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A Continuation Problem for Computing Solutions of Discretised Evolution Problems. Part I – Abstract Frame.

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Abstract

A continuation problem for finding successive solutions of discretised abstract evolution problems of the first order is proposed and a general piecewise C^1 continuation problem is studied. A condition ensuring local existence and uniqueness of its solution curves is given. An analogy of the first-order system for smooth problems is derived and results of existence and uniqueness of its solutions are stated. Possibility of continuation of a solution curve along a direction from the first-order system is discussed. A technique for numerical continuation of solution curves is developed.

Keywords: discretized evolution problem, continuation method, piecewise-smooth function, first-order system, predictor-corrector.

1 Introduction

When time-stepping schemes are used to solve quasi-static problems in solid mechanics numerically, one can encounter situations where usual solvers (for instance, the Newton method with the initial approximation chosen to be a solution from the previous time step) fail to compute any solution. Typically, this can happen when a snap-through instability is present and even a small change in loading leads to a dramatic change of the solution. This has lead us to construct a suitable continuation problem for dealing with such situations. Although our motivation has originated from solving quasi-static problems with the

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particularity that the time derivative appears only in a nonlinear term, our approach can be applied to first-order evolution problems generally. The idea how to do it is explained in an abstract frame in Section 2.

Whereas continuation is well-established for problems involving a continuously differentiable map (see [3], for example), a little work has been done for problems with non-smooth maps and it is oriented mainly to homotopy methods to author's knowledge [2, 12]. That is why the next ambition of this paper is to give a rigorous analysis of a general continuation problem. In particular, a problem involving an arbitrary piecewise C^1 (PC^1) map is considered in Section 3, and a result guaranteeing local existence and uniqueness of its solution curves is stated. Furthermore, an analogy of the first-order system for smooth problems is introduced, which gives the possibility of studying tangent behaviour of solution curves near a given solution point.

Let us mention that the reason why we confine ourselves to the framework of PC^1 -functions is that it seems to be well-suited for plane contact problems. These lead to mappings that are not Gâteaux-differentiable in general. Nevertheless, other problems from engineering or economics are covered, as well [11].

Finally, a method of numerical continuation for tracing PC^1 solution curves of the problem from Section 3 is described in Section 4. It is well-known that the standard Newton method fails when folds occur on the curve, even in the smooth case. Hence, our proposed technique is based on the predictor-corrector continuation method for smooth maps sketched in [4], which is capable of traversing such types of points. Here, we shall modify it to our PC^1 -case similarly as it is done in [7, 6], yet with an important difference: whereas the cited works essentially use the so-called test functions, which require a quite detailed specification of the PC^1 -function involved, there is no such need in the present strategy. This makes it more straightforward and easier to implement.

The companion paper [9] deals with a continuation problem for quasi-static plane contact problems with friction. The theory from the general case is developed and the method of numerical continuation is tested on finite-element models.

Throughout the present paper, the following notation is employed: $\mathbf{x} \cdot \mathbf{y} = \mathbf{x}^\top \mathbf{y}$ is the scalar product of vectors \mathbf{x} and \mathbf{y} and $B(\mathbf{x}, r)$ stands for a closed ball centred at \mathbf{x} with radius r . The gradients of a real-valued function f and a vector-valued function \mathbf{f} at a point \mathbf{x} are denoted by $\nabla f(\mathbf{x})$ and $\nabla \mathbf{f}(\mathbf{x})$, respectively, and the partial gradients of f and \mathbf{f} with respect to \mathbf{y} at (\mathbf{x}, \mathbf{y}) are denoted by $\nabla_{\mathbf{y}} f(\mathbf{x}, \mathbf{y})$ and $\nabla_{\mathbf{y}} \mathbf{f}(\mathbf{x}, \mathbf{y})$, respectively.

2 Construction of the Continuation Problem

Let us consider a nonlinear evolution mathematical model whose spatial semi-discretisation leads to a problem of the type:

$$\begin{aligned} & \text{Find } \mathbf{x}: [0, T] \rightarrow \mathbb{R}^N \text{ such that} \\ & \mathbf{G}(\mathbf{x}(t), \dot{\mathbf{x}}(t)) = \mathbf{F}(t, \mathbf{x}(t)) \text{ in } (0, T), \quad \mathbf{x}(0) = \mathbf{x}^0 \end{aligned}$$

with $N \in \mathbb{N}$, $T > 0$, $\mathbf{G}: \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}^N$, $\mathbf{F}: \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$ and $\mathbf{x}_0 \in \mathbb{R}^N$ given. Here, $\dot{\mathbf{x}} \equiv d\mathbf{x}/dt$ stands for the time derivative of \mathbf{x} .

To illustrate the idea how to construct the announced continuation problem for a particular time discretisation, we divide the interval $[0, T]$ into n_T sub-intervals $[t_k, t_{k+1}]$, $k = 0, \dots, n_T - 1$, and use the backward difference

$$\dot{\mathbf{x}}(t_{k+1}) \approx \frac{\mathbf{x}(t_{k+1}) - \mathbf{x}(t_k)}{t_{k+1} - t_k}.$$

In this way, we obtain a sequence of incremental problems for $k = 0, \dots, n_T - 1$:

$$\left. \begin{array}{l} \text{Find } \mathbf{x}^{k+1} \in \mathbb{R}^N \text{ such that} \\ \mathbf{G}\left(\mathbf{x}^{k+1}, \frac{\mathbf{x}^{k+1} - \mathbf{x}^k}{t_{k+1} - t_k}\right) = \mathbf{F}(t_{k+1}, \mathbf{x}^{k+1}). \end{array} \right\} \quad (\mathcal{P}_{k+1})$$

Now, let $k \geq 1$ be fixed. We introduce the continuation problem with an additional scalar parameter γ as follows:

$$\left. \begin{array}{l} \text{Find } (\gamma, \mathbf{x}) \in \mathbb{R} \times \mathbb{R}^N \text{ such that} \\ \mathbf{H}(\gamma, \mathbf{x}) = \mathbf{0}, \end{array} \right\} \quad (\mathcal{P})$$

where $\mathbf{H}: \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$ is defined as

$$\mathbf{H}(\gamma, \mathbf{x}) := \mathbf{G}\left(\mathbf{x}, \frac{\mathbf{x} - \mathbf{x}^k}{t_{k+1} - t_k} + (1 - \gamma) \frac{\mathbf{x}^k - \mathbf{x}^{k-1}}{t_k - t_{k-1}}\right) - (\gamma \mathbf{F}(t_{k+1}, \mathbf{x}) + (1 - \gamma) \mathbf{F}(t_k, \mathbf{x})).$$

It is readily seen that any \mathbf{x}^k solving (\mathcal{P}_k) satisfies $\mathbf{H}(0, \mathbf{x}^k) = \mathbf{0}$ and \mathbf{x} solves (\mathcal{P}_{k+1}) if and only if $\mathbf{H}(1, \mathbf{x}) = \mathbf{0}$. Hence, if we are able to continue solutions of (\mathcal{P}) numerically, we are furnished with the following method for finding solutions of (\mathcal{P}_{k+1}) : starting with $(0, \mathbf{x}^k)$ as the initial point, any couple (γ, \mathbf{x}) with $\gamma = 1$ found during the continuation gives \mathbf{x} solving the problem (\mathcal{P}_{k+1}) .

Let us note that the term $(1 - \gamma)(\mathbf{x}^k - \mathbf{x}^{k-1})/(t_k - t_{k-1})$ in the definition of \mathbf{H} approximates a multiple of the time derivative of \mathbf{x} at t_k . Thus, it not only makes $(0, \mathbf{x}^k)$ a solution of (\mathcal{P}) , but also adds a kind of viscosity and makes the continuation problem more coherent.

Remark 1. The backward difference used in the time discretisation corresponds to the backward Euler method. Nevertheless, our approach can be easily modified for other classical time discretisation schemes like the θ -method or midpoint rule. Indeed, when using any time-stepping scheme, one can always introduce a parameter γ so that problems on successive time levels are recovered for γ equal to 0 and 1, respectively. Clearly, our approach can be applied also to any second-order evolution problem after rewriting it as a system of the first order.

In the remaining part of the paper, we shall suppose that the function \mathbf{H} in the problem (\mathcal{P}) is an arbitrary PC^1 -function as defined in the appendix.

3 Analysis of the Continuation Problem

One would expect that the solution set of $\mathbf{H}(\gamma, \mathbf{x}) = \mathbf{0}$ could be described as a curve. We shall show that under assumptions of an appropriate implicit function theorem, this is indeed, at least locally, the case. In particular, we shall use the notion of a completely coherently oriented function, which is introduced in the appendix for functions that are PC^1 .

Let \mathbf{H} be a PC^1 -function and $(\bar{\gamma}, \bar{\mathbf{x}}) \in \mathbb{R} \times \mathbb{R}^N$ be such that

$$\left. \begin{array}{l} \text{(i) } \mathbf{H}(\bar{\gamma}, \bar{\mathbf{x}}) = \mathbf{0}; \\ \text{(ii) } \mathbf{H} \text{ is completely coherently oriented with respect to } \mathbf{x} \text{ at } (\bar{\gamma}, \bar{\mathbf{x}}). \end{array} \right\} \quad (1)$$

Then it follows from Proposition 5 in the appendix that the equation $\mathbf{H}(\gamma, \mathbf{x}) = \mathbf{0}$ determines a unique implicit PC^1 -function $\mathbf{x}(\gamma)$ in a neighbourhood of $(\bar{\gamma}, \bar{\mathbf{x}})$ with $\mathbf{x}(\bar{\gamma}) = \bar{\mathbf{x}}$. Defining a curve \mathbf{c} as

$$\mathbf{c}: s \mapsto (s, \mathbf{x}(s))$$

on the corresponding neighbourhood of $\bar{\gamma}$, we arrive immediately at the following proposition:

Proposition 1. *Let $\mathbf{H}: \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a PC^1 -function and $(\bar{\gamma}, \bar{\mathbf{x}}) \in \mathbb{R} \times \mathbb{R}^N$ satisfy (1). Then there exist an open interval J and a PC^1 -curve $\mathbf{c}: J \rightarrow \mathbb{R} \times \mathbb{R}^N$ such that*

$$\left. \begin{array}{l} \text{(j) } \exists \bar{s} \in J: \mathbf{c}(\bar{s}) = (\bar{\gamma}, \bar{\mathbf{x}}); \\ \text{(jj) } \forall s \in J: \mathbf{H}(\mathbf{c}(s)) = \mathbf{0}. \end{array} \right\} \quad (2)$$

Moreover, the solution set of $\mathbf{H}(\gamma, \mathbf{x}) = \mathbf{0}$ coincides with the image of \mathbf{c} in a neighbourhood of $(\bar{\gamma}, \bar{\mathbf{x}})$.

Keeping this result in mind, we shall suppose in the following that we are given a zero $(\bar{\gamma}, \bar{\mathbf{x}})$ of \mathbf{H} and there exists a PC^1 -curve $\mathbf{c}: s \mapsto \mathbf{c}(s) = (\gamma(s), \mathbf{x}(s))$ satisfying (2). Since any PC^1 -function is locally Lipschitz continuous and B-differentiable, we can compute the right-hand side derivative of (2)(jj) at \bar{s} according to Proposition 3 from the appendix (for any function \mathbf{f} of a real variable, \mathbf{f}' denotes its right-hand side derivative for brevity of notation here and in what follows):

$$\mathbf{H}'(\mathbf{c}(\bar{s})) = \mathbf{H}'(\mathbf{c}(\bar{s}); \mathbf{c}'(\bar{s})) = \mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); (\gamma'(\bar{s}), \mathbf{x}'(\bar{s}))) = \mathbf{0}.$$

Thus, if \mathbf{c} is a curve passing through $(\bar{\gamma}, \bar{\mathbf{x}})$ whose course we do *not* know completely, we can recover its tangent behaviour at $(\bar{\gamma}, \bar{\mathbf{x}})$ by solving the problem:

$$\left. \begin{array}{l} \text{Find } (\gamma', \mathbf{x}') \in \mathbb{R} \times \mathbb{R}^N \text{ such that} \\ \mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); (\gamma', \mathbf{x}')) = \mathbf{0}. \end{array} \right\} \quad (\mathcal{P}')$$

By analogy with continuation of smooth curves, we call this problem a *first-order system*.

It is known that the derivative $\mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); (\gamma', \mathbf{x}'))$ is a piecewise-linear function of (γ', \mathbf{x}') for any PC^1 -function \mathbf{H} . Invoking theory of piecewise-linear functions, we have results of existence and uniqueness of solutions of (\mathcal{P}') .

Proposition 2. *Let $\mathbf{H}: \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a PC^1 -function that is coherently oriented with respect to \mathbf{x} at $(\bar{\gamma}, \bar{\mathbf{x}})$. Then for any $\gamma' \in \mathbb{R}$, there exists at least one $\mathbf{x}' \in \mathbb{R}^N$ such that (γ', \mathbf{x}') solves (\mathcal{P}') . If \mathbf{H} is even completely coherently oriented with respect to \mathbf{x} at $(\bar{\gamma}, \bar{\mathbf{x}})$, the vector \mathbf{x}' is determined uniquely.*

Proof. Under the given assumptions, the mapping $\tilde{\mathbf{H}}: \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R} \times \mathbb{R}^N$ introduced as

$$\tilde{\mathbf{H}}: (\gamma', \mathbf{x}') \mapsto \begin{pmatrix} \mathbf{H}((\bar{\gamma}, \bar{\mathbf{x}}); (\gamma', \mathbf{x}')) \\ \gamma' \end{pmatrix}$$

is piecewise-linear and (completely) coherently oriented and the assertions follow directly from Proposition 4 in the appendix. \square

For other criteria guaranteeing unique solvability of (\mathcal{P}') , see [10, Section 4], [1] and the references therein.

So far, we have shown that any one-sided tangent vector of a solution curve of (\mathcal{P}) is a solution of the first-order system (\mathcal{P}') . Now, we shall deal with the converse: Having a solution (γ', \mathbf{x}') of (\mathcal{P}') at our disposal, we shall give conditions under which it corresponds to a tangent to a solution branch of (\mathcal{P}) emanating from that point. We shall obtain even uniqueness of such a solution branch.

The first result complements Proposition 1.

Theorem 1. *Let the assumptions of Proposition 1 be fulfilled and $(\gamma', \mathbf{x}') \in \mathbb{R} \times \mathbb{R}^N$ solve (\mathcal{P}') . Then there are $\delta > 0$ and a PC^1 -curve $\mathbf{c}: [\bar{s}, \bar{s} + \delta) \rightarrow \mathbb{R} \times \mathbb{R}^N$ such that*

$$\left. \begin{array}{l} \text{(j)} \quad \mathbf{c}(\bar{s}) = (\bar{\gamma}, \bar{\mathbf{x}}); \\ \text{(jj)} \quad \forall s \in [\bar{s}, \bar{s} + \delta): \quad \mathbf{H}(\mathbf{c}(s)) = \mathbf{0}; \\ \text{(jjj)} \quad \mathbf{c}'(\bar{s}) = (\gamma', \mathbf{x}'). \end{array} \right\} \quad (3)$$

Moreover, if $(\gamma', \mathbf{x}') \neq (0, \mathbf{0})$, the image of any other curve $\tilde{\mathbf{c}}: [\bar{s}, \bar{s} + \tilde{\delta}) \rightarrow \mathbb{R} \times \mathbb{R}^N$ with $\tilde{\delta} > 0$ and such that

$$\left. \begin{array}{l} \text{(j)} \quad \tilde{\mathbf{c}}(\bar{s}) = (\bar{\gamma}, \bar{\mathbf{x}}); \\ \text{(jj)} \quad \forall s \in [\bar{s}, \bar{s} + \tilde{\delta}): \quad \mathbf{H}(\tilde{\mathbf{c}}(s)) = \mathbf{0}; \\ \text{(jjj)} \quad \tilde{\mathbf{c}}'(\bar{s}) \in \bigcup_{r>0} r(\gamma', \mathbf{x}') \end{array} \right\} \quad (4)$$

coincides with the image of \mathbf{c} in a neighbourhood of $(\bar{\gamma}, \bar{\mathbf{x}})$.

Proof. As we already know, $\mathbf{H}(\gamma, \mathbf{x}) = \mathbf{0}$ determines a unique implicit PC^1 -function $\mathbf{x}(\gamma)$ in a neighbourhood of $(\bar{\gamma}, \bar{\mathbf{x}})$. Let us define \mathbf{c} as

$$\mathbf{c}: s \mapsto (\gamma'(s - \bar{s}) + \bar{\gamma}, \mathbf{x}(\gamma'(s - \bar{s}) + \bar{\gamma})).$$

Then (3)(j) and (jj) are clearly satisfied for sufficiently small $\delta > 0$ and

$$\mathbf{c}'(\bar{s}) = (\gamma', \gamma' \mathbf{x}'(\bar{\gamma})).$$

From the derivation of (\mathcal{P}') , we know that $(\gamma', \gamma' \mathbf{x}'(\bar{\gamma}))$ belongs to its solutions and the uniqueness result of Proposition 2 implies that

$$\gamma' \mathbf{x}'(\bar{\gamma}) = \mathbf{x}',$$

which completes (3). The second part of the assertion follows from the uniqueness of the implicit function $\mathbf{x}(\gamma)$ in a neighbourhood of $(\bar{\gamma}, \bar{\mathbf{x}})$. \square

Due to the implicit function theorem used in the proof, the previous theorem can be applied only to cases where exactly two one-sided solution branches $s \mapsto (\gamma(s), \mathbf{x}(s))$ emanate from $(\bar{\gamma}, \bar{\mathbf{x}})$ – one with γ increasing and the other one with γ decreasing. The next theorem covers also situations with more solution branches.

Theorem 2. *Let $\mathbf{H}: \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a PC^1 -function and $(\bar{\gamma}, \bar{\mathbf{x}}), (\gamma', \mathbf{x}') \in \mathbb{R} \times \mathbb{R}^N$ satisfy $\mathbf{H}(\bar{\gamma}, \bar{\mathbf{x}}) = \mathbf{0}$ and $\mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); (\gamma', \mathbf{x}')) = \mathbf{0}$. If $\{\mathbf{H}^{(i)}\}_{i \in I}$ is a family of C^1 selection functions of \mathbf{H} at $(\bar{\gamma}, \bar{\mathbf{x}})$ and there exists $i_0 \in I$ such that*

$$\left. \begin{array}{l} \text{(i) } \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}) = \mathbf{H}(\bar{\gamma}, \bar{\mathbf{x}}); \\ \text{(ii) } \nabla \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}})(\gamma', \mathbf{x}') = \mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); (\gamma', \mathbf{x}')) \neq \nabla \mathbf{H}^{(i)}(\bar{\gamma}, \bar{\mathbf{x}})(\gamma', \mathbf{x}'), \quad \forall i \neq i_0; \\ \text{(iii) } \nabla_{\mathbf{x}} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}) \text{ is non-singular,} \end{array} \right\} \quad (5)$$

then all the conclusions of Theorem 1 hold and the solution curve \mathbf{c} is even of the class C^1 .

Proof. By the classical implicit function theorem, the equation $\mathbf{H}^{(i_0)}(\gamma, \mathbf{x}) = \mathbf{0}$ determines a unique implicit function $\mathbf{x}(\gamma)$ around $(\bar{\gamma}, \bar{\mathbf{x}})$. In this case, $\mathbf{x}(\gamma)$ is continuously differentiable and its (two-sided) derivative is:

$$\mathbf{x}'(\bar{\gamma}) = -(\nabla_{\mathbf{x}} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}))^{-1} \nabla_{\gamma} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}). \quad (6)$$

Let us define a curve \mathbf{c} by

$$\mathbf{c}: s \mapsto (\gamma'(s - \bar{s}) + \bar{\gamma}, \mathbf{x}(\gamma'(s - \bar{s}) + \bar{\gamma})).$$

Then (3)(j) clearly holds. By (5)(ii) and (iii),

$$\begin{aligned} \nabla \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}})(\gamma', \mathbf{x}') &= \nabla_{\gamma} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}) \gamma' + \nabla_{\mathbf{x}} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}) \mathbf{x}' = \mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); (\gamma', \mathbf{x}')) = \mathbf{0}, \\ \mathbf{x}' &= -\gamma' (\nabla_{\mathbf{x}} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}))^{-1} \nabla_{\gamma} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}). \end{aligned}$$

This combined with (6) yields

$$\mathbf{c}'(\bar{s}) = (\gamma', \gamma' \mathbf{x}'(\bar{\gamma})) = (\gamma', -\gamma' (\nabla_{\mathbf{x}} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}))^{-1} \nabla_{\gamma} \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}})) = (\gamma', \mathbf{x}'), \quad (7)$$

that is, (3)(jjj) is fulfilled, as well. Moreover, $\mathbf{H}^{(i_0)}(\mathbf{c}(s)) = \mathbf{0}$ and to prove (3)(jj), we have to show:

$$\mathbf{H}(\mathbf{c}(s)) = \mathbf{H}^{(i_0)}(\mathbf{c}(s)) \text{ for } s \geq \bar{s}, s \text{ close to } \bar{s}. \quad (8)$$

Hereafter, we shall suppose that

$$\forall i \in I: \mathbf{H}^{(i)}(\bar{\gamma}, \bar{\mathbf{x}}) = \mathbf{H}(\bar{\gamma}, \bar{\mathbf{x}}) \quad (9)$$

(the other indices may be omitted from I by virtue of continuity of \mathbf{H}).

Making use of (5)(ii), one can find for any $i \neq i_0$ an index $j(i)$ such that

$$\nabla H_{j(i)}^{(i)}(\bar{\gamma}, \bar{\mathbf{x}}) \cdot (\gamma', \mathbf{x}') \neq \nabla H_{j(i)}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}) \cdot (\gamma', \mathbf{x}'),$$

which ensures ϵ defined by

$$\epsilon := \min_{i \neq i_0} |(\nabla H_{j(i)}^{(i)}(\bar{\gamma}, \bar{\mathbf{x}}) - \nabla H_{j(i)}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}})) \cdot (\gamma', \mathbf{x}')|$$

to be positive. Continuous differentiability of $\mathbf{H}^{(i)}$ implies that there is $\bar{\delta} > 0$ such that

$$\forall i \neq i_0 \forall (\gamma, \mathbf{x}) \in B((\bar{\gamma}, \bar{\mathbf{x}}), \bar{\delta}): |(\nabla H_{j(i)}^{(i)}(\gamma, \mathbf{x}) - \nabla H_{j(i)}^{(i_0)}(\gamma, \mathbf{x})) \cdot (\gamma', \mathbf{x}')| \geq \frac{\epsilon}{2}$$

and

$$\begin{aligned} \forall i \neq i_0 \forall (\gamma, \mathbf{x}) \in B((\bar{\gamma}, \bar{\mathbf{x}}), \bar{\delta}) \forall (u, \mathbf{v}) \in B((\gamma', \mathbf{x}'), \delta'): \\ |(\nabla H_{j(i)}^{(i)}(\gamma, \mathbf{x}) - \nabla H_{j(i)}^{(i_0)}(\gamma, \mathbf{x})) \cdot (u, \mathbf{v})| \\ \geq |(\nabla H_{j(i)}^{(i)}(\gamma, \mathbf{x}) - \nabla H_{j(i)}^{(i_0)}(\gamma, \mathbf{x})) \cdot (\gamma', \mathbf{x}')| \\ - |(\nabla H_{j(i)}^{(i)}(\gamma, \mathbf{x}) - \nabla H_{j(i)}^{(i_0)}(\gamma, \mathbf{x})) \cdot (u - \gamma', \mathbf{v} - \mathbf{x}')| \\ \geq \frac{\epsilon}{2} - \|\nabla H_{j(i)}^{(i)}(\gamma, \mathbf{x}) - \nabla H_{j(i)}^{(i_0)}(\gamma, \mathbf{x})\| \|(u - \gamma', \mathbf{v} - \mathbf{x}')\| > 0 \end{aligned}$$

for some $\delta' > 0$ by boundedness of $\nabla H_{j(i)}^{(i)}(\gamma, \mathbf{x}) - \nabla H_{j(i)}^{(i_0)}(\gamma, \mathbf{x})$. Therefore, there is $\bar{r} > 0$ such that

$$\begin{aligned} \forall i \neq i_0 \forall (u, \mathbf{v}) \in B((\gamma', \mathbf{x}'), \delta') \forall r \in [0, \bar{r}): \\ |(\nabla H_{j(i)}^{(i)}(\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v}) - \nabla H_{j(i)}^{(i_0)}(\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v})) \cdot (u, \mathbf{v})| > 0 \quad (10) \end{aligned}$$

and due to (5)(ii) and continuity of $\mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); \cdot)$,

$$\begin{aligned} \forall i \neq i_0 \forall (u, \mathbf{v}) \in B((\gamma', \mathbf{x}'), \delta'): \\ \mathbf{H}'((\bar{\gamma}, \bar{\mathbf{x}}); (u, \mathbf{v})) = \nabla \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}})(u, \mathbf{v}) \neq \nabla \mathbf{H}^{(i)}(\bar{\gamma}, \bar{\mathbf{x}})(u, \mathbf{v}). \quad (11) \end{aligned}$$

Now, let us take $(u, \mathbf{v}) \in B((\gamma', \mathbf{x}'), \delta')$ arbitrary but fixed and define $\phi, \phi^{(i)}: \mathbb{R} \rightarrow \mathbb{R}^N$ by

$$\phi: r \mapsto \mathbf{H}(\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v}), \quad \phi^{(i)}: r \mapsto \mathbf{H}^{(i)}(\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v}).$$

Clearly,

$$\boldsymbol{\phi}'(r) = \mathbf{H}'((\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v}); (u, \mathbf{v})), \quad (\boldsymbol{\phi}^{(i)})'(r) = \nabla \mathbf{H}^{(i)}(\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v})(u, \mathbf{v})$$

and by virtue of (9), (10) and (11),

$$\forall i \in I: \boldsymbol{\phi}^{(i)}(0) = \boldsymbol{\phi}(0), \quad (12)$$

$$\forall i \neq i_0 \forall r \in [0, \bar{r}): |(\boldsymbol{\phi}_{j(i)}^{(i)})'(r) - (\boldsymbol{\phi}_{j(i)}^{(i_0)})'(r)| > 0,$$

$$\forall i \neq i_0: \boldsymbol{\phi}'(0) \neq (\boldsymbol{\phi}^{(i)})'(0). \quad (13)$$

As $\boldsymbol{\phi}^{(i)}$ are of the class C^1 , we obtain

$$\begin{aligned} \forall i \neq i_0 \forall r \in (0, \bar{r}): |\boldsymbol{\phi}_{j(i)}^{(i)}(r) - \boldsymbol{\phi}_{j(i)}^{(i_0)}(r)| &= \left| \int_0^r (\boldsymbol{\phi}_{j(i)}^{(i)})'(t) - (\boldsymbol{\phi}_{j(i)}^{(i_0)})'(t) dt \right| \\ &= \int_0^r |(\boldsymbol{\phi}_{j(i)}^{(i)})'(t) - (\boldsymbol{\phi}_{j(i)}^{(i_0)})'(t)| dt > 0 \end{aligned} \quad (14)$$

because $(\boldsymbol{\phi}_{j(i)}^{(i)})'(t) - (\boldsymbol{\phi}_{j(i)}^{(i_0)})'(t)$ may not change its sign due to continuity.

On the basis of these relations, we shall prove that

$$\forall r \in [0, \bar{r}): \boldsymbol{\phi}(r) = \boldsymbol{\phi}^{(i_0)}(r). \quad (15)$$

Firstly, let us suppose that one can find $\{r_n\}_{n \in \mathbb{N}}$, $r_n \rightarrow 0_+$, and $\{i_n\}_{n \in \mathbb{N}}$, $i_0 \neq i_n \in I$, such that $\boldsymbol{\phi}(r_n) = \boldsymbol{\phi}^{(i_n)}(r_n)$. Since I is finite by definition, we may suppose that r_n are chosen so that $i_n = \tilde{i}$ for some $i_0 \neq \tilde{i} \in I$ fixed. From here and (12),

$$\boldsymbol{\phi}'(0) = \lim_{n \rightarrow \infty} \frac{\boldsymbol{\phi}(r_n) - \boldsymbol{\phi}(0)}{r_n} = \lim_{n \rightarrow \infty} \frac{\boldsymbol{\phi}^{(\tilde{i})}(r_n) - \boldsymbol{\phi}^{(\tilde{i})}(0)}{r_n} = (\boldsymbol{\phi}^{(\tilde{i})})'(0),$$

which contradicts (13). Hence, there exists $\tilde{r} > 0$ such that

$$\forall r \in [0, \tilde{r}): \boldsymbol{\phi}(r) = \boldsymbol{\phi}^{(i_0)}(r).$$

From continuity of $\boldsymbol{\phi}$ and $\boldsymbol{\phi}^{(i)}$ and (14), it is readily seen that we can take $\tilde{r} = \bar{r}$, that is, (15) holds. By definition of $\boldsymbol{\phi}$ and $\boldsymbol{\phi}^{(i_0)}$, this means that

$$\forall r \in [0, \bar{r}) \forall (u, \mathbf{v}) \in B((\gamma', \mathbf{x}'), \delta'): \mathbf{H}(\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v}) = \mathbf{H}^{(i_0)}(\bar{\gamma} + ru, \bar{\mathbf{x}} + r\mathbf{v}). \quad (16)$$

Let us define a cone \mathcal{C} and a number $\hat{\delta}$ by

$$\begin{aligned} \mathcal{C} &:= \bigcup_{r \geq 0} rB((\gamma', \mathbf{x}'), \delta'), \\ \hat{\delta} &:= \bar{r} \min\{\|(u, \mathbf{v})\|; (u, \mathbf{v}) \in B((\gamma', \mathbf{x}'), \delta')\}. \end{aligned}$$

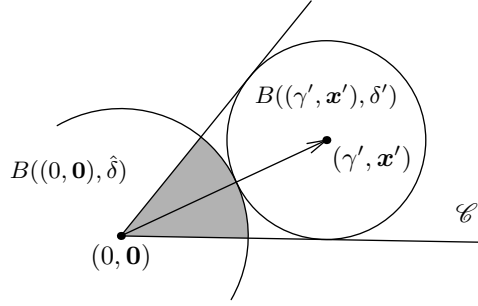


Figure 1: Intersection $\mathcal{C} \cap B((0, \mathbf{0}), \hat{\delta})$.

Obviously, $\hat{\delta}$ is positive (by (11), for example) and from (16), it follows that

$$\forall (u', v') \in \mathcal{C} \cap B((0, \mathbf{0}), \hat{\delta}): \mathbf{H}(\bar{\gamma} + u', \bar{\mathbf{x}} + v') = \mathbf{H}^{(i_0)}(\bar{\gamma} + u', \bar{\mathbf{x}} + v') \quad (17)$$

(see Figure 1). Having this result at hand, it is now easy to verify (8).

Indeed, (7) furnishes us with $\delta > 0$ such that

$$\begin{aligned} \forall s \in (\bar{s}, \bar{s} + \delta): \frac{\mathbf{c}(s) - \mathbf{c}(\bar{s})}{s - \bar{s}} &\in B((\gamma', \mathbf{x}'), \delta'), \\ \forall s \in [\bar{s}, \bar{s} + \delta): \mathbf{c}(s) - \mathbf{c}(\bar{s}) &\in (s - \bar{s})B((\gamma', \mathbf{x}'), \delta') \subset \mathcal{C}. \end{aligned}$$

Taking into account continuity of \mathbf{c} and reducing δ if necessary, we also have:

$$\forall s \in [\bar{s}, \bar{s} + \delta): \mathbf{c}(s) - \mathbf{c}(\bar{s}) \in B((0, \mathbf{0}), \hat{\delta}).$$

Hence, invoking (3)(j) and (17), we arrive at (8):

$$\begin{aligned} \forall s \in [\bar{s}, \bar{s} + \delta): \mathbf{H}^{(i_0)}(\mathbf{c}(s)) &= \mathbf{H}^{(i_0)}(\mathbf{c}(\bar{s}) + \mathbf{c}(s) - \mathbf{c}(\bar{s})) = \mathbf{H}^{(i_0)}((\bar{\gamma}, \bar{\mathbf{x}}) + \mathbf{c}(s) - \mathbf{c}(\bar{s})) \\ &= \mathbf{H}((\bar{\gamma}, \bar{\mathbf{x}}) + \mathbf{c}(s) - \mathbf{c}(\bar{s})) = \mathbf{H}(\mathbf{c}(s)). \end{aligned}$$

Finally, for any curve $\tilde{\mathbf{c}}$ satisfying (4), the same arguments give

$$\mathbf{H}^{(i_0)}(\tilde{\mathbf{c}}(s)) = \mathbf{H}(\tilde{\mathbf{c}}(s)) = \mathbf{0} \text{ for } s \geq \bar{s}, s \text{ close to } \bar{s},$$

and uniqueness of the implicit function determined by the equation $\mathbf{H}^{(i_0)}(\gamma, \mathbf{x}) = \mathbf{0}$ in a vicinity of $(\bar{\gamma}, \bar{\mathbf{x}})$ completes the claim. \square

The following examples of scalar functions of two variables show what can happen when the assumptions (5)(ii) or (iii) of the previous theorem are not fulfilled.

Example 1 (the null direction of the derivative of \mathbf{H} is in the kernel of gradients of more than one selection function). Let G and H be defined by

$$G(\gamma, x) := \begin{cases} G^{(1)}(\gamma, x) := -x + \gamma & \text{if } \gamma \leq 0, x \leq 0; \\ G^{(2)}(\gamma, x) := -x + \gamma^2 & \text{if } \gamma \geq 0, x \leq 0; \\ G^{(3)}(\gamma, x) := x + \gamma^2 & \text{if } \gamma \geq 0, x \geq 0; \\ G^{(4)}(\gamma, x) := x + \gamma & \text{if } \gamma \leq 0, x \geq 0; \end{cases}$$

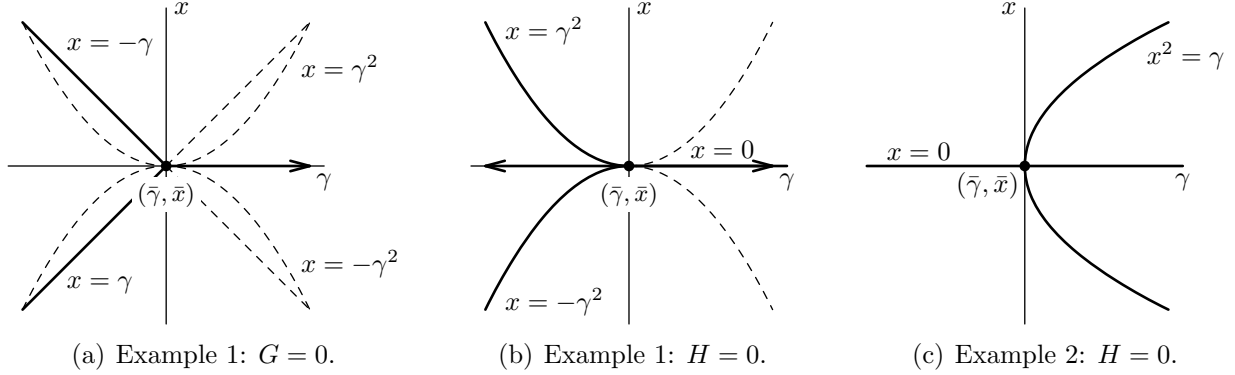


Figure 2: Violation of the assumptions in (5): (a), (b) the null direction in the kernel of two selection functions; (c) singularity of the partial gradient with respect to x .

$$H(\gamma, x) := \begin{cases} H^{(1)}(\gamma, x) := x + \gamma^2 & \text{if } \gamma \leq 0, x \leq 0; \\ H^{(2)}(\gamma, x) := x & \text{if } \gamma \geq 0, x \leq 0; \\ H^{(3)}(\gamma, x) := -x & \text{if } \gamma \geq 0, x \geq 0; \\ H^{(4)}(\gamma, x) := -x + \gamma^2 & \text{if } \gamma \leq 0, x \geq 0 \end{cases}$$

and $(\bar{\gamma}, \bar{x}) := (0, 0)$. Then

$$\begin{aligned} G'((\bar{\gamma}, \bar{x}); (1, 0)) &= 0 = \nabla G^{(2)}(\bar{\gamma}, \bar{x}) \cdot (1, 0) = \nabla G^{(3)}(\bar{\gamma}, \bar{x}) \cdot (1, 0), \\ H'((\bar{\gamma}, \bar{x}); (1, 0)) &= 0 = \nabla H^{(2)}(\bar{\gamma}, \bar{x}) \cdot (1, 0) = \nabla H^{(3)}(\bar{\gamma}, \bar{x}) \cdot (1, 0), \\ H'((\bar{\gamma}, \bar{x}); (-1, 0)) &= 0 = \nabla H^{(1)}(\bar{\gamma}, \bar{x}) \cdot (-1, 0) = \nabla H^{(4)}(\bar{\gamma}, \bar{x}) \cdot (-1, 0). \end{aligned}$$

However, no solution branch of $G = 0$ emanates from $(\bar{\gamma}, \bar{x})$ in the direction $(1, 0)$, one solution branch of $H = 0$ emanates from $(\bar{\gamma}, \bar{x})$ in the direction $(1, 0)$ and two solution branches of $H = 0$ emanate from $(\bar{\gamma}, \bar{x})$ in the direction $(-1, 0)$ (see Figures 2(a) and (b)). From here, one can see that neither uniqueness nor existence of solution branches can be either guaranteed or excluded in the null direction of the derivative on the basis of the first-order analysis only.

Example 2 (singularity of the partial gradient with respect to \mathbf{x}). Let $H: \mathbb{R}^2 \rightarrow \mathbb{R}$ be a smooth function defined by $H(\gamma, x) := x(x^2 - \gamma)$ (that is, $H^{(1)} = H$ is the only selection function) and $(\bar{\gamma}, \bar{x}) := (0, 0)$. Then $\nabla H(\bar{\gamma}, \bar{x}) = (0, 0)^\top$ and $H'((\bar{\gamma}, \bar{x}); (\gamma', x')) = 0$ for any $(\gamma', x') \in \mathbb{R}^2$. On the other hand, $H^{-1}(0)$ is formed by two curves that intersect at $(\bar{\gamma}, \bar{x})$ and their tangents at $(\bar{\gamma}, \bar{x})$ are linearly independent (see Figure 2(c)).

Let us note that this example is a case of a (smooth) bifurcation (for its definition, see, for instance, [3, Section 24]). In general, if (5)(iii) does not hold, a bifurcation can occur in the solution set of $\mathbf{H}^{(i_0)} = \mathbf{0}$, whose subset can form a part of the solution set of $\mathbf{H} = \mathbf{0}$.

Remark 2. Apparently, solution curves of $\mathbf{H}(\gamma, \mathbf{x}) = \mathbf{0}$ do not have to be always parametrizable by γ (this will not be considered even in the next section). Nevertheless, it is readily

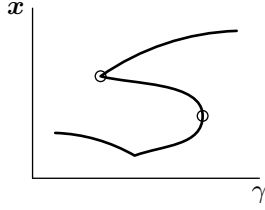


Figure 3: A PC^1 -curve with smooth and non-smooth folds.

seen that one can interchange the role of γ and \mathbf{x} with the role of x_j and the N -tuple $(\gamma, x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_N)$, respectively, for any $j = 1, \dots, N$ in the previous analysis and all the results can be generalised in this way. In particular, the assumption (5)(iii) in Theorem 2 can be replaced by the following weaker assumption:

$$(iii) \quad \nabla \mathbf{H}^{(i_0)}(\bar{\gamma}, \bar{\mathbf{x}}) \text{ has } N \text{ linearly independent columns.} \quad (5')$$

4 Numerical Continuation

This section describes a numerical method for tracing PC^1 solution curves of (\mathcal{P}) . It is capable of traversing folds (also called turning points) with respect to the parameter γ , where it is not possible to parametrise the curve by γ . Let us note that apart from folds known from theory of classical continuations, we have to deal with folds where \mathbf{H} is not Gâteaux-differentiable, as well (see Figure 3 for illustration).

We shall not make an explicit difference between the state variable \mathbf{x} and the parameter γ and we shall consider a uniform formulation of (\mathcal{P}) , namely,

$$\mathbf{H}(\mathbf{y}) = \mathbf{0}$$

with $\mathbf{y} = (\gamma, \mathbf{x})$. Nevertheless, to avoid bad scaling when calculating tangents, for example, we shall use the following weighted scalar product and norm:

$$(\mathbf{y}, \tilde{\mathbf{y}})_w := y_\gamma \tilde{y}_\gamma + \kappa \mathbf{y}_x^\top \tilde{\mathbf{y}}_x, \quad \|\mathbf{y}\|_w := \sqrt{(\mathbf{y}, \mathbf{y})_w}, \quad \mathbf{y} = (y_\gamma, \mathbf{y}_x), \quad \tilde{\mathbf{y}} = (\tilde{y}_\gamma, \tilde{\mathbf{y}}_x)$$

as proposed in [8, pp. 86 and 87]. Here, κ should be chosen so that $\kappa \mathbf{y}_x^\top \tilde{\mathbf{y}}_x$ is proportional to the scalar product of the corresponding spatial variables, usually in L^2 . One can take, for instance, $\kappa = h^d$, where h is the mesh size and d stands for the dimension of the underlying problem. Alternatively, κ can be chosen as $1/N$, for simplicity.

The principal idea of our continuation strategy is the same as the one proposed in [7, 6], namely, to continue smooth pieces of solution curves by a predictor-corrector method and to join the smooth pieces continuously.

The predictor-corrector method employed here is a slight modification of the inexact Moore-Penrose continuation implemented in MATCONT [4], which can be viewed as an approximation of a continuation routine making use of the Moore-Penrose pseudo-inverse. It computes a sequence of points $\{\mathbf{y}_k\}$ lying approximately on a solution curve and a

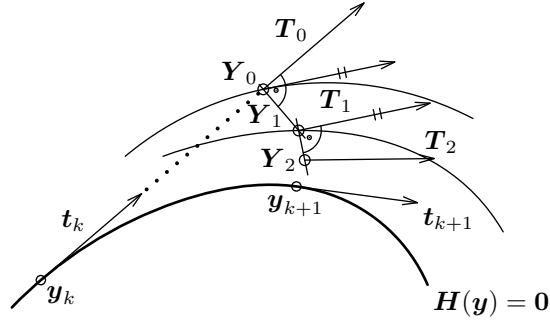


Figure 4: Inexact Moore-Penrose predictor-corrector.

sequence of the corresponding unit tangent vectors $\{\mathbf{t}_k\}$. The method consists of two different steps: A predictor step generates an initial approximation of a new point in the direction of the tangent vector. Corrector steps, which are iterative steps of Newton's type, bring the predicted point back to the curve as illustrated in Figure 4. Since points of non-differentiability of \mathbf{H} may be encountered in this procedure, the adaptation of the Newton steps for piecewise-smooth functions [5, 7.2.14 Algorithm] is used and gradients of active selection functions of \mathbf{H} are taken, in general. The following algorithm sketches our implementation.

Algorithm 1 (*Piecewise-smooth inexact Moore-Penrose predictor-corrector*).

Input data: $\varepsilon, \varepsilon' > 0$, $c_{\min} \leq 1$, $h_{\max} \geq h \geq h_{\min} > 0$, $h_{\text{inc}} > 1 > h_{\text{dec}} > 0$, $j_{\max} \geq j_{\text{thr}} > 0$ and $\mathbf{y}_0, \mathbf{t}_0 \in \mathbb{R}^{N+1}$ satisfying:

$$\|\mathbf{H}(\mathbf{y}_0)\| \leq \varepsilon, \quad \mathbf{H}'(\mathbf{y}_0; \mathbf{t}_0) = \mathbf{0}, \quad \|\mathbf{t}_0\|_w = 1.$$

Step 1: Set $k := 0$.

Step 2: Set $n_{\text{dec}} := 0$.

Step 3 (*predictor step*): Set $j := 0$ and

$$\mathbf{Y}_0 := \mathbf{y}_k + h\mathbf{t}_k, \quad \mathbf{T}_0 := \mathbf{t}_k.$$

Step 4 (*corrector step*): Select an index i_j from $I_{\mathbf{H}}(\mathbf{Y}_j)$, find \mathbf{Y}_{j+1} and $\tilde{\mathbf{T}}$ such that

$$\begin{aligned} \nabla \mathbf{H}^{(i_j)}(\mathbf{Y}_j)(\mathbf{Y}_{j+1} - \mathbf{Y}_j) &= -\mathbf{H}(\mathbf{Y}_j), & \nabla \mathbf{H}^{(i_j)}(\mathbf{Y}_j)\tilde{\mathbf{T}} &= \mathbf{0}, \\ \mathbf{T}_j^\top(\mathbf{Y}_{j+1} - \mathbf{Y}_j) &= 0, & (\tilde{\mathbf{T}}, \mathbf{T}_j)_w &= 1 \end{aligned}$$

and set

$$\mathbf{T}_{j+1} := \tilde{\mathbf{T}} / \|\tilde{\mathbf{T}}\|_w.$$

Step 5: If $\|\mathbf{H}(\mathbf{Y}_{j+1})\| \leq \varepsilon$ and $\|\mathbf{Y}_{j+1} - \mathbf{Y}_j\|_w \leq \varepsilon'$, go to Step 8.

Step 6: If $j < j_{\max}$, set $j := j + 1$ and go to Step 4.

Step 7: If $h > h_{\min}$, set $h := \max\{h_{\text{dec}}h, h_{\min}\}$, $n_{\text{dec}} := n_{\text{dec}} + 1$ and go to Step 3. Otherwise, break; predictor-corrector has failed.

Step 8: If $\mathbf{T}_{j+1}^\top \mathbf{t}_k < c_{\min}$, go to Step 7. Otherwise, set

$$\begin{aligned} \mathbf{y}_{k+1} &:= \mathbf{Y}_{j+1}, & \mathbf{t}_{k+1} &:= \mathbf{T}_{j+1}, \\ \text{if } j < j_{\text{thr}} \text{ and } n_{\text{dec}} = 0, & \text{ then } h &:= \min\{h_{\text{inc}}h, h_{\max}\}. \end{aligned}$$

Set $k := k + 1$ and go to Step 2.

Here, ε and ε' are convergence tolerances and c_{\min} serves for controlling changes of direction between the tangent vectors at two consecutive points. Further, h_{\max} and h_{\min} are the maximal and the minimal step lengths used in the predictor step, respectively, and h_{inc} and h_{dec} are scale factors for adjusting the step length h . It is shortened in the case of non-convergence of the corrector or too large deviation between the newly computed tangent and the previous one. On the other hand, it is elongated for the next predictor step if the last computed couple is accepted, the number of corrector steps does not reach j_{thr} and the number n_{dec} of step length reductions of h for the current value of k is zero. Finally, j_{\max} stands for the maximal number of corrector steps allowed.

We have chosen the inexact Moore-Penrose predictor-corrector for our continuation technique because it is an efficient path-following method that can traverse smooth folds with respect to the parameter. From our experience, it may pass also over points of non-differentiability if the test on the tangent direction is satisfied. However, we have encountered points of non-differentiability where our predictor-corrector failed to converge and its improvement was needed to overcome this difficulty.

Let $\bar{\mathbf{y}}$ be a point of non-differentiability on the solution curve that we want to pass over. The analysis in the previous section suggests to compute $\bar{\mathbf{y}}$, solve $\mathbf{H}'(\bar{\mathbf{y}}; \mathbf{t}) = \mathbf{0}$ for a new tangent direction \mathbf{t} and restart the predictor-corrector with $\bar{\mathbf{y}}$ and \mathbf{t} . However, this approach requires an explicit knowledge of sub-domains where \mathbf{H} coincides with its individual selection functions, which does not have to be always at one's disposal.

To avoid this requirement, we shall present another approach that consists in restarting the predictor-corrector with an approximation of the couple $(\bar{\mathbf{y}}, \mathbf{t})$. It is applicable in the most probable case when only two selection functions of \mathbf{H} are active at $\bar{\mathbf{y}}$, $\mathbf{H}^{(1)}$ and $\mathbf{H}^{(2)}$, and the adjacent smooth pieces of the solution curve \mathbf{c} solve $\mathbf{H}^{(1)} = \mathbf{0}$ and $\mathbf{H}^{(2)} = \mathbf{0}$, respectively. Moreover, we shall restrict ourselves to the case when the one-sided tangent directions to the solution curve, say $\mathbf{t}^{(1)}$ and $\mathbf{t}^{(2)}$, do not lie on a line (otherwise, we would have no problem with the tangent predictor). In addition, we shall suppose that

$$\nabla \mathbf{H}^{(1)}(\bar{\mathbf{y}}) \text{ and } \nabla \mathbf{H}^{(2)}(\bar{\mathbf{y}}) \text{ have both the maximal rank } N \quad (18)$$

(compare (5')). For the sake of simplicity of our exposition, we shall also assume that the set $\{\mathbf{y} \in \mathbb{R}^{N+1}; \mathbf{H}(\mathbf{y}) = \mathbf{H}^{(1)}(\mathbf{y}) = \mathbf{H}^{(2)}(\mathbf{y})\}$ forms an N -dimensional C^1 -manifold in a

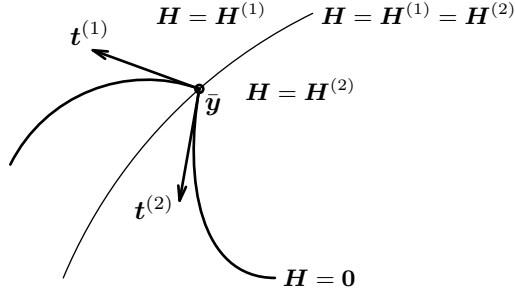


Figure 5: Transition between smooth pieces of the solution curve.

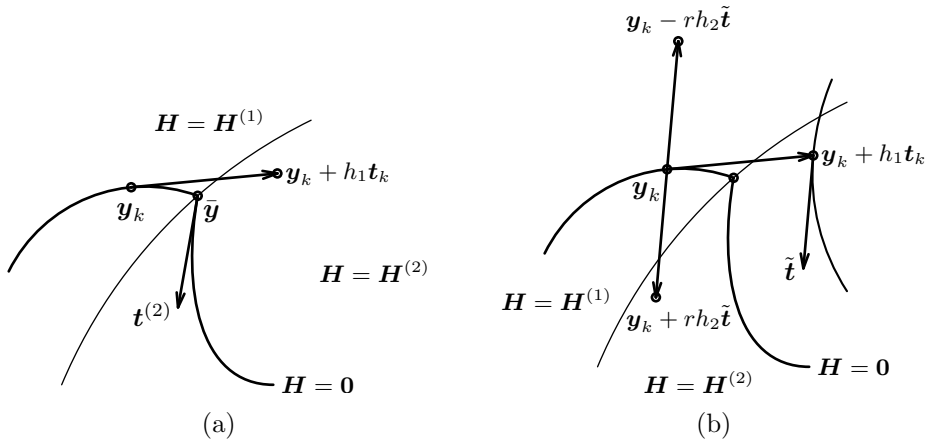


Figure 6: Approximation of a new tangent direction.

neighbourhood of $\bar{\mathbf{y}}$ (this is satisfied, for example, when there exists a function $\rho: \mathbb{R}^{N+1} \rightarrow \mathbb{R}$ of the class C^1 such that $\rho(\mathbf{y}) = 0$ iff $\mathbf{H}^{(1)}(\mathbf{y}) = \mathbf{H}^{(2)}(\mathbf{y})$ in a vicinity of $\bar{\mathbf{y}}$ and $\nabla \rho(\bar{\mathbf{y}}) \neq \mathbf{0}$). The overall considered situation is depicted in Figure 5.

Now, let an approximation of the solution piece $\{\mathbf{y} \in \mathbb{R}^{N+1}; \mathbf{H}(\mathbf{y}) = \mathbf{H}^{(1)}(\mathbf{y}) = \mathbf{0}\}$ be known from the predictor-corrector run through till $h = h_{\min}$, $(\mathbf{y}_k, \mathbf{t}_k)$ denotes the last computed couple and we want to pass to the piece $\{\mathbf{y} \in \mathbb{R}^{N+1}; \mathbf{H}(\mathbf{y}) = \mathbf{H}^{(2)}(\mathbf{y}) = \mathbf{0}\}$. To do this, we seek approximations of $\bar{\mathbf{y}}$ and $\mathbf{t}^{(2)}$ as suggested before.

Firstly, let us observe that when we choose the minimal step length h_{\min} sufficiently small, the predictor-corrector follows the first part of the solution curve corresponding to $\mathbf{H}^{(1)}(\mathbf{y}) = \mathbf{0}$ very close to $\bar{\mathbf{y}}$ as it generates points from the sub-domain $\{\mathbf{y} \in \mathbb{R}^{N+1}; \mathbf{H}(\mathbf{y}) = \mathbf{H}^{(1)}(\mathbf{y})\}$ of smooth behaviour if the step length h in the predictor step is small enough. Hence, \mathbf{y}_k can be supposed to be a good approximation of $\bar{\mathbf{y}}$.

Secondly, to compute an approximation of $\mathbf{t}^{(2)}$, we shall make use of the equality

$$\mathbf{H}'(\bar{\mathbf{y}}; \mathbf{t}^{(2)}) = \nabla \mathbf{H}^{(2)}(\bar{\mathbf{y}}) \mathbf{t}^{(2)} = \mathbf{0}$$

(see Figure 5). Figure 6(a) shows that taking h_1 sufficiently large in comparison with the value of h_{\min} (but not too large to remain in the neighbourhood of $\bar{\mathbf{y}}$ where Figure 5 is relevant), the point $\mathbf{y}_k + h_1 \mathbf{t}_k$ belongs to the interior of the sub-domain $\{\mathbf{y} \in \mathbb{R}^{N+1}; \mathbf{H}(\mathbf{y}) =$

$\mathbf{H}^{(2)}(\mathbf{y})\}$. Therefore, \mathbf{H} is Fréchet-differentiable there and

$$\nabla \mathbf{H}(\mathbf{y}_k + h_1 \mathbf{t}_k) = \nabla \mathbf{H}^{(2)}(\mathbf{y}_k + h_1 \mathbf{t}_k) \approx \nabla \mathbf{H}^{(2)}(\bar{\mathbf{y}})$$

if $\mathbf{y}_k + h_1 \mathbf{t}_k$ remains sufficiently close to $\bar{\mathbf{y}}$. According to (18), $\nabla \mathbf{H}(\mathbf{y}_k + h_1 \mathbf{t}_k)$ has still rank N for h_1 not too large and $\text{span}\{\mathbf{t}^{(2)}\}$ can be approximated by $\text{span}\{\tilde{\mathbf{t}}\}$ if $\tilde{\mathbf{t}}$ solves

$$\nabla \mathbf{H}(\mathbf{y}_k + h_1 \mathbf{t}_k) \tilde{\mathbf{t}} = \mathbf{0}, \quad \|\tilde{\mathbf{t}}\|_w = 1.$$

Finally, we have to determine an appropriate direction of $\tilde{\mathbf{t}}$. Figure 6(b) illustrates that there exists $r \in \{\pm 1\}$ such that $\mathbf{y}_k - rh_2 \tilde{\mathbf{t}}$ remains in $\{\mathbf{y} \in \mathbb{R}^{N+1}; \mathbf{H}(\mathbf{y}) = \mathbf{H}^{(1)}(\mathbf{y})\}$ for any h_2 positive (restricting ourselves to the values of h_2 such that $\mathbf{y}_k \pm h_2 \tilde{\mathbf{t}}$ is in the neighbourhood of $\bar{\mathbf{y}}$). This can be recognised by the fact that $\frac{|\mathbf{t}_-^\top \tilde{\mathbf{t}}|}{\|\mathbf{t}_-\| \|\tilde{\mathbf{t}}\|}$ is observably smaller than 1 for \mathbf{t}_- with $\nabla \mathbf{H}(\mathbf{y}_k - rh_2 \tilde{\mathbf{t}}) \mathbf{t}_- = \mathbf{0}$. By $\|\cdot\|$, we denote the Euclidean norm here and in what follows.

On the other hand, $\mathbf{y}_k + rh_2 \tilde{\mathbf{t}}$ appears in $\{\mathbf{y} \in \mathbb{R}^{N+1}; \mathbf{H}(\mathbf{y}) = \mathbf{H}^{(2)}(\mathbf{y})\}$ for h_2 larger than some positive threshold. For such values, $\frac{|\mathbf{t}_+^\top \tilde{\mathbf{t}}|}{\|\mathbf{t}_+\| \|\tilde{\mathbf{t}}\|}$ is close to 1 for \mathbf{t}_+ from the kernel of $\nabla \mathbf{H}(\mathbf{y}_k + rh_2 \tilde{\mathbf{t}})$.

This suggests the following procedure for selecting the desired direction of $\tilde{\mathbf{t}}$: Increase the values of h_2 successively and when you arrive at h_2 and $r \in \{\pm 1\}$ such that

$$\frac{|\mathbf{t}^\top \tilde{\mathbf{t}}|}{\|\mathbf{t}\| \|\tilde{\mathbf{t}}\|} \approx 1, \quad \nabla \mathbf{H}(\mathbf{y}_k + rh_2 \tilde{\mathbf{t}}) \mathbf{t} = \mathbf{0}, \quad \|\mathbf{t}\|_w = 1,$$

take $r\tilde{\mathbf{t}}$ as an approximation of $\mathbf{t}^{(2)}$.

The overall algorithm for finding a new tangent direction can be sketched as follows.

Algorithm 2 (*Simple tangent switch*).

Input data: $h_1, h_2 > 0$, $c_{\min} \leq 1$ and $\mathbf{y}, \mathbf{t} \in \mathbb{R}^{N+1}$ with $\|\mathbf{t}\|_w = 1$.

Step 1: Compute $\tilde{\mathbf{t}}$ such that

$$\nabla \mathbf{H}(\mathbf{y} + h_1 \mathbf{t}) \tilde{\mathbf{t}} = \mathbf{0}, \quad \|\tilde{\mathbf{t}}\|_w = 1.$$

Step 2: Find \mathbf{t}_+ and \mathbf{t}_- such that

$$\nabla \mathbf{H}(\mathbf{y} \pm h_2 \tilde{\mathbf{t}}) \mathbf{t}_\pm = \mathbf{0}, \quad \|\mathbf{t}_\pm\|_w = 1.$$

Step 3: If $\frac{|\mathbf{t}_+^\top \tilde{\mathbf{t}}|}{\|\mathbf{t}_+\| \|\tilde{\mathbf{t}}\|} \geq c_{\min}$, then set $\mathbf{t} := \tilde{\mathbf{t}}$.

Otherwise, if $\frac{|\mathbf{t}_-^\top \tilde{\mathbf{t}}|}{\|\mathbf{t}_-\| \|\tilde{\mathbf{t}}\|} \geq c_{\min}$, set $\mathbf{t} := -\tilde{\mathbf{t}}$.

Otherwise, increase h_2 and go to Step 2.

The value of c_{\min} should be chosen the same or close to the one in Algorithm 1 whereas the value of h_1 should be a bit greater than h_{\min} from Algorithm 1. In our computations, $h_1 = 1.5h_{\min}$ showed to be reliable. Finally, in our test examples in [9], we take $h_2 = h_{\min}$ at the beginning and we increase the values of h_2 by adding $h_{\min} \cdot 10^{\lfloor \log_{10}(h/h_{\min}) \rfloor}$ to it in Step 3. Here, $\lfloor \cdot \rfloor$ stands for the lower integer part.

To sum up, the whole numerical continuation of (\mathcal{P}) is started with the predictor-corrector (Algorithm 1) with a point \mathbf{y}_0 approximating a solution and the corresponding unit tangent \mathbf{t}_0 in the direction of desired continuation. If the predictor-corrector fails for some value of k , the simple tangent switch is run with the last computed couple $(\mathbf{y}_k, \mathbf{t}_k)$. After finding a new tangent direction \mathbf{t} , one restarts the predictor-corrector with $(\mathbf{y}_k, \mathbf{t})$ and continues tracing a solution curve. Let us point out that this method shows to work well even for curves involving non-smooth folds in our test examples.

5 Conclusion

We have proposed a continuation problem for finding solutions of discretised abstract first-order evolution problems with the property that any solution from one time level of the discretised problem furnishes us with an initial point for computing solutions on the next time level. Confining ourselves to a PC^1 continuation problem, we have proved local existence and uniqueness of solution curves under assumptions required by an appropriate implicit function theorem. Moreover, we have derived a first-order system characterising one-sided tangents to curves solving the continuation problem and we have stated criteria guaranteeing existence and uniqueness of solutions of this system.

Possibility of continuation in the direction of a null vector of the first-order system has been deeply discussed. In particular, it has been shown that if the null vector is directed at the interior of a sub-domain of smooth behaviour and if the corresponding selection function has the maximal rank, then there exists a unique solution curve emanating in that direction (Theorem 2). In addition, it has been demonstrated on simple examples what can happen when one of these two assumptions is violated. We believe that this analysis gives insight into possible scenarios during piecewise-smooth continuation.

Finally, an easy-to-implement restarted predictor-corrector continuation method of PC^1 solution curves has been described. It is capable of passing over points on transitions between two different selection functions and of traversing smooth as well as non-smooth folds. Numerical tests will be presented in the companion paper [9].

A Piecewise-Differentiable Functions

For the sake of completeness of our exposition, we introduce basic notions and results from theory of piecewise-differentiable functions here. Our presentation is extracted from [11, 10].

Definition 1. (i) A function $\mathbf{H}: \mathbb{R}^M \rightarrow \mathbb{R}^N$ is PC^1 if it is continuous and for every

$\bar{\mathbf{y}} \in \mathbb{R}^M$, there exist an open neighbourhood O of $\bar{\mathbf{y}}$ and a finite family of C^1 -functions $\mathbf{H}^{(i)}: O \rightarrow \mathbb{R}^N$, $i \in I$, such that

$$\forall \mathbf{y} \in O: \mathbf{H}(\mathbf{y}) \in \{\mathbf{H}^{(i)}(\mathbf{y}); i \in I\}.$$

The functions $\mathbf{H}^{(i)}$ are termed *selection functions* of \mathbf{H} at $\bar{\mathbf{y}}$.

(ii) A selection function $\mathbf{H}^{(i)}$ of a PC^1 -function \mathbf{H} is called *active* at $\bar{\mathbf{y}}$ if

$$\mathbf{H}^{(i)}(\bar{\mathbf{y}}) = \mathbf{H}(\bar{\mathbf{y}})$$

and *essentially active* at $\bar{\mathbf{y}}$ if

$$\bar{\mathbf{y}} \in \overline{\text{Int}\{\mathbf{y} \in O; \mathbf{H}^{(i)}(\mathbf{y}) = \mathbf{H}(\mathbf{y})\}}.$$

The set of indices of active and essentially active selection functions of \mathbf{H} at $\bar{\mathbf{y}}$ are denoted by $I_{\mathbf{H}}(\bar{\mathbf{y}})$ and $I_{\mathbf{H}}^e(\bar{\mathbf{y}})$, respectively.

Due to continuity, selection functions can be chosen at every point $\bar{\mathbf{y}}$ so that they are all active there. One can also show that every PC^1 -function is locally Lipschitz continuous and Bouligand-differentiable (B-differentiable). Let us recall that the B-derivative of \mathbf{H} at \mathbf{y} in the direction \mathbf{z} is the directional derivative $\mathbf{H}'(\mathbf{y}; \mathbf{z})$ that satisfies:

$$\lim_{\mathbf{z} \rightarrow \mathbf{0}} \frac{\|\mathbf{H}(\mathbf{y} + \mathbf{z}) - \mathbf{H}(\mathbf{y}) - \mathbf{H}'(\mathbf{y}; \mathbf{z})\|}{\|\mathbf{z}\|} = 0.$$

The following chain rule holds for B-derivatives:

Proposition 3. *Let $\mathbf{G}: \mathbb{R}^M \rightarrow \mathbb{R}^N$ and $\mathbf{H}: \mathbb{R}^N \rightarrow \mathbb{R}^P$ be locally Lipschitz continuous and B-differentiable at \mathbf{y} and $\mathbf{G}(\mathbf{y})$, respectively. Then the composite function $\mathbf{H} \circ \mathbf{G}$ is B-differentiable at \mathbf{y} and*

$$(\mathbf{H} \circ \mathbf{G})'(\mathbf{y}; \mathbf{z}) = \mathbf{H}'(\mathbf{G}(\mathbf{y}); \mathbf{G}'(\mathbf{y}; \mathbf{z})).$$

The following definition introduces two important notions for PC^1 -functions.

Definition 2. Let $\mathbf{H}: \mathbb{R}^N \times \mathbb{R}^M \rightarrow \mathbb{R}^N$ be a PC^1 -function with essentially active selection functions $\mathbf{H}^{(1)}, \dots, \mathbf{H}^{(n)}$ at $(\bar{\mathbf{x}}, \bar{\mathbf{y}})$.

(i) The function \mathbf{H} is called *coherently oriented* with respect to \mathbf{x} at $(\bar{\mathbf{x}}, \bar{\mathbf{y}})$ iff the partial gradients $\nabla_{\mathbf{x}} \mathbf{H}^{(i)}(\bar{\mathbf{x}}, \bar{\mathbf{y}})$, $i = 1, \dots, n$, have the same non-vanishing determinantal sign.

(ii) The function \mathbf{H} is *completely coherently oriented* with respect to \mathbf{x} at $(\bar{\mathbf{x}}, \bar{\mathbf{y}})$ if all matrices of the form

$$\begin{pmatrix} \nabla_{\mathbf{x}} H_1^{(i_1)}(\bar{\mathbf{x}}, \bar{\mathbf{y}})^\top \\ \nabla_{\mathbf{x}} H_2^{(i_2)}(\bar{\mathbf{x}}, \bar{\mathbf{y}})^\top \\ \vdots \\ \nabla_{\mathbf{x}} H_N^{(i_N)}(\bar{\mathbf{x}}, \bar{\mathbf{y}})^\top \end{pmatrix},$$

where $i_1, i_2, \dots, i_N \in \{1, \dots, n\}$, have the same non-vanishing determinantal sign.

We say that \mathbf{H} is (completely) coherently oriented with respect to \mathbf{x} if it is (completely) coherently oriented with respect to \mathbf{x} on $\mathbb{R}^N \times \mathbb{R}^M$. Besides, if $M = 0$, that is, if the dimensions of the preimage and image space of \mathbf{H} coincide, then we simply speak of (complete) coherent orientation of \mathbf{H} .

A special case of a PC^1 -function is a *piecewise-linear* function. It is a continuous function whose selection functions are linear, that is, of the form $\mathbf{y} \mapsto \mathbf{A}^{(i)}\mathbf{y}$ for some matrices $\mathbf{A}^{(i)}$. It is known that the B-derivative $\mathbf{H}'(\mathbf{y}; \cdot)$ of a PC^1 -function \mathbf{H} is a piecewise-linear function. In fact, $\mathbf{H}'(\mathbf{y}; \cdot)$ is Lipschitz-continuous and

$$\mathbf{H}'(\mathbf{y}; \mathbf{z}) \in \{\nabla \mathbf{H}^{(i)}(\mathbf{y})\mathbf{z}; i \in I_{\mathbf{H}}^c(\mathbf{y})\}$$

in this case.

Proposition 4. *A coherently oriented piecewise-linear function is surjective. If it is in addition completely coherently oriented, it is a homeomorphism.*

Proposition 5. *Let $\mathbf{H}: \mathbb{R}^N \times \mathbb{R}^M \rightarrow \mathbb{R}^N$ be a PC^1 -function. If \mathbf{H} is completely coherently oriented with respect to \mathbf{x} at a zero $(\bar{\mathbf{x}}, \bar{\mathbf{y}})$ of \mathbf{H} , then the equation $\mathbf{H}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$ determines a unique implicit PC^1 -function $\mathbf{x}(\mathbf{y})$ in a neighbourhood of $(\bar{\mathbf{x}}, \bar{\mathbf{y}})$.*

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