

On the numerical calculation of topological turning point

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On the numerical calculation of topological turning points

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We introduce the definition of topological turning point of a function $\mathcal{F}(x, \lambda) : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$, then we propose a numerical method for calculating it. This new definition does not require any regularity for \mathcal{F} but its continuity, moreover topological turning point coincides with turning point when \mathcal{F} is sufficiently smooth. The numerical method that we introduce has linear rate of convergence and it is of secure convergence.

Keywords: Critical point; Turning point; Direct method.

AMS Subject Classification: 2000 MSC: Primary: 65H10; Secondary: 58K05

1. Introduction

An open issue in applied mathematics is finding the *turning points* of the equation

$$\mathcal{F}(x, \lambda) = 0 \quad (1)$$

where \mathcal{F} maps \mathbb{R}^{n+1} in \mathbb{R}^n , $x \in \mathbb{R}^n$ is a variable and $\lambda \in \mathbb{R}$ is a parameter. The search for turning points arises in many physical problems as soon as the mathematical description of phenomena leads to (1). This problem has a long history but it is still of interest today, as it is shown by recent works on this topic and on related arguments [1, 2]. In studying equation (1) other interesting questions may arise such as the search for bifurcation points or the individual solution arcs to name but a few. For a description of these problems we refer to [3, 4] and references therein. A solution (x_c, λ_c) of (1) is said to be a turning point if the Jacobian of \mathcal{F} with respect to x is singular at that point, whereas the complete Jacobian of \mathcal{F} has maximum rank [5]. Turning points can be further classified by taking into account the number of successive null-derivatives (calculated at the turning point) of the curve solution of (1) [6]. This number identifies the order of the turning point and we can distinguish *simple* (first order) and *double* (second order) turning points and so on. In [6] *simple* turning points are distinguished from *non-simple* turning points.

We can identify two basic strategies for finding turning points, based on direct and indirect methods. The first one consists in completing (1) with some additional equations, which characterize turning points, in order to obtain a determined system that can be solved by Newton method (or its modification): this strategy is proposed in [5, 7–9] where different examples of characterizing equations for

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1 turning points are given (see also [10] and references therein). The second strat-
2 egy essentially applies methods developed for the arc following problem: one varies
3 the parameter λ and calculates the respective value of x such that (1) holds. This
4 is the strategy used, for example, in [3, 4, 11, 12] where the Newton method or
5 its modification is used to approximate the value of x . Another basic difference
6 between methods is in the use of derivatives of \mathcal{F} . Derivatives of \mathcal{F} are involved
7 in the definition of turning points and hence all the methods previously discussed
8 require certain data from them. However, it is possible to devise methods which in-
9 volve only suitable approximations when dealing with derivatives. These are called
10 *free-derivative methods* (see, for example, [3, 4]).

11 In this work we suggest the definition of *topological turning points*. The topolog-
12 ical approach to problems related to singular solution of (1) is not new: in [13],
13 this kind of problem is approached with linearization methods and differential-
14 topology arguments. We follow a different method, we base our investigations on
15 general-topology arguments we avoid any requests of regularity for \mathcal{F} apart from
16 its continuity. We consider the variable x of $\mathcal{F}(x, \lambda)$ as a scalar variable: although
17 this choice is actually a limitation with respect to the general case where x is a
18 **vector**, it turns out to be useful to handle the new definition. The reason for this
19 new definition is that a topological turning point is a turning point (of odd order)
20 if \mathcal{F} is sufficiently smooth and, conversely, any odd order turning point is a topo-
21 logical turning point. In particular, simple turning points are topological turning
22 points. Moreover, we introduce a numerical method for calculating a topological
23 turning point which represents the main result of the paper.

24 The method for calculating topological turning points inherits its properties from
25 traditional bisection: it has linear **rate of convergence** and it is of secure conver-
26 gence. It can be applied for the calculation of turning points **and** it requires fewer
27 conditions for \mathcal{F} to be applied. As we shall see, it avoids derivatives of \mathcal{F} as well as
28 their approximations, actually no data are required from derivatives of \mathcal{F} neither
29 the existence of same derivatives. This feature is useful in several contexts: in [14]
30 the analytical definition of the function \mathcal{F} is such involved that discourages the
31 computation of its derivatives so an earlier version of the method is employed to
32 overcome this difficulty.

33 We note that it is possible to apply the method to calculate cusp points and
34 other kind of singular points. Typical approach for calculating cusp points is to
35 augment the original equation with defining equations to obtain a specific type of
36 bifurcation points [15]. This strategy require the existence of Jacobian matrix in a
37 neighborhood of the cusp point and hence it fails when the involved function has
38 non differentiable points in any punctured neighborhood of the singular point. We
39 suggest some examples in the following of the paper.

40 The paper is organized as follows: in **Section 2** we define the topological turning
41 point, in **Section 3** we state theorems for its existence and uniqueness. In **Section 4**
42 we develop the iterative method for calculating a topological turning point and in
43 **Section 5** we introduce a pseudo-code which elaborates the algorithm. In **Section**
44 **6** we provide several examples of the method. Finally, in **Section 7** we come to the
45 conclusions.

46 2. Defining Topological Turning Points

47 In the following we formally define topological turning points and motivate this
48 definition in a geometrical context. **Before** going on let us briefly recall the definition
49 of turning points.

1 DEFINITION 2.1 Let us suppose \mathcal{F} is sufficiently smooth. A turning point (x_c, λ_c)
 2 solves the system of equations

$$3 \mathcal{F}(x, \lambda) = 0 \quad (2)$$

$$4 \partial_x \mathcal{F}(x, \lambda) = 0 \quad (3)$$

$$5 \partial_\lambda \mathcal{F}(x, \lambda) \neq 0 \quad (4)$$

6 Equations (2)-(4) are the univariate case of more general conditions which identify
 7 turning points for \mathcal{F} . To distinguish simple turning points from turning points of
 8 a different type a further condition is needed:

$$9 \partial_{x^2} \mathcal{F}(x_c, \lambda_c) \neq 0. \quad (5)$$

10 If equation (5) does not hold, the turning point is called non-simple. In this case
 11 the condition

$$12 \partial_{x^i} \mathcal{F}(x_c, \lambda_c) = 0 \quad (6)$$

13 holds for every $i = 2, \dots, n$ but $i = n + 1$ and the turning point has order n .

14 The idea behind the definition of a topological turning point is to characterize a
 15 special solution of the critical point connection problem [16].

16 Problem 2.2 Critical-point connection problem: In a certain interval X , a one-
 17 parameter family of functions $\{\mathcal{F}_\lambda\}_\lambda$ is cut in half by the x -axis resulting in at
 18 most two intersections with each function \mathcal{F}_λ . The aim is to find, if it exists, the
 19 value of parameter $\lambda \in \Lambda$ in correspondence of the coalescence of two intersections
 20 and the value of x where the two intersections actually coalesce.

21 A complete characterization of the solutions of the critical-point connection prob-
 22 lem is beyond the scope of the paper, it is possible that even a point of horizontal
 23 inflection for \mathcal{F}_λ could solve the problem: hypotheses on the family of functions play
 24 a key role in determining the solutions of the problem. If we let $\mathcal{F}(x, \lambda) := \mathcal{F}_\lambda(x)$,
 25 the special solution which rouses our interest is defined as follows:

26 DEFINITION 2.3 Let $\mathcal{F}(x, \lambda)$ be a continuous function in a domain D . The point
 27 $(x_c, \lambda_c) \in D$ is said to be a topological turning point for \mathcal{F} if there exists a compact
 28 rectangular domain $X \times \Lambda \subset D$ such that:

- 29 i) $(x_c, \lambda_c) \in \overset{\circ}{X} \times \overset{\circ}{\Lambda}$ ($\overset{\circ}{X}$ is the interior of X);
 30 ii) x_c is a global minimizer (maximizer) for $\mathcal{F}(x, \lambda_c)$ in X ;
 31 iii) the equation

$$32 \mathcal{F}(x_c, \lambda_c) = 0$$

33 holds.

34 It is clear that a turning point of odd order is a topological turning point. In
 35 particular, a simple turning point satisfies the Conditions (2)-(5) and, therefore,
 36 it also satisfies conditions in Definition 2.3. On the other hand, the regularity of
 37 \mathcal{F} ensures that a topological turning point is an odd order turning point, but this
 38 is not enough to ensure that it is a simple turning point. We build up this trivial
 39 counter-example:

$$40 \mathcal{F}(x, \lambda) = x^4 + \lambda$$

in this case the point $(0, 0)$ is a topological turning point and also a turning point but it is not a simple turning point since (5) does not hold. As long as no derivatives for \mathcal{F} are required in the definition, also cusp points can be a topological turning point.

The critical point connection problem also lies behind the basic idea of the numerical method, we compute the distance between the two intersections and we recursively operate to reduce it. The difference in the order of magnitude for the approximations in λ and in x is remarkable (see Tables 1, 2). When the topological turning point is a turning point, we should be able to recognize its order taking into account the approximation ratio between λ and x , that is the polynomial degree of their functional dependence. This will be investigated elsewhere.

3. Existence and uniqueness results

Before continuing with the discussion we give some definitions and notations. Let $X \times \Lambda$ be a compact rectangular domain in \mathbb{R}^2 and

$$\begin{aligned} \mathcal{F} : X \times \Lambda &\longrightarrow \mathbb{R} \\ (x, \lambda) &\longmapsto y \end{aligned}$$

In the following we adopt the notation \mathcal{F}_λ to emphasize the dependence of \mathcal{F} on x and \mathcal{F}_x to emphasize the dependence of \mathcal{F} on λ . We denote the graph of a generic function $\varphi : X \rightarrow \mathbb{R}$ by

$$\mathcal{G}_X(\varphi) = \{(x, \varphi(x)) \mid x \in X\}$$

and its epigraph by

$$\mathcal{E}_X(\varphi) := \{(x, y) \mid x \in X, y \geq \varphi(x)\}.$$

With regard to the one-parameter family of functions \mathcal{F}_λ , we set

$$E_n(X, \Lambda) = \{\lambda \in \Lambda : \#(\mathcal{G}_X(\mathcal{F}_\lambda) \cap \mathcal{G}_X(y=0)) = n\}, \quad n \in \mathbb{N}.$$

We note that $E_n(X, \Lambda)$ is the set of $\lambda \in \Lambda$ for which the graph of \mathcal{F}_λ has exactly n intersections with the x -axis and the process of counting the intersections does not take into account their multiplicity. We now recall two equivalent definitions, widely used in the following.

DEFINITION 3.1 [17, Definition 4.2.5] *A function $\varphi : [a, b] \subset \mathbb{R} \rightarrow \mathbb{R}$ is strictly quasiconvex on $[a, b]$ if, for any $t_1, t_2 \in [a, b]$, $t_1 \neq t_2$*

$$\varphi(\tau t_1 + (1 - \tau)t_2) < \max\{\varphi(t_1), \varphi(t_2)\}, \quad \forall \tau \in (0, 1).$$

DEFINITION 3.2 [17, Definition 8.7.1] *A function $\varphi : [a, b] \subset \mathbb{R} \rightarrow \mathbb{R}$ is strictly unimodal on $[a, b]$ if there exists a $t^* \in [a, b]$ such that $\varphi(t^*) = \min\{\varphi(t) \mid t \in [a, b]\}$, and if, for any $a \leq t_1 < t_2 \leq b$,*

$$\begin{cases} t_2 \leq t^* \text{ implies that } \varphi(t_1) > \varphi(t_2), \\ t^* \leq t_1 \text{ implies that } \varphi(t_2) > \varphi(t_1). \end{cases}$$

A result of Elkin [18], remarked in [17, 4.2.5], shows that the class of strictly quasiconvex functions coincides with the class of strictly unimodal functions: we will

use them without distinction, depending on suitability. Clearly the strict convexity implies the strict quasiconvexity but the converse is not true; we also remark that a strictly quasiconvex function is not, in general, a continuous function [19].

THEOREM 3.3 *Let us suppose that the function \mathcal{F} is continuous in $\Lambda \times X$ and that*

$$\begin{aligned} \mathcal{F}_\lambda : X &\rightarrow \mathbb{R}, \quad x \in X \text{ is strictly unimodal for each } \lambda \in \Lambda, \\ \mathcal{F}_x : \Lambda &\rightarrow \mathbb{R}, \quad \lambda \in \Lambda \text{ is strictly monotone for each } x \in X. \end{aligned} \quad (7)$$

If there exists a topological turning point in $\Lambda \times X$, then it is unique.

Proof For each $\lambda \in \Lambda$ the functions \mathcal{F}_λ are strictly quasi convex (concave) and have a global minimizer (or maximizer) in X : recalling the **Definition 2.3** a topological turning point (x_c, λ_c) identifies a function \mathcal{F}_{λ_c} where x_c is its global minimizer (or maximizer) and the following equation holds

$$\mathcal{F}_{\lambda_c}(x_c) = 0.$$

Using reductio ad absurdum, we can suppose (x_c, λ_c) and (x'_c, λ'_c) are two different topological turning points in $\Lambda \times X$: x_c and x'_c are the minimum for \mathcal{F}_{λ_c} and $\mathcal{F}_{\lambda'_c}$ respectively. The strict unimodality of \mathcal{F}_λ excludes that $\lambda_c = \lambda'_c$ and $x_c \neq x'_c$ whereas the strict monotonicity of \mathcal{F}_x excludes that $\lambda_c \neq \lambda'_c$ and $x_c = x'_c$: hence we have to discuss the case where $\lambda'_c \neq \lambda_c$ and $x'_c \neq x_c$. Without loss of generality, we can suppose $\lambda'_c < \lambda_c$ and that all functions \mathcal{F}_x are strictly increasing for each $x \in X$. Consequently

$$0 = \mathcal{F}_{\lambda'_c}(x'_c) < \mathcal{F}_{\lambda'_c}(x_c) < \mathcal{F}_{\lambda_c}(x_c) = 0$$

which is absurd since the first inequality follows from the strict unimodality of \mathcal{F}_λ and the second from the strict monotonicity of \mathcal{F}_x . ■

Remark 1 We can compare the hypothesis of **Theorem 3.3** with the conditions required by the Newton method. More precisely, in order to apply the Newton method to compute a simple turning point, among other conditions, it is required that \mathcal{F} is of class C^2 and

$$\begin{vmatrix} \frac{\partial \mathcal{F}}{\partial \lambda} \Big|_{(\lambda, x)} & \frac{\partial \mathcal{F}}{\partial x} \Big|_{(\lambda, x)} \\ \frac{\partial^2 \mathcal{F}}{\partial \lambda \partial x} \Big|_{(\lambda, x)} & \frac{\partial^2 \mathcal{F}}{\partial x^2} \Big|_{(\lambda, x)} \end{vmatrix} \neq 0 \quad (8)$$

for each (x, λ) in a neighborhood $X \times \Lambda$ of its solution (x_c, λ_c) [20]. Basically, we note that condition (8) is equivalent to the following

$$\frac{\partial^2 \mathcal{F}}{\partial x^2} \Big|_{(x_c, \lambda_c)} \neq 0 \quad (9)$$

and

$$\frac{\partial \mathcal{F}}{\partial \lambda} \Big|_{(x_c, \lambda_c)} \neq 0 \quad (10)$$

when evaluated at the point (x_c, λ_c) . **Condition (9)** implies the strict unimodality of functions \mathcal{F}_λ and condition (10) implies the strict monotony of functions \mathcal{F}_x at least in the neighborhood of (x_c, λ_c) .

From the definition of unimodality each horizontal line intersects the graph of a unimodal function at least twice, eventually by reducing the domain (X, Λ) and in virtue of **Theorem 3.3** we assume

$$E_n(X, \Lambda) = \emptyset, \quad n > 2. \quad (11)$$

On the other hand, the existence of a topological turning point is not ensured even if the conditions

$$E_n(X, \Lambda) \neq \emptyset, \quad n = 0, 2$$

are added to the hypothesis of **Theorem 3.3**, as in the counter example in **Figure 1**. In order to ensure the existence of a topological turning point we need a further

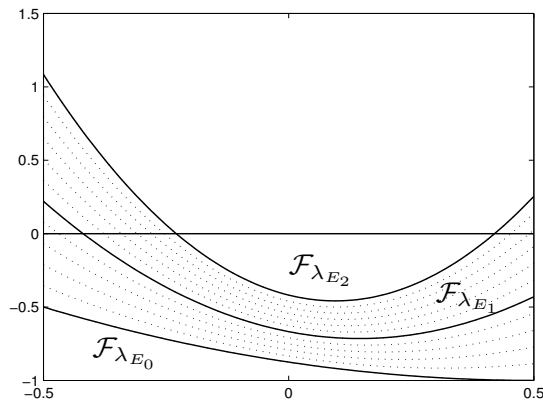


Figure 1. $E_0(\Lambda, X) \neq \emptyset$, $E_1(\Lambda, X) \neq \emptyset$, $E_2(\Lambda, X) \neq \emptyset$ but there is no topological turning point.

condition on the mutual position of the graphs of the functions \mathcal{F}_λ , as the following theorem shows.

THEOREM 3.4 *Let the function \mathcal{F} satisfy the hypothesis of **Theorem 3.3**; moreover let $E_n(X, \Lambda) \neq \emptyset$ be for $n = 0, 2$. If in addition there exist $\lambda_{E_0} \in E_0(X, \Lambda)$ and $\lambda_{E_2} \in E_2(X, \Lambda)$ such that*

$$\mathcal{G}_X(\mathcal{F}_{\lambda_{E_0}}) \subset \mathcal{E}_X(\mathcal{F}_{\lambda_{E_2}}), \quad (12)$$

then there exists a topological turning point in $X \times \Lambda$.

Before demonstrating **Theorem 3.4** we state the following

LEMMA 3.5 *In the hypothesis of **Theorem 3.4** the sets $E_0(X, \Lambda)$, $E_2(X, \Lambda)$ are open with respect to the topology induced by the Euclidean topology on $\Lambda = [\min\{\lambda_{E_0}, \lambda_{E_2}\}, \max\{\lambda_{E_0}, \lambda_{E_2}\}]$.*

Proof **Without loss of generality, suppose** that all functions \mathcal{F}_x are strictly increasing functions for each $x \in X$.

In order to prove that $\lambda_{E_0} \in \mathring{E}_0(X, \Lambda)$ (\mathring{E}_0 is the interior of E_0) we set

$$\delta := \min_{x \in X} \{\mathcal{F}_{\lambda_{E_0}}\}$$

and therefore

$$\mathcal{F}_{\lambda_{E_0}}(x) \geq \delta > 0, \quad \forall x \in X.$$

We consider the open covering of $\mathcal{G}_X(\mathcal{F}_{\lambda_{E_0}})$ generated by the open balls with center $(x, \mathcal{F}_{\lambda_{E_0}}(x))$ and radius δ , for each $x \in X$. Let λ be such that the graph $\mathcal{G}_X(\mathcal{F}_\lambda)$ lies entirely in the open covering above: then $\lambda \in E_0(X, \Lambda)$ and the set of such λ is an open interval in Λ by the hypothesis on \mathcal{F} . An analogous argument can be repeated for each $\lambda'_{E_0} \in E_0(X, \Lambda)$. **Consequently** $E_0(X, \Lambda)$ is open in Λ .

In order to prove that $\lambda_{E_2} \in \overset{\circ}{E}_2(X, \Lambda)$ we denote by $x_m \in \overset{\circ}{X}$ the abscissa of the global minimum of $\mathcal{F}_{\lambda_{E_2}}$. As long as $\lambda_{E_2} \in E_2(X, \Lambda)$, then

$$\mathcal{F}_{\lambda_{E_2}}(x_m) < 0$$

because of the strict unimodality of the function. **On** the other hand

$$\mathcal{F}_{\lambda_{E_0}}(x_m) > 0$$

since $\lambda_{E_0} \in E_0(X, \Lambda)$ and condition (12) holds. Because of the continuity of \mathcal{F}_{x_m} there exists a $\bar{\lambda} \in (\lambda_{E_2}, \lambda_{E_0})$ such that

$$\mathcal{F}_{\bar{\lambda}}(x_m) = 0.$$

Since $\mathcal{F}_{\lambda_{E_2}}$ is **nonnegative** at the boundary points of X we find that $[\lambda_{E_2}, \bar{\lambda}) \subset E_2(X, \Lambda)$ by the hypothesis on \mathcal{F} . An analogous argument can be repeated for each $\lambda'_{E_2} \in E_2(X, \Lambda)$. **Consequently** $E_2(X, \Lambda)$ is open in Λ . ■

Now we can prove **Theorem 3.4**.

Proof Taking into account the fact that Λ is an interval and that $E_0(X, \Lambda) \cap E_2(X, \Lambda) = \emptyset$, in virtue of **Lemma 3.5** there must exist a $\lambda_c \in E_1(X, \Lambda) \subset \overset{\circ}{\Lambda}$.

Let $x_c \in X$ be the unique zero of the function \mathcal{F}_{λ_c} . Due to the strict monotonicity of \mathcal{F}_{x_c} , **the** point x_c lies between the two zeros of $\mathcal{F}_{\lambda_{E_2}}$ and hence $x_c \in \overset{\circ}{X}$. Now we have to prove that x_c is the global minimizer of \mathcal{F}_{λ_c} . **Through *reductio ad absurdum***, let x_m be the global minimizer of \mathcal{F}_{λ_c} : it would satisfy the condition

$$\mathcal{F}_{\lambda_c}(x_m) < 0$$

and consequently, from the hypothesis on \mathcal{F} , there would exist two distinct zeros of \mathcal{F}_{λ_c} which is a contradiction. Therefore the pair (λ_c, x_c) is a topological turning point. ■

Remark 2 Theorem 3.4 only claims explicitly the existence of a topological turning point. However, under the same hypotheses, **Theorem 3.3** holds and hence the topological turning point is also unique.

Remark 3 We can compare the hypothesis of **Theorem 3.4** with the conditions required by the Newton method. More precisely, in order to apply the Newton method to compute a simple turning point we assume \mathcal{F} is sufficiently smooth and

we expand it using Taylor series centered at (λ_c, x_c) :

$$\begin{aligned} \mathcal{F}(x, \lambda) \approx & -\frac{\partial \mathcal{F}}{\partial \lambda} \Big|_{(\lambda_c, x_c)} (\lambda - \lambda_c) + \frac{1}{2} \frac{\partial^2 \mathcal{F}}{\partial x^2} \Big|_{(\lambda_c, x_c)} (x - x_c)^2 \\ & - \frac{\partial^2 \mathcal{F}}{\partial x \partial \lambda} \Big|_{(\lambda_c, x_c)} (x - x_c) (\lambda - \lambda_c) - \frac{1}{2} \frac{\partial^2 \mathcal{F}}{\partial \lambda^2} \Big|_{(\lambda_c, x_c)} (\lambda - \lambda_c)^2 \end{aligned} \quad (13)$$

where the constant as well as the linear term in $x - x_c$ are zero by (2) and (3) respectively. We note that the right hand side of (13) can be read as a polynomial in x and its discriminant is a function in λ :

$$\begin{aligned} \Delta(\lambda - \lambda_c) = & \left[\left(\frac{\partial^2 \mathcal{F}}{\partial x \partial \lambda} \Big|_{(\lambda_c, x_c)} \right)^2 + \frac{\partial^2 \mathcal{F}}{\partial x^2} \Big|_{(\lambda_c, x_c)} \frac{\partial^2 \mathcal{F}}{\partial \lambda^2} \Big|_{(\lambda_c, x_c)} \right] (\lambda - \lambda_c)^2 \\ & + \frac{\partial^2 \mathcal{F}}{\partial x^2} \Big|_{(\lambda_c, x_c)} \frac{\partial \mathcal{F}}{\partial \lambda} \Big|_{(\lambda_c, x_c)} (\lambda - \lambda_c). \end{aligned} \quad (14)$$

Because of Conditions (9) and (10), required by the Newton method, this discriminant has a single zero at λ_c . In turn the number of zeroes of the quadratic polynomial, with respect to the variable $x \in X$ at the r.h.s. of (13), ranges from 0 to 2 in the neighborhood Λ of λ_c . Consequently, $E_0(X, \Lambda)$ and $E_2(X, \Lambda)$ are non-empty sets while the critical value λ_c is an isolated point of E_1 and it lies in the closure of E_n $n = 0, 2$: as required in Theorem 3.4.

4. The converging sequences

This section is devoted to introducing sequences $\{(x_n, \lambda_n)\}$ which converge to a topological turning point (x_c, λ_c) in the hypotheses of Theorem 3.4. We prove that if (x_1, x_2) is the open interval between the two roots x_1, x_2 of a certain \mathcal{F}_λ , then $x_c \in (x_1, x_2)$: an *ad hoc* modification of the bisection method (which is further discussed in Section 5) ensures the linear convergence to x_c . At the same time we take into account the convergence of λ towards λ_c . Finally, a map C links together every $x \in (x_1, x_2)$ with a uniquely determined value of λ .

Before going on with the discussion we shall introduce some notations. Let $\lambda_{E_0} \in E_0(X, \Lambda)$, $\lambda_{E_2} \in E_2(X, \Lambda)$ and without loss of generality assume $\lambda_{E_0} < \lambda_c < \lambda_{E_2}$. For each $\lambda \in E_2(X, \Lambda)$ we denote by x_1^λ, x_2^λ , with $x_1^\lambda < x_2^\lambda$, the two roots of the equation $\mathcal{F}_\lambda = 0$. Finally, by reducing the rectangle, we assume $X = [x_1^{\lambda_{E_2}}, x_2^{\lambda_{E_2}}]$ and $\Lambda_c = (\lambda_c, \lambda_{E_2}] \subset \Lambda = [\lambda_{E_0}, \lambda_{E_2}]$. In the following we suppose the hypotheses of Theorem 3.4 hold.

LEMMA 4.1 *Let be $\lambda \in \Lambda_c \subset E_2(X, \Lambda)$, let x_1^λ and x_2^λ be the two roots of $\mathcal{F}_\lambda = 0$. Then:*

$$x_c \in (x_1^\lambda, x_2^\lambda), \quad (15)$$

$$\lim_{\lambda \rightarrow \lambda_c^+} |x_2^\lambda - x_1^\lambda| = 0^+ \Leftrightarrow \lim_{|x_2^\lambda - x_1^\lambda| \rightarrow 0^+} \lambda = \lambda_c^+ \quad (16)$$

and for each $\lambda_1, \lambda_2 \in \Lambda_c$

$$|\lambda_1 - \lambda_c| < |\lambda_2 - \lambda_c| \Leftrightarrow (x_1^{\lambda_1}, x_2^{\lambda_1}) \subsetneq (x_1^{\lambda_2}, x_2^{\lambda_2}) \subset X. \quad (17)$$

Proof In order to prove (15) let us assume by *reductio ad absurdum* that $x_c \notin [x_1^\lambda, x_2^\lambda]$. Let $x_m^\lambda \in [x_1^\lambda, x_2^\lambda]$ be s.t. $\mathcal{F}_\lambda(x_m^\lambda) = \min \{\mathcal{F}_\lambda(x) : x \in [x_1^\lambda, x_2^\lambda]\}$. The strict unimodality yields

$$\mathcal{F}_\lambda(x_m^\lambda) < 0 < \mathcal{F}_{\lambda_c}(x_m^\lambda) \implies \mathcal{F}_\lambda(x_m^\lambda) - \mathcal{F}_{\lambda_c}(x_m^\lambda) < 0$$

and the strict monotony yields

$$\mathcal{F}_\lambda(x_c) > \mathcal{F}_{\lambda_c}(x_c) = 0 \implies \mathcal{F}_\lambda(x_c) - \mathcal{F}_{\lambda_c}(x_c) > 0.$$

Hence there exists a point $\bar{x} \in (\min \{x_m^\lambda, x_c\}, \max \{x_m^\lambda, x_c\})$ such that

$$\mathcal{F}_\lambda(\bar{x}) = \mathcal{F}_{\lambda_c}(\bar{x})$$

against the monotony of \mathcal{F}_x .

The proofs of conditions (16) and (17) are straightforward if we recall that (16) follows from **Theorem** 3.3 while (17) can be proven analogously to condition (15). ■

We define the map

$$C : \Lambda_c \rightarrow \bar{\Lambda}_c = \Lambda_c \cup \{\lambda_c\}$$

as follows: let $\lambda \in \Lambda_c$, x_1^λ and x_2^λ be the associated roots. We select the middle point $\bar{x} \in (x_1^\lambda, x_2^\lambda)$ and determine the unique $\bar{\lambda}$ such that $\mathcal{F}_{\bar{\lambda}}(\bar{x}) = 0$. We set

$$C(\lambda) = \bar{\lambda}.$$

We remark that $\bar{\lambda}$ is actually unique for the **monotonicity** of the functions \mathcal{F}_x , then we can prove the following:

THEOREM 4.2 For each $\lambda \in \Lambda_c$ and for each $\varepsilon > 0$ there exists $n \in \mathbb{N}$ such that

$$|C^n(\lambda) - \lambda_c| < \varepsilon. \quad (18)$$

Proof For each couple $\lambda_1, \lambda_2 \in \bar{\Lambda}_c$ we associate the positive real number

$$d(\lambda_1, \lambda_2) = \left| \left| x_1^{\lambda_1} - x_2^{\lambda_1} \right| - \left| x_1^{\lambda_2} - x_2^{\lambda_2} \right| \right|.$$

We can state that function d is a distance and $(\bar{\Lambda}_c, d)$ is a metric space. In fact, the **nonnegativity** and the **symmetry** of d follows from its definition, the **identity of indiscernible** follows by (17) and by the strict **monotonicity** of \mathcal{F}_x ; finally, the **triangle inequality** follows from the fact that from (17) each set $\{\lambda_1, \lambda_2, \lambda_3\}$ is strictly ordered by distance $d(\lambda_i, \lambda_c)$.

We conclude the proof remarking that if $C(\lambda) = \lambda_c$ condition (18) is trivial; otherwise, if $C^{n-1}(\lambda)$ belongs to Λ_c , the iterates of map C satisfy the inequality

$$d(C^n(\lambda), \lambda_c) \leq \frac{1}{2} d(C^{n-1}(\lambda), \lambda_c).$$

■

The above discussion shows that the map C has an attractive fixed point in λ_c and more importantly:

$$x_1^\lambda < x_1^{C(\lambda)} \leq x_c \leq x_2^{C(\lambda)} < x_2^\lambda \quad \forall \lambda \in \Lambda_c. \tag{19}$$

Hence to attain sequences $\{(x_n, \lambda_n)\}$ which converge to a topological turning point it is sufficient to set $\lambda_0 = \lambda_{E_2}$ and to pair the terms of the sequence $\{C^n(\lambda_0)\}$, $n \geq 0$, with the corresponding ones in sequences $\{x_1^{C^n(\lambda_0)}\}$, $\{x_2^{C^n(\lambda_0)}\}$.

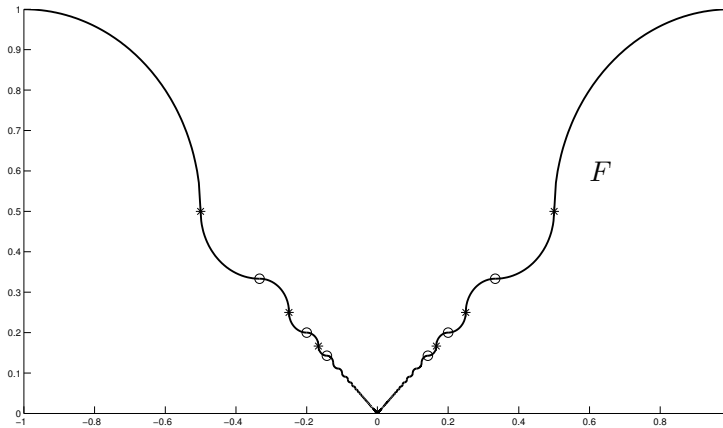


Figure 2. \mathcal{F}_{λ_c} is neither convex nor concave and it has a countable number of points with horizontal (circle) or vertical (star) tangent line in any punctured neighborhood of $x_c = 0$.

5. The pseudocode

Here we introduce a pseudo-code which elaborates the method: to help the reader we split it into three macro-steps and discuss, separately, the procedures involved in each one of them. Then we shall introduce the main procedure which actually yields the topological turning point.

step 1 Given λ_n and the roots $x_1^{\lambda_n}$, $x_2^{\lambda_n}$ of the equation $\mathcal{F}_{\lambda_n}(x) = 0$, we set \bar{x} the midpoint of $(x_1^{\lambda_n}, x_2^{\lambda_n})$.

PROCEDURE: **firstx**
 $x_1^{\lambda_n}, x_2^{\lambda_n}$ (input)
 $\bar{x} \leftarrow x_1^{\lambda_n} + (x_2^{\lambda_n} - x_1^{\lambda_n}) / 2$
 \bar{x} (output)

step 2 We determine the unique λ_{n+1} such that $\mathcal{F}_{\lambda_{n+1}}(\bar{x}) = 0$.

PROCEDURE: **nextlambda**
 $\mathcal{F}, \lambda_{E_0}, \lambda_n, \bar{x}$ (input)
 $\lambda_{n+1} \leftarrow \text{Solve}[\mathcal{F}_\lambda(\bar{x}) = 0]$
 λ_{n+1} (output)

The procedure **Solve** is a zero finding method and a standard bisection can be used in order to achieve λ_{n+1} . In fact, the assumptions on the function \mathcal{F} assure that $\lambda_{n+1} \in [\min \{\lambda_{E_0}, \lambda_n\}, \max \{\lambda_{E_0}, \lambda_n\}]$, where $\lambda_{E_0} \in E_0(X, \Lambda)$, and the computation of λ_{n+1} can be realized in order to assure that $\lambda_{n+1} \in E_2(X, \Lambda)$. Moreover, if $\mathcal{F}_\lambda(x)$ is algebraic in λ , it may be possible to compute the value λ_{n+1} directly. In this case the input datum λ_{E_0} is not really needed.

step 3 We approximate the second root z of the equation $\mathcal{F}_{\lambda_{n+1}}(x) = 0$ by \bar{x} ; then we renominate \bar{x} and \bar{x} as $x_1^{\lambda_{n+1}}$ and $x_2^{\lambda_{n+1}}$ from the left to the right.

The variable \mathcal{C} in input assumes the values 1, -1 according to the assignment in the procedure **tpoint**; as a consequence of its definition, the value of \mathcal{C} is the opposite of the sign of (9) when it is meaningful.

PROCEDURE: **nextx**

$\mathcal{F}, \lambda_{n+1}, x_1^{\lambda_n}, x_2^{\lambda_n}, \bar{x}, \mathcal{C}$ (input)

$x_l \leftarrow x_1^{\lambda_n} + (\bar{x} - x_1^{\lambda_n}) / 2;$

$x_r \leftarrow \bar{x} + (x_2^{\lambda_n} - \bar{x}) / 2;$

$l \leftarrow \mathcal{F}_{\lambda_{n+1}}(x_l);$

$r \leftarrow \mathcal{F}_{\lambda_{n+1}}(x_r);$

while $l \cdot r > 0$

$x_1^{\lambda_n} \leftarrow x_l;$

$x_2^{\lambda_n} \leftarrow x_r;$

$x_l \leftarrow x_1^{\lambda_n} + (\bar{x} - x_1^{\lambda_n}) / 2;$

$x_r \leftarrow \bar{x} + (x_2^{\lambda_n} - \bar{x}) / 2;$

$l \leftarrow \mathcal{F}_{\lambda_{n+1}}(x_l);$

$r \leftarrow \mathcal{F}_{\lambda_{n+1}}(x_r);$

end

If $l \cdot r = 0$

If $l = 0$

$x_1^{\lambda_{n+1}} \leftarrow x_l;$

$x_2^{\lambda_{n+1}} \leftarrow \bar{x};$

else

$x_1^{\lambda_{n+1}} \leftarrow \bar{x};$

$x_2^{\lambda_{n+1}} \leftarrow x_r;$

end

else

if $\mathcal{C} \cdot l < 0$

$x_1^{\lambda_{n+1}} \leftarrow x_1^{\lambda_n}$

$x_2^{\lambda_{n+1}} \leftarrow \bar{x};$

else

$x_1^{\lambda_{n+1}} \leftarrow \bar{x};$

$x_2^{\lambda_{n+1}} \leftarrow x_2^{\lambda_n}$

end

end

$x_1^{\lambda_{n+1}}, x_2^{\lambda_{n+1}}$ (output)

The choice of \bar{x} as approximation of the zero z is a critical issue: here an *ad hoc* modification of the standard bisection is needed. The zero z must belong to the interval with end-points \bar{x}, \bar{x} , i.e. z must belong to the calculated interval. **This**

feature ensures that the sequence of intervals bounded by the exact zeroes of $\mathcal{F}_{\lambda_{n+1}}$ converges to x_c when $|x_2^{\lambda_{n+1}} - x_1^{\lambda_{n+1}}|$ tends to zero. For this reason point \bar{x} must be a left or a right approximation of z depending on the position of z with respect to \bar{x} . The point \bar{x} can be considered an exact approximation of the corresponding zero.

We note that the error $|\bar{x} - z|$ need not be small with respect to $|x_2^{\lambda_n} - x_1^{\lambda_n}|$: the algorithm improves its efficiency by decreasing the quantity $|\bar{x} - z|$ but, at the same time, the amount of evaluations of the function $\mathcal{F}_{\lambda_{n+1}}$ increases together with this precision. On the other hand, knowledge of the mutual position of the zeros *per se* allows us to choose the values $x_1^{\lambda_n}$ or $x_2^{\lambda_n}$ as left or right approximation of z respectively. In fact, it follows that

$$|\bar{x} - x_1^{\lambda_n}| = |\bar{x} - x_2^{\lambda_n}| = \frac{1}{2} (x_2^{\lambda_n} - x_1^{\lambda_n})$$

which still ensures a linear speed of convergence. To determine a value between $x_1^{\lambda_n}$ and $x_2^{\lambda_n}$ which may approximate z , the procedure **nextx** determines if z is greater than or equal to \bar{x} in order to choose a narrow interval, namely $(x_1^{\lambda_n}, x_l)$ or $(x_r, x_2^{\lambda_n})$, containing z . The procedure fixes the auxiliary points

$$x_l = (x_1^{\lambda_n} + \bar{x}) / 2, \quad x_r = (\bar{x} + x_2^{\lambda_n}) / 2$$

and considers the product of evaluations $l \cdot r$ where

$$l := \mathcal{F}_{\lambda_{n+1}}(x_l), \quad r := \mathcal{F}_{\lambda_{n+1}}(x_r).$$

From the unimodality of \mathcal{F}_λ , in the interval $(x_1^{\lambda_n}, x_2^{\lambda_n})$, the function $\mathcal{F}_{\lambda_{n+1}}$ can be approximated by a certain parabola with zeroes in \bar{x} and in z : if x_l and x_r are both outside the interval (\bar{x}, z) , then $l \cdot r$ is positive so that we may consider only the narrower interval (x_l, x_r) and proceed along the same line of reasoning. Conversely, if the sign of $l \cdot r$ is negative, only one among x_l, x_r lies between \bar{x}, z : this case ensures that the root z lies outside the interval (x_l, x_r) whereas $\bar{x} \in (x_l, x_r)$. Hence z is the only root in the interval $(x_1^{\lambda_n}, x_l)$ or in $(x_r, x_2^{\lambda_n})$ depending on the sign of \mathcal{C} and the sign of l (or r): consequently the procedure assigns to \bar{x} the value of $x_1^{\lambda_n}$ or $x_2^{\lambda_n}$.

Finally we introduce the procedure **tpoint** which calculates the topological turning point; in fact, we employ all the procedures previously introduced. Recalling the definition of $\Lambda_c \times X$ (see Section 4) we initialize the variables.

PROCEDURE: **tpoint**

$\mathcal{F}, \lambda_{E_0}, \lambda_{E_2}, x_1^{\lambda_{E_2}}, x_2^{\lambda_{E_2}}$ (input)

$x_1^\lambda \leftarrow x_1^{\lambda_{E_2}}$

$x_2^\lambda \leftarrow x_2^{\lambda_{E_2}}$

$\lambda_{old} \leftarrow \lambda_{E_0}$

$\lambda \leftarrow \lambda_{E_2}$

$\bar{x} \leftarrow \mathbf{firstx}$

$\mathcal{C} \leftarrow -\mathit{sign}(\mathcal{F}_\lambda(\bar{x}))$

while $|\lambda - \lambda_{old}| > \mathit{eps}$

$\bar{x} \leftarrow \mathbf{firstx}$

Table 1. Numerical results for the two-bar Framework

Iterations	λ	$ \lambda - \lambda_{old} $	$(x_1^\lambda + x_2^\lambda) / 2$	$ x_1^\lambda - x_2^\lambda $
26	3.079201435678002	1.7E-15	0.845299444414370	1.0E-07
27	-3.079201435678005	1.7E-15	3.154700516871277	2.6E-08

```

 $\lambda_{old} \leftarrow \lambda$ 
 $\lambda \leftarrow \text{nextlambda}$ 
 $x_1^\lambda \leftarrow \text{nextx}((1))$ 
 $x_2^\lambda \leftarrow \text{nextx}((2))$ 
end
 $\lambda, x_1^\lambda, x_2^\lambda$  (output)

```

6. Numerical experiments

In this section we test the method in several cases. The first two examples are well-known in the literature; in particular, Example 1 is reported also in [21] and can serve as a comparison with other methods. Example 3 introduces several cases of cusp point. Example 4 introduces a function with non differentiable points in any punctured neighborhood of the topological turning point. Examples 3 and 4 are especially chosen in order to emphasize the peculiarity of the proposed method. A Matlab code is **developed** to run the method.

Example 1. Oden [22] introduced an example of a two bar framework constructed of an isotropic Hookean material. A standard finite element approximation leads to the equilibrium equations for the displacement vector $y = (y_1, y_2) \in \mathbb{R}^2$. The equilibrium equations $F(y, t) = (0, 0)$ are linear in parameter t and also depend on the given load vector $p = (p_1, p_2) \in \mathbb{R}^2$ as well as on a further scalar parameter μ which must be fixed. We test our method on the first component of F :

$$(y_1^2 - 3\mu y_1 + 2\mu^2) y_1 + (y_1 y_2 - \mu y_2) y_2 - t p_1 = 0$$

in correspondence of $p_1 = 1$, $\mu = 2$ (as in [21]) and we set $y_2 = 0$ in order to make the problem unidimensional. We run the Matlab code of the algorithm two times with the initial values $\lambda_{E_0} = \frac{16}{3\sqrt{3}} + 1$, $\lambda_{E_2} = -\frac{16}{3\sqrt{3}}$, $x_1^{\lambda_{E_2}} = 2 - \frac{4}{\sqrt{3}}$, $x_2^{\lambda_{E_2}} = 2 + \frac{2}{\sqrt{3}}$ and $\lambda_{E_0} = -\frac{16}{3\sqrt{3}} - 1$, $\lambda_{E_2} = \frac{16}{3\sqrt{3}}$, $x_1^{\lambda_{E_2}} = 2 - \frac{2}{\sqrt{3}}$, $x_2^{\lambda_{E_2}} = 2 + \frac{4}{\sqrt{3}}$.

The two runs generate the output values given in Table 1. These values correspond to turning points $T_1 = \left(2 - \frac{2}{\sqrt{3}}, 0, +\frac{16}{3\sqrt{3}}\right)$, $T_2 = \left(2 + \frac{2}{\sqrt{3}}, 0, -\frac{16}{3\sqrt{3}}\right)$ reported in [21].

Example 2. Spence and Werner [6] study nonlinear operators motivated by two parameter problems which arise from physical applications, such as the theory of thermal ignition. In introducing the notion of simple and double turning points they discuss the map

$$\mathcal{F}(x, \lambda) := x^3 - \mu x + \lambda$$

where μ is a fixed constant. This map is the polynomial realization of the so called *cusp catastrophe* [23, p. 174]. For $\mu > 0$ there are two simple turning points (λ_c, x_c) ,

Table 2. Numerical results for the one parameter family $\mathcal{F}(\lambda, x) = x^3 - \mu x + \lambda$, $\mu = 1$

Iterations	λ	$ \lambda - \lambda_{old} $	$(x_1^\lambda + x_2^\lambda) / 2$	$ x_1^\lambda - x_2^\lambda $
15	0.384900179459748	0.0E-16	5.773503035306931E-01	1.5E-07
15	-0.384900179459748	0.0E-16	-5.773503035306931E-01	1.5E-07

$\lambda_c = \pm 2(\mu/3)^{3/2}$, $x_c = \pm(\mu/3)^{1/2}$. We tested our method on

$$\mathcal{F}(x, \lambda) = 0$$

for the special case $\mu = 1$ (see Figure 3).

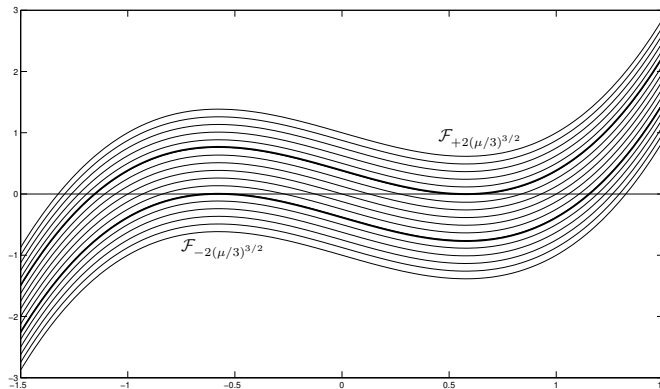


Figure 3. The one parameter family $\mathcal{F}(\lambda, x) = x^3 - \mu x + \lambda$, $\mu = 1$

We run the Matlab code of the algorithm two times, with the initial values $\lambda_{E_0} = 1$, $\lambda_{E_2} = 0$, $x_1^{\lambda_{E_2}} = -.5$, $x_2^{\lambda_{E_2}} = 2$ and $\lambda_{E_0} = -1$, $\lambda_{E_2} = 0$, $x_1^{\lambda_{E_2}} = -2$, $x_2^{\lambda_{E_2}} = .5$. The outcomes are reported in the first and in the second line of the Table 2, respectively.

Example 3. For each $(\alpha, \beta) \in \mathbb{N} \times \mathbb{N}$ we set:

$$F_{\alpha, \beta}(x) := |x|^{\frac{\alpha}{\beta}} \tag{20}$$

and

$$P(x) := -1 + (x - .5)^2.$$

The one-parameter family of functions

$$\mathcal{F}_{\alpha, \beta}(x, \lambda) := F_{\alpha, \beta}(x) - \lambda(F_{\alpha, \beta}(x) - P(x)), \quad (\alpha, \beta) \in \mathbb{N} \times \mathbb{N}$$

are linear homotopies between the functions $y = F_{\alpha, \beta}(x)$ (obtained in correspondence with the value $\lambda = 0$ of the parameter) and the parabola $y = P(x)$ (which corresponds to $\lambda = 1$). We have tested the method on

$$\mathcal{F}_{\alpha, \beta}(\lambda, x) = 0$$

for different values of α, β and their graphic representations are given in Figures 4, 5, 6: if $\alpha > \beta$ the point $(0, 0)$ is a turning point, but if $\alpha \leq \beta$ the point $(0, 0)$ is only a topological turning point (a cusp, in these cases). The Matlab code of the algorithm with the initial values $\lambda_{E_0} = 0.2, \lambda_{E_2} = 1, x_1^{\lambda_{E_2}} = -.5, x_2^{\lambda_{E_2}} = 1$ generates the output values with their respective number of iterations given in Table 3

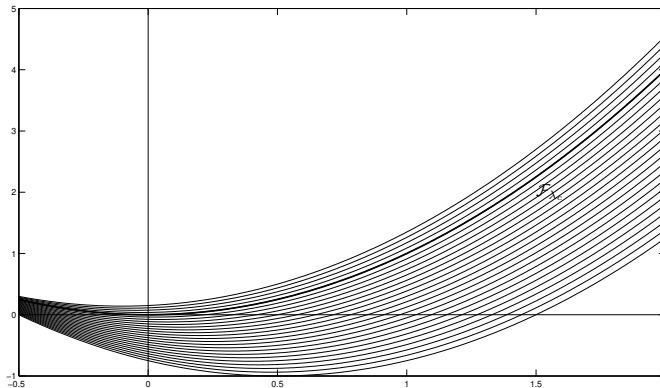


Figure 4. The one parameter family $F_{2,1} - \lambda(P - F_{2,1})$ with $F_{2,1}$ defined as in eq. (20)

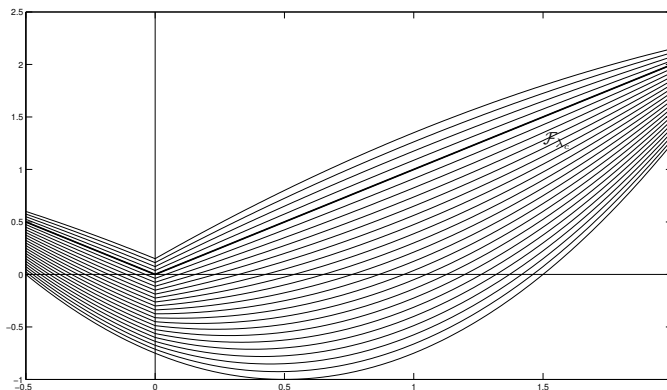


Figure 5. The one parameter family $F_{1,1} - \lambda(P - F_{1,1})$ with $F_{1,1}$ defined as in eq. (20)

Example 4. For each $x \in \mathbb{R} \setminus \{0\}$ we set $n(x) = (1/|x|)$ and consider the function F on $[-1, 1]$ defined as

$$F(x) = \begin{cases} \frac{1}{n(x)+1} + \sqrt{\frac{1}{n(x)^2(n(x)+1)^2} - \left(|x| - \frac{1}{n(x)}\right)^2}, & (n(x), 2) = 1 \\ \frac{1}{n(x)} - \sqrt{\frac{1}{n(x)^2(n(x)+1)^2} - \left(|x| - \frac{1}{n(x)+1}\right)^2}, & (n(x), 2) = 0 \\ 0, & x = 0 \end{cases} \quad (21)$$

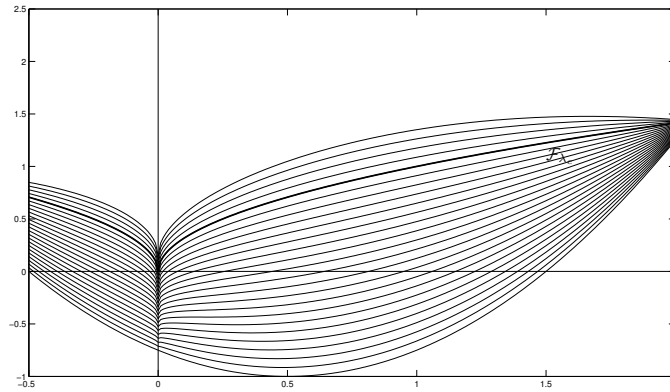


Figure 6. The one parameter family $F_{1,2} - \lambda(P - F_{1,2})$ with $F_{1,2}$ defined as in eq. (20)

Table 3. Numerical results for the sheaf $F_{\alpha,\beta} - \lambda(P - F_{\alpha,\beta})$, $\alpha + \beta \leq 5$

(α, β)	Iterations	λ	$ \lambda - \lambda_{old} $	$(x_1^\lambda + x_2^\lambda)/2$	$ x_1^\lambda - x_2^\lambda $
(1, 1)	52	3.0E-16	0.0E-16	-1.1E-16	6.6E-16
(2, 1)	26	1.6E-16	1.8E-16	-7.5E-09	4.5E-08
(1, 2)	100	7.1E-16	1.8E-16	2.0E-31	1.2E-30
(3, 1)	18	1.1E-16	0.0E-16	-1.9E-06	1.1E-05
(1, 3)	150	7.7E-16	1.8E-16	1.7E-46	1.0E-45
(4, 1)	14	6.3E-17	0.0E-16	-2.9E-05	1.8E-04
(3, 2)	35	7.5E-17	1.8E-16	1.4E-11	8.7E-11
(2, 3)	76	6.2E-16	1.8E-16	-6.5E-24	3.9E-23
(1, 4)	197	1.6E-15	1.8E-16	-1.2E-60	7.5E-60

Table 4. Numerical results for the one parameter family $F - \lambda(P - F)$

Iterations	λ	$ \lambda - \lambda_{old} $	$(x_1^\lambda + x_2^\lambda)/2$	$ x_1^\lambda - x_2^\lambda $
52	3.0E-16	0.0E-16	-1.1E-16	6.6E-16

whose graph is given in Figure 2. This function does not satisfy conditions of convexity or differentiability in any punctured neighborhood of 0; outside the interval $[-1, 1]$ the function F is extended by two arc of parabola in order to preserve the continuity and the strict unimodality. The one parameter family

$$\mathcal{F}(x, \lambda) = F(x) - \lambda \left(F(x) + 1 - (x - .5)^2 \right) \quad (22)$$

is a linear homotopy between the function $y = F(x)$ and the parabola $y = 1 - (x - .5)^2$. The graphic representation of the one parameter family is given in Figure 7. In this case $(0, 0)$ is only a topological turning point and the Matlab code of the algorithm with the initial values $\lambda_{E_0} = 0.2$, $\lambda_{E_2} = 1$, $x_1^{\lambda_{E_2}} = -.5$, $x_2^{\lambda_{E_2}} = 1$ generates the output values with their respective number of iterations given in Table 4.

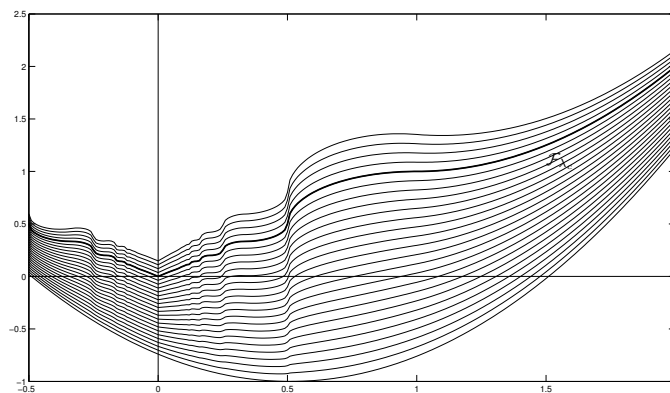


Figure 7. The one parameter family $F - \lambda(P - F)$ with F defined as in eq. (21)

7. Conclusions

The main result of the paper is a numerical method of linear **convergence rate** and of secure convergence for calculating turning points, as well as cusp points and other kind of singular points. This wide range of applicability is due to the definition of topological turning point, which is introduced in the **Section 2** of the paper.

The numerical method proposed here belongs to the class of free derivative methods **since** it does not only avoids the use of derivatives, but also their approximation and even their existence. In particular, this last feature is a novelty in dealing with turning points. Numerical examples are provided and confirm theoretical results.

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