practical terms it is clear that we do not obtain derivative objects in the sense of a vectors and matrices or a collection thereof, but rather algorithms for evaluating a piecewise linear function. As we have noted before the Bouligand derivative $F'(\mathring{x}; \Delta x)$ already has essentially the same structure, except that it is homogeneous. At least in a conceptual sense the piecewise linearization can be simplified a little in the following way.

4.1 *Reduced representation*

Even though that may not be always the most efficient approach in terms of overall linear algebra operations, we can preaccumulate all smooth partials $\mathring{c}_{ij}$ at the current argument $\mathring{x}$ such that the evaluation of $\Delta F(\mathring{x}; \Delta x)$ can be performed on a *reduced computational graph* with exactly $n + 2s + m$ vertices.

More precisely, after renumbering the intermediate variables and modifying the precedence relation $\prec$ accordingly the piecewise linearized procedure takes the form

$$\begin{aligned}
\Delta v_{i-n} &= \Delta x_i \quad \text{for } i = 1 \cdots n,\\
\Delta u_i &= \sum_{j \prec i} \mathring{c}_{ij} \Delta v_j,\\
\sigma_i &= \textbf{sign}(\mathring{u}_i + \Delta u_i) \quad \text{for } i = 1 \cdots s,\\
\Delta v_i &= \sigma_i \cdot (\mathring{u}_i + \Delta u_i) - \mathring{v}_i,\\
\Delta y_{i-s} &= \sum_{j \prec i} \mathring{c}_{ij} \Delta v_j \quad \text{for } i = s+1 \cdots s+m.
\end{aligned} \tag{11}$$

Here and throughout we omit the argument $\mathring{x}$, whenever we consider it as constant. The signature vector $\sigma = \sigma(\Delta x) \in \{-1, 0, 1\}^s$ characterizes the control flow. The above procedure can be visualized as a computational graph of the special structure shown in Figure 5.

As we see below, our domain is successively cut into finer and finer polyhedral pieces as we pass the s absolute value functions, which we may think of as sign-switches. In the end

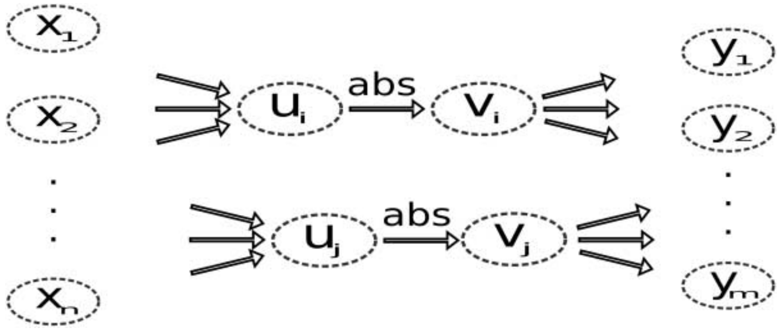

Figure 5. Reduced computational graph in piecewise differentiable case.

each element

$$S_\sigma = \{\Delta x \in \mathbb{R}^n : \sigma(\Delta x) = \sigma\}$$

of this polyhedral decomposition is uniquely defined by the signature vector with the components $\sigma_i \equiv \sigma_i(\Delta x) = \mathbf{sign}(u_i + \Delta u_i) \in \{-1, 0, 1\}$. There are 3^s distinct signature vectors, but we hope that most of the corresponding exponentially many facets are in fact empty. We will call signatures *critical* if they contain zeros, $\sigma_i = 0$, for some i, and otherwise call *definite*. Correspondingly, we call all points Δx at which no switches are critical *noncritical* and their closed complement the critical set.

4.2 *Structural properties*

The connection between the evaluation of the individual linear functions and their selection seems to distinguish our approach from previous treatments. Otherwise, our observations regarding piecewise linear functions and the polyhedral decomposition of their domain are in principal standard, but they get a much more constructive flavour in our context. Assuming still that there are s absolute value calls one obtains by induction on the intermediate quantities v_i the following results.

PROPOSITION 2 *Piecewise linear model*

(i) *At any* $\mathring{x} \in \mathcal{D}$ *the function* $\Delta F(\mathring{x}; \Delta x)$ *is defined for all* $\Delta x \in \mathbb{R}^n$.
(ii) $\mathbb{R}^n$ *is the disjoint union of relatively open convex polyhedra* S_σ *for* $\sigma \in \{-1, 0, 1\}^s$.
(iii) *On the closures* $\bar{S}_\sigma$, *the function* $\Delta F(\mathring{x}; \Delta x)$ *is linear with Jacobians* $J_\sigma \in \mathbb{R}^{m\times n}$.
(iv) *If the common facet* $\bar{S}_\sigma \cap \bar{S}_{\tilde{\sigma}}$ *has the maximal dimension* $n - 1$ *then* $J_\sigma - J_{\tilde{\sigma}} = 2ba^\top$, *where* *a is some nonzero normal of the facet and* $b \in \mathbb{R}^n$.

Proof The first assertion (i) follows from the fact that the recurrences (1)–(3) and also (4) can be executed for arbitrary inputs Δx. Moreover, we note immediately that $\Delta F(\mathring{x}; \Delta x)$ as a composition of globally Lipschitz piecewise linear functions has the same property.

To prove the second assertion (ii) let us consider two points $\Delta\check{x}$ and $\Delta\hat{x} \in S_\sigma$ for some common σ. Then it follows immediately by induction on i that for any convex combination

$$\Delta x = (1 - t)\Delta\check{x} + t\Delta\hat{x}$$

with $0 \le t \le 1$ we have for the same t also

$$\Delta v_i = (1 - t)\Delta\check{v}_i + t\Delta\hat{v}_i$$

for $i = 1 \cdots l$ and in particular

$$\mathbf{sign}(v_j + \Delta\check{v}_j) = \mathbf{sign}(v_j + \Delta v_j) = \mathbf{sign}(v_j + \Delta\hat{v}_j).$$

Here the $\Delta\check{v}_i$ and $\Delta\hat{v}_j$ are the increment values attained at $\Delta\check{x}$ and $\Delta\hat{x}$, respectively. Hence the signature vector is the same and we have $\Delta x \in S_\sigma$. Thus, we have shown that the S_σ are convex and that $\Delta F(\mathring{x}; \Delta x)$ is linear on them. Its linearity on the closure (iii) then follows immediately from its Lipschitz continuity. The final assertion (iv) follows from the fact that the Jacobians must agree in directions that are parallel to the common facets. ■

The last assertion means that on crossing from one polyhedron to another one can do a cheap update of the Jacobian since the vectors $b \in \mathbb{R}^m$ and $a \in \mathbb{R}^n$ can be computed at an effort similar to that of evaluating F itself in the forward and reverse mode of algorithmic differentiation, respectively. We will obtain algebraic expressions for them in Section 6. We will call the Jacobians J_σ that apply on polyhedral subdomains S_σ with nonempty interior *proper Jacobians* of the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$.

4.3 *Model generation using ADOL-C*

ADOL-C like other AD tools [20] can evaluate the directional derivatives $F'(\mathring{x}; \Delta x)$. In fact for fixed x the ADOL-C routine *first-order-forward* represents exactly the Bouligand mapping from Δx to $\Delta y = F'(\mathring{x}; \Delta x)$. However, this functionality is not widely understood and suffers from the predicament that it differs from Fréchet differentiation only at rather special arguments $\mathring{x}$. Moreover, near these values we have discontinuity and thus strong volatility with respect to perturbations in $\mathring{x}$. Finally, the piecewise linear structure of $F'(\mathring{x}; \Delta x)$ is of course currently not accessible or exploitable via ADOL-C. We show here how $\Delta F(\mathring{x}; \Delta x)$ can be precomputed at a given x and then can be used by separate routines for optimization, equation solving, etc.

The s vector u_i and the $(s + m) \times (n + s)$ sparse matrix $C = (c_{ij}) \in \mathbb{R}^{(s+m)\times(n+s)}$ represent the piecewise linearization at the current base point x. These data may be generated by ADOL-C as follows. Using a macro we may redefine **fabs**(u) globally to **swabs**(u) and define this new function for adoubles and doubles as arguments

```
adouble swabs(adouble u)
  {static double udum;
   u >>= udum;
   v <<= fabs(udum);
   return v; }

double swabs(double u)
  {return fabs(u);}
```

In the adouble version we first mark the arguments of all absolute value evaluations, as new dependent variables with the corresponding $\gg=$ operator of ADOL-C. Similarly we mark all the results as new independents using $\ll=$. During the so-called *tracing* of the overall evaluation there will be $s \geq 0$ such pairs (u_i, v_i) of artificial dependents u_i and independents v_i. The key observation is that the mapping $\tilde{F}(x, v) \mapsto (y, u)$ is smooth so that its Jacobian can be evaluated using standard ADOL-C calls. Note that the values of the artificial independents v_i are internally computed on the fly during the tracing and can be recomputed from the artificial dependents u_i by just taking their absolute values afterwards. They are needed for subsequent calls to **jacobian**, **gradient** and other utilities for computing derivatives, sparsity patterns, etc.

The constants in the reduced piecewise linearization can be obtained as $c_{i,j} \equiv \tilde{J}_{i,j-n}$, where

$$\tilde{F}'(x, v) \equiv \tilde{J} = (\tilde{J}_{i,j})_{j=0\cdots n+s}^{i=0\cdots s+m} \equiv \begin{bmatrix} U & L \\ J & V \end{bmatrix} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial v} \\ \frac{\partial y}{\partial x} & \frac{\partial y}{\partial v} \end{bmatrix}. \tag{12}$$

The blocks have the formats $U \in \mathbb{R}^{s\times n}, J \in \mathbb{R}^{m\times n}, V \in \mathbb{R}^{m\times s}$ and $L \in \mathbb{R}^{s\times s}$ with the latter being strictly lower triangular. When none of the nonsmooth elementals depends on another one the matrix L vanishes completely.

In terms of these matrices we can rewrite the procedure (11) as

$$\begin{bmatrix} \Delta u \\ \Delta y \end{bmatrix} = \begin{bmatrix} U\Delta x + L(|\mathring{u} + \Delta u| - |\mathring{u}|) \\ J\Delta x + V(|\mathring{u} + \Delta u| - |\mathring{u}|) \end{bmatrix} = \begin{bmatrix} U & L \\ J & V \end{bmatrix} \begin{bmatrix} \Delta x \\ |\mathring{u} + \Delta u| - |\mathring{u}| \end{bmatrix}.$$

The truly dependent values $\mathring{y}$ do not directly enter into the incremental piecewise linearization but will most likely play a role in whatever calculation one wishes to perform on the model. That will usually involve a sequence of *current points* x starting from the *base point* $\mathring{x}$ at which the piecewise linearization was generated. For that purpose the vector triplet $(\mathring{x}, \mathring{u}, \mathring{y})$ can be updated for any step $\Delta x \in \mathbb{R}^n$ to

$$\mathring{x} += \Delta x; \quad \mathring{u} += \Delta u; \quad \mathring{y} += \Delta y, \tag{13}$$

where Δu and Δy are calculated as above. The extended Jacobian $\tilde{J}$ remains completely unchanged.

5. Applications of piecewise linearization

Here we sketch straightforward generalizations of steepest descent for unconstrained optimization, the midpoint rule for numerical integration and Newton's method for equation solving. We present their theoretical properties, but we do not discuss the algorithmic details of solving the corresponding piecewise linear model problems. As we noted in Section 1, the complexity of this task is an important consideration in judging a particular differentiation concept. For example in the context of optimization we arrive at disjunctive quadratic programming problems, which are certainly NP hard in their global versions. This can be seen quite easily by reduction from SAT3 (Satisfiability 3). We conjecture that the task of just finding a local minimum, the inner loop of the following algorithm, is already NP hard.

5.1 *Optimization with quadratic overestimation*

Suppose with x_0 the starting point, our objective function $f : \mathbb{R}^n \mapsto \mathbb{R}$ has a bounded level set $\mathcal{N}_0 \equiv \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$ and satisfies the assumptions of Section 2 on an open neighbourhood $\tilde{\mathcal{N}}_0$ of $\mathcal{N}_0$. Then there exists a monotonic mapping $\bar{q}(\delta)$ of $[0, \infty)$ into itself such that for all $x \in \mathcal{N}_0$ and $\Delta x \in \mathbb{R}^n$

$$\hat{q}(x, \Delta x) \equiv \frac{|f(x + \Delta x) - f(x) - \Delta f(x; \Delta x)|}{\|\Delta x\|^2} \leq \bar{q}(\|\Delta x\|).$$

Here the scalar $\bar{q}(\rho)$ denotes essentially the constant on the RHS of Proposition 1 in $\tilde{\mathcal{N}}_0$. Since the base points x are restricted to $\mathcal{N}_0$, those steps Δx for which the line segment $[x, x + \Delta x]$ is not fully contained in $\tilde{\mathcal{N}}_0$ must have a certain minimal size. Then the denominators in the expressions above are bounded away from zero so that $\bar{q}(\|\Delta x\|)$ does indeed exist.

Of course $\bar{q}$ will generally not be known. Hence we approximate it by an estimate q, which we will refer to as the *quadratic coefficient*. Now suppose we generate sequences of iterates $x \in \mathcal{N}_0$, potential steps $\Delta x \in \mathbb{R}^n$ and consistently update the quadratic coefficient starting from some $q = q_0 > 0$ according to

$$q_+ = \max(q, \hat{q}(x, \Delta x)).$$

Then we must obviously have monotonic convergence of the bounds q to some limit $q_* \in (0, \infty]$.

Throughout this section, most mathematical symbols represent an infinite sequence of values generated by our iterative optimization algorithm. As in the recursion for q above, successors will be denoted by subscript $+$ of scalars, vectors and matrices alike. Initial values will be labelled by subscript $_0$ and limits or cluster points by the subscript $*$, as we have already done for q. Our first goal is to show that the values q and all tentative steps Δx are uniformly bounded so that in particular $q_* < \infty$.

By minimizing the supposed upper bound $\Delta f(x; \Delta x) + q\|\Delta x\|^2$ on $f(x + \Delta x) - f(x)$ at least locally we always obtain a step

$$\Delta x \equiv \underset{\tilde{s}}{\mathbf{argmin}}(\Delta f(x; \tilde{s}) + q\|\tilde{s}\|^2).$$

A globally minimizing step Δx must exist since $\Delta f(x; \tilde{s})$ can only decrease linearly so that the positive quadratic term always dominates for large $\|\tilde{s}\|$.

Moreover, Δx vanishes only at first order minimal points x where $\Delta f(x; \tilde{s})$ and $f'(x; \tilde{s})$ have the local minimizer $\tilde{s} = 0$. Of course this is extremely unlikely to happen and for the sake of consistency we will then consider a sequence of trivial steps $\Delta x = \Delta\mathring{x} = 0$ and thus a stationary iterates $x = \mathring{x}$ to be generated.

Generally, we simply accept any kind of function value reduction and therefore set

$$x_+ = x + \Delta x \quad \text{if } f(x + \Delta x) < f(x) \quad \text{and} \quad x_+ = x \ \text{ otherwise}.$$

Whenever the step is unsuccessful so that $x_+ = x$ the new q_+ must be bigger than the current value q. This extremely simple scheme involves no method parameters and has the following convergence property.

PROPOSITION 3 Optimization by piecewise linearization with overestimation *Under the general assumptions of this section, all cluster points $\mathring{x}$ of the infinite sequence x generated by the scheme above satisfy the first order minimality condition $f'(\mathring{x}; \cdot) \geq 0$ for composite piecewise differentiable problems.*

Proof It follows from $q \geq q_0 > 0$ and Proposition 1 by continuity of all quantities on the compact set $\mathcal{N}_0$ that the step size $\delta \equiv \|\Delta x\|$ must be uniformly bounded by some $\bar{\delta}$. This means that the $\hat{q}$ are uniformly bounded by $\bar{q} \equiv \bar{q}(\bar{\delta})$. Consequently, the function

$$\psi(x) \equiv \min_{\tilde{s}}(\Delta f(x; \tilde{s}) + \bar{q}\|\tilde{s}\|^2) \leq 0$$

is lower semi-continuous with respect to $x \in \mathcal{N}_0$. Unless x satisfies first order optimality condition the step Δx satisfies $\Delta f(x; \Delta x) + q\|\Delta x\|^2 \leq \psi(x) < 0$. Then we find after the evaluation of $f(x + \Delta x)$ that

$$f(x + \Delta x) - f(x) = \Delta f(x; \Delta x) + \hat{q}(x, \Delta x)\|\Delta x\|^2 \leq \psi(x) + [\hat{q}(x, \Delta x) - q]\|\Delta x\|^2.$$

Now suppose the sequence x had no first order minimizers as cluster points. Then $\sup \psi(x)$ would be negative, the other term on the right tends to zero since $\hat{q} \to q_* \leftarrow q$ and thus the left hand side would have a negative supremum too. Obviously, within the bounded level set $\mathcal{N}_0$ infinitely many significant reductions are impossible so that the x must have a first order minimizer as cluster point. The same argument applies to any other subsequence which completes the proof. ■

Of course, this strikingly simple theoretical result is somewhat unsatisfactory from a practical point of view. In particular the monotonic growth in the quadratic coefficient q must lead to rather slow final convergence, except when there are at least n critical switches at the limiting first order minimizer, so that one may have in fact quadratic convergence. An efficient implementation of successive piecewise linearization must certainly allow the estimate q to be reduced when things are going well. Moreover, one may replace the Euclidean norm by an ellipsoidal one, ideally defined by a positive definite matrix approximating the curvature in an 'active' subspace. If a local minimizer happens to lie in a neighbourhood where f is differentiable the method should then reduce to a variant of the well-established BFGS method.

The result remains true if the Δx are defined and computed as local rather than global minima of the bounding functions $\Delta f(x, \Delta s) + q\|\Delta x\|^2$. That local minimization can certainly be performed by a finite number of reduction steps with some kind of active critical switch strategy. As a very special case one may wind up with the simplex algorithm for linear programming, which may of course take an exponential number of steps as in the case of the Klee Minty example. Nevertheless, some successive pivoting strategy is probably the best we can do since we may not assume any kind of convexity.

5.2 *Numerical integration of ODEs with Lipschitzian RHS*

A more challenging, but also promising, application is the numerical integration of a differential equation $\dot{x} = F(x)$ with $F : \mathbb{R}^n \mapsto \mathbb{R}^n$ being composite piecewise differentiable as discussed above. Such ODEs with Lipschitzian RHSs arise for example through the space discretization of PDEs using sign conditions, flux limiters and other nonsmooth elements. In the ODE community dealing with kinks, jumps and even impulse on the RHS is sometimes called *event handling*. Higher order convergence can only be preserved if these events can be specified by the user or computed exactly. In an attempt to avoid this effort we may use the following generalizations of standard methods for the smooth case. Simply replacing the RHS of the ODE by its piecewise linearization at the current point $\mathring{x}$ we obtain the local initial value problem

$$\dot{x} = F(\mathring{x}) + \Delta F(\mathring{x}; x - \mathring{x}) \quad \text{with} \;\; x(0) = \mathring{x}.$$

Its exact solution would require eigenvalue decompositions of the Jacobians J_σ occurring in our piecewise linearizations and some nontrivial calculations to determine when and where the solution trajectory crosses from one polyhedral subdomain S_σ into another. The local truncation error would certainly be of third order so that the global convergence order of this generalized Rosenbrock method would be 2.

Alternatively, with $h > 0$ the step size, $\check{x}$ the current point, $\hat{x}$ the next point to be computed and $\mathring{x} = (\check{x} + \hat{x})/2$ the corresponding one might apply the midpoint rule

$$\hat{x} - \check{x} = h \int_{-1/2}^{1/2} [F(\mathring{x}) + \Delta F(\mathring{x}; (\hat{x} - \check{x})t)] \, \mathrm{d}t. \tag{14}$$

If F and its evaluation procedure are smooth, the approximating model will be linear so that in fact

$$\Delta F(\mathring{x}; (\hat{x} - \check{x})t) = F'(\mathring{x})(\hat{x} - \check{x})t,$$

whose integral over $t \in [-\frac{1}{2}, \frac{1}{2}]$ will drop out so that the rule reduces to the familiar form $(\hat{x} - \check{x}) = hF(\mathring{x})$. Otherwise, we can use the piecewise linearity of $\Delta F(\mathring{x}; \Delta x)$ with respect to Δx and its internal representation to evaluate the integral for given $\check{x}$ and $\hat{x}$ exactly.

To analyse the general case, we assume that after a variable shift the initial point $\check{x}$ is the origin and setting $x \equiv \hat{x}$ we may rewrite (14) in the fixed point form

$$x = hG(x) \equiv h \int_{-1/2}^{1/2} \left[\mathring{F} + \Delta F\left(\frac{x}{2}; xt\right)\right] \mathrm{d}t$$
$$= hF\left(\frac{x}{2}\right) + h \int_{-1/2}^{1/2} \Delta F\left(\frac{x}{2}; xt\right) \mathrm{d}t.$$

PROPOSITION 4 *Suppose our assumptions are satisfied in an open neighbourhood $\mathcal{D}$ of the origin $\check{x} = 0$. Then there is a step size bound $\bar{h} > 0$ such that for all $h < \bar{h}$ the function $hG(x)$ maps some closed ball $B_\rho(0) \subset \mathcal{D}$ into itself and is contractive. Moreover, the unique fixed point $x_h \in B_\rho(0)$ satisfies*

$$x_h - x(h) = \mathcal{O}(h^3) \quad \textit{where } x(t) \textit{ solves } \dot{x}(t) = F(x(t)) \textit{ from } x(0) = 0.$$

Proof Since F is under our assumptions locally Lipschitz and since the piecewise linearization is Lipschitz continuous with respect to the base point, we have in some ball with radius ρ about the origin some $L > 0$

$$\|F(x)\| \leq \|F(0)\| + L\rho \quad \text{and} \quad \|\Delta F(0, x, tx)\| \leq \|\Delta F(0, 0, tx)\| + L\rho \quad \text{for } \|x\| \leq \rho.$$

Assuming that the constant L is also a Lipschitz constant of $\Delta F(x; \Delta x)$ with respect to Δx and selected larger than the $\tilde{\gamma}$ in Proposition 1 we obtain the Lipschitz constant

$$\begin{aligned}
\|G(\tilde{x}) - G(x)\| &\leq \|F(\tilde{x}/2) - F(x/2)\| + \int_{-1/2}^{1/2} \|\Delta F(\tilde{x}/2; \tilde{x}t) - \Delta F(x/2; xt)\| \,\mathrm{d}t \\
&\leq L\|\tilde{x} - x\|/2 + \int_{-1/2}^{1/2} \|\Delta F(\tilde{x}/2; \tilde{x}t) - \Delta F(x/2; \tilde{x}t)\| \,\mathrm{d}t \\
&\quad + \int_{-1/2}^{1/2} \|\Delta F(x/2; \tilde{x}t) - \Delta F(x/2; xt)\| \,\mathrm{d}t \\
&\leq \frac{L}{2}\|\tilde{x} - x\| \left[1 + \int_{-1/2}^{1/2} (1 + |t|\|\tilde{x}\|) \,\mathrm{d}t\right] + L\|\tilde{x} - x\| \int_{-1/2}^{1/2} |t| \,\mathrm{d}t \\
&\leq \tilde{L}\|\tilde{x} - x\| \equiv L\|\tilde{x} - x\|(5 + \rho)/4.
\end{aligned}$$

Hence we have obvious contraction if $h\tilde{L} < 1$ and since $G(0) = F(0)$ we can also ensure that $\|hG(x)\| \leq \|hF(0)\| + h\tilde{L}\|x\| < \rho$ for h sufficiently small. Then Banach's fixed point theorem yields a unique solution $x_h \in B_\rho(0)$. The exact solution trajectory $x(\tau)$ is by definition $C^{1,1}$. Hence, its deviation from the straight secant line $(t + 0.5)x(h)$ for $-0.5 \leq t \leq 0.5$ is bounded by

$$\|x((t + 0.5)h) - (t + 0.5)x(h)\| \leq \hat{\gamma}\left(\frac{1}{4} - t^2\right) h^2$$

for some constant $\hat{\gamma}$. Consequently, we have due to the Lipschitz continuity of F

$$\begin{aligned}
0 &= \left\| x(h) - h \int_{-1/2}^{1/2} F(x((t + 0.5)h)) \,\mathrm{d}t \right\| \\
&= \left\| x(h) - h \int_{-1/2}^{1/2} F((t + 0.5)x(h)) \,\mathrm{d}t \right\| - \mathcal{O}(h^3) = \|x(h) - hG(x(h))\| - \mathcal{O}(h^3),
\end{aligned}$$

where the last equality follows from the approximation property established in Proposition 1 of the piecewise linearization at $\mathring{x} = x/2$. Now since the mapping $x - hG(x)$ has locally a Lipschitz continuous inverse we can conclude that x_h as its preimage for the value 0 is only $\mathcal{O}(h^3)$ apart from $x(h)$ its preimage for a right hand perturbation of size $\mathcal{O}(h^3)$. ∎

Obviously, a sequence of such midpoint steps represents indeed a numerical integration method of global convergence order 2 as we claimed before. The steps can be computed by the Picard like fixed point iteration $x = hG(x)$ provided h is significantly smaller than the reciprocal of the Lipschitz constant L of the RHS. That is not very desirable in the stiff case, where L may be very large due to large negative or largely complex eigenvalues of the system Jacobian, where it does exist.

The advantage of the generalized midpoint method for piecewise smooth systems is that one can step through several kinks without loss of order and without identifying them for the RHS function itself. We only need to identify them along a straight line in the piecewise linearization during the evaluation of a trapezoidal quadrature rule. Naturally that is no significant computational expense. While certainly symmetric with respect to time, the nonsmooth version (14) of the midpoint rule seems unlikely to also inherit the highly desirable property of symplecticness for Hamiltonian dynamical systems [22].

Third, we may also construct a generalized trapezoidal rule

$$\hat{x} - \check{x} = h \int_{-1/2}^{1/2} [\mathring{F} + \Delta F(\check{x}, \hat{x}; (\hat{x} - \check{x})t)]\, \mathrm{d}t. \tag{15}$$

Under the integral we have the secant-based piecewise linearization $\mathring{F} + \Delta F(\check{x}, \hat{x}; \Delta x)$, to be described in Section 7. With $\mathring{F} = (\check{F} + \hat{F})/2$ it interpolates $F(x)$ at $\check{x}$ and $\hat{x}$.

When F and its evaluation procedure are smooth, the approximating model will be linear so that in fact

$$\Delta F(\check{x}, \hat{x}; (\hat{x} - \check{x})t) = [F(\hat{x}) - F(\check{x})]t,$$

and then the integration scheme reduces to the trapezoidal rule. Otherwise, we can again use the piecewise linearity of the secant-based approximation to evaluate the integral exactly. The corresponding fixed point formulation with $\check{x} = 0$ and $x = \hat{x}$ is

$$\begin{aligned} x = hG(x) &\equiv h \int_{-1/2}^{1/2} [\mathring{F} + \Delta F(0, x; tx)]\, \mathrm{d}t \\ &= \frac{h}{2}[F(0) + F(x)] + h \int_{-1/2}^{1/2} \Delta F(0, x; tx)\, \mathrm{d}t. \end{aligned}$$

By a slight adaption of the proof of the last proposition one can show that the generalized trapezoidal rule has also global order 2. The only significant difference in the argument is that we now have to use the bilinear approximation result in Proposition 10 of Section 7 rather than the second order result in Proposition 1.

Of course, both the midpoint and the trapezoidal rule are implicit, so that computing the new point $\hat{x}$ requires the solution of a nonsmooth system of algebraic equations. In the nonstiff case that can be done by a Picard-like iteration. Otherwise, one may have to bring in variants of the equation solver discussed in the following subsection to compute the steps from $\check{x}$ to $\hat{x}$ efficiently.

5.3 *Nonsmooth equation solving by piecewise linearization*

We consider the square case of $m = n$ equations $F(x) = 0$ in as many unknowns. When F is semismooth [23] in some neighbourhood of some root $\mathring{x} \in F^{-1}(0)$ and some regularity condition on generalized Jacobians is satisfied, then the generalized Newton's method converges locally and superlinearly. However, the radius of contraction is well known to be rather small. Geometrically, the radius is bounded by the distance to the next Jacobian discontinuity to which $\mathring{x}$ does not belong.

Consequently, unless F is differentiable at $\mathring{x}$, the convergence radii for the perturbed systems $F(x) = y \approx 0$ have the infimum zero with respect to y. This stems from the fact that the Newton step $-J^{-1}F(x)$ with $J \in \nabla^C F(x)$ takes absolutely no notice of nearby discontinuities in the generalized Jacobian. We will discuss in the next section how such J can be computed constructively, but that does not fix the basic difficulties with Newton's method in the nonsmooth case.

Instead, in the spirit of Ralphs path search proposal [5,33] we consider for fixed x the parametrized equation

$$\Delta F(x; \Delta x) = -tF(x) \quad \text{for } t \in (0, 1].$$

When it can be solved for $t = 1$ we have a full Newton-like step and can expect local quadratic convergence. The equation can be solved for arbitrary but fixed residual $F(x)$ on the RHS and sufficiently small t if and only if the piecewise linear approximation $\Delta F(x; \Delta x)$ is open with respect to Δx at $\Delta x = 0$. Now we can draw on the following characterizations from [36].

Proposition 5 *Coherent orientation, openness and surjectivity*

(i) *The piecewise linear model $\Delta F(\mathring{x}; \Delta x)$ is open at $\Delta x \in \mathbb{R}^n$ if and only if all Jacobians J_σ for which $\Delta x \in S_\sigma$ and $\dim(S_\sigma) = n$ have the same nonzero sign.*
(ii) *(Global) injectivity of $\Delta F(\mathring{x}; \Delta x)$ implies coherent orientation in the sense of (i) at all Δx, which in turn implies (global) surjectivity of $\Delta F(\mathring{x}; \Delta x)$.*
(iii) *If $\Delta F(\mathring{x}; \Delta x)$ and equivalently $F'(\mathring{x}; \Delta x)$ are open at $\Delta x = 0$ then there exists some constant γ such that $\Delta F(\mathring{x}; \Delta x) = c$ implies $\|\Delta x\| \le \gamma(\|c\|)$.*

The last property is called metric regularity. The natural question whether or not $\Delta F(\mathring{x}; \Delta x)$ has coherent orientation in that (i) holds is not that easy to answer. Moreover, we have already seen in example (10) that coherent orientation of the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$ is not a stable property. Rather, it may be satisfied at a point $\mathring{x}$ but violated at points x arbitrary close.

Moreover, since in that example $\Delta F(0; \Delta x)$ is in fact linear and nonsingular it follows immediately that the stronger property of the piecewise linearization being a homeomorphism is not stable with respect to perturbation of the base point. Nevertheless, according to Theorem 3.2.3 in [34] coherent orientation of $F'(\mathring{x}; \Delta x)$ implies that the underlying $F(x)$ is open at $\mathring{x}$, which means that $F(x) = y$ has solutions near $\mathring{x}$ for all $y \approx \mathring{y} = F(\mathring{x})$.

However, we do not as yet have a straight forward and realistic regularity condition on $\Delta F(\mathring{x}; \Delta x)$ at and near a root $x_* \in F^{-1}(0)$ that would allow us to conclude that some of these preimages can be safely calculated by piecewise linearization as suggested here. Ralph has proved convergence of his closely related path search method in [33]. He had to assume uniform Lipschitz invertibility of the approximations, which we denote here by $\Delta F(\mathring{x}; \Delta x)$. While he could establish that this assumption holds for certain classes of problems including KKT conditions and other nonlinear complementarity problems, one would wish that a more general solution strategy could be guaranteed to converge at least locally from within neighbourhoods of in some sense regular roots. Nevertheless, let us analyse the solvability of the local model problem in a little detail.

For fixed $\mathring{x}$ and abbreviating $z \equiv \Delta x$ we will consider in the remainder of this section the piecewise linear function

$$G(z) \equiv F(\mathring{x}) + \Delta F(\mathring{x}; z),$$

whose roots are exactly the Newton-like steps. Also note that G being just a shifted version of $\Delta F(\mathring{x}; \Delta x)$ has the same polyhedral subdivision S_σ and the same Jacobians J_σ discussed in

Proposition 2. To solve it we consider a homotopy approach, which is described in a more general setting by Allgower and Georg [1].

We can derive from Scholtes an interesting result concerning the equivalence classes

$$[z] \equiv \{\tilde{z} \in \mathbb{R}^n : G(\tilde{z}) = \lambda G(z), 0 < \lambda \in \mathbb{R}\},$$

which are inverse images of the rays generated by any particular residual value $G(z)$ in $\mathbb{R}^n$. If there exists at least one root $z_* \in G^{-1}(0)$ the class $[z_*] = G^{-1}(0)$ plays a special role. It is always closed and the same is true for its union with any other class $[z] \neq [z_*]$. We will call $[z] \neq [z_*]$ regular if G is a homeomorphism at all its elements. Otherwise, we call $[z]$ *critical* and all its elements *critically connected*.

Regular classes are continuous manifolds of dimension 1, which consist in the coherently oriented case of a fixed number p of connected components [36]. In contrast, critical classes may contain bifurcations and endpoints, but their number of connected components is also bounded by the same p. Due to the piecewise linearity of $G(z)$ the closure of any regular class $[z] = G^{-1}\{\lambda G(z), \lambda > 0\}$ must contain all roots in $[z_*]$. One of them can be reached from any of its elements by successively reducing the multiplier λ from 1 towards 0. We will call this method piecewise Newton (apparently already suggested by Robinson). See also the damped Newton method of Peng for complementarity problems. Critical classes are exceptional and cannot contain full polynomials.

PROPOSITION 6 Polynomial escape *Assume $G(z)$ is coherently oriented in that all its Jacobians have the same nonzero sign. Consider the set of critically connected points C, which is exactly the union of all critical classes $[z]$. Then C is closed and contained in a union of finitely many polyhedra of dimension less than n. Consequently, for any set of basis vectors $e_j \in \mathbb{R}^n$ and some suitable bound $\bar{\tau} > 0$ the polynomial arc*

$$z(\tau) \equiv z_0 + \sum_{j=1}^{n} e_j \tau^j \quad \text{for} \ \tau \in (0, \bar{\tau})$$

is disjoint from C and thus contains no critically connected points.

Proof As observed by Scholtes $\Delta F(\Delta x)$ is a local homeomorphism at all points in the union R of the relatively open polyhedra S_σ of dimension n and $n-1$. Consequently, the complement $R^n \setminus R$ is a finite union of the remaining polyhedra S_σ, which have dimensions less than $n-1$ and its closure V is contained in the union of all closed polyhedra S_σ of dimension $n-2$. By continuity and piecewise linearity its range $F(V)$ is also a union of closed polyhedra of dimension $n-2$. Consequently, the cone $K \equiv \{\lambda r : r \in F(V); 0 < \lambda \in R\}$ is contained in the finite union of polyhedra of dimension $n-1$ and the same must be true for the inverse image $F^{-1}(K)$. Since clearly $C \subset F^{-1}(K)$ we have thus proven the first assertion. By assumption of linear independence of the e_j the arc $x(t)_{0<t<\bar{t}}$ spans for any $\bar{t}$ the whole of $\mathbb{R}^n$ and can therefore not be contained in any one of the $(n-1)$ dimensional polyhedra covering C. Hence it lies outside C for a sufficiently small positive $\bar{t}$. ■

The proof actually establishes the same property for the union of C with all classes $[z]$ containing any points in polyhedra S_σ of dimension less than $n-1$. We are then left with starting points $z_0 \in \mathbb{R}^n \setminus C$ for solving $G(z) = 0$ for which $[z_0]$ contains only a finite number of points in polyhedra of dimension $n-1$ and none of the dimension below that. Then we may simply follow the piecewise linear paths in $[z_0]$ that starts at z_0 and moves through the polyhedral subdivision $\{S_\sigma\}$ until a root is reached. To see that such $[z_0]$ cannot get trapped in a hypersurface we note the following consequence of Proposition 2.

LEMMA 1 Coherent orientation ensures transversal of interfaces *Suppose the Newton direction* $\Delta z_- \equiv -J_-^{-1}G(z_-)$ *computed at some point* z_- *in the interior of a full dimensional polyhedron* S_- *reaches a point* $z_+ = z_- + \tau\Delta z_-$ *with* $\tau < 1$ *at the boundary to a neighbouring polyhedron with the normal* $a \in \mathbb{R}^n$. *Then the new Newton direction* $\Delta z_+ \equiv -J_+^{-1}G(z_+)$ *satisfies in relation to the old* Δz_-

$$[(a^\top \Delta z_+)\det(J_+)][(a^\top \Delta z_-)\det(J_-)] \geq 0.$$

Here J_- *and* J_+ *are of course the Jacobians of* G *valid in* S_- *and* S_+.

Proof If either determinant is zero the assertion holds trivially. Otherwise, it follows from Proposition 2 and the Sherman–Morrison–Woodbury formula that

$$\det(J_+) = \det(J_-)(1 + 2a^\top J_-^{-1}b) \quad \text{and} \quad J_+^{-1} = J_-^{-1}\left[\frac{I - 2ba^\top J_-^{-1}}{1 + 2a^\top J_-^{-1}b}\right].$$

Multiplying the second equation from the left by $a^\top$ and the right by $G(z_+)$ we obtain

$$a^\top J_+^{-1}G(z_+) = a^\top J_-^{-1}G(z_+) - \frac{2a^\top J_-^{-1}ba^\top J_-^{-1}G(z_+)}{1 + 2a^\top J_-^{-1}b}$$
$$= \frac{a^\top J_-^{-1}G(z_+)}{1 + 2a^\top J_-^{-1}b} = \frac{a^\top J_-^{-1}G(z_+)\det(J_-)}{\det(J_+)}.$$

Here the second equality is obtained by bringing the two terms over the common denominator. $\mathring{v}_i = v_i(\mathring{x})$ implies the result since $G(z_+) = (1 - \tau)G(z_-)$ with $\tau < 1$. ■

In other words, as long as we have coherent orientation, successive Newton directions and thus the regular classes $[z]$ will penetrate joint interfaces rather than being turned back or staying within lower dimensional polyhedra. However, if one starts from within the extended excluded set C effects like cycling in linear programming may occur. Rather than discussing possible remedies, we finish this section by giving an example where piecewise Newton works perfectly.

The underlying function $G : \mathbb{R}^2 \mapsto \mathbb{R}^2$ depicted in Figure 6 is itself piecewise linear and homogeneous. On the left we see the unit circle in the domain space of G, and on the right the unit

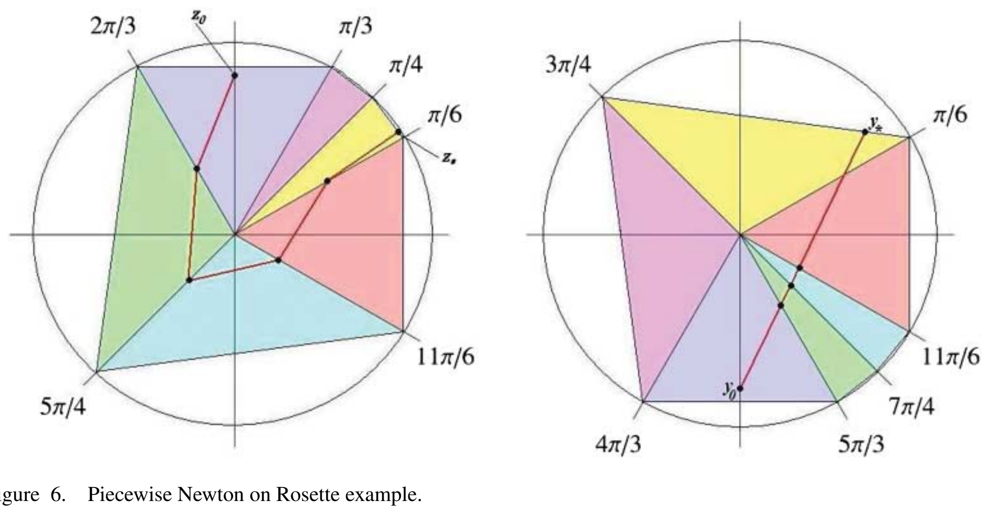

Figure 6. Piecewise Newton on Rosette example.

circle in its range. The pairs of equally coloured triangles represent preimages and images. They are mapped into each other linearly with positive determinant, which completely determines F as a global homeomorphism from $\mathbb{R}^2$ onto itself.

Now suppose we pick the starting point z_0 in the purple triangle of the domain and the RHS vector y_* at the boundary of the yellow triangle of the range. With respect to the residual $G(z) - y_*$ the class $[z_0]$ is the piecewise linear path on the left connecting z_0 to the inverse image $z_* = G^{-1}(y_*)$. The corresponding residuals form a straight line connecting $y_0 = G(z_0)$ to $y_* = G(z_*)$ in the range. Extending all open triangles to cones and their separating lines to rays we obtain the decomposition of the domain of F into six polyhedra of dimension 2, the cones; six polyhedra of dimension 1, the rays; and the origin $\{0\}$ as the only polyhedron of dimension $0 < n - 1 = 1$.

6. Jacobians

Another use of piecewise linearization is generalized differentiation in the sense of computing Jacobian matrices of some sort. In Section 2, we have already discussed the purposes and desirable properties of derivative concepts from a more philosophical point of view. At first we will ignore our key recommendation that methods for producing such generalized derivatives should kick in generically, i.e. not just return the standard Fréchet derivative at almost all arguments. We will use the following terminology and notation:

Jacobians:	$\nabla_x F(\mathring{x}) \equiv \partial F(x)/\partial x\|_{x=\mathring{x}}$	$: \mathcal{D} \mapsto \mathbb{R}^{m\times n} \cup \emptyset$
Limiting Jacobians:	$\nabla_x^L F(\mathring{x}) \equiv \overline{\lim}_{x\to\mathring{x}} \nabla F(x)$	$: \mathcal{D} \rightrightarrows \mathbb{R}^{m\times n}$
Clarke Jacobians:	$\nabla_x^C F(\mathring{x}) \equiv \mathbf{c}onv(\nabla^L F(\mathring{x}))$	$: \mathcal{D} \rightrightarrows \mathbb{R}^{m\times n}$
Conical Jacobians:	$\nabla_x^K F(\mathring{x}) \equiv \nabla_z^L F'(\mathring{x}; z)\|_{z=0}$	$: \mathcal{D} \rightrightarrows \mathbb{R}^{m\times n}$

Here $\overline{\lim}$ denotes the outer limit and $\rightrightarrows$ a multi-function. Hence both $\nabla_x^L F(\mathring{x})$ and $\nabla_x^C F(\mathring{x})$ are by definition outer semicontinuous set-valued functions.

We use the corresponding singular terms limiting Jacobian, Clarke Jacobian and conical Jacobian to denote single elements of the sets $\nabla_x^L F(\mathring{x})$, $\nabla_x^C F(\mathring{x})$ and $\nabla_x^K F(\mathring{x})$, respectively. The limiting Jacobians are sometimes called Bouligand Jacobians, but we will continue to use this name for the directional derivative mapping first defined in (5).

The main goal of this sections is to compute conical Jacobians as limiting Jacobians of the Bouligand derivative $F'(\mathring{x}; \Delta x)$ at the origin $\Delta x = 0$ and to show that they are in fact limiting Jacobians of the underlying $F(x)$ at $x = \mathring{x}$. In other words, we establish constructively that

$$\emptyset \neq \nabla^K F(\mathring{x}) \subset \nabla^L F(\mathring{x}) \subset \nabla^C F(\mathring{x}),$$

where the last inclusion is of course well known. That both inclusions, may be proper, can be seen from example (10), where $\nabla^L F(0)$ contains two elements but $\nabla^K F(0)$ reduces to the Jacobian $\{\nabla F(0)\}$ as always when and where F is differentiable.

The computation of elements in $\nabla^K F(\mathring{x})$ is an important achievement, since hitherto there has been no generally applicable methodology for computing limiting or more generally Clarke Jacobians, due to the lack of proper chain rules.

Because of (7) the conical Jacobians at $\mathring{x}$ as defined above are exactly those matrices J_σ for which the corresponding domain S_σ of the piecewise linearization $\Delta F(\mathring{x}, \Delta x)$ is open in $\mathbb{R}^n$ and contains 0 in its closure. Sufficient but not necessary for S_σ to be open and thus of full dimension is that σ is definite, i.e. contains no zero components.

At any Δx in an open S_σ the procedure (11) is differentiable and yields thus with $\sigma = \sigma(\Delta x) \in \{-1, 0, -1\}^s$ the Jacobian $J_\sigma = (\nabla y_{i-s}^\top)_{i=1\cdots m}$ row-wise by

$$\begin{aligned} \nabla v_{i-n} &= e_i && \text{for } i = 1\cdots n, \\ \nabla u_i &= \textstyle\sum_{j\prec i} \mathring{c}_{ij} \nabla v_j && \text{for } i = 1\cdots s, \\ \nabla v_i &= \sigma_i \nabla u_i && \\ \nabla y_{i-s} &= \textstyle\sum_{j\prec i} \mathring{c}_{ij} \nabla v_j && \text{for } i = s+1\cdots s+m. \end{aligned} \tag{16}$$

Here the e_i represents for the time being the Cartesian basis vectors.
Moreover, if the closure of S_σ contains zero we get for all small Δx the linear relation

$$\Delta u_i(\Delta x) = \nabla u_i^\top \Delta x \quad \text{for } i = 1\cdots s,$$

which we will use frequently below.

6.1 *Explicit representation as Schur complements*

Now let us express the Jacobians J_σ by block elimination on the AD-generated extended Jacobian (12). For any set of directions $\dot{x}, \dot{v}, \dot{u}, \dot{y}$ that are feasible in that they maintain the linearization of $\tilde{F}$ we must have the compatibility conditions

$$\dot{u} = U\dot{x} + L\dot{v} \quad \text{and} \quad \dot{y} = J\dot{x} + V\dot{v}.$$

With $\dot{v} = \Sigma\dot{u}$ for $\Sigma = \mathbf{diag}(\sigma)$ a signature matrix, we obtain by eliminating $\dot{v}$

$$\dot{u} = (I - L\Sigma)^{-1}U\dot{x} \quad \text{and} \quad \dot{y} = J_\sigma \dot{x},$$

where J_σ is the selection Jacobian

$$J_\sigma \equiv J + V\Sigma(I - L\Sigma)^{-1}U. \tag{17}$$

Note that due to the strict lower singularity of L the inverse $(I - L\Sigma)^{-1}$ always exists and is even polynomial in the entries of $L\Sigma$.

The row vector $e_i^\top (I - L\Sigma)^{-1}U$ can be interpreted as the gradient $\partial u_i/\partial x$ of the (i)th absolute value argument u_i with respect to x. Combining them in a matrix we obtain the relation

$$\frac{\partial u}{\partial x} = (I - L\Sigma)^{-1}U \in \mathbb{R}^{s\times n} \quad \text{when } v \equiv \Sigma u.$$

Similarly, we can compute the tangent $\partial y/\partial v_i$ of the dependent vector y with respect to the (i)th absolute value v_i as follows. Let us set that $\sigma_i = 0$ but $\dot{v}_i = 1$ and again $\dot{v}_j = \sigma_j \dot{u}_j$ for $j \neq i$. Then we have $\dot{v} = e_i + \Sigma\dot{u}$ and thus obtain for $\dot{x} = 0$ the tangents

$$\dot{u} = (I - L\Sigma)^{-1}Le_i \quad \text{and} \quad \dot{y} = V[I + \Sigma(I - L\Sigma)^{-1}L]e_i.$$

Again we can combine that to the matrix equation

$$\frac{\partial y}{\partial v} = V[I + \Sigma(I - L\Sigma)^{-1}L] \in \mathbb{R}^{m\times s}.$$

It is interesting to note what happens when the ith entry of σ is zero and changes to ± 1 so that we obtain the definite signature vector $\sigma_\pm = \sigma \pm e_i$. Then it follows that

$$J_\pm = J + V(\Sigma \pm e_i e_i^\top)(I - L\Sigma \mp l_i e_i^\top)^{-1}U,$$

where $l_i = Le_i$. After some more elementary calculations we find that

$$J_\pm - J_\sigma = \pm V[I + \Sigma(I - L\Sigma)^{-1}L]e_i e_i^\top (I - L\Sigma)^{-1}U = \pm \frac{\partial y}{\partial v_i}\frac{\partial u_i}{\partial x}.$$

This implies obviously

$$J_+ - J_- = 2V[I + \Sigma(I - L\Sigma)^{-1}L]e_i e_i^\top (I - L\Sigma)^{-1}U = 2\frac{\partial y}{\partial v_i}\frac{\partial u_i}{\partial x}.$$

Hence we have an explicit representation of the rank one change established in Proposition 2. As we noted before the tangent $\partial y/\partial v_i$ and the gradient $\partial u_i/\partial x$ can be computed cheaply in the forward and reverse mode of algorithmic differentiation, respectively.

6.2 *Forward mode with lexicographic branching*

For arbitrary $\sigma \in \{-1, 0, 1\}^s$ we may interpret the J_σ computed in (16) and expressed explicitly in (17) as the Jacobian of $F'_\sigma(\mathring{x})$ of the function $y = F_\sigma(x)$ defined by

$$\begin{array}{rll} v_{i-n} = x_i & \text{for } i = 1 \cdots n, & \\ u_i = \psi_i(v_j)_{j \prec i} & \multirow{2}{*}{for } i = 1 \cdots s, & \\ v_i = \sigma_i u_i & & \\ y_{i-s} = v_i & \text{for } i = s+1 \cdots s+m, & \end{array} \tag{18}$$

where the ψ_i for $i = 1 \cdots s$ are the compositions of the smooth elementary functions that lead up to the arguments u_i of the s switches.

By a suitable reduction of the domain $x \in \mathcal{D}$ we can make sure that all F_σ are well defined and Lipschitz-continuously differentiable on $x \in \mathcal{D}$. For theoretical investigations in the vicinity in the neighbourhood of a particular point $\mathring{x}$ we can furthermore assume that all arguments $u_i(\mathring{x})$ are zero so that $\sigma(0) = 0$, since all nonvanishing absolute values can be subsumed locally into the smooth parts. Hence, we have in any case for $x \in \mathcal{D}$ the piecewise differentiability property

$$F(x) \in \{F_\sigma(x) : \sigma \in \{-1, 0, 1\}^s\} \quad \text{with } F_\sigma \in \mathcal{C}^{1,1}(\mathcal{D}).$$

It is well known [34] that the limiting Jacobians $\partial^L F(\mathring{x})$ are contained in the union of the Jacobians $J_\sigma(\mathring{x})$ with $\sigma \in \{-1, 0, 1\}^s$. Fortunately, most of these 3^s matrices are quite likely not contained in $\nabla^L F(\mathring{x})$ and therefore need not be touched in practical calculations if that can be avoided. Scholtes has shown that one needs only to consider those J_σ for which F_σ is *essentially active* at $\mathring{x}$ in that it coincides with F on a set whose interior has $\mathring{x}$ as a cluster point. On the scalar example (8) this includes near the origin the function $y^2 - x$ on the slither $y^2 > x > 0$ whose gradient $(-1, 2y)$ is not part of the piecewise linearization $f'(0; \Delta x) \equiv 0$. We will restrict ourselves to an even smaller subset namely, the *conically active* selection functions and their Jacobians. To establish the key relationship (6) we first disregard indefinite signatures.

PROPOSITION 7 *If the origin* 0 *belongs to the closure of* S_σ *and* σ *is definite in that it contains no zeros, then there is an open subset* $\tilde{S}_\sigma \subset S_\sigma$ *with the same tangent cone as* S_σ *at* 0 *such that*

$$F(x) = F_\sigma(x) \quad \text{for } x \in \mathring{x} + \tilde{S}_\sigma,$$

and the J_σ *computed according to* (16) *belongs to* $\nabla^L \Delta F(\mathring{x}; 0) \cap \nabla^L F(\mathring{x})$.

Proof Let us consider F in the reduced representation (18). As in the proof of Proposition 1 we note that for any $\Delta x \in S_\sigma$, each i, and arbitrary $t \in \mathbb{R}$

$$u_i(x + t\Delta x) = u_i + \Delta u_i(t\Delta x) + \mathcal{O}(t^2\|\Delta x\|^2) = u_i + t\nabla u_i^\top \Delta x + \mathcal{O}(t^2\|\Delta x\|^2),$$

where both order terms are uniform in $\|\Delta x\|$. Hence, definiteness ensures that for all small $t > 0$ the sign of $u_i(x + t\Delta x)$ agrees with that of $u_i + \Delta u_i(t\Delta x)$ and also that of $u_i + t\nabla u_i^\top \Delta x$, namely $\sigma_i \neq 0$. This means that $F(\mathring{x} + t\Delta x) = F_\sigma(\mathring{x} + t\Delta x)$ for $\mathring{x} + t\Delta x$ in an open neighbourhood $\tilde{S}_\sigma$, which intersects all rays $\mathring{x} + t\Delta x$ and whose closure contains $\mathring{x}$. Obviously, J_σ is a Bouligand derivative of both the underlying function and its piecewise linearization. ■

Normally, one does not know a priori to which S_σ a given *increment* $\Delta x \in \mathbb{R}^n$ belongs. Then the natural approach to computing a limiting Jacobian is to apply (16) with the signatures

$$\sigma_i = \textbf{firstsign}(u_i, \nabla u_i^\top \Delta x) = \textbf{sign}(u_i + \Delta u_i(t\Delta x)) \quad \text{for } 0 < t \approx 0.$$

Here and throughout, **firstsign**(z) of a vector z is defined as the **sign** of the first nonvanishing component of z if that exists; otherwise the value is set to zero. If one finds that all σ_i obtained are nonzero one can be sure that the resulting J_σ is indeed a Bouligand derivative of the underlying function and its linearization on the corresponding open S_σ. Theoretically, both u_i and the directional derivatives $\nabla u_i^\top \Delta x$ may vanish exactly for some i. That happens if and only if Δx belongs to a polyhedron S_σ that is critical in that the s-vector σ has a first zero component.

Unless the corresponding gradient ∇u_i vanishes altogether the set S_σ has an empty interior and one may try to remedy the situation by slightly perturbing Δx, of course making sure that previous sign decisions are unaffected. This is the strategy used by Khan and Barton [26] to compute conical Jacobians.

We pursue more systematic approach by setting $e_1 = \Delta x$ and then complementing it with $n - 1$ additional vectors e_i for $i = 2 \cdots n$, such that together they form a nonsingular basis matrix $E \in \mathbb{R}^{n\times n}$. With this initialization of the $\nabla v_{i-n} = e_i$ we may then apply the procedure (16) using the lexicographic signature rule

$$\sigma_i = \textbf{firstsign}(u_i, \nabla u_i).$$

Of course one may permute the components of ∇u_i that have not yet determined any one of the σ_j with $j < i$, for example by bringing the component with the largest modulus to the front. Any one such *permuted lexicographic* definitions of σ_i yields a conical Jacobian as shown below.

PROPOSITION 8 *Suppose we initialize* $(\nabla x_i^\top)_{i=1\cdots n} = E$ *with* $\det(E) \neq 0$ *and define* σ *lexicographically as described above. Then the recurrence* (16) *yields a matrix, say* $J_\sigma^E = (\nabla y_{i-s}^\top)_{i=1\cdots m}$, *whose backtransformation*

$$J_\sigma \equiv J_\sigma^E E^{-1} \in \nabla^L \Delta F(\mathring{x}; 0)$$

is a limiting Jacobian of both $F'(\mathring{x}, \Delta x)$ *and* $\Delta F(\mathring{x}, \Delta x)$ *at the current argument* $\mathring{x}$.

Proof Let us consider the transformed vector function $\tilde{F}(\tilde{x}) \equiv F(E\tilde{x})$. Then we have a special case of the chain rule discussed in Section 3.5

$$\Delta\tilde{F}(\tilde{x}; \Delta\tilde{x}) = \Delta F(E\tilde{x}; E\Delta\tilde{x}) = \Delta F(x; \Delta x).$$

Consequently, for fixed $\tilde{x}$ and $x = E\tilde{x}$ a matrix J^E is a limiting Jacobian of $\Delta\tilde{F}(\tilde{x}; \Delta\tilde{x})$ at $\Delta\tilde{x} = 0$ if and only if $J^E E^{-1}$ is a limiting Jacobian of $\Delta F(x; \Delta x)$ at $\Delta x = 0$. Hence, we may assume without loss of generality that $E = I$ and σ is an unpermuted lexicographic ordering. Then define the polynomial path

$$\Delta x(t) = (t, t^2, t^3, \ldots, t^n) = \sum_{i=1}^{n} e_i t^i.$$

For each intermediate variable the resulting vector curve $\Delta u(t)$ is also piecewise polynomial and continuous with respect to the variable t. Hence, there is a small interval $t \in (0, \tau)$ on which all s components of $\Delta u(t)$ are in fact polynomial, and a possibly even smaller interval $(0, \tilde{\tau})$ on which the signature vector $\sigma \equiv \mathbf{sign}(u + \Delta u(t))$ is constant. Consequently, the initial path segment $\Delta x(t)_{t\in(0,\tilde{\tau})}$ is contained in the corresponding facet S_σ, which must have the full dimension n because the coefficient vectors of the monomials t^j were chosen linearly independent.

Hence, the piecewise linearization will be differentiable with the constant Jacobian J_σ at all points $\Delta x(t)$ for $t \in (0, \tilde{\tau})$. Obviously that means that J_σ is indeed a limiting Jacobian. We may easily compute the coefficients of the resulting polynomials $\Delta u_i(t)$ and $\Delta v_i(t) = \sigma_i \Delta u_i(t)$ by propagating them forward. Then $\mathbf{sign}(u_i + \Delta u_i(t))$ is always determined by the lowest order nonvanishing coefficient. Due to linearity the j-th order coefficient of these polynomials depends only on the corresponding coefficients of the preceding variables. Hence we may omit the powers t^j and interpret the coefficients as directional derivatives w.r.t. Δx_j. In other words, we obtain exactly the Jacobian accumulation procedure described above. ■

The main idea of the construction we are using is what we called polynomial escape in the nondegeneracy result for the piecewise Newton solver. In both cases singularities and other trouble may only arise on finite unions of subspaces, which can be avoided by moving along polynomials of degree n. Again this approach is familiar from strategies to avoid cycling in linear programming.

The complement vectors e_i for $i = 2 \cdots n$ to a given preferred direction Δx can be chosen such that solving a linear system in the resulting E can be done in $\mathcal{O}(n)$ operations, e.g. using the Sherman–Morrison–Woodbury formula. Then the *unscaling* of J^E_σ by E^{-1} can be achieved at a cost of order $\mathcal{O}(n^2)$. In practice one might prefer an iterative procedure where the *higher order directions* e_i are added for $i = 2 \cdots n$ one-by-one until the resulting signature vector is definite for the first time. That will typically happen for $m \ll n$.

By repeatedly choosing different directions Δx and their complementations, one can compute several limiting Jacobians of the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$ at the origin. Of course there may be an exponential number of such conic Jacobians, and enumerating all of them systematically would appear quite costly, and probably not really worth the effort. It seems more realistic to assume that the user indicates Δx as a *preferred direction* in which he might want to move and then obtains a Jacobian that is active on a cone whose closure contains the given Δx.

Even more useful would be a mode where the AD tool first determines the smallest positive $\tau > 0$ at which the ray $\tau\Delta x$ reaches a kink of the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$, then applies the shift $\mathring{x}\mathrel{+}= \tau\Delta x$ and finally computes a limiting Jacobian in the way described above, still in the preferred direction Δx. In this way the user would obtain useful information (based on linearization) of how far the next kink of F lies along the ray $\mathring{x} + \tau\Delta x$ with $\tau > 0$, and what the Jacobian looks like on the far side of the kink. Of course this could also be repeated for several preferred directions Δx.

The provision of such a procedure for *stabilized generalized* differentiation in a preferred direction would satisfy one of our key requirement on practical differentiation concepts. Namely, that they not just reduce to returning the conventional Jacobian at almost all input arguments, here $\mathring{x}$ and Δx. This calculation would then really be based on the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$ rather than just the Bouligand derivative $F'(\mathring{x}; \Delta x)$, which already yields the exactly conical Jacobians.

6.3 *Proof of conic activity on underlying function*

Since the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$ is an $\mathcal{O}(\|\Delta x\|^2)$ approximation of the underlying function $F(\mathring{x} + \Delta x) - F(\mathring{x})$, one would expect that its limiting Jacobians at $\Delta x = 0$ are always also limiting Jacobians of F at $\mathring{x}$ as we claim in (6). This is indeed the case as we prove below without the noncriticality assumption used in Proposition 7.

Considering once more the example (8) displayed in Figure 3 we find that there may be indefinite signature vectors σ for which the corresponding domain S_σ has nevertheless full dimension, i.e. is open in $\mathbb{R}^n$. More specifically at the origin we can have for $\sigma \in \{-1, 0, 1\}$ only the combinations $(-1, 0)$, $(0, 0)$ and $(1, 0)$ out of the theoretically possible $9 = 3^2$ signature vectors. The corresponding S_σ are the open left half plane, the vertical axis and the open right half plane for $(-1, 0)$, $(0, 0)$ and $(1, 0)$, respectively. The second component of σ is always zero, yet the problem is even differentiable with the gradients of the function and its piecewise linearization coinciding.

That the inclusion (6) holds even in this case with some critical but open S_σ is no coincidence as we see from the following generalization of Proposition 7. To state it we abbreviate by

$$\tilde{\sigma} \succ \sigma \quad \Leftrightarrow \quad \tilde{\sigma}_i \sigma_i \geq \sigma_i^2 \quad \text{for } i = 1 \cdots s$$

the fact that $\tilde{\sigma}_i$ agrees with σ_i whenever the latter is nonzero and is arbitrary otherwise. One can easily check that this determinacy relation is indeed a reflexive partial ordering.

PROPOSITION 9 *If the origin* 0 *belongs to the closure of an open* S_σ *then there is an open subset* $\tilde{S}_\sigma \subset S_\sigma$ *with the same tangent cone as* S_σ *at* 0 *such that*

$$F(x) \in \{F_{\tilde{\sigma}}(x) : \tilde{\sigma} \succ \sigma\} \quad \text{for } x \in \mathring{x} + \tilde{S}_\sigma,$$

and the J_σ *computed according to (16) belongs to* $\nabla^L \Delta F(\mathring{x}; 0) \cap \nabla^L F(\mathring{x})$.

Proof To simplify the notation we may assume the locally reduced representation (18) of $F \in \mathcal{C}^{1,1}(\mathcal{D})$ and moreover $u_i(\mathring{x}) = 0$ for all i and also $F_\sigma \in \mathcal{C}^{1,1}(\mathcal{D})$ for arbitrary σ. This means firstly that $\sigma_i(\Delta x) = \mathbf{sign}(\nabla u_i^\top \Delta x)$ for all i. Moreover, as S_σ has full dimension the criticality property $\sigma_i = 0$ implies for any i that also $\nabla u_i = 0$. Consequently, the piecewise linearizations $\Delta F_{\tilde{\sigma}}(\mathring{x}, \Delta x)$ of all $F_{\tilde{\sigma}}$ for which $\tilde{\sigma} \succ \sigma$ coincide on S_σ with $\Delta F_\sigma(\mathring{x}, \Delta x)$. Since they are continuously differentiable on some neighbourhood of $\mathring{x}$ and are second order approximations to the common piecewise linearization on S_σ, their Jacobians $F'_{\tilde{\sigma}}(\mathring{x})$ must coincide with J_σ. Hence all that is left to show is that $F(x) = F_{\tilde{\sigma}}(x)$ for some $\tilde{\sigma} \succ \sigma$ for $\Delta x = x - \mathring{x} \in \tilde{S}_\sigma$ with an $\tilde{S}_\sigma$ of the asserted quality. Given any $\Delta x \in S_\sigma$ all multiples $t\Delta x$ for $0 < t \leq 1$ must also belong to S_σ because 0 is contained in its closure. Since $u_i = 0$ it follows as in the proof of Proposition 1 that the intermediate values generated by the original nonlinear procedure satisfy

$$u_i(x + t\Delta x) - u_i - \Delta u_i(t\Delta x) = u_i(x + t\Delta x) - t\nabla u_i^\top \Delta x = \mathcal{O}(t^2).$$

Now if $\sigma_i(\Delta x) = \mathbf{sign}(\nabla u_i^\top \Delta x) = 0$ the sign of $u_i(x + t\Delta x)$ and thus the value $\tilde{\sigma}_i$ for which

$$v_i(x + t\Delta x) = \mathbf{abs}(u_i(x + t\Delta x)) = \tilde{\sigma}_i u_i(x + t\Delta x)$$

may vary depending on t. However, if $\sigma_i(\Delta x) = \mathbf{sign}(\nabla u_i^\top \Delta x) \neq 0$ then this relation enforces $\tilde{\sigma}_i = \sigma_i$ for all sufficiently small t. Over all there is a bound $\bar{t}$ for each given $\Delta x \in S_\sigma$ such that at all $x = \mathring{x} + t\Delta x$ the value $F(x)$ equals $F_{\tilde{\sigma}}(x)$ for some $\tilde{\sigma} \succ \sigma$. This completes the proof. ∎

From the last two results we obtain the following corollary.

COROLLARY 1 *The subset of conical Jacobians*

$$\nabla^K F(\mathring{x}) \subset \nabla^L F(\mathring{x}) \subset \nabla^C F(\mathring{x})$$

consists exactly of those limiting Jacobians J of F at $\mathring{x}$ for which there exists a signature vector $\sigma \in \{-1, 0, 1\}^s$ such that $J = F'_\sigma(\mathring{x})$ and the coincidence set $\{x \in \mathcal{D} : F(x) = F_\sigma(x)\}$ at $\mathring{x}$ has at $\mathring{x}$ a tangent cone with nonzero interior.

One important observation is that wherever F is Fréchet differentiable there is only one conically active Jacobian, whereas the Clarke derivatives need not reduce to a singleton ∇F.

7. Piecewise linearization in secant mode

As a generalization of $\Delta F(\mathring{x}; \Delta x)$ we construct in this section a *piecewise secant linearization* $\Delta F(\check{x}, \hat{x}; \Delta x)$ of F at the pair $\check{x}$ and $\hat{x}$, such that for the midpoints $\mathring{x} = (\check{x} + \hat{x})/2$ and $\mathring{F} = (\check{F} + \hat{F})/2$ with $\check{F} = F(\check{x})$ and $\hat{F} = F(\hat{x})$

$$F(x) = \mathring{F} + \Delta F(\check{x}, \hat{x}; x - \mathring{x}) + \mathcal{O}(\|x - \check{x}\| \|x - \hat{x}\|).$$

Here we have $\mathring{F} \neq F(\mathring{x})$ in general, except when F is linear altogether. The new $\Delta F(\check{x}, \hat{x}; \Delta x)$ has the same homogeneity properties as $\Delta F(\mathring{x}; \Delta x)$ and reduces to it when the two sample points $\check{x}$ and $\hat{x}$ coalesce at $\mathring{x}$.

Our motivation for constructing $\Delta F(\check{x}, \hat{x}; \Delta x)$ is that, sometimes, one might look for a piecewise linear generalization of the first order Hermite interpolation to a function between the sample points $\check{x}$ and $\hat{x}$. For example, when $m = 1$, one may wish to perform a line-search to approximately minimize $\varphi(\alpha) \equiv F(x + \alpha s)$ with respect to the step multiplier α. When F and thus φ are smooth, one typically uses a quadratic or cubic Hermite interpolant between values of φ, its derivatives at $\alpha = 0$ and a current trial value $\alpha_c > 0$. However, this makes only limited sense when F and thus φ are nonsmooth, typically because they contain penalty terms of the form $\| \max(c(x), 0)\|_p$, with $c(x) \leq 0$ a set of constraints and $p \in \{1, \infty\}$ defining the norm. We exclude the Euclidean norm where $p = 2$ because that elemental function is well known to destroy piecewise differentiability. An exploratory line-search based on generalized Taylor expansion at single points for nonsmooth problems has been implemented in [15].

A more challenging, but also promising, application is the generalized trapezoidal method for differential equation $\dot{x} = F(x)$ with $F : \mathbb{R}^n \mapsto \mathbb{R}^n$ as discussed already in Section 5.

7.1 *Defining relations for secant approximation*

In the tangent approximation the reference point was always the evaluation point $\mathring{x}$ and the resulting values $\mathring{v}_i = v_i(\mathring{x})$. Now we will make reference to the midpoints

$$\mathring{v}_i \equiv \check{v}_i + \hat{v}_i/2 \quad \text{with} \quad \check{v}_i \equiv v_i(\check{x}) \quad \text{and} \quad \hat{v}_i \equiv v_i(\hat{x}). \tag{19}$$

Therefore we have really the functional dependence $\mathring{v}_i = \mathring{v}_i(\check{x}, \hat{x})$, which is at least Lipschitz continuous under our assumptions. Now the amazing observation is that the recurrences (1) and (2) for arithmetic operations can stay just the same, and the recurrence (3) for nonlinear univariates is still formally valid, except that the tangent slope $\varphi'(\mathring{v}_j)$ must be generalized to the secant slope

$$\mathring{c}_{ij} \equiv \begin{cases} \varphi_i'(\mathring{v}_j) & \text{if } \check{v}_j = \hat{v}_j, \\ \dfrac{\hat{v}_i - \check{v}_i}{\hat{v}_j - \check{v}_j} & \text{otherwise.} \end{cases} \tag{20}$$

Theoretically, some $\check{v}_i$ and $\hat{v}_i$ may coincide, even if the underlying sample points $\check{x}$ and $\hat{x}$ are not selected identically, in which case the secant-based model would reduce to the tangent-based model. While exact coincidence of any pair $\check{v}_i$ and $\hat{v}_i$ is rather unlikely, one should make sure that the divided difference is not taken over too small an increment and then use a univariate Taylor expansion instead. Finally, the nonsmooth rule (4) can stay unchanged except that we set now

$$\mathring{v}_i \equiv \tfrac{1}{2}(\check{v}_i + \hat{v}_i) = \tfrac{1}{2}[\mathbf{abs}(\check{v}_j) + \mathbf{abs}(\hat{v}_j)]. \tag{21}$$

Hence, it is immediately clear that the new secant approximation reduces to the old tangent approximation when $\check{x} = \hat{x}$. In general, we will denote the mapping between the input increments $\Delta x \in \mathbb{R}^n$ and the resulting values $\Delta y \in \mathbb{R}^m$ by

$$\Delta y = \Delta y(\Delta x) = \Delta F(\check{x}, \hat{x}; \Delta x) : \mathbb{R}^n \mapsto \mathbb{R}^m.$$

Its piecewise linear structure is very much the same as that of the tangent-based model, which is described in Section 3. Here we emphasize its quality in approximating the underlying nonlinear and nonsmooth F. The geometry of the tangent and secant-based piecewise linearization of a function $F(x) = \max(F_1(x), F_2(x))$ with the F_i smooth is already depicted in Figures 1 and 2.

The rules for propagating the increments Δv_i according to (1)–(4) are formally identical to the tangent case, the only difference lies in the definition of the midpoints $\mathring{v}_i$ and the multipliers $\mathring{c}_{ij}$. In other words, the elemental functions φ_i and their derivative c_{ij} must be defined for pairs of arguments $(\check{v}_j, \hat{v}_j)$. It is obvious how this can be generated by operator overloading through a modification of ADOL-C and other AD tools, but this variation is much more substantial than in that tangent case considered above.

7.2 *Interpolation, approximation and stability*

First, we verify by induction that the approximation reproduces the values at the sample points $\check{x}$ and $\hat{x}$.

LEMMA 2 Interpolation property *The rules (1), (2), (4) and (3) with (20) and (21) ensure that for all $i = 1 \cdots l$*

$$\Delta x = \hat{x} - \mathring{x} = \hat{x} - \check{x}/2 \Longrightarrow \Delta v_i = \hat{v}_i - \mathring{v}_i \Longrightarrow F(\hat{x}) = \mathring{F} + \Delta F(\check{x}, \hat{x}; \Delta x)$$

and

$$\Delta x = \check{x} - \mathring{x} = \check{x} - \hat{x}/2 \Longrightarrow \Delta v_i = \check{v}_i - \mathring{v}_i \Longrightarrow F(\check{x}) = \mathring{F} + \Delta F(\check{x}, \hat{x}; \Delta x).$$

Proof Due to the complete symmetry of the situation we only need to prove the first identity. For addition and subtraction we have

$$\begin{aligned} \mathring{v}_i + \Delta v_i &= \frac{\check{v}_i + \hat{v}_i}{2} + \Delta v_i \\ &= \frac{\check{v}_j \pm \check{v}_k}{2} + \frac{\hat{v}_j \pm \hat{v}_k}{2} + (\Delta v_j \pm \Delta v_k) \end{aligned}$$

$$= \frac{\check{v}_j + \hat{v}_j}{2} \pm \frac{\check{v}_k + \hat{v}_k}{2} + (\Delta v_j \pm \Delta v_k)$$
$$= (\mathring{v}_j + \Delta v_j) \pm (\mathring{v}_k + \Delta v_k) = \hat{v}_j \pm \hat{v}_k = \hat{v}_i,$$

where the next to last equality holds by induction hypothesis. For the multiplication things are a little bit more involved since

$$\begin{aligned}
\mathring{v}_i + \Delta v_i &= \frac{\check{v}_i + \hat{v}_i}{2} + \Delta v_i \\
&= \frac{\check{v}_j * \check{v}_k}{2} + \frac{\hat{v}_j * \hat{v}_k}{2} + \mathring{v}_j * \Delta v_k + \Delta v_j * \mathring{v}_k \\
&= (\mathring{v}_j - \Delta v_j) * \frac{\mathring{v}_k - \Delta v_k}{2} + (\mathring{v}_j + \Delta v_j) * \frac{\mathring{v}_k + \Delta v_k}{2} + \mathring{v}_j * \Delta v_k + \Delta v_j * \mathring{v}_k \\
&= \mathring{v}_j * \mathring{v}_k + \Delta v_j * \mathring{v}_k + \Delta v_k * \mathring{v}_j + \Delta v_j * \Delta v_k \\
&= (\mathring{v}_j + \Delta v_j) * (\mathring{v}_k + \Delta v_k) = \hat{v}_j * \hat{v}_k = \hat{v}_i,
\end{aligned}$$

where the next to last equality holds again by induction hypothesis. For the univariate elementals we simply have

$$\begin{aligned}
\mathring{v}_i + \Delta v_i &= \frac{\check{v}_i + \hat{v}_i}{2} + \left[\frac{\hat{v}_i - \check{v}_i}{\hat{v}_j - \check{v}_j}\right] \Delta v_j \\
&= \frac{\check{v}_i + \hat{v}_i}{2} + \frac{\Delta v_j (\hat{v}_i - \check{v}_i)}{2\Delta v_j} = \hat{v}_i.
\end{aligned}$$

Finally, we obtain for the absolute value function trivially

$$\mathring{v}_i + \Delta v_i = \mathbf{abs}(\mathring{v}_j + \Delta v_j) = \mathbf{abs}(\hat{v}_j) = \hat{v}_i,$$

which completes the proof. ■

The Lemma says that the values of F at $\check{x}$ and $\hat{x}$ are reproduced exactly by our approximation as one would expect from a secant approximation. This property clearly nails down the piecewise linearization rules (4) and (3) with (20) for all univariate functions. Also, there is no doubt that addition and subtraction should be linearized according to (1) and that multiplications $v_i = cv_j$ by constants c should yield the differentiated version $\Delta v_i = c\Delta v_j$, which is a special case of (2).

For general multiplications $v_i = v_j * v_k$ the two values $\check{v}_i = \check{v}_j * \check{v}_k$ and $\hat{v}_i = \hat{v}_j * \hat{v}_k$ could also be interpolated by other linear functions than the one defined by (2). However, we currently see no possible gain in that flexibility, and maintaing the usual product rule form seems rather attractive. After these preparations we can now prove our main result, which in fact strengthens the statement of the Lemma.

PROPOSITION 10 Bilinear Approximation and Lipschitz continuity *Suppose F is composite piecewise differentiable on some open neighbourhood $\mathcal{D}$ of a closed convex domain $\mathcal{K} \subset \mathbb{R}^n$. Then there exists a constant γ such that for all triples $\check{x}, \hat{x}, x \in \mathcal{K}$ with $\mathring{x}$ and $\mathring{F}$ again the midpoints of arguments and functions values*

$$\|F(x) - \mathring{F} - \Delta F(\check{x}, \hat{x}; x - \mathring{x})\| \le \gamma(\|x - \check{x}\| \|x - \hat{x}\|).$$

Moreover, there exists another constant $\tilde{\gamma}$ such that for any pair of pairs $(\check{x}, \hat{x}), (\check{z}, \hat{z}) \in \mathcal{K}^2$ and $\Delta x \in \mathbb{R}^n$

$$\frac{\|\Delta F(\check{z}, \hat{z}; \Delta x) - \Delta F(\check{x}, \hat{x}; \Delta x)\|}{1 + \|\Delta x\|} = \tilde{\gamma}(\|\check{z} - \check{x}\| + \|\hat{z} - \check{x}\|).$$

Proof For proving the first assertion, we proceed again by induction to show that for all $i = 1 - n \cdots l$

$$\mathring{v}_i + \Delta v_i = v_i(\mathring{x} + \Delta x) + \mathcal{O}(\|x - \check{x}\|\|x - \hat{x}\|).$$

For $i = 1 - n \cdots 0$ these relations hold by definition with $v_{i-n} \equiv x_i$. For addition and subtraction $v_i = v_j \pm v_k$ that property is obviously inherited from the summands. In preparation for the other operations we note first that by the assumed Lipschitz continuous differentiability of all nonlinear functions on the compact domain $\mathcal{K}$ and because of the preceding Lemma

$$\Delta\mathring{v}_i \equiv \hat{v}_i - \check{v}_i/2 = v_i(\hat{x}) - v_i(\check{x})/2 = \mathcal{O}(\|\hat{x} - \check{x}\|).$$

Here the order term on the right is, like others that will follow, uniform on the triples in $\mathcal{K}$. Moreover, we will assume in the following without loss of generality that for the given x we have $\|x - \hat{x}\| \le \|x - \check{x}\|$ and, consequently, $\|\hat{x} - \check{x}\| \le 2\|x - \check{x}\|$, which can be ensured by exchanging $\check{x}$ and $\hat{x}$ if necessary.

Also, since the Lipschitz continuous difference $\Delta v_i - \Delta\mathring{v}_i$ vanishes if $x = \hat{x}$ and thus $\mathring{v}_i + \Delta v_i = \hat{v}_i$ we have always $\Delta v_i - \Delta\mathring{v}_i = \mathcal{O}(\|x - \hat{x}\|) = \mathcal{O}(\|x - \check{x}\|)$. Now we find for the multiplication using the definition of Δv_i in (2)

$$\begin{aligned}
&\mathring{v}_i + \Delta v_i - v_i(\mathring{x} + \Delta x)\\
&\quad = \frac{\check{v}_i + \hat{v}_i}{2} + \Delta v_i - v_j(\mathring{x} + \Delta x) * v_k(\mathring{x} + \Delta x)\\
&\quad = \frac{\check{v}_i + \hat{v}_i}{2} + \mathring{v}_j * \Delta v_k + \Delta v_j * \mathring{v}_k - (\mathring{v}_j + \Delta v_j) * (\mathring{v}_k + \Delta v_k) + \mathcal{O}(\|x - \check{x}\|\|x - \hat{x}\|).
\end{aligned}$$

The last term follows from the induction hypothesis and the fact that all continuous quantities are uniformly bounded on $\mathcal{K}$. Quite a few terms in the middle cancel and we find by elementary manipulations that

$$\begin{aligned}
&\mathring{v}_i + \Delta v_i - v_i(\mathring{x} + \Delta x) - \mathcal{O}(\|x - \check{x}\|\|x - \hat{x}\|)\\
&\quad = \frac{\check{v}_i + \hat{v}_i}{2} - \mathring{v}_j * \mathring{v}_k - \Delta v_j * \Delta v_k\\
&\quad = \frac{\check{v}_j * \check{v}_k}{2} + \frac{\hat{v}_j * \hat{v}_k}{2} - (\check{v}_j + \hat{v}_j) * \frac{\check{v}_k + \hat{v}_k}{4} - \Delta v_j * \Delta v_k\\
&\quad = (\hat{v}_j - \check{v}_j) * \frac{\hat{v}_k - \check{v}_k}{4} - \Delta v_j * \Delta v_j = \Delta\mathring{v}_j * \Delta\mathring{v}_k - \Delta v_j * \Delta v_k.
\end{aligned}$$

Now we can use the estimates at the beginning of the proof to obtain finally that

$$\begin{aligned}
&\mathring{v}_i + \Delta v_i - v_i(\mathring{x} + \Delta x) - \mathcal{O}(\|x - \check{x}\|\|x - \hat{x}\|)\\
&\quad = (\Delta\mathring{v}_j - \Delta v_j) * \Delta\mathring{v}_k + \Delta v_j * (\Delta\mathring{v}_k - \Delta v_k)\\
&\quad = 2\mathcal{O}(\|x - \hat{x}\|) * \mathcal{O}(\|\hat{x} - \check{x}\|) = \mathcal{O}(\|x - \hat{x}\|\|x - \check{x}\|).
\end{aligned}$$

All of this is again uniform on $\mathcal{K}$, which completes the induction argument for the multiplication operation $*$.

As third class of operations we have to consider the nonlinear univariate functions $v_i = \varphi_i(v_j)$. Then we obtain the difference

$$\mathring{v}_i + \Delta v_i - v_i(\mathring{x} + \Delta x) = \frac{1}{2}(\check{v}_i + \hat{v}_i) + \frac{\hat{v}_i - \check{v}_i}{\hat{v}_j - \check{v}_j} * \Delta v_j - \varphi_i\left(\frac{1}{2}(\check{v}_j + \hat{v}_j) + \Delta v_j\right),$$

which vanishes for $\Delta v_j = \pm\Delta\mathring{v}_j$ by the interpolation property we have established before. It is well known [21] that for any φ with a Lipschitz continuous derivative the difference to its secant interpolant for $\Delta v_j \in [-\Delta\mathring{v}_j, \Delta\mathring{v}_j]$ is of order

$$\mathcal{O}(\|\Delta v_j + \Delta\mathring{v}_j\|\|\Delta v_j - \Delta\mathring{v}_j\|) = \mathcal{O}(\|\hat{x} - \check{x}\|)\mathcal{O}(\|x - \hat{x}\|) = \mathcal{O}(\|x - \check{x}\|\|x - \hat{x}\|),$$

where we have again used the convention that $\|x - \hat{x}\| \leq \|x - \check{x}\|$.

Finally, we find for the absolute value function

$$\mathring{v}_i + \Delta v_i - v_i(\mathring{x} + \Delta x) = \mathbf{abs}(\mathring{v}_j + \Delta v_j) - \mathbf{abs}(v_j(\mathring{x} + \Delta x)) = \mathcal{O}(\|x - \check{x}\|\|x - \hat{x}\|),$$

where the last relation follows from the induction hypothesis and the Lipschitz continuity of the absolute value function. Hence the proof by induction is complete.

The second assertion is also proved by induction. Since $v_i(\check{z}) - v_i(\check{x}) = \mathcal{O}(\|\check{z} - \check{x}\|)$ and $v_i(\hat{z}) - v_i(\hat{x}) = \mathcal{O}(\|\hat{z} - \hat{x}\|)$ we have

$$\mathring{v}_i(\check{z}, \hat{z}) - \mathring{v}_i(\check{x}, \hat{x}) = \tfrac{1}{2}[v_i(\check{z}) - v_i(\check{x}) + v_i(\hat{z}) - v_i(\hat{x})] = \mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \hat{x}\|).$$

Moreover, we have $\|\Delta v_i(\check{x}, \hat{x}; \Delta x)\| \leq c_i\|\Delta x\|$ where c_i is a suitable constant. The first property implies for all smooth elementals by assumption of Lipschitz continuous differentiability of all elementals that also

$$\mathring{c}_{ij}(\check{z}, \hat{z}) - \mathring{c}_{ij}(\check{x}, \hat{x}) = \mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \hat{x}\|) \quad \text{for } j \prec i.$$

Now we can derive the second assertion by showing that for all i

$$\frac{|\Delta v_i(\check{z}, \hat{z}; \Delta x) - \Delta v_i(\check{x}, \hat{x}; \Delta x)|}{1 + \|\Delta x\|} = \mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \hat{x}\|).$$

This is obviously true for the independent values v_i for $i = 1 - n \cdots 0$ whose increments $\Delta v_i = \Delta x_{i+n}$ are chosen independently of $\check{x}$ and $\hat{x}$. Then it follows by induction for smooth elementals $v_i = \varphi_i(v_j)_{j\prec i}$ that

$$\begin{aligned}
&\frac{|\Delta v_i(\check{z}, \hat{z}; \Delta x) - \Delta v_i(\check{x}, \hat{x}; \Delta x)|}{1 + \|\Delta x\|} \\
&\quad \leq \frac{|\sum_{j\prec i}(\mathring{c}_{ij}(\check{z}, \hat{z}) - \mathring{c}_{ij}(\check{x}, \hat{x}))\Delta v_j(\check{z}, \hat{z}; \Delta x) + \sum_{j\prec i}\mathring{c}_{ij}(\check{x}, \hat{x})(\Delta v_j(\check{z}, \hat{z}; \Delta x) - \Delta v_j(\check{x}, \hat{x}; \Delta x))|}{1 + \|\Delta x\|} \\
&\quad \leq \sum_{j\prec i}\mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \check{x}\|)\frac{c_j\|\Delta x\|}{1 + \|\Delta x\|} + \sum_{j\prec i}|\mathring{c}_{ij}(\check{z}, \hat{z})|\frac{|\Delta v_j(\check{z}, \hat{z}; \Delta x) - \Delta v_j(\check{x}, \hat{x}; \Delta x)|}{1 + \|\Delta x\|} \\
&\quad \leq \mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \check{x}\|) + \sum_{j\prec i}|\mathring{c}_{ij}(\check{z}, \hat{z})|\mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \check{x}\|) = \mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \check{x}\|).
\end{aligned}$$

Hence we only have to prove the assertion for the absolute value where

$$\begin{aligned}
&|\Delta v_i(\check{z}, \hat{z}; \Delta x) - \Delta v_i(\check{x}; \hat{x}; \Delta x)| \\
&\quad = |\mathbf{abs}(\mathring{v}_j(\check{z}, \hat{z}) + \Delta v_j(\check{z}, \hat{z}; \Delta x)) - \mathring{v}_i(\check{z}, \hat{z}) - [\mathbf{abs}(\mathring{v}_j(\check{x}, \hat{x}) + \Delta v_j(\check{x}, \hat{x}; \Delta x)) - \mathring{v}_i(\check{x}, \hat{x})]| \\
&\quad \leq |\mathring{v}_j(\check{z}, \hat{z}) + \Delta v_j(\check{z}, \hat{z}; \Delta x) - [\mathring{v}_j(\check{x}, \hat{x}) + \Delta v_j(\check{x}, \hat{x}; \Delta x)]| + |\mathring{v}_i(\check{z}, \hat{z}) - \mathring{v}_i(\check{x}, \hat{x})| \\
&\quad \leq |\mathring{v}_j(\check{z}, \hat{z}) - \mathring{v}_j(\check{x}, \hat{x})| + |\Delta v_j(\check{z}, \hat{z}; \Delta x) - \Delta v_j(\check{x}, \hat{x}; \Delta x)| + |\mathring{v}_i(\check{z}, \hat{z}) - \mathring{v}_i(\check{x}, \hat{x})| \\
&\quad = (2 + \|\Delta x\|)\mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \check{x}\|) = (1 + \|\Delta x\|)\mathcal{O}(\|\check{z} - \check{x}\| + \|\hat{z} - \check{x}\|),
\end{aligned}$$

which completes the proof. ■

The key assertion is the uniformity of the bilinear error term on the RHS, even when $\check{x}$ and $\hat{x}$ come arbitrarily close to each other. If they stay apart by a certain minimal distance the assertion follows already from the interpolation property and the Lipschitz continuity. The typical contours of the bilinear error term are depicted in Figure 7.

The bilinear approximation property is crucial in proving second order convergence of the generalized trapezoidal rule that was already discussed together with a generalization of the midpoint rule in Section 6. Moreover, we have also shown that the linearization varies Lipschitz continuously with respect to the two sample points. In other words the model $\Delta F(\check{x}, \hat{x}; \Delta x)$ is like the tangent version stable with respect to the sample points. Finally, one can easily check that the exact composition rules that we derived for the tangent approximation generalize to the secant extension. The connection between the secant linearization and slopes [31] remains to be explored. A big difference is certainly that the piecewise secant linearization is a global approximation rather than a rigorous inclusion on certain interval domain.

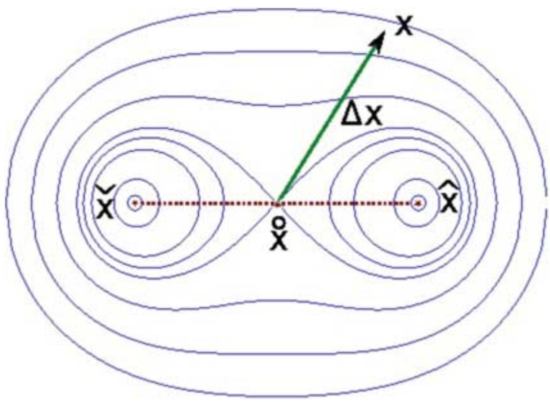

Figure 7. Bilinear error function $\|x - \check{x}\|\|x - \hat{x}\|$.

8. Summary, conclusions and outlook

For dealing with piecewise smoothness brought about by the absolute value function min() and max() we have proposed and analysed an AD like piecewise linearization and also a secant-based variant. We have demonstrated how these local approximations can be provided and utilized for the basic computation tasks of unconstrained optimization, ODE integration and equation solving. We have also shown that they can be used to calculate conically active generalized Jacobians. However, we also demonstrated by example that the radius of convergence of the generalized Newton's method can be tiny even on coherently oriented piecewise linear functions. Since they are naturally semi-smooth, we conclude that simple successive linearization is generally not a promising strategy for the treatment of nonsmooth systems of equations.

Let us briefly discuss the results in the light of the criteria for rating derivative concepts discussed in Section 1. For the purpose of the three basic tasks considered here the fit between the underlying piecewise smooth functions and their tangent or secant linearizations seem reasonably good. However, as already observed by Scholtes the Bouligand derivative $F'(\mathring{x}; \Delta x)$ at some point $\mathring{x}$ may be a global homeomorphism with the underlying function being only open but not invertible at $\mathring{x}$ and $F(\mathring{x})$. This is related to the fact that coherent orientation of $F'(\mathring{x}; \Delta x)$ or $\Delta F(\mathring{x}; \Delta x)$ is not a stable property with respect to perturbations in $\mathring{x}$. As far as simplicity is concerned we argue that the piecewise linearization $\Delta F(\mathring{x}; \Delta x)$ and its secant-based generalization $\Delta F(\check{x}, \hat{x}; \Delta x)$ are really not much more complicated than the Bouligand derivative mapping $F'(\mathring{x}; \Delta x)$, which is used frequently in theoretical investigations though probably not as often in the computational practice.

From the computer science point of view implementing $\Delta F(\mathring{x}; \Delta x)$ is a minute variation of the forward AD mode, but realizing the secant variation $\Delta F(\check{x}, \hat{x}; \Delta x)$ is little more substantial. As far as the reverse mode is concerned it should play a major role in walking the polyhedral decomposition, where active normals should be computed backward as discussed in Section 7. The key challenge for the AD community is to develop suitable interfaces between AD tool and the user and his or her algorithms.

Apart from implementation issues there are many questions to be examined both theoretically and algorithmically. That concerns for example the relation to slopes and the issue of mesh dependence for families of discretizations. Possible extensions concern the handling of discontinuities and branching with or without the assurance of overall continuity. Without, one would arrive at piecewise linear approximations $\Delta F(\mathring{x}, \Delta x)$, which are discontinuous and thus have a set valued convex outer semi-continuous envelope. One then faces amongst others the challenge of solving generalized equations, i.e. finding points Δx, where 0 belongs to the image of that envelope function.

A somewhat less thorny issue is the treatment of the Euclidean norm, where some adaptive piecewise linear approximation should be computable. More interesting would be an extension to fractional piecewise linear approximations, where all intermediates are approximated by quotients of piecewise linear functions. The corresponding propagation rules are not a priori unique, even if one maintains the second order approximation property. Of course, such fractional piecewise linear models would also greatly impact the theory and algorithmics of optimization, ODE integration and equation solving. For the solution of those classical numerical tasks we have given some preliminary observations, but they need to be elaborated and experimentally validated. Finally, we expect algorithmic piecewise linearization to be useful on many other computational tasks.

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