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NUMERICAL STABILITY OF ITERATIONS FOR SOLUTION
OF NONLINEAR EQUATIONS AND LARGE LINEAR SYSTEMS

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ABSTRACT

We survey some recent results on the problem of numerical stability of iterations for the solution of nonlinear equations $F(x) = 0$ and large linear systems $Ax + g = 0$ where $A = A^*$ is positive definite.

For systems of nonlinear equations we assume that the function F depends on a so called data vector $F(x) = F(x; d)$. We define the condition number $\text{cond}(F; d)$, numerical stability and well-behavior of iterations for the solution of $F(x) = 0$. Necessary and sufficient conditions for a stationary iteration to be numerically stable and well-behaved are presented. We show that Newton iteration for the multivariate case and secant iteration for the scalar case are well-behaved.

For large linear systems we present the rounding error analysis for the Chebyshev iteration and for the successive approximation iterations. We show that these iterations are numerically stable and that the condition number of A is a crucial parameter.

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1. INTRODUCTION

Any iterative algorithm for the solution of nonlinear equations or large linear systems should satisfy a number of criteria such as good convergence properties, numerical stability and as small complexity as possible. Since any iteration is implemented in floating point arithmetic, due to rounding errors one can at best count on approximate properties of this iteration.

In this paper we survey some recent results on the problem of numerical stability of iterations for solving nonlinear equations or large linear systems. Section 2, which deals with numerical stability of iterations for nonlinear equations, is primarily based on the author's paper [75a]. Section 3, which deals with numerical stability of iterations for large linear systems, is based on the author's papers [75b] and [75d].

It might seem that the problem of numerical stability of iterations is not as important as for direct methods. We show that the condition number of the problem is crucial and if the problem is ill-conditioned, then it is impossible to compute a good approximation of the solution no matter how sophisticated an iteration is used. Furthermore, if the problem is well-conditioned, then we can compute a good approximation whenever the iteration used is numerically stable.

2. NUMERICAL STABILITY OF ITERATIONS FOR NONLINEAR EQUATIONS

We approximate a simple zero α of the nonlinear function F ,

$$(2.1) \quad F(x) = 0$$

where $F: D \subset \mathbb{C}^N \rightarrow \mathbb{C}^N$ and \mathbb{C}^N is the N dimensional complex

space. Throughout this section we assume that F depends parametrically on a vector d which will be called a data vector, $F(x) = F(x;d)$, and $d \in \mathbb{C}^m$. For many problems d is given explicitly, e.g., $F(x) = \sum_{i=0}^n a_i x^i$ for $N = 1$. For certain F it is not obvious how to define d , e.g. $F(x) = x^2 - e^x$.

One idea how to determine d is as follows. We solve (2.1) by iteration and most practical iterations use the value of $F(x)$ to get the next approximation to α . We compute $F(x;d)$ in floating point binary arithmetic (fl), see Wilkinson [63], and at best we can expect that a slightly perturbed computed value $fl(F(x;d))$ is the exact one for a slightly perturbed function at slightly perturbed inputs (see Kahan [71]), i.e.,

$$(2.2) \quad fl(F(x;d)) = (I - \Delta F)F(x + \Delta x; d + \Delta d)$$

for $\|\Delta F\| \leq K_1 2^{-t} \|I\|$, $\|\Delta x\| \leq K_2 2^{-t} \|x\|$ and $\|\Delta d\| \leq K_3 2^{-t} \|d\|$ where $K_i = K_i(N;m)$ and 2^{-t} is the relative computer precision.

The condition (2.2) can be treated as an equation on a data vector.

We have to represent the data vector d in fl. Let $\tilde{d} = rd(d)$ denote t digit representation of d in fl. Then

$$(2.3) \quad \|\tilde{d} - d\| \leq K_4 2^{-t} \|d\| \quad \text{where } K_4 = K_4(m).$$

Due to this unavoidable change of the data vector instead of the problem $F(x;d) = 0$ we can at best approximate a solution of the problem $F(x;\tilde{d}) = 0$. Let $\tilde{\alpha}$ be a simple zero of $F(x;\tilde{d}) = 0$. It is easy to verify that for sufficiently smooth F we get

$$(2.4) \quad \tilde{\alpha} - \alpha = -F'_x(\alpha;d)^{-1} F'_d(\alpha;d)(\tilde{d} - d) + O(2^{-2t})$$

where F'_x and F'_d denote the first derivative with respect to x and d . For $\alpha \neq 0$ we have

$$(2.5) \quad \frac{\|\tilde{\alpha} - \alpha\|}{\|\alpha\|} \leq K_4 2^{-t} \text{cond}(F;d) + O(2^{-2t})$$

where

$$(2.6) \quad \text{cond}(F;d) = \left\| F'_x(\alpha;d)^{-1} F'_d(\alpha;d) \right\| \frac{\|d\|}{\|\alpha\|}$$

is called the condition number of F with respect to the data vector d.

The condition number measures the relative sensitivity of the solution with respect to a small relative perturbation of the data vector.

Note that in general $\text{cond}(F;d)$ is not related to the condition number $H(F'(\alpha))$ of the first derivative $F'(\alpha)$, $H(F'(\alpha)) = \|F'(\alpha)\| \|F(\alpha)^{-1}\|$ which occurs in linear analysis.

Having the concept of the condition number we define numerical stability and well-behavior of iterations for the solution of $F(x;d) = 0$.

Let $\{x_k\}$ be a computed sequence of the successive approximations of α by an iteration φ in fl.

An iteration φ is called numerically stable if

$$(2.7) \quad \overline{\lim}_k \frac{\|x_k - \alpha\|}{\|\alpha\|} \leq 2^{-t} (K_5 + K_6 \text{cond}(F;d)) + O(2^{-2t})$$

where $K_i = K_i(N,m)$ for $i = 5,6$.

An iteration φ is called well-behaved if

$$(2.8) \quad \overline{\lim}_k \|F(x_k + \delta x_k; d + \delta d_k)\| = O(2^{-2t})$$

where $\|\delta x_k\| \leq K_7 2^{-t} \|\tilde{x}_k\|$, $\|\delta d_k\| \leq K_8 2^{-t} \|d\|$.

Numerical stability states that the relative error of the computed x_k is of order $2^{-t} \text{cond}(F;d)$. Well-behavior states that a slightly perturbed computed x_k , k large, is an almost exact solution of a slightly perturbed problem.

Note that if φ is well-behaved, then φ is numerically

stable but not vice versa except the scalar case $N = 1$ (see Lemma 4.1 in Wozniakowski [75a]).

Assume that φ is a stationary iteration which produces in exact arithmetic the next approximation x_{k+1} equal to

$$(2.9) \quad x_{k+1}^* = \varphi(x_k, \dots, x_{k-n}, \mathfrak{N}(x_k, \dots, x_{k-n}, F))$$

where n denotes the size of the iteration memory (see Traub [64]) and \mathfrak{N} is information of F at x_k, \dots, x_{k-n} . Next suppose that

$$\|x_{k+1}^* - \alpha\| \leq C \prod_{j=0}^n \|x_{k-j} - \alpha\|^{P_j}$$

where $P_j \geq 0$, $\sum_{j=0}^n P_j \geq 2$ and $C = C(F)$ whenever $\|x_k - \alpha\| \leq \dots \leq \|x_{k-n} - \alpha\| \leq \Gamma$ for sufficiently small Γ .

In floating point arithmetic instead of (2.9) we have

$$(2.10) \quad x_{k+1} = x_{k+1}^* + \xi_k$$

where ξ_k is the computer error in one iterative step. The value of ξ_k depends mainly on the computed error of the information \mathfrak{N} and on the computed error of an algorithm which is used to perform one iterative step.

It is possible to find a form of ξ_k to ensure numerical stability and well-behavior of the stationary iteration φ . Namely, φ is numerically stable iff

$$(2.11) \quad \lim_k \frac{\|\xi_k\|}{\|\alpha\|} \leq 2^{-t} (K_9 + K_{10} \text{cond}(F;d)) + O(2^{-2t})$$

where $K_i = K_i(N, m)$ for $i = 9, 10$, and φ is well-behaved iff

$$(2.12) \quad \xi_k = \Delta x_k + F'_x(x_k; d)^{-1} F'_d(x_k; d) \Delta d_k + O(2^{-2t})$$

where $\|\Delta x_k\| \leq K_{11} 2^{-t} \|x_k\|$, $\|\Delta d_k\| \leq K_{12} 2^{-t} \|d\|$ for large k and

$K_i = K_i(N, m)$, $i = 11$ and 12 . (See Theorem 4.1 and Corollary 4.2 in Wozniakowski [75a].)

Using (2.11) and (2.12) one can verify that Newton iteration is well-behaved under the following assumptions:

- (i) $F(x_k; d)$ is computed by a well-behaved algorithm (see (2.2))
- (ii) $fl(F'(x_k; d)) = F'(x_k) + O(2^{-t})$
- (iii) the computed z_k , ($z_k = -F'(x_k)^{-1}F(x_k)$ and $x_{k+1} = x_k + z_k$) satisfies $(fl(F'(x_k; d)) + E_k)z_k = -fl(F(x_k; d))$, $E_k = O(2^{-t})$.

The first two conditions require a certain accuracy in $F(x_k)$ and $F'(x_k)$ whereas the last conditions mean that z_k is the exact solution of a perturbed system which holds if Gaussian elimination with pivoting or the Householder method is used.

An interesting question is whether the secant iteration is well-behaved. For the scalar case secant iteration produces

$$x_{k+1}^* = x_k - \frac{x_k - y_k}{F(x_k) - F(y_k)} F(x_k)$$

where $y_k = x_{k-1}$ (with memory) or $y_k = x_k + \gamma_k F(x_k)$ (two-point iteration) for a certain γ_k .

It is shown in Wozniakowski [75a] that secant iteration is well-behaved whenever

$$(2.13) \quad \left| \frac{F(x_k)}{F(x_k) - F(y_k)} \right| \leq Q$$

for all $k \geq k_0$ and a positive constant Q independent of F . Note that (2.13) does not hold for the Steffenson iteration, $y_k = x_k + F(x_k)$. It may be shown that with this choice of

y_k , secant iteration is unstable. For secant iteration with memory

$$\frac{F(x_k)}{F(x_k) - F(x_{k-1})} \cong O(x_{k-2}^{-\alpha}) + O\left(\frac{2^{-t}}{x_{k-1}^{-\alpha}}\right).$$

Thus (2.13) holds as long as $|x_{k-1}^{-\alpha}| \gg 2^{-t}$.

Numerical stability of the multivariate secant iteration was proved by Jankowska [75] under some assumptions on a suitable distance and position of successive approximations. Well-behavior of the multivariate secant iteration is open.

There are several classes of iterations of practical interest for which the problem of numerical stability is open. Examples are interpolatory iterations $I_{n,s}$ for the scalar case and $I_{0,s}$ for the multivariate one, integral-interpolatory iterations $I_{-1,s}$ and hermitian multipoint iterations (see Traub [64], Kacwicz [75a] and [75b], Kung and Traub [74] and Wozniakowski [75c] respectively). One interesting question is how to use iterations with memory in a stable way. There are some reasons to believe that at least some of the mentioned classes of iterations are numerically stable under certain assumptions but further research is needed.

3. NUMERICAL STABILITY OF ITERATIONS FOR LARGE LINEAR SYSTEMS

Direct methods of numerical interest for the solution of linear systems $Ax+g = 0$ where A is $N \times N$ matrix and g is $N \times 1$ vector are well-behaved. Specifically they produce an approximation y to the exact solution α such that y is the exact solution for a slightly perturbed A ,

$$(3.1) \quad (A+E)y + g = 0$$

where $\|E\| \leq C_1 2^{-t} \|A\|$ and $C_1 = C_1(N)$.

Examples of well-behaved direct methods include Gaussian elimination with pivoting, the Householder method and the Gram-Schmidt reorthogonalization method. Note that a method is well-behaved iff the residual vector $r = Ay + g$ is small, i.e.

$$(3.2) \quad \|r\| \leq c_2 2^{-t} \|A\| \|y\|, \quad c_2 = c_2(N).$$

Furthermore, for any well-behaved method we get

$$(3.3) \quad \frac{\|y - \alpha\|}{\|\alpha\|} \leq c_3 2^{-t} H(A)$$

where $H(A) = \|A\| \|A^{-1}\|$ denotes the condition number of A and $c_3 = c_3(N)$. In general (3.3) is sharp which indicates that the condition number $H(A)$ is a crucial parameter. (Note that (3.3) also holds for any numerically stable method.)

It might seem that the numerical accuracy of iterations for solving large linear systems might be better than for direct methods. However, this is not true. We shall discuss some iterations to see that $H(A)$ is still crucial and moreover, we shall show that for some very efficient iterations well-behavior does not hold in general.

Two reasons why the condition number is still crucial are as follows:

- (i) No matter which iteration is used we have to represent (not necessarily store!) all entries of A and g in floating point arithmetic. Thus, instead of the problem $Ax + g = 0$ we can at best approximate the solution $\tilde{\alpha}$ of

$$(3.4) \quad (A + \delta A)x + (g + \delta g) = 0$$

where $\|\delta A\| \leq c_4 2^{-t} \|A\|$, $\|\delta g\| \leq c_5 2^{-t} \|g\|$ and

and $C_i = C_i(N)$ for $i = 4, 5$. The relative error $\frac{\|\tilde{\alpha} - \alpha\|}{\|\alpha\|}$ is of order $2^{-t} H(A)$. Thus, once more the condition number is important.

(ii) Let us assume that all entries of A and g can be exactly represented in fl, $A = rd(A)$, $g = rd(g)$. For many iterations the only known information of the system is given by a procedure which for a given x computes $z = Ax$. Since Ax is computed in fl then at best we can get

$$(3.5) \quad z = fl(Ax) = (A+E)x$$

where $E = E(x)$ and $\|E\| \leq C_5 2^{-t} \|A\|$, $C_5 = C_5(N)$. Thus all information derives from perturbed systems and the computed solution x_k can be at best the exact solution of a slightly perturb problem $(A+E_k) x_k + g = 0$. Then

$$(3.6) \quad x_k - \alpha = -A^{-1} E_k x_k.$$

As long as we do not require any special property of E_k then $\|A^{-1} E_k x_k\|$ can be close to $\|A^{-1}\| \|E\| \|x_k\|$ which is of order $2^{-t} H(A) \|x_k\|$.

We are now in a position to discuss numerical properties of some particular iterations. First we consider successive approximation iterations which are defined as follows:

(i) Transform $Ax+g = 0$ to the equivalent system

$$(3.7) \quad x = Bx + h.$$

Sometimes B is chosen to minimize the spectral radius $\rho(B)$ of B , $\rho(B) < 1$.

(ii) Solve (3.7) by the iteration

$$(3.8) \quad x_{k+1} = Bx_k + h, \quad k = 0, 1, \dots$$

where x_0 is a given initial approximation.

For different transformations we get different iterations; for instance, the Jacobi (J), Richardson (R), Gauss-Seidel (GS) or successive overrelaxation (SOR) iterations, see Young [71]. Note that for $e_k = x_k - \alpha$ we get $e_k = B^k e_0$ and the character of convergence mainly depends on the spectral radius $\rho(B)$.

Suppose that in fl we have

$$(3.9) \quad fl(Bx_k + h) = (B + E_k)x_k + (I + \delta I_k)h = Bx_k + h + \xi_k$$

where $\|E_k\| \leq C_6 2^{-t} \|B\|$, $\|\delta I_k\| \leq C_7 2^{-t}$ and $C_i = C_i(N)$, $i = 6, 7$ and

$$\xi_k = E_k x_k + \delta I_k (I - B)\alpha.$$

Thus, instead of (3.8) we get in fl,

$$x_{k+1} = Bx_k + h + \xi_k$$

which has the solution

$$(3.10) \quad x_{k+1} - \alpha = B^{k+1}(x_0 - \alpha) + \sum_{i=0}^k B^{k-i} \xi_i.$$

Suppose that $\|B\| < 1$. From (3.3) we get

$$\overline{\lim}_k \|x_k - \alpha\| \leq \frac{1}{1 - \|B\|} \overline{\lim}_k \|\xi_k\| \leq C_8 2^{-t} \frac{\|B\| + \|I - B\|}{1 - \|B\|} \|\alpha\| + O(2^{-2t})$$

where $C_8 = \max(C_6, C_7)$. Hence if

$$(3.11) \quad q = (\|B\| + \|I - B\|) / (1 - \|B\|) \text{ is of order } \|A\| \|A^{-1}\|$$

then this iteration is numerically stable.

For instance, for the Richardson iteration we get

$$B = I - cA \quad \text{where } A = A^* > 0$$

$$\text{and } c = \frac{2}{\lambda_1 + \lambda_2} \quad \text{for } \lambda_1 = \|A^{-1}\|_2^{-1}, \lambda_2 = \|A\|_2.$$

$$\text{Then } \|B\|_2 = (\lambda_2 - \lambda_1) / (\lambda_2 + \lambda_1) \text{ and}$$

$$q = \frac{3}{2} H(A) - 1$$

which proves that the Richardson iteration is stable. (For more examples see Wozniakowski [75d].) However, it is very easy to find a counter example where (3.11) does not hold even for $N = 1$. (Note that for $N = 1$, $H(A) = 1$.) Let us consider

$$(2-c)x = 1 \quad \text{for } 0 < c < 1$$

with the transformation $x = (-1+c)x + 1$. Thus $B = -1+c$ and $q = q(c) = \frac{3-2c}{c}$. Note that $\lim_{c \rightarrow 0^+} q(c) = +\infty$ which indicates that for small c (3.11) does not hold. Numerical tests confirm this observation. For instance using the PD10 where $2^{-t} \doteq 10^{-8}$ with $c = 10^{-4}$ we get x_k such that $|x_k - \alpha| / |\alpha| \doteq 10^{-4}$.

It is possible to prove that if B is diagonalizable then (3.11) ensures well-behavior (Stewart [73]). Note that for the SOR iteration B is not diagonalized and the problem of well-behavior is open.

We pass to the second class of iterations for large linear systems $Ax + g = 0$ where $A = A^*$ is positive definite. We construct a sequence $\{x_k\}$ of the successive approximation of α such that

$$(3.12) \quad x_k - \alpha = W_k(A)(x_0 - \alpha)$$

where $W_k(0) = 1$ and W_k is a polynomial of degree at most k .

In the Chebyshev iteration W_k is defined by

$$(3.13) \quad \|W_k\| = \inf_{P \in P_k(0,1)} \|P\|$$

where $\|P\| = \sup_{a \leq x \leq b} |P(x)|$, $P_k(0,1)$ denotes a class of polynomials of degree at most k which has the value 1 at zero and $[a,b]$ contains all eigenvalues of matrix A .

The solution of (3.13) is given by the Chebyshev polynomials of the first kind and using the three-terms recurrence formula we get

$$(3.14) \quad x_{k+1} = x_k + \left\{ p_{k-1}(x_k - x_{k-1}) - r_k \right\} / q_k, \quad r_k = Ax_k + g$$

for certain coefficients p_{k-1} and q_k .

Assuming that

$$(3.15) \quad f(Ax) = (A+E)x, \quad \|E\|_2 \leq C_9 2^{-t} \|A\|_2$$

and $a = \|A^{-1}\|_2^{-1}$, $b = \|A\|_2$ it is possible to show that the computed sequence $\{x_k\}$ by the Chebyshev iteration satisfies

$$(3.16) \quad \overline{\lim}_k \|x_k - \alpha\| \leq (1+4C_9)2^{-t} H(A) + O(2^{-2t})$$

which means numerical stability. Unfortunately the Chebyshev iteration is, in general, not well-behaved since the computed residual vector r_k can be of order $2^{-t} \|A\| \|\alpha\| H(A)$, see Wozniakowski [75b]. It seems to us that for any numerically stable iteration based on (3.12), the norm $\max_k \|W_k\|$ has to be relatively small. Note that in conjugate gradient iterations W_k is defined as the polynomial which minimizes a certain norm of $x_k - \alpha$, see Stiefel [58]. This need not imply that $\|W_k\|$ is small. This might explain why conjugate gradient iterations are numerically unstable.

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