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On a Numerical Treatment for the Curve-Tracing of the Homotopy Method

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Summary. A Newton-like iteration scheme is proposed for the tracing of an implicitly defined smooth curve. This scheme originates from the study of the continuous Newton-Raphson method for underdetermined systems and, hence, inherits the characteristic property of orthogonality. Its domain of attraction is formed and makes it possible to trace this curve more efficiently.

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1. Introduction

The problem to be considered is the following: Suppose that a smooth curve $\Gamma \subset \mathbb{R}^{n+1}$ is implicitly defined by the equation

$$H(x,t)=0 \tag{1.1}$$

where H: $\mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is a C^2 function. We would like to numerically trace this curve Γ from the point (x_0, t_0) to the point (x^*, t^*). For the simplicity of discussion we shall assume that $0 \in \mathbb{R}^n$ is a regular value for H, i.e., the $n \times (n+1)$ Jacobian matrix $DH(x,t)$ has full rank at every point on Γ.

In recent years a number of approaches have been proposed for the numerical computation of this curve-tracing problem [1, 2, 5, 6–9, 11, 13]. Essentially all these techniques are of the predictor-corrector type. A prototype algorithm usually takes steps of the following form:

(i) Let $Y_i=(x_i, t_i) \in \mathbb{R}^{n+1}$ be a point being accepted as an approximating point for Γ. Choose a predictor for the next approximating point. Usually this is done by setting

$$Z_0 = Y_i + h_i T_i \tag{1.2}$$

where h_i is an appropriate step length and T_i is the (unit) tangent vector of Γ at Y_i.

(ii) Starting from Z_0, take a sequence of Newton iterations by requiring Z_k to lie on the hyperplane normal to a certain prescribed vector (usually the tangent vector T_i).

(iii) Set $Y_{i+1}=Z$ where Z is the point of convergence from the sequence $\{Z_k\}$.

In this paper we study one of the many possible variations upon the above general frame. The aim is to establish a uniform domain of attraction for a Newton-like iteration scheme while this scheme, without specifying any normal vector, automatically will have the desired property of orthogonality as stated in (ii). Moreover, with this domain of attraction it is possible to use the secant vector S_i joining the previously computed Y_{i-1} and Y_i to replace the tangent vector T_i at Y_i in the predictor process (1.2). This approach, which somehow is ignored by most authors in the references, usually will save at least $O\left(\frac{n^3}{6}\right)$ "flops" per step while we still maintain a comparable accuracy.

This short paper consists of two major parts. We begin in the next section with a heuristic background by reviewing some theoretic results of the continuous Newton method. This consideration more or less justifies the property of orthogonality. Then in the last section we establish the domain of attraction along the curve Γ which, in essence, is equivalent to the well-known Newton-Kantorovich theorem.

2. Preliminaries

Henceforth we shall denote the point (x,t) in $\mathbb{R}^{n+1}$ by Y. If we introduce a parameter σ, say the arc length, along the curve Γ, then an initial value problem is implicitly defined by

$$DH(Y)\cdot \dot{Y}=0; \qquad Y(0)=Y_0 \tag{2.1}$$

where $\dot{} = \frac{d}{d\sigma}$. It can be shown [9] that the vector field $\dot{Y}$ is locally Lipschizian. Thus nowadays highly developed IVP-solvers certainly can be utilized to help solve this problem, see e.g., [13]. In doing so, however, no advantages is taken of the fact that the curve Γ satisfies the Eq. (1.1).

On the other hand, if the continuous Newton method is applied to solve this underdetermined system (1.1), we will have to consider the differential system

$$DH(Y)\cdot Y' = -H(Y) \tag{2.2}$$

where $' = \frac{d}{d\tau}$ and τ is a certain appropriate parameter. It is obvious that any solution to (2.2) satisfies the equation

$$H(Y(\tau)) = e^{-\tau} H(Y(0)). \tag{2.3}$$

Furthermore, if we assume that $DH(Y)$ is always of full rank along the solution curve, then (2.2) can be reduced to

$$Y' = -DH^{+}(Y)H(Y) \tag{2.4}$$

where $DH^{+}(Y) = DH^{T}(Y)[DH(Y)DH^{T}(Y)]^{-1}$ is the Moore-Penrise generalized inverse of $DH(Y)$. From the well-known fact that

$$\mathrm{Range}(DH^{+}) = \mathrm{Range}(DH^{T}) = \mathrm{Kernel}(DH)^{\perp} \tag{2.5}$$

and the fact (2.3), we see that the solution $Y(\tau)$ to (2.4) always moves in such a way not only to reduce the magnitude of $H(Y)$ but also to remain perpendicular to the 1-dimensional kernel space of $DH(Y)$.

Consider now an Euler step of (2.4). This corresponds to the following Newton-like iteration scheme

$$Y_{k+1} = Y_k - DH^{+}(Y_k)H(Y_k). \tag{2.6}$$

The above arguments for the continuous case certainly are in favor of this discrete case as well. In particular, the resulting point Y_{k+1} lies on the hyperplane normal to the tangent vector of the curve $\{Y \in \mathbb{R}^{n+1};\ H(Y) = H(Y_k)\}$.

Since these tangent vectors form a Lipschizian vector field on Y, we can expect the desired property of orthogonality from the scheme (2.6), provided the sequence $\{Y_k\}$ converges to a point on Γ. This fact will be justified in the next section. To get enough motivations, however, we conclude this section with the modification of two theorems proved by Tanabe [10] concerning the convergence of the continuous scheme (2.4).

Theorem 2.1. *The set* $\Gamma = \{Y \in \mathbb{R}^{n+1};\ H(Y) = 0\}$ *is a stable centre manifold* (*see* [4]) *for the system* (2.4).

Theorem 2.2. *If the initial value* $Y(0)$ *is close enough to the curve* Γ, *then the solution* $Y(\tau)$ *to* (2.4) *stays close to* Γ. *Indeed,* $Y(\tau)$ *converges to a point on* Γ *exponentially as* $\tau \to \infty$.

3. Domain of Attraction

In this section we analyze the local convergence behavior of the scheme (2.6). In fact, a modified version

$$Y_{k+1} = Y_k - DH^{+}(Y_0)H(Y_k) \tag{3.1}$$

has already been proposed by Ben-Israel [3] as early as 1965, and its convergence property is a consequence of a classical implicit function theorem. Recently, other versions of scheme (2.6), such as the least change secant update of $DH(Y_k)$, have also been proposed [5, 6]. Although no theoretic work has been done for these methods at the present time, the reported numerical testing results apparently evidence the success.

We first generalize the Banach perturbation lemma.

Lemma 3.1. *Suppose that the matrix $A \in \mathbb{R}^{n\times(n+1)}$ is of full rank and the matrix $B \in \mathbb{R}^{n\times(n+1)}$ is such that $\|A-B\|\,\|A^+\|<1$. Then*

(i) *B is of full rank and*

$$\text{(ii)}\quad \|B^+\| \leqq \frac{\|A^+\|}{1-\|A-B\|\,\|A^+\|} \tag{3.2}$$

where $\|\ \|$ is the $\mathscr{L}^2$-norm.

Proof. Observe that, since A is of full rank,

$$B = A(I + A^+(B-A)) \tag{3.3}$$

where I is the identity matrix in $\mathbb{R}^{(n+1)\times(n+1)}$. Classical Banach lemma implies that $I+A^+(B-A)$ is invertible. Part (i) follows. Furthermore, we have the estimate

$$\|[I+A^+(B-A)]^{-1}\| \leqq \frac{1}{1-\|B-A\|\,\|A^+\|}. \tag{3.4}$$

Recall that

$$B^+ B = P_{B^T} \tag{3.5}$$

where P_{B^T} is the projection onto the row space of B. Multiplying both sides of (3.5) by A^+, we obtain

$$B^+ = P_{B^T} A^+ [I + (B-A)A^+]^{-1}. \tag{3.6}$$

Since $\|P_{B^T}\|=1$, (3.2) follows from (3.4).

The next very useful lemma is a classical result in advanced calculus. We simply state it without proof.

Lemma 3.2. *Let $F\colon D\subset\mathbb{R}^m \to \mathbb{R}^n$ be a continously differentiable function such that*

$$\|DF(Y)-DF(Z)\| \leqq \gamma\,\|Y-Z\| \tag{3.7}$$

for every $Y, Z\in D$. Then for every $Y, Z \in D$, we have

$$\|F(Y)-F(Z)-DF(Z)(Y-Z)\| \leqq \frac{\gamma}{2}\,\|Y-Z\|^2. \tag{3.8}$$

We now establish the main result.

Theorem 3.1. *Let $H\colon D\subset\mathbb{R}^{n+1}\to\mathbb{R}^n$ be a C^2 function such that*

$$\|DH(Y)-DH(Z)\| \leqq \gamma\,\|Y-Z\| \tag{3.9}$$

for every $Y, Z\in D$. Suppose $H(Z^*)=0$ and $DH(Z^*)$ is of full rank. Choose $0<\delta<\frac{3-\sqrt{5}}{2}$ and define

$$M = \min\left\{\frac{2}{3\gamma\,\|DH^+(Z^*)\|}, \operatorname{dist}(Z^*, \partial D)\right\}. \tag{3.10}$$

If $0<r<\delta M$ is such that for every $Z\in B(Z^*, r)$ we have

$$\|H(Z)\| < \frac{\delta \gamma M^2}{2}, \tag{3.11}$$

then with any $Z_0 \in B(Z^*, r) \subset D$, *the scheme* (2.6) *is well-defined and converges geometrically to a point in* $\Gamma \cap B(Z^*, M)$.

Proof. For any $Z \in B(Z^*, M)$, observe that

$$\|DH(Z) - DH(Z^*)\| \, \|DH^+(Z^*)\| \leqq \gamma \|Z - Z^*\| \, \|DH^+(Z^*)\| < \tfrac{2}{3} < 1. \tag{3.12}$$

It follows from Lemma 3.1 that $DH(Z)$ is of full rank and

$$\|DH^+(Z)\| \leqq 3 \|DH^+(Z^*)\|. \tag{3.13}$$

Using the condition (3.11) we then have

$$\|Z_1 - Z_0\| = \|DH^+(Z_0) H(Z_0)\| < \delta M. \tag{3.14}$$

It follows from the choice of δ that $\|Z_1 - Z^*\| < M$ and, thus, Z_2 is well-defined. Furthermore, applying Lemma 3.2, we have

$$\begin{aligned} \|Z_2 - Z_1\| &= \|DH^+(Z_1) H(Z_1)\| \\ &\leqq \|DH^+(Z_1)\| \, \|H(Z_1) - H(Z_0) - DH(Z_0)(Z_1 - Z_0)\| \\ &< \|DH^+(Z_1)\| \frac{\gamma}{2} \|Z_1 - Z_0\|^2. \end{aligned} \tag{3.15}$$

With the help of (3.10) and (3.14), it follows that

$$\|Z_2 - Z_1\| < \delta \|Z_1 - Z_0\| \tag{3.16}$$

and

$$\|Z_2 - Z^*\| < \frac{1}{1-\delta} \|Z_1 - Z_0\| + \|Z_0 - Z^*\| < M. \tag{3.17}$$

Now suppose that we have shown the following

$$\|Z_k - Z_{k-1}\| < \delta \|Z_{k-1} - Z_{k-2}\| \tag{3.18}$$

and

$$3 \|DH^+(Z^*)\| \frac{\gamma}{2} \|Z_{k-1} - Z_{k-2}\| < \delta \tag{3.19}$$

for all $k = 2, 3, \ldots, n$. Then

$$\begin{aligned} \|Z_n - Z^*\| &\leqq \sum_{j=1}^{n} \|Z_j - Z_{j-1}\| + \|Z_0 - Z^*\| \\ &\leqq \frac{1}{1-\delta} \|Z_1 - Z_0\| + \|Z_0 - Z^*\| < M \end{aligned} \tag{3.20}$$

by our choice of δ. Using (3.13) and (3.18), we also have

$$\|DH^{+}(Z_n)\| \frac{\gamma}{2} \|Z_n - Z_{n-1}\| < \delta^2 < \delta. \tag{3.21}$$

But then

$$\begin{aligned} \|Z_{n+1} - Z_n\| &\leqq \|DH^{+}(Z_n)\| \, \|H(Z_n) - H(Z_{n-1}) - DH(Z_{n-1})(Z_n - Z_{n-1})\| \\ &\leqq \|DH^{+}(Z_n)\| \frac{\gamma}{2} \|Z_n - Z_{n-1}\|^2 < \delta \|Z_n - Z_{n-1}\| \end{aligned} \tag{3.22}$$

By induction we see that $\{Z_k\} \subset B(Z^*, M)$ and

$$\|Z_{k+p} - Z_k\| \leqq \frac{\delta^k(1-\delta^p)}{1-\delta} \|Z_1 - Z_0\|. \tag{3.23}$$

If $\hat{Z}$ is the limit point of this Cauchy sequence, then $DH^{+}(\hat{Z})H(\hat{Z}) = 0$. Since $DH^{+}(\hat{Z})$ is of full rank, it is necessary to have $H(\hat{Z}) = 0$.

Remark. Geometrically the condition (3.11) is used merely to monitor the magnitude of the projection of $Z_0 - Z^*$ onto the kernel space of $DH(Z_0)$. It is possible to have other alternatives instead of (3.11).

Remark. Suppose Y_{k-1} and Y_k are two consecutive points which have been accepted as approximating points for Γ. Let

$$S_k = Y_k - Y_{k-1}. \tag{3.24}$$

The predictor (1.2) can be replaced by

$$Z_0 = Y_k + r \frac{S_k}{\|S_k\|} \tag{3.25}$$

where the scalar r may be regarded as the acceleration or deceleration factor taking place along the curve Γ. This adaptive procedure is quite nature and practical now since it has been shown that the curve Γ is enveloped in a (uniform) domain of attraction. As long as Z_0 stays in this envelope, this r can be adapted to be as large as possible.

Remark. Although the rate of convergence of scheme (2.6) is shown to be geometric only, one should note that the strength of a proposed method also depends upon the strength of its computer implementation. For example, the introduction of the Broyden secant update with special Powell steps and other special controls into our method have been proved to be able to reduce the total overhead significantly, see e.g. [5] and [6]. It is hoped that besides being of theoretical interest in itself, our result will be further developed and implemented.

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