Mathematical Programming 39 (1987) 181-188
North-Holland

ON THE GLOBAL CONVERGENCE OF PATH-FOLLOWING METHODS TO DETERMINE ALL SOLUTIONS TO A SYSTEM OF NONLINEAR EQUATIONS

Immo DIENER

Institut für Numerische und Angewandte Mathematik, Georg-August Universität Göttingen, D-3400 Göttingen, FR Germany

Received 23 August 1985
Revised manuscript received 6 April 1987

In this paper we prove a general theorem stating a sufficient condition for the inverse image of a point under a continuously differentiable map from $\mathbb{R}^n$ to $\mathbb{R}^k$ to be connected. This result is applied to the trajectories generated by the Newton flow. Several examples demonstrate the applicability of the results to nontrivial problems.

AMS(MOS) Subject Classification: 65K05, 65H10, 26B10, 90C30, 90A14.

Key words: Global optimisation, trajectory methods, continuous Newton method, global implicit function theorem.

1. Introduction

We consider the problem of determining $Z(F)$, the set of all zeros of a continuously differentiable map $F:\mathbb{R}^n\to\mathbb{R}^n$. Only during the last decade has this problem been investigated in the literature and still there are only a few papers on this subject. Most of these papers describe various methods which might in some cases yield success, but results concerning the above problem have only been obtained for certain classes of polynomial-like functions (cf. [5, 6]). Among the path-following algorithms there are basically two distinct approaches, namely homotopy methods and trajectory methods, but various connections exist between these two methods [4].

A procedure that finds all solutions to a system of nonlinear equations has numerous applications for instance in physics, in engineering and in economics. Also, with such a procedure, the global optimum of a scalar function can be found by considering the gradient equations and by determining all stationary points. In this paper we prove a general theorem, which can be applied to several path-following methods to yield global convergence results. Some examples are given in Section 3.

2. A global convergence theorem

The following theorem states sufficient conditions, such that the inverse images of points under a map $F:\mathbb{R}^n\to\mathbb{R}^k$, $k\leq n$, are all connected $(n-k)$-dimensional

This work was supported by the Deutsche Forschungsgemeinschaft.

submanifolds of R^n. The idea is to construct a retraction from R^n onto $F^{-1}(0)$. The conditions are rather restrictive but, however, are satisfied in a number of cases. Some examples are given in Section 3.

Theorem 2.1. *For $k \leqslant n$ let F be a function in $C^2(\mathbb{R}^n, \mathbb{R}^k)$ such that*

$$\sup\{\|(DF(x)D^{\mathrm{T}}F(x))^{-1}\| \,|\, x \in \mathbb{R}^n\} \leqslant K < \infty.$$

Then $F^{-1}(0)$ is a connected $(n-k)$-dimensional submanifold in $\mathbb{R}^n$.

Proof. By the regularity condition, $F^{-1}(0)$ is trivially a $(n-k)$-submanifold in $\mathbb{R}^n$. Only the connectedness needs to be proved. Consider the C^1-vectorfield on $\mathbb{R}^n$, given by

$$V : x \mapsto -D^{\mathrm{T}}F(x)(DF(x)D^{\mathrm{T}}F(x))^{-1}\frac{F(x)}{1+\|F(x)\|}.$$

For all $x \in \mathbb{R}^n$ we have (with $\|\cdot\|$ denoting the euclidean norm)

$$\|V(x)\| \leqslant \sqrt{K}\frac{\|F(x)\|}{(1+\|F(x)\|)} < \sqrt{K}.$$

Thus the vectorfield is defined on the whole $\mathbb{R}^n$ and bounded. It follows that V determines a global C^1 flow $\Phi(t, x)$ such that

$$\frac{\partial \Phi(t, x)}{\partial t} = V(\Phi(t, x)) \quad \text{and} \quad \Phi(0, x) = x.$$

Therefore we have

$$\frac{\partial}{\partial t} F(\Phi(t, x)) = -\frac{F(\Phi(t, x))}{1+\|F(\Phi(t, x))\|}$$

and

$$\frac{\partial}{\partial t}\|F(\Phi(t, x))\|^2 = -2\frac{\|F(\Phi(t, x))\|^2}{1+\|F(\Phi(t, x))\|} \leqslant 0.$$

Thus for any $x_0 \in \mathbb{R}^n$ and any $t \geqslant 0$:

$$\begin{aligned}\|F(\Phi(t, x_0))\|^2 &= \|F(x_0)\|^2 \exp\left(-2\int_0^t \frac{\mathrm{d}\tau}{1+\|F(\Phi(\tau, x_0))\|}\right)\\ &\leqslant \|F(x_0)\|^2 \exp\left(\frac{-2t}{1+\|F(x_0)\|}\right).\end{aligned}$$

It follows that

$$\lim_{t\to\infty} \|F(\Phi(t, x_0))\| = 0.$$

Next we show that all trajectories are bounded. For any $x \in \mathbb{R}^n$ we obtain

$$\begin{aligned}
\|\Phi(T, x) - \Phi(0, x)\| &= \left\| \int_0^T V(\Phi(t, x))\, \mathrm{d}t \right\| \\
&\leq \int_0^T \|V(\Phi(t, x))\|\, \mathrm{d}t \\
&\leq \sqrt{K} \int_0^T \frac{\|F(\Phi(t, x))\|}{1 + \|F(\Phi(t, x))\|}\, \mathrm{d}t \\
&\leq \sqrt{K} \int_0^T \|F(\Phi(t, x))\|\, \mathrm{d}t \\
&\leq \sqrt{K}\|F(x)\| \int_0^T \exp\left(\frac{-t}{1 + \|F(x)\|}\right) \mathrm{d}t.
\end{aligned}$$

Therefore, for all $x_0 \in \mathbb{R}^n$ and $T \geq 0$ we have

$$\|\Phi(T, x_0) - x_0\| \leq \sqrt{K}\|(x_0)\|(1 + \|F(x_0)\|$$

and thus the trajectories are bounded and reach $F^{-1}(0)$ for $t \to \infty$. So we can define a continuous, surjective mapping $\Phi_\infty : \mathbb{R}^n \to F^{-1}(0)$ which leaves $F^{-1}(0)$ fixed. Since R^n is connected, it follows that $F^{-1}(0)$ is connected. $\square$

Remark. The reader might convince himself that the condition rank $DF(x) = k$ for all $x \in \mathbb{R}^n$ is not sufficient in general for $F^{-1}(0)$ to be connected.

3. Applications

Consider the curves generated by the Newton flow, that is, the flow generated by the well known Newton equation

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = -(DF(x(t)))^{-1} F(x(t)) \tag{1}$$

In this context it is customary to study, instead of (1), the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = -\mathrm{adj}\ DF(x(t)) F(x(t)) \tag{2}$$

where adj A denotes the adjoint of a matrix A. The phase portrait of (1) "equals" the phase portrait of (2) on the subset of $\mathbb{R}^n$ where both equations are defined. System (2) and similar equations have recently been studied by several authors (cf. Branin [1], Gomulka [7], Jongen, Jonker and Twilt [10], Smale [12] and others) in connection with the determination of the global minimum of a function $f : \mathbb{R}^n \to \mathbb{R}$. Also, since the usual Newton method can be viewed as a numerical integration of

(1), the study of these trajectories might yield new insight into the global convergence behavior of the Newton method (cf. [9]).

The related set of solutions to

$$G(x, t) = F(x) - tF(x_0) = 0, \quad x \in \mathbb{R}^n, \ t \in \mathbb{R}, \tag{3}$$

has been studied for instance in [3, 4, 11 and 12]. The projection of $G^{-1}(0)$ onto the first n components yields a point set "equal" to the phase portrait of (2). Moreover, $G^{-1}(0)$ can be traced by using a scalar labeling simplicial pivoting algorithm instead of integrating (1) or (2).

We shall introduce one more description of the relevant point set:

Definition. We write $x \| y$ if x and y are linearly dependent. Let $F: \mathbb{R}^n \to \mathbb{R}^n$ be continuous, and $0 \neq g \in \mathbb{R}^n$ be a fixed direction. Then we call the set

$$T_g(F) := \{x \in \mathbb{R}^n \mid F(x) \| g\}$$

a *Newton trajectory* of F. Let $A_g : \mathbb{R}^n \to \mathbb{R}^{n-1}$ be a linear map of rank $n-1$ such that $A_g g = 0$. Then we define the continuous map F_g by

$$F_g : \mathbb{R}^n \to \mathbb{R}^{n-1}, \qquad x \mapsto A_g F(x).$$

Obviously we have $F_g^{-1}(0) = T_g(F)$.

$T_g(F)$ is just the projection of $G^{-1}(0)$, where $F(x_0) = g$, onto $\mathbb{R}^n$. The nice property of these trajectories are expressed by the following obvious.

Lemma. *Let g_1, $g_2 \in \mathbb{R}^n$ be linearly independent and $F \in C(\mathbb{R}^n, \mathbb{R}^n)$. Then $Z(f) = T_{g_1}(F) \cap T_{g_1}(F)$.*

Thus if $T_g(F)$ is connected for some $g \in \mathbb{R}^n$, we could find all zeros of F by tracing $T_g(F)$. However, in general $T_g(F)$ can have many components and no one knows how these can be detected. Theorem 2.1 gives sufficient conditions, such that $T_g(F)$ has only one component:

Theorem 3.1. *Let $F \in C^2(\mathbb{R}^n, \mathbb{R}^n)$, $0 \neq g \in \mathbb{R}^n$. If*

$$\sup\{\|(AgDF(x)D^\top F(x)A_g^\top)^{-1}\| \,|\, x \in \mathbb{R}^n\} < \infty$$

then the Newton trajectory $T_g(F)$ is a connected, 1-dimensional submanifold in $\mathbb{R}^n$ containing all zeros of F.

Proof. Apply Theorem 2.1 to the map F_g. $\square$

Defining the trajectories by (3) yields an equivalent condition which is, however, a condition on the inverse of an n by n-matrix whereas the above theorem is about $n-1$ by $n-1$-matrices. In general the above condition is easier to work with. Thus, if Theorem 3.1 applies (3) can be used to numerically trace all zero points of F.

Let $f \in C^2(\mathbb{R}^n, \mathbb{R})$. By $\nabla f(x)$ we denote the usual gradient vector and $H_f(x)$ denotes the Hessian matrix of f at x. We define $T_g(f)$ to be $T_g(\nabla f)$. Since the Hessian matrix is symmetric we have

Theorem 3.2. *Let f be a function from $C^3(\mathbb{R}^n, \mathbb{R})$ and $0 \neq g \in \mathbb{R}^n$. If*

$$\sup\{\|(A_g H_f^2(x) A_g^\top)^{-1}\| \mid x \in \mathbb{R}^n\} < \infty$$

then the Newton trajectory $T_g(f)$ is a connected 1-dimensional submanifold in $\mathbb{R}^n$, containing all critical points of f.

In order to apply these theorems it is often useful to know some of the transformation properties of Newton trajectories. The next theorem summarizes some easily established facts.

Theorem 3.3. (a) *If $f \in C^1(\mathbb{R}^n, \mathbb{R})$ and $h \in C^1(\mathbb{R}, \mathbb{R})$ with $h'(x) > 0$ for all $x \in \mathbb{R}$, then we have $T_g(h \circ f) = T_g(f)$.*

(b) *If F, $B \in C(\mathbb{R}^n, \mathbb{R}^n)$ and $B^{-1}(x)$ exists for all $x \in \mathbb{R}^n$, then we have $T_g(F \circ B) = B^{-1} T_g(F)$.*

(c) *If $f \in C^1(R^n, \mathbb{R})$ and B is a linear isomorphism of $\mathbb{R}^n$, then we have $T_g(f) = B \cdot T_{B^\top g}(f \circ B)$.*

(d) *If G denotes the constant function which maps every x to g, we have $T_g(F) = T_g(F+G)$ although $Z(F) \cap Z(F+G)$ is empty. Likewise, if $\hat{G}$ sends x to $g^\top x$, it follows that $T_g(f) = T_g(f + \hat{G})$ although the two functions have no critical point in common.*

Proof. (a) and (d) are obvious. (b) follows from

$$\begin{aligned} T_g(F \circ B) &= \{x \in \mathbb{R}^n \mid g \| F(B(x))\} \\ &= \{B^{-1}(y) \in \mathbb{R}^n \mid g \| F(y)\} \\ &= B^{-1} T_g(F). \end{aligned}$$

In case (c) we calculate

$$\begin{aligned} T_g(f) &:= T_g(\nabla f) \\ &= B \cdot T_g(\nabla f \circ B) \\ &= B \cdot T_g(B^{\top -1} \nabla (f \circ B)) \\ &= B \cdot T_{B^\top g}(\nabla (f \circ B)) \\ &= B \cdot T_{B^\top g}(f \circ B). \end{aligned}$$

This proves the theorem. $\square$

We illustrate the application of these theorems by some examples

Example 1. Let $f:\mathbb{R}^2\to\mathbb{R}$ be given such that $f_{xy}(x,y)\geqslant\varepsilon>0$ for all $(x,y)^{\mathrm{T}}\in\mathbb{R}^2$ (for instance the notorious six hump camel-back function is of this type [8]). Choosing $A_g=(0,1)$, i.e. $g=(1,0)^{\mathrm{T}}$, we get

$$A_gH^2(x,y)A_g^{\mathrm{T}}=f_{yy}^2+f_{xy}^2\geqslant\varepsilon^2$$

for all $(x,y)^{\mathrm{T}}\in\mathbb{R}^2$. Thus $T_g(f)$ is connected and contains all critical points of f. (Thus, for instance, $T_g(f)$ strings all 15 critical points of the six hump-camel back function.) Applying Theorem 3.3 yields that $T_{B^{\mathrm{T}}g}(h\circ f\circ B)$ is connected, where $h:\mathbb{R}\to\mathbb{R}$, $h'(t)>0$ for all $x\in\mathbb{R}$, and B is a linear isomorphism of $\mathbb{R}^n$.

A whole class of examples of this type is obtained by considering (discrete or continuous) nonlinear L_2-approximation problems with approximating family $\{u(x,t)+v(y,t)\,|\,x,y\in\mathbb{R}\}$ such that $(u'(x),v'(y))\geqslant\varepsilon\geqslant0$ for all $x,y\in\mathbb{R}$ (for instance $u(x,t)=v(x,t)=\mathrm{e}^{xt}$). Then the Newton trajectory corresponding to $g=(1,0)^{\mathrm{T}}$ strings all critical points of the error function $f(x,y):=\|u(x)+v(x)-h\|^2$ no matter which function h is approximated and despite the fact that there may be any number of critical points (cf. [2]).

The functions in the next two examples were taken from [1], where the corresponding Newton trajectories have been computed only numerically. In either case there are numerous solutions depending on the choice of parameters.

Example 2. Let $F:\mathbb{R}^2\to\mathbb{R}^2$ be defined by

$$F(x,y)=\begin{pmatrix} a+(b-1)y+c\sin(d(x-y))-x(b+x^2)\\ x-y-e\sin(f(x^3+y))\end{pmatrix}$$

where a, b, c, d, e and f are arbitrary real parameters. Using Theorem 3.3 and substituting $x\leftarrow x^3+y$ and $y\leftarrow x-y$ we get

$$F(x,y)=\begin{pmatrix} a-by+c\sin(dy)-x\\ y-e\sin(fx)\end{pmatrix}$$

Choosing $A_g:=(\alpha,\beta)\neq(0,0)$, we obtain

$$A_gDF(x,y)D^{\mathrm{T}}F(x,y)A_g^{\mathrm{T}}=\|(-\alpha-\beta ef\cos(fx),\beta-\alpha(b-cd\cos(dy)))\|_2^2.$$

Theorem 3.2 applies if one of the following conditions holds:

(a) $|\alpha|>|\beta ef|$

(b) $|\beta-\alpha b|>|\alpha cd|$.

Given parameters $a,b,\ldots,f$ it is always possible to fulfill (a) or (b) by a suitable choice of α, and β.

Example 3. We consider the function $F:\mathbb{R}^3\to\mathbb{R}^3$ defined by

$$F(x,y,z)=\begin{pmatrix} a\sin(bx)\sin(bz)-y \\ c-dz+ey\sin(fz)-x \\ g+hy\sin(kx)-z \end{pmatrix}$$

where a, b, c, d, s, f, g, h and k are arbitrary real parameters. Calculating DF yields

$$DF(x,y,z)=\begin{pmatrix} ab\cos(bx)\sin(bz) & -1 & ab\sin(bx)\cos(bz) \\ -1 & e\sin(fz) & -d+efy\cos(fz) \\ hky\cos(kx) & h\sin(kx) & -1 \end{pmatrix}.$$

If we take, for instance,

$$A_g=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

i.e. $g=(0,0,1)^{\mathrm{T}}$, we get, after some calculation, for the determinant det of $A_gDF(x,y,z)D^{\mathrm{T}}F(x,y,z)A_g^{\mathrm{T}}$:

$$\begin{aligned}\det &= ((efy\cos(fz)-d)+abe\sin(fz)\sin(bx)\cos(bz))^2 \\ &\quad +a^2b^2(\cos(bx)\sin(bz)(efy\cos(fz)-d)+\sin(bx)\cos(bz))^2 \\ &\quad +(1-abe\sin(fz)\cos(bx)\sin(bz))^2.\end{aligned}$$

Clearly, if $|abe|=\varepsilon<1$, then $\det(x,y,z)\geqslant(1-\varepsilon)^2>0$ for all $(x,y,z)^{\mathrm{T}}\in\mathbb{R}^3$. Thus, in this case, $T_g(F)$ strings all zeros of F.

References

[1] F.H. Branin, Jr., "A widely convergent method for finding multiple solutions of simultaneous nonlinear equations," *IBM Journal of Research and Development* (1972) 504–522.

[2] I. Diener, "On Nonuniqueness in Nonlinear L_2-Approximation," *Journal of Approximation Theory* (to appear).

[3] C.B. Garcia and F.J. Gould, "A theorem on homotopy paths," *Mathematics of Operations Research* 3 (1978) 282–289.

[4] C.B. Garcia and F.J. Gould, "Relations between several path following algorithms and local and global Newton methods," *SIAM Review* 22 (1980) 263–274.

[5] C.B. Garcia and W.I. Zangwill, "Determining all solutions to certain systems of nonlinear equations," *Mathematics Operations Research* 4 (1979) 1–14.

[6] C.B. Garcia and W.I. Zangwill, "Finding all solutions to polynomial systems and other systems of equations," *Mathematical Programming* **16** (1979) 159–176.

[7] J. Gomulka, "Remarks on Branin's method for solving nonlinear equations," in: L.C. Dixon and G.P. Szegö, eds., *Towards Global Optmisation* (North-Holland Publishing Company, Amsterdam, 1975) pp. 96–106.

[8] J.W. Hardy, "An implemented extension of Branin's method," in: L.C. Dixon and G.P. Szegö, eds., *Towards Global Optimisation* (North-Holland Publishing Company, Amsterdam, 1975) p. 140.

[9] M.W. Hirsch and S. Smale, "On algorithms for solving $f(x)=0$," *Communications in Pure Applied Mathematics* 32 (1979) 281–312.

[10] H.Th. Jongen, P. Jonker and F. Twilt, "On Newton flows in optimisation," *Methods of Operations Research* 31 (1979) 345-359.

[11] H.B. Keller, "Global Homotopies and Newton Methods," in: C. De Boor and G.H. Golub, eds., *Recent Advances in Numerical Analysis* (Academic Press, 1978) pp. 73-94.

[12] S. Smale, "A convergent process of price adjustment and global Newton methods," *Journal of Mathematical Economics* 3 (1976) 107-120.