

اصلاحی بر حرکت روی منحنی در روش هموتوپی پیوسته

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چکیده

پیدا نمودن جوابهای معادلات تحلیلی از قدیم الایام مورد توجه و بحث ریاضی دانان بوده و روشها مختلفی برای حل اینگونه مسائل ارائه شده است. در این مورد از اوائل دهه ۱۹۳۰ روشی بنام هموتوپی ارائه شده که هنوز هم زمینه بحث فراوان دارد. اصول این روش به اختصار چنین است: فرض کنیم $F(x)$ معادله‌ای است که در شرایط خاصی صدق می‌کند. برای پیدا نمودن صفرهای این معادله ابتدا معادله‌ای ارائه می‌شود که صفرهای آن به سهولت قابل محاسبه است و به طریقی در ارتباط با $F(x)$ می‌باشد. سپس یک هموتوپی بین $F(x)$ و معادله اخیر برقرار می‌نمائیم. از این مرحله به بعد روش کار به این صورت است که از جوابهای معادله اخیر بکمک هموتوپی داده شده بطور پیوسته حرکت نموده و انتظار می‌رود که نهایتاً به جوابهای $F(x)$ برسیم. اما چگونگی تعریف هموتوپی مورد بحث، تعیین معادله‌ای که جوابهای آن به سهولت قابل محاسبه‌اند، چگونگی حرکت بطور پیوسته، امکان حرکت، و نهایتاً راههای مقرون به صرفه چنین حرکتی متضمن مسائل و مشکلات عدیده‌ای می‌باشد. در این مقاله سعی شده است که جهت حرکت روی منحنی در هر لحظه تعیین شود. عبارت دیگر ثابت شده است که این جهت در ارتباط با حاصلضرب میدان برداری جوابهای معادله دیفرانسیل متناظر با هموتوپی مفروض پیدا می‌شود.

An improvement on the path following technique of the homotopy continuation method

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Abstract

In order to approximate the solution of an analytic function by homotopy continuation method, one follows a curve starting from a trivial system and numerically moves along this curve to find the solution of the given function.

In this paper a new technique is developed to determine the orientation of the movement along the path by computing of the vector field of the corresponding differential equation. Namely as a main result we show that the orientation is derived from computation of the corresponding vector field.

1. Introduction

Let F be a smooth function from \mathbf{R}^n to \mathbf{R}^n . In this paper we shall first consider the problem of finding the solution of $F(x)=0$, by homotopy continuation method. The term «continuation method» is derived from a class of numerical methods dating at least back to Lahaye (1934 & 1935), and also known as «embedding method». Detailed discussion of these methods can be found in articles by Wacker (1978), and Allgower & George (1980). One starts with a trivial equation, one to which the solution is obvious and immediately known. Then the system is deformed continuously to $F(x)=0$. In general, the solution of the trivial system will prescribe under this deformation, a smooth curve which is connected to the solution of $F(x)=0$. Our discussion here is limited to following the curve. As a main result, we show the determination of the orientation of the curve is a by-product of the computation of the vector field of the ordinary differential equation.

2. Homotopy and path existence

In early 1950's, Davidenko (1953a & b) introduced a method of solving $F(x)=0$, where F is a smooth function from \mathbf{R}^n to \mathbf{R}^n . Let $H : \mathbf{R}^n \times [0, 1] \rightarrow \mathbf{R}^n$ be defined as

$$H(x, t) = (1 - t)(x - a) + tF(x) \quad (2.1)$$

with $a \in \mathbf{R}^n$ given. It is clear that $H(x, 0) = x - a$ and $H(x, 1) = F(x)$, Suppose.

(A): the partial derivative H_x is always nonsingular. Then by application of the Implicit Function Theorem, there exists a curve $x(t)$, as a function of t , such that

$$H(x(t), t) = 0. \quad (2.2)$$

we differentiate (2.2) with respect to t , to get the differential equation

$$\frac{dx}{dt} = -H_x^{-1} H_t, \quad (2.3)$$

$$x(0) = a.$$

Thus, finding a zero of $F(x)$ is equivalent to solving the initial value problem (2.3), and finding its value at

$t=1$. The assumption (A) is rather strong, and hence the power of Davidenko's method is restricted.

Let us consider the homotopy

$$H : \mathbf{R}^n \times \mathbf{R}^n \times (0, 1) \rightarrow \mathbf{R}^n \quad (2.4)$$

defined by

$$H(x, a, t) = (1 - t)(x - a) + tF(x)$$

with $x \in \mathbf{R}^n$, $a \in \mathbf{R}^n$, $t \in (0, 1)$. For a fixed $a \in \mathbf{R}^n$, define

$$H_a : \mathbf{R}^n \times (0, 1) \rightarrow \mathbf{R}^n \quad (2.5)$$

by $H_a(x, t) = H(x, a, t)$.

The following theorem may be found in Transversal mapping and flows, by Abraham and Robbin (1967).

Theorem 2.1 (Generalized Sard's Theorem)

Let $V \subset \mathbf{R}^n$, $W \subset \mathbf{R}^m$ be open and let

$$G : V \times W \rightarrow \mathbf{R}^p$$

be smooth. If $0 \in \mathbf{R}^p$ is a regular value for G , then for almost every $a \in V$ (in the sense of either Baire category or Lebesgue measure), 0 is a regular value for $G_a(\cdot) \equiv G(a, \cdot)$.

For our homotopy defined in (2.4) we have the following.

Lemma 2.2

For almost every $a \in \mathbf{R}^n$, zero is a regular value of

$$H_a : \mathbf{R}^n \times (0, 1) \rightarrow \mathbf{R}^n$$

Where H_a is given in (2.5).

The overall idea is to start from a trivial solution of $H_a(\cdot, 0) = 0$, and follow the path generated in $H_a(\cdot, t)$ as t goes from zero to one. We hope the trivial solution deforms into the solution of the original system, and hence we would be able to follow the connected path from the trivial system to the solution of $F(x) = 0$.

Of course this is quite an idealized process, and there are a number of difficulties. First of all, in general, a path need not exist. Second, if one exists, it might be very ill-behaved. In other words the set

$$\{(x, t) : x \in \mathbf{R}^n, t \in (0, 1), H_a(x, t) = 0\}$$

may consist of different solutions, such as isolated points, self-convergings, bifurcations, endless spirals, closed

orbit, and smooth paths. But we are interested only in smooth paths,

Let a be chosen so that 0 is a regular value for $H_a(x, t)$ (because of Lemma (2.2) this can be done with probability one). Then repeated use of the Implicit function Theorem implies that $H_a^{-1}(0)$ consists of one dimensional manifolds. Detailed discussion for the existence of paths are given by Garcia and Zangwill (1978), Garcia (1979a & b) and Chow, Mallet - Paret and Yorke (1978). Let Γ_a be the component of $H_a^{-1}(0)$ with a as one endpoint. Also let us assume this component is parameterized by s . For notational convenience we refer to $H_a(x, t)$ by $H(x, t)$. Therefore,

$$\begin{aligned} H(x(s), t(s)) &= 0, \\ x(0) &= a. \end{aligned} \quad (2.6)$$

Differentiation of H with respect to parameter s yields

$$\begin{aligned} H_x(x(s), t(s)) \cdot \dot{x} + H_t(x(s), t(s)) \cdot \dot{t} &= 0, \\ x(0) &= a. \end{aligned} \quad (2.7)$$

Here H_x and H_t are respectively the partial derivative of H with respect to x and t . The ordinary differential equations (2.7) can be written in the following matrix form

$$\begin{aligned} [H_x \ H_t] \begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix} &= 0, \\ \begin{bmatrix} x(0) \\ t(0) \end{bmatrix} &= \begin{bmatrix} a \\ 0 \end{bmatrix}. \end{aligned} \quad (2.8)$$

The integral curve of this differential equation, namely $(x(s), t(s))$ is a simple curve starting from $(a, 0)$. In the next section we carefully examine the movement along this curve.

3. Movement along the Path

We have seen that $H_a^{-1}(0)$ consists of only arcs and closed curves. These curves are the solutions of the ordinary differential equations

$$[H_x \ H_t] \begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix} = 0,$$

$$\begin{bmatrix} x(0) \\ t(0) \end{bmatrix} = \begin{bmatrix} a \\ 0 \end{bmatrix}, \quad (3.1)$$

where H_x is an $n \times n$ matrix, H_t is an $n \times 1$ matrix and $\dot{H} = d/ds$ for some parameter s . For the remainder of this section, we will let s be the arc length. Since 0 is a regular value of H , $[H_x \ H_t]$ is of full rank. Hence the kernel of $[H_x \ H_t]$ is one - dimensional, by above the vector $\begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix}$ lies in this kernel.

$$\begin{aligned} \text{Let } A &= [H_x \ H_t] \text{ and } y = \begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix}. \text{ Then (3.1) simplifies to} \\ Ay &= 0, \quad y(0) = \begin{bmatrix} a \\ 0 \end{bmatrix}. \end{aligned} \quad (3.2)$$

with $\|\dot{y}\|_2 = 1$, where $\|\cdot\|_2$ is the ordinary Euclidean norm. The equation $Ay = 0$ means that \dot{y} is perpendicular to the row space of A . Let $A^t = QR$ where Q is an $(n+1) \times (n+1)$ orthogonal matrix and R is an $(n+1) \times n$ upper triangular matrix with $r_{ii} \geq 0$ ($i=1, \dots, n$).

Suppose for some s , $\dot{y}(s)$ is known, hence A is known.

The following lemma enables us to find $\dot{y}(s+\Delta s)$ and trace the path by an ordinary differential equation solver.

Lemma 3.1

Let q_{n+1} be the last column of the orthogonal matrix Q , then

$$\dot{y} = \pm q_{n+1}. \quad (3.3)$$

Proof :

Since $A^t = QR$, and $Ay = 0$, we have

$$R^t Q^t \dot{y} = 0.$$

Since matrix R has rank n , we get

$$r_{ii} \neq 0 \quad i=1, 2, \dots, n.$$

Suppose $Q^t \dot{y} = (\beta_1, \beta_2, \dots, \beta_{n+1})^t$, then we have

$$\begin{aligned} r_{11}\beta_1 &= 0 \\ r_{12}\beta_1 + r_{22}\beta_2 &= 0 \\ &\vdots \\ r_{1n}\beta_1 + r_{2n}\beta_2 + \dots + r_{nn}\beta_n &= 0. \end{aligned}$$

Because of (3.4) this system implies

$$\beta_1 = \beta_2 = \dots = \beta_n = 0.$$

Hence

$$Q^t \dot{y} = (0, 0, \dots, \beta_{n+1})^t.$$

So

$$\dot{y} = Q(0, 0, \dots, \beta_{n+1}).$$

Therefore \dot{y} is a scalar multiple of the last column of Q .

Since $\|\dot{y}\|_2 = 1$, we get

$$\dot{y} = \pm q_{n+1}.$$

In order to determine the orientation of \dot{y} , we give the following theorem which can be found in Garcia and Gould (1978).

Theorem 3.2

Let $H : \mathbf{R}^{n+1} \rightarrow \mathbf{R}^n$ be a C^1 map, and let $z(s) = (z_1(s), \dots, z_{n+1}(s))$ be a C^1 curve in \mathbf{R}^{n+1} satisfying $H(z(s)) = 0$.

Then for all s either

$$\text{sgn } z'_i(s) = \text{sgn } \det H^i(z(s)) \quad (3.5)$$

or

$$\text{sgn } z'_i(s) = -\text{sgn } \det H^i(z(s)) \quad (3.5.1)$$

where $z'_i(s) = \frac{dz}{ds}$ and H^i is the Jacobian of H with

i th column deleted.

Applying this theorem to our homotopy, we get either

$$\text{sgn } \dot{t}(s) = \text{sgn } \det H_x(x(s), t(s)) \quad (3.6)$$

or

$$\text{sgn } \dot{t}(s) = -\text{sgn } \det H_x(x(s), t(s)) \quad (3.6.1)$$

for all s . However at $s = 0$, H_x is the $n \times n$ identity matrix and hence $\det H = 1$. We may assume $\dot{t}(0) > 0$, therefore (3.6) holds for all s . Thus $\text{sgn } \dot{y}$ in (3.3) is determined as soon as we know $\text{sgn } \dot{t}(s)$, and to this end we prove the following proposition :

Proposition 3.3

Let $Q = (q_{ij})$, then

$$\text{sgn } \dot{t}(s) = (-1)^n \text{sgn } (q_{n+1, n+1}), \quad (3.7)$$

Proof

Let $e_{n+1} \in \mathbf{R}^{n+1}$ be the $(n+1)$ th unit vector.

That is

$$e_{n+1} = (0, 0, \dots, 1)$$

then

$$Q^t[A^t e_{n+1}] = Q^t[QR e_{n+1}] = [R Q^t e_{n+1}].$$

By property of the Housholder transformations (For detail see Raleston, 1978)

$$\det Q^t = \det p_n \det p_{n-1} \dots \det p_1 = (-1)^n.$$

Where p_1, \dots, p_n is a sequence of Housholder transformations such that

$$P_n P_{n+1}, \dots, P_1 A^t = R.$$

Hence

$$\begin{aligned} \det [R Q^t e_{n+1}] &= \det Q^t \cdot \det [A^t e_{n+1}] \\ &= (-1)^n \det \begin{bmatrix} H_x^t & 0 \\ H_t^t & 0 \end{bmatrix} = (-1)^n \det H_x^t. \end{aligned}$$

On the other hand, since R is an upper triangular matrix with $r_{ii} > 0$, we have

$$\text{sgn } \det [R Q^t e_{n+1}] = \text{sgn } (q_{n+1, n+1}). \quad (3.8)$$

Therefore

$$\text{sgn } \dot{t} = \text{sgn } \det H_x^t = (-1)^n \text{sgn } (q_{n+1, n+1}) \quad (3.9)$$

From the above discussion we see that in order to follow the curve Γ_a , namely, finding the solution of homotopy equation (2.6) at $t=1$ can be summarized as follows :

We start at $t=0$ and compute H_x , H_t and factorize

$$A^t = \begin{bmatrix} H_x^t \\ H_t^t \end{bmatrix}$$

as a product of an $(n+1) \times (n+1)$ orthogonal matrix

$Q = (q_{ij})$ and an $(n+1) \times n$ upper triangular

matrix R . Then $\begin{bmatrix} x(s) \\ t(s) \end{bmatrix}$ is given by the last column of

Q with a possible sign change, and the sign of this vector is given by (3.7). Next we solve the differential equation (2.8) and continue this process until $t=1$.

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