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AN ACCELERATION METHOD IN THE HOMOTOPY NEWTON'S CONTINUATION FOR NONLINEAR SINGULAR PROBLEMS*

YANG ZHONG-HUA (杨忠华)
(Shanghai University of Science and Technology, Shanghai, China)

Abstract

The nonlinear singular problem $f(u)=0$ is considered. Here f is a C^3 mapping from E^n to E^n. The Jacobian matrix $f'(u)$ is singular at the solution u^* of $f(u)=0$. A new acceleration method in the homotopy Newton's continuation is proposed. The quadratic convergence of the new algorithm is proved. A numerical example is given.

§ 1. Introduction

We consider the nonlinear singular problem

$$f(u)=0. \tag{1.1}$$

Here f is a C^3 mapping from E^n to E^n and u^* is a singular solution of (1.1), i.e. $f(u^*)=0$ and the Jacobian matrix $f'(u^*)$ is singular.

Newton's method and its acceleration in the neighborhood of a singular solution have been studied by many authors (see [2]—[9], [11], [13]—[15] for details), under the requirement that the initial guess not only is near u^* but also belongs to a special cone

$$W(\rho, \theta)=\{u \mid 0<\|u-u^*\|<\rho, \ \|P_x(u-u^*)\|\leqslant\theta\|P_N(u-u^*)\|\}$$

for small ρ, θ, where N is the null space of $f'(u^*)$, X is the complement of N in E, P_N is the projection onto N and P_x is the projection onto X.

We assume the dimension of N is one, i.e. rank $f'(u^*)=n-1$. This is the case we usually meet. Denote

$$N=\{\alpha\phi \mid \alpha\in R\}, \quad \phi\in E^n, \phi\neq 0,$$

$$M=\mathrm{Range}(f'(u^*))=\{y\in E^n \mid \psi y=0\}, \quad \psi\in E^n, \psi\neq 0.$$

We introduce a homotopy continuation mapping $G(u, \lambda)=f(u)-\lambda f(u^0)$ from E^{n+1} to E^n. A point $(u, \lambda)\in E^{n+1}$ is called a regular point for G if DG: $E^{n+1}\to E^n$ is surjective. A point $v\in E^n$ is a regular value of G if each point of $G^{-1}(v)$ is a regular point for G.

Our idea is to transform the singularity in the original problem into the singularity in a scalar equation which is simply treated by an acceleration method. Compared with the other algorithms ours does not require that the initial guess must lie in a special cone $W(\rho, \theta)$ for small ρ, θ. Also, some combination of our

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algorithm with the other algorithms is possible. The initial guess for other algorithms can be obtained by our method.

§ 2. Pseudo-Arclength Continuation

We construct a homotopy

$$G(u, \lambda) = f(u) - \lambda f(u^0), \tag{2.1}$$

where u^0 is chosen in such a way that 0 is a regular value of $G(u, \lambda)$. According to Lemma 2.15 in [10], we can choose such u^0 with probability one.

Our purpose is to find a path $u(\lambda)$ from $\lambda=1$ to $\lambda=0$. Obviously $u(1)=u^0$, and $u(0)$ is just a solution of $f(u)=0$ that we want to solve. An auxiliary equation introduced in the pseudo-arclength continuation method is

$$N(u, \lambda; \sigma) = \dot{u}_*^T(u-u_*) + \dot{\lambda}_*(\lambda-\lambda_*) - (\sigma-\sigma_*), \tag{2.2}$$

where (u_*, λ_*) is a point on the homotopy path at $\sigma=\sigma_*$, $\dot{u}_*=du(\sigma_*)/d\sigma$, $\dot{\lambda}_*=d\lambda(\sigma_*)/d\sigma$, $\dot{u}_*^T$ is the transpose of $\dot{u}_*$.

§ 3. Computing the Root σ^* of $\lambda(\sigma)=0$

In order to get the solution of $f(u)=0$ we are concerned only with the root σ^* of $\lambda(\sigma)=0$ and the corresponding computation for $u(\sigma^*)$, rather than the whole homotopy path $\Gamma(\sigma)$: $[\lambda(\sigma), u(\sigma)]$.

Keller [9] proposed the secant iteration

$$\sigma_{j+1} = \sigma_j - \frac{\sigma_j - \sigma_{j-1}}{\lambda(\sigma_j) - \lambda(\sigma_{j-1})} \cdot \lambda(\sigma_j) \tag{3.1}$$

after σ_0 and σ_1, which satisfy $\lambda(\sigma_0)\cdot\lambda(\sigma_1)<0$, are computed. Of course we can use Newton's iteration for $\lambda(\sigma)=0$,

$$\sigma_{j+1} = \sigma_j - \lambda(\sigma_j)/\dot{\lambda}(\sigma_j). \tag{3.2}$$

The practical computations show that both methods converge slowly in our singular case because of

Theorem 1. *Along with the homotopy path $\Gamma(\sigma)$: $[u(\sigma), \lambda(\sigma)]$, $\dot{\lambda}(\sigma^*)=0$ if $\lambda(\sigma^*)=0$.*

Proof. u^0 was chosen in Section 1 such that

$$DG(u, \lambda) = (f'(u), f(u^0)) \tag{3.3}$$

is a surjective mapping from E^{n+1} to E^n. So

$$\text{Rank}(f'(u), f(u^0)) = n \quad \forall (u, \lambda) \in \Gamma. \tag{3.4}$$

Noticing

we have $$\text{Rank}\, f'(u^*) = n-1 \text{ at } \sigma=\sigma^*$$

$$f(u^0) \overline{\in} \text{Range}\, f'(u^*).$$

Otherwise $f(u^0)$ is a linear combination of each column of the matrix $f'(u^*)$, and therefore

$$\text{Rank}(f'(u^*), f(u^0)) = \text{Rank}\, f'(u^*) = n-1.$$

That contradicts (3.4).

Differentiating (2.1) with respect to σ at $\sigma=\sigma^*$, we get

$$f'(u^*)\dot{u}(\sigma^*)-\dot{\lambda}(\sigma^*)f(u^0)=0.$$

So

$$\begin{aligned}&\dot{\lambda}(\sigma^*)=0,\\ &\dot{u}(\sigma^*)=\alpha\phi\in N(f'(u^*)) \text{ for some } \alpha(\neq 0)\in\mathbb{R}.\end{aligned} \tag{3.5}$$

Q.E.D.

Theorem 2. *Assume* $f''(u^*)\phi\phi\overline{\in}\mathrm{Range}(f'(u^*))$. *Then*

$$\ddot{\lambda}(\sigma^*)\equiv\left.\frac{d^2\lambda(\sigma)}{d\sigma^2}\right|_{\sigma=\sigma^*}=\alpha^2\psi[f''(u^*)\phi\phi]/\psi[f(u^0)]\neq 0. \tag{3.6}$$

Proof. Differentiating (2.1) with respect to σ at $\sigma=\sigma^*$ twice, we get

$$f''(u^*)\dot{u}(\sigma^*)\dot{u}(\sigma^*)+f'(u^*)\ddot{u}(\sigma^*)-\ddot{\lambda}(\sigma^*)f(u^0)=0. \tag{3.7}$$

Substituting (3.5) into (3.7) and multiplying ψ on both sides we have

$$\ddot{\lambda}(\sigma^*)=\alpha^2\psi[f''(u^*)\phi\phi]/\psi[f(u^0)]\neq 0$$

because $f(u^0)$ and $f''(u^*)\phi\phi$ are not in $\mathrm{Range}(f'(u^*))$. Q.E.D.

Expanding (3.2) at $\sigma=\sigma^*$ we get

$$\begin{aligned}&\sigma_{j+1}-\sigma^*\\ &=\sigma_j-\sigma^*-\left[\frac{1}{2}\ddot{\lambda}(\sigma^*)(\sigma_j-\sigma^*)^2+0((\sigma_j-\sigma^*)^3)\right]\Big/[\ddot{\lambda}(\sigma^*)(\sigma_j-\sigma^*)+0((\sigma_j-\sigma^*)^2)]\\ &=\frac{1}{2}(\sigma_j-\sigma^*)+0((\sigma_j-\sigma^*)^2).\end{aligned}$$

Newton's iteration (3.2) converges at most linearly, and it is the same with the secant iteration (3.1).

§ 4. A New Acceleration Algorithm

Naturally, an acceleration iteration

$$\sigma_{j+1}=\sigma_j-2\lambda(\sigma_j)/\dot{\lambda}(\sigma_j) \tag{4.1}$$

is proposed.

Lemma 1. *There exists an inequality*

$$|\sigma_{j+1}-\sigma^*|\leq C|\sigma_j-\sigma^*|^2 \tag{4.2}$$

for the iteration (4.1) *provided* σ_0 *is near* σ^*; *here* C *is a constant.*

Proof. Expanding (4.1) at $\sigma=\sigma^*$ we have

$$\begin{aligned}&\sigma_{j+1}-\sigma^*\\ &=\sigma_j-\sigma^*-2\left[\frac{1}{2}\ddot{\lambda}(\sigma^*)(\sigma_j-\sigma^*)^2+0((\sigma_j-\sigma^*)^3)\right]\Big/[\ddot{\lambda}(\sigma^*)(\sigma_j-\sigma^*)+0((\sigma_j-\sigma^*)^2)]\\ &\leq C|\sigma_j-\sigma^*|^2.\end{aligned}$$

Q.E.D.

Lemma 1 shows that the iteration sequence $\{\sigma_j\}$ of (4.1) converges to σ^* quadratically.

Now we summarize our new acceleration algorithm as follows:

1° Choose $u_*=u^0$, $\lambda_*=1$.

2° Compute $\dot{\lambda}_* = \pm(1+\|f'(u_*)^{-1}f(u^0)\|^2)^{-1/2}$, (4.3)

$$\dot{u}_* = \dot{\lambda}_* f'(u_*)^{-1}f(u^0),$$

where the sign of $\dot{\lambda}_*$ depends on the sign of det $(f'(u_*)^{-1}f(u_*))$.

3° Set $i=0$, $\sigma_i=1$.

4° Predict
$$\lambda_0(\sigma_i) = \lambda_* + \sigma_i\dot{\lambda}_*,$$
$$u_0(\sigma_i) = u_* + \sigma_i\dot{u}_*.$$

5° Use $[u_0(\sigma_i), \lambda_0(\sigma_i)]$ as an initial guess for the solution $[u(\sigma_i), \lambda(\sigma_i)]$ of (2.1), (2.2) by Newton's method, which is called inner iteration.

6° Compute $\dot{\lambda}(\sigma_i)$ and $\dot{u}(\sigma_i)$ by
$$\dot{\lambda}(\sigma_i) = 1/(\dot{\lambda}_* + \dot{u}_*^T \cdot f'(u(\sigma_i))^{-1}f(u^0)),$$
$$\dot{u}(\sigma_i) = \dot{\lambda}(\sigma_i)f'(u(\sigma_i))^{-1}f(u^0).$$

7° Compute
$$\delta\sigma_i = -2\lambda(\sigma_i)/\dot{\lambda}(\sigma_i), \quad \sigma_{i+1} = \sigma_i + \delta\sigma_i,$$
which is called the outer iteration, and a new initial guess for the solution $\lambda(\sigma_{i+1})$, $u(\sigma_{i+1})$ of (2.1), (2.2) is
$$\lambda_0(\sigma_{i+1}) = \lambda(\sigma_i) + \delta\sigma_i\dot{\lambda}(\sigma_i),$$
$$u_0(\sigma_{i+1}) = u(\sigma_i) + \delta\sigma_i\dot{u}(\sigma_i). \tag{4.4}$$

8° If $|\delta\sigma_i| < 10^{-10}$, then $u(\sigma_i)$ is the approximate solution of $f(u)=0$. Otherwise set $i=i+1$, and go to step 5.

Note 1. (u_*, λ_*) is fixed in our algorithm.

Note 2. The initial guess (4.4) in step 7 by using the update data without any additional work is increasingly better during the computation.

§ 5. Combination Procedure

If the initial guess does not lie in a cone $W(\rho, \theta)$ for small ρ, θ, the algorithms in [2]—[9], [11] and [13]—[15] do not work generally.

The combination of our algorithm with those algorithms is possible. The reason is that the point $u(\sigma)$ on the homotopy path near σ^* can be expressed as
$$u(\sigma) = u(\sigma^*) + (\sigma-\sigma^*)\dot{u}(\sigma^*) + \text{h.o.t. of } (\sigma-\sigma^*).$$
We can deduce $u(\sigma) \in W(\rho, \theta)$ for small ρ, θ, provided $|\sigma-\sigma^*|$ is small enough, because $u(\sigma^*) = u^*$ is the solution of $f(u)=0$ and $\dot{u}(\sigma^*)$ lies in the null space N of $f'(u^*)$.

No matter where the point of departure is, a few points on the homotopy path can be got by our algorithm. Such a point on the path can be used as an initial guess for the previous algorithms (e.g., the Kelley–Suresh method in [11]).

§ 6. Numerical Example

We consider the Chandrasekhar H-equation (see [1], [11], [12] for details)
$$F(H)(\mu) = H(\mu) - \left(1 - \frac{1}{2}\int_0^1 \frac{\mu}{\mu+\nu}H(\nu)d\nu\right)^{-1} = 0. \tag{6.1}$$
According to [12], (6.1) has a unique solution $H \geqslant 1$ and $F'(H)$ is a Fredholm operator of index 0 with one-dimensional null space N spanned by $\phi(\mu) = \mu H(\mu)$.

Moreover, the range of $F'(H)$ is given by

$$\left\{f\in C[0, 1]\,\middle|\,\int_0^1 f(\mu)H^{-1}(\mu)d\mu=0\right\}.$$

We approximate the integral $LH=\frac{1}{2}\int_0^1\frac{\mu}{\mu+\nu}H(\nu)d\nu$ by the eight-point Gaussian quadrature formula. This reduces (6.1) to a system of eight nonlinear algebraic equations in eight unknowns. If LH is reinterpreted in this setting, N still has dimension one (see [12]). To compare with the results in [1], [11], [12] we tabulate $\overline{H}=(I-LH)^{-1}(\mu)$ for $\mu=0, 0.1, \cdots, 0.9, 1$ with $H^0(\mu)=H_*(\mu)\equiv 1$ as a point of departure on the homotopy path.

λ	the times of inner iteration	μ	values of $\overline{H}(\mu)$	μ	values of $\overline{H}(\mu)$
1.0 $E+0$		0.0	1.00000	0.6	2.19414
0.56459 $E+0$	3	0.1	1.24735	0.7	2.37398
0.29564 $E-1$	4	0.2	1.45036	0.8	2.55271
0.25450 $E-4$	3	0.3	1.64253	0.9	2.73060
0.62199 $E-9$	2	0.4	1.82928	1.0	2.90782
	total 12	0.5	2.01278		

The total times of inner iterations by Newton's method for $\lambda(\sigma)=0$ are 38, which is much more than 12.

Simple calculation shows that $H_0(\mu)\equiv 1.843053$ does not lie in $W(\rho, \theta)$ for any ρ, θ because

$$\int_0^1 (H_0(\mu)-H(\mu))H^{-1}(\mu)d\mu=0.$$

But we take $H_0(\mu)\equiv 1.843053$ as a point of departure on the path. One outer iteration of our algorithm leads to a point $(1.45624, 1.54819, 1.67929, 1.83323, 1.99169, 2.13555, 2.24746, 2.31420)^T$ whose components are the values of $H(\mu)$ at the Gaussian points in the interval $(0, 1)$, on the homotopy path. Such a point can be used as an initial point for the Kelley–Suresh algorithm. The combination procedure works very well in this case.

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