

A quasi-Newton method with optimal r-order without independence assumption*

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Abstract

Quasi-Newton methods based on least change secant updating formulas that solve linear equations $Ax = b$ in $n = \dim(x) = \dim(b)$ steps can be expected to solve corresponding smooth nonlinear systems n -step quadratically, i.e. with an r -order of $\rho = 2^{1/n} = 1 + 1/n + O(1/n^2)$. The best rate one can possibly expect on general problems is given by the positive root ρ_n of $\rho^n(\rho - 1) = 1$, for which $\rho_n - 1 = \ln(n)/n + O(1/n^2)$. To show that this upper bound is actually achieved one usually has to impose a priori some kind of linear independence condition on the sequence of steps taken by the quasi-Newton iteration in question. Without any such assumptions we establish in this paper the convergence order ρ_n for the two-sided rank one formula proposed by Schlenkrich et al in [SGW06]. It requires the evaluation of adjoint vectors, is invariant with respect to linear transformations on the variable domain and combines the properties of bounded deterioration and heredity.

Keywords: nonlinear equations, R-order, quasi-Newton methods, adjoint based update, Automatic Differentiation

1 Convergence of quasi-Newton methods

For the iterative solution of a system of nonlinear equations

$$F(x_*) = 0,$$

where $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is continuously differentiable and F' is Lipschitz-continuous in $x_* \in \mathbb{R}^n$, we consider the following general algorithm:

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Algorithm 1 (Quasi-Newton Algorithm) Suppose $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $\{A_i\}_{i \in \mathbb{N}_0} \subset \mathbb{R}^{n \times n}$ with A_i non-singular, $x_0 \in \mathbb{R}^n$, and $x_* \in \mathbb{R}^n$ with $F(x_*) = 0$ are given, then the algorithm

$$\begin{aligned} s_i &= -A_i^{-1}F(x_i) \\ x_{i+1} &= x_i + s_i \end{aligned} \quad \text{for } i = 0, 1, 2, \dots$$

is called a full-step quasi-Newton iteration to locate x_* .

Here the matrix A_i is an approximation to the Jacobian $F'(x_i)$. There are several approaches for choosing A_i . To avoid the repeated evaluation and factorization of an approximated Jacobian, low-rank least-change secant updates are of particular interest. For general nonlinear problems Broyden's update formula [Bro65] is well studied. Burmeister (cf. [Sch79, B. 5.5.1.]) and Gay [Gay79] proved for this method $2n$ -step q -quadratic convergence for smooth nonlinear problems. That corresponds to an r -order of $\sqrt[2n]{2} = 1 + 1/(2n) + O(1/n^2)$. The same result with $2n$ replaced by m can be expected for any method that depends smoothly on function values and solves linear problems exactly in at most m steps. For example this would be true with $m = n$ for direct generalizations of the one-dimensional secant method that ensure uniform linear independence of the last n steps. By enforcing the validity of the last n secant conditions simultaneously one then finds that $A_i - F'(x_*) = O(\|x_{i-n} - x_*\|)$, which can be shown to imply that the r -order of the sequence of errors $\{\|x_i - x_*\|\}$

$$\rho \equiv \liminf \sqrt[i]{\|x_i - x_*\|}$$

is no less than the positive root ρ_n of the polynomial $\rho^{n+1} = \rho^n + 1$. In general one has exactly $\rho = \rho_n$ and it is hard to imagine how any rank one updating method could converge faster, since its Jacobian must still be effected by function information from n steps back. We will therefore refer to ρ_n as the maximal r -order. To prove that it is actually attained one usually has to assume that the steps are in some sense uniformly linearly independent. To enforce this property requires a considerable extra computational effort and introduces more scaling dependence, which is usually avoided in quasi-Newton methods.

In the case of unconstrained minimization, A_i is an approximation to a Hessian and is therefore maintained to be symmetric. In particular the symmetric rank-2 update formulas of the (restricted) Broyden class can be applied. These methods have the property of heredity on strongly convex quadratic problems, provided the line-searches are exact. The previous secant conditions remain valid. In [Sto75] Stoer proved for these methods, combined with an asymptotically exact line search, an r -order of at least $\sqrt[n]{2}$. Furthermore Schuller [Sch74] proved for the BFGS method under the assumptions, that the steps are uniformly linear independent that the maximal order ρ_n is in fact attained. [Sch74].

One particular member of the unrestricted Broyden class update, the symmetric rank-1 (SR1) update is a rank one update that preserves previous secant conditions for quadratic problems without any line search. However, it does not

share the least change property of the members in the restricted class. Consequently updating must be suspended or severely damped when some denominator becomes small or zero and even proofs of mere superlinear convergence assume uniform linear independent steps [CGT91] or combine the updating with a trust-region algorithm [BKS96]. An estimation of the r -order of convergence is not yet available.

In this paper, we consider the adjoint tangent rank-1 (ATR1) update, that combines the fixed scale least change property with heredity. It was introduced in [SGW06] and is given below:

Definition 2 (Adjoint tangent rank-1 update) *Let $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be differentiable, $x_{i+1} \in \mathbb{R}^n$. For a given matrix $A_i \in \mathbb{R}^{n \times n}$ and a given direction $\sigma_i \in \mathbb{R}^n$, the formula*

$$A_{i+1} = A_i + \frac{\sigma_i \sigma_i^T}{\sigma_i^T \sigma_i} (F'(x_{i+1}) - A_i) \quad (1)$$

is called 'adjoint tangent rank-1 (ATR1) update' of A_i . Particular choices of σ_i are

- (i) $\sigma_i = F(x_{i+1})$ as Residual update and
- (ii) $\sigma_i = (F'(x_{i+1}) - A_i)s_i$ for a tangent direction $s_i \in \mathbb{R}^n \setminus \{0\}$ as transposed tangent Broyden update.

We suppose that the tangents $F'(x)s$ and gradients $\sigma^T F'(x)$ are evaluated exactly. This can be done, for example, by using the forward and reverse mode of Automatic Differentiation (AD). Details on AD are described in [Gri00]. For the quasi-Newton algorithm with ATR1 updates, given by Definition 2 (i) and (ii), one can verify the following properties:

Lemma 3 *Let $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be differentiable and F' Lipschitz-continuous in $x_* \in \mathbb{R}^n$ with constant $L < \infty$. Suppose $F(x_*) = 0$ and $F'(x_*)$ is non-singular. Then for the quasi-Newton Algorithm 1 with ATR1 updates (i) and (ii) holds:*

- (i) *For any $r \in (0, 1)$ there are constants $\epsilon, \delta > 0$, so that if $\|x_0 - x_*\| < \epsilon$ and $\|A_0 - F'(x_*)\| < \delta$ then the sequence $\{x_i\}$ is well defined and converges to x_* . Moreover*

$$\|x_{i+1} - x_*\| \leq r \|x_i - x_*\|$$

and $\|A_i\|$ and $\|A_i^{-1}\|$ are uniformly bounded.

- (ii) *If the sequence $\{x_i\}$ converges to x_* , so that $\sum_{i=0}^{\infty} \|x_i - x_*\| < \infty$, then*

$$\lim_{i \rightarrow \infty} \frac{\|(A_i - F'(x_i))s_i\|}{\|s_i\|} = 0,$$

i.e., $\{x_i\}$ converges q -superlinear.

(iii) For any sequence $\{x_i\}$ and any previous quasi-Newton step s_j with $j < i$, we have non-linear heredity, i.e., for a constant $C < \infty$

$$\frac{\|(A_i - F'(x_*))s_j\|}{\|s_j\|} \leq C \sum_{k=j}^i \|x_k - x_*\|. \quad (2)$$

Here, in particular C equals the Lipschitz-constant L .

For a proof of these statements we refer to [SGW06].

Since the left side of inequality (2) depends only on the direction of s_j but not on its length, we consider from now on $\tilde{s}_i = s_i/\|s_i\|$. Moreover, we set $\delta_i = \|(A_i - F'(x_*))\tilde{s}_i\|$, and $\varepsilon_i = \|x_i - x_*\|$. If the direction \tilde{s}_i , can be represented as a linear combination of previous directions \tilde{s}_j with $j < i$, i.e.,

$$\tilde{s}_i = \sum_{j < i} \lambda_{i,j} \tilde{s}_j,$$

we get from (2), that

$$\delta_i \leq \sum_{j < i} |\lambda_{i,j}| \|(A_i - F'(x_*))\tilde{s}_j\| \leq \sum_{j < i} |\lambda_{i,j}| L \sum_{k=j}^i \varepsilon_k.$$

Since we are interested in the asymptotic rate of convergence, we assume, that the sequence $\{x_i\}$, generated by Algorithm 1 already converges to x_* , so that $\sum_{k=j}^i \varepsilon_k \leq C_0 \varepsilon_j$ for any pair of indices j and i . This is in particular the case, if ε_i converges q -linear as ensured by Lemma 3. Then we derive that

$$\delta_i \leq L C_0 \sum_{j < i} |\lambda_{i,j}| \varepsilon_j, \quad \text{where} \quad \tilde{s}_i = \sum_{j < i} \lambda_{i,j} \tilde{s}_j. \quad (3)$$

This estimation of δ_i is crucial for the proof in the following section. Since (3) holds for any linear combination, the idea is to consider (3) as a constrained minimization problem.

2 Main Result

In this section we state and prove that the ATR1 formula and all other updates satisfying the non-linear heredity condition (2) ensure convergence at the maximal r-order ρ_n , which is asymptotically equivalent to the expressions $1 + \ln(n)/n$ and $\sqrt[n]{n}$. In other words we get n -step order n rather than n -step order 2 or $\sqrt{2}$, which is obtained for Broyden. The asymptotic equivalence is established in the following auxiliary result.

Lemma 4 For $n \in \mathbb{N}$, be $\rho_n > 1$ with $\rho_n^n(\rho_n - 1) = 1$, then

$$\lim_{n \rightarrow \infty} \frac{\rho_n - 1}{\frac{\log n}{n}} = \lim_{n \rightarrow \infty} \frac{\rho_n - 1}{\sqrt[n]{n} - 1} = 1$$

Proof: Substituting $\eta_n = \rho_n - 1$ yields

$$(1 + \eta_n)^n \eta_n = 1 \quad \text{with} \quad 1 > \eta_n > 0 \quad (4)$$

and we prove, that

$$\lim_{n \rightarrow \infty} \frac{\eta_n}{\frac{\log(n)}{n}} = 1.$$

Since η_n decreases monotonically and $\eta_n \rightarrow 0$ for $n \rightarrow \infty$, we have that

$$\lim_{n \rightarrow \infty} \frac{\eta_n}{\frac{\log(n)}{n}} = \lim_{\eta_n \rightarrow 0} \frac{n \eta_n}{\log(n)}.$$

From equation (4), we get that $n = \frac{-\log(\eta_n)}{\log(1+\eta_n)}$. Thus using Bernoulli-l'Hospitales rule yields

$$\lim_{\eta_n \rightarrow 0} \frac{n \eta_n}{\log(n)} = \lim_{\eta_n \rightarrow 0} \frac{-\log(\eta_n)}{\log(n)} \cdot \underbrace{\lim_{\eta_n \rightarrow 0} \frac{\eta_n}{\log(1+\eta_n)}}_{=1} = \lim_{\eta_n \rightarrow 0} \frac{-\log(\eta_n)}{\log(n)}.$$

Furthermore $\log(n) = \log(-\log(\eta_n)) - \log(\log(1 + \eta_n))$ and

$$\frac{\log(n)}{-\log(\eta_n)} = \frac{\log(\log(1 + \eta_n)) - \log(-\log(\eta_n))}{\log(\eta_n)} = \frac{\log(\log(1 + \eta_n))}{\log(\eta_n)} - \frac{\log(-\log(\eta_n))}{\log(\eta_n)}.$$

Applying again Bernoulli-l'Hospitales rule gives

$$\lim_{\eta_n \rightarrow 0} \frac{\log(\log(1 + \eta_n))}{\log(\eta_n)} = \lim_{\eta_n \rightarrow 0} \frac{\eta_n}{\log(1 + \eta_n)(1 + \eta_n)} = 1$$

and

$$\lim_{\eta_n \rightarrow 0} \frac{\log(-\log(\eta_n))}{\log(\eta_n)} = \lim_{\eta_n \rightarrow 0} \frac{1}{\log(\eta_n)} = 0,$$

which finally yields $\lim_{\eta_n \rightarrow 0} \frac{-\log(\eta_n)}{\log(n)} = 1$ and

$$\lim_{n \rightarrow \infty} \frac{\rho_n - 1}{\frac{\log n}{n}} = 1.$$

To prove the second part consider a differentiable positive function $g(x)$ with $\lim_{x \rightarrow \infty} g(x) = 0$. Then Bernoulli-l'Hospitale yields

$$\lim_{x \rightarrow \infty} \frac{g(x)}{e^{g(x)} - 1} = \lim_{x \rightarrow \infty} \frac{g'(x)}{g'(x)e^{g(x)}} = 1.$$

This holds in particular for $g(x) = \log(x)/x$. With $x^{1/x} = e^{\log(x)/x}$ it follows, that

$$\lim_{n \rightarrow \infty} \frac{\log(n)/n}{\sqrt[n]{n} - 1} = \lim_{x \rightarrow \infty} \frac{\log(x)/x}{x^{1/x} - 1} = 1.$$

Thus, with the first part of the proof, we also get that

$$\lim_{n \rightarrow \infty} \frac{\rho_n - 1}{\sqrt[n]{n} - 1} = 1,$$

which concludes the proof. \square

The main convergence result is given in the following theorem:

Theorem 5 *Suppose Algorithm 1 is applied to find $x_* \in \mathbb{R}^n$ with $F(x_*) = 0$, F is Lipschitz continuously differentiable at x_* , and $F'(x_*)$ is non-singular. If the sequence $\{x_i\}$ converges q -linearly and the sequence $\{A_i\}$ satisfies the non-linear heredity property (2) then the rate of convergence is q -superlinear with an r -order of*

$$\rho = \liminf_{i \rightarrow \infty} \sqrt[i]{|\log \|x_i - x_*\||} \geq \rho_n,$$

where ρ_n is the positive root of $\rho^n(\rho - 1) = 1$.

Proof: The proof consists of four parts. In the first part we consider the constrained minimization problem as in (3) and bound the optimal solution. This is followed by an auxiliary result in the second part. The third part uses the previous results to estimate the current error by a product of previous errors. Finally in the fourth part we derive the r -order of convergence.

Part 1 Analogously as for the ATR1 updates in the previous section, we define $\tilde{s}_i = s_i/\|s_i\|$, $\delta_i = \|(A_i - F'(x_*))\tilde{s}_i\|$, and $\varepsilon_i = \|x_i - x_*\|$. Without loss of any generality we may assume that the first n steps are linearly independent. For example we may precede the actual quasi-Newton iteration by n conceptual steps along the coordinate axes, which may or may not be used to update the A_i . In any case we can compute corresponding quantities δ_i and ε_i for $i = 1 \dots n$, which may be quite large but do not effect the asymptotic rate of convergence of course. Then we have, that for a positive constant $C_3 < \infty$,

$$\delta_i \leq C_3 \sum_{j < i} |\lambda_{i,j}| \varepsilon_j, \quad \text{where} \quad \tilde{s}_i = \sum_{j < i} \lambda_{i,j} \tilde{s}_j.$$

From this, we derive with Cauchy-Schwartz

$$\delta_i^2 \leq C_3^2 i \sum_{j < i} \lambda_{i,j}^2 \varepsilon_j^2.$$

By combining $\lambda_i = (\lambda_{i,0}, \dots, \lambda_{i,i-1})^T \in \mathbb{R}^i$, $S_i = [\tilde{s}_0, \dots, \tilde{s}_{i-1}] \in \mathbb{R}^{n \times i}$, and $E_i = \text{diag}(\varepsilon_0, \dots, \varepsilon_{i-1}) \in \mathbb{R}^{i \times i}$, we get that

$$\delta_i^2 \leq C_3^2 \cdot i \cdot \lambda_i^T E_i^2 \lambda_i, \quad \text{where} \quad \tilde{s}_i = S_i \lambda_i.$$

This can be considered as equality constrained quadratic program

$$\min_{\lambda_i} \frac{1}{2} \lambda_i^T E_i^2 \lambda_i \quad \text{s.t.} \quad \tilde{s}_i = S_i \lambda_i.$$

The first-order necessary optimality condition yields the system

$$\begin{bmatrix} E_i^2 & S_i^T \\ S_i & 0 \end{bmatrix} \begin{bmatrix} \lambda_i \\ \eta_i \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{s}_i \end{bmatrix}, \quad (5)$$

for a Lagrange-multiplier $\eta_i \in \mathbb{R}^n$. Since $\varepsilon_i > 0$, the matrix E_i^2 is positive definite. Moreover, since we may assume without loss of generality the first n steps to be linear independent, we get that for $i \geq n$, the matrix S_i has full row-rank. Therefore there is a unique solution of the system (5) and

$$\lambda_i = -E_i^{-2} S_i^T \eta_i \quad \text{and} \quad S_i \lambda_i = \tilde{s}_i.$$

Thus, we find that $-S_i E_i^{-2} S_i^T \eta_i = \tilde{s}_i$. With the same arguments as before, this system has a unique solution. Therefore we get, that $\eta_i = -(S_i E_i^{-2} S_i^T)^{-1} \tilde{s}_i$ and

$$\lambda_i = E_i^{-2} S_i^T (S_i E_i^{-2} S_i^T)^{-1} \tilde{s}_i.$$

This yields, that

$$\begin{aligned} \lambda_i^T E_i^2 \lambda_i &= \tilde{s}_i^T (S_i E_i^{-2} S_i^T)^{-1} S_i E_i^{-2} E_i^2 E_i^{-2} S_i^T (S_i E_i^{-2} S_i^T)^{-1} \tilde{s}_i \\ &= \tilde{s}_i^T \underbrace{(S_i E_i^{-2} S_i^T)^{-1}}_{M_i} \tilde{s}_i \end{aligned}$$

and thus

$$\delta_i^2 \leq C_3^2 i \tilde{s}_i^T M_i^{-1} \tilde{s}_i. \quad (6)$$

Before considering the third part of the proof, we state and proof an auxiliary result.

Part 2 Let $S = [s_1, \dots, s_n] \in \mathbb{R}^{n \times n}$ with $\|s_k\| \leq 1$, $D = \text{diag}(d_1, \dots, d_n) \in \mathbb{R}^{n \times n}$ be positive definite, and $c > 0$. Then

$$\det [SDS^T + cI] \leq \det [nD + cI]. \quad (7)$$

Without loss of generality we may assume that the elements of D are in descending order. Then there is an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$, so that $\tilde{S} = QS$ is an upper triangular matrix with the first row being $[\rho, r^T]$. So we have

$$\tilde{S}D\tilde{S}^T + cI = \begin{bmatrix} \rho^2 d_1 + r^T D' r + c & r^T D' S'^T \\ S' D' r & S' D' S'^T + cI \end{bmatrix},$$

where $\tilde{S}' = [\tilde{s}'_1, \dots, \tilde{s}'_{n-1}] \in \mathbb{R}^{(n-1) \times (n-1)}$ is the matrix \tilde{S} without the first row and column. Hence \tilde{S}' is also an upper triangular matrix and $\|\tilde{s}'_k\| \leq 1$. Moreover $D' = \text{diag}(d_2, \dots, d_n) \in \mathbb{R}^{(n-1) \times (n-1)}$. Since $SDS^T + cI$ is positive definite and Q is orthogonal we have

$$\det [SDS^T + cI] = \det [\tilde{S}D\tilde{S}^T + cI]$$

and $\left[\tilde{S}D\tilde{S}^T + cI\right]$ is positive definite. Omitting $S'D'r$ and its corresponding transposed increases the determinant (see for example [Ber05, Fact 2.13.4]). Moreover, since the norm of the columns of \tilde{S} is less or equal to one, so is the absolute value of each element in $[\rho, r^T]$ and thus

$$\begin{aligned}\det[SDS^T + cI] &\leq (\rho^2 d_1 + r^T D'r + c) \det[S'D'S'^T + cI] \\ &\leq (nd_1 + c) \det[S'D'S'^T + cI].\end{aligned}$$

By induction follows now that

$$\det[SDS^T + cI] \leq \prod_{k=1}^n nd_k + c = \det[nD + cI].$$

With this, we continue with the next part of the proof of Theorem 5.

Part 3 Considering the matrix $M_i \in \mathbb{R}^{n \times n}$, we find, that $M_i = \sum_{j=0}^{i-1} \tilde{s}_j \tilde{s}_j^T / \varepsilon_j^2$ or recursively $M_{i+1} = M_i + \tilde{s}_i \tilde{s}_i^T / \varepsilon_i^2$. For $i \geq n$ the matrices M_i are non-singular and we get by Sherman Morrison

$$\det(M_{i+1}) = \det(M_i) \left(1 + \frac{\tilde{s}_i^T M_i^{-1} \tilde{s}_i}{\varepsilon_i^2}\right) = \det(M_n) \prod_{j=n}^i \left(1 + \frac{\tilde{s}_j^T M_j^{-1} \tilde{s}_j}{\varepsilon_j^2}\right).$$

Combining this with the estimate in (6) yields

$$\det(M_{i+1}) \geq \det(M_n) \underbrace{\prod_{j=n}^i \left(1 + \frac{\delta_j^2}{C_3^2 j \varepsilon_j^2}\right)}_{t_j}.$$

For the further derivation we have to consider the term t_j . Since $\{x_i\}$ converges to x_* , there are, according to [DS96] and [SGW06, Lemma 19], an index i_0 and constants C_4 and C_5 , so that for all $j \geq i_0$

$$\varepsilon_{j+1} \leq C_4 \delta_j (\varepsilon_j + \varepsilon_{j+1}) + C_5 (\varepsilon_j + \varepsilon_{j+1})^2 \leq (C_4 \delta_j + C_5 \varepsilon_j) \varepsilon_j.$$

Choosing a $C < \infty$, we have that either $\varepsilon_j \leq C\delta_j$ or $\delta_j < \frac{1}{C}\varepsilon_j$. In the latter case, we get in particular, that $\frac{\varepsilon_{j+1}}{\varepsilon_j^2} < \infty$. This yields for t_j , that there is a constant $C_{3,1}$, so that

$$t_j \geq 1 \geq \frac{1}{C_{3,1} \cdot j} \cdot \frac{\varepsilon_{j+1}^2}{\varepsilon_j^4}.$$

In the case that $\varepsilon_j \leq C\delta_j$, we get $\varepsilon_{j+1} \leq (C_4 + C_5 C) \delta_j \varepsilon_j$, which gives

$$\frac{\delta_j^2}{\varepsilon_j^2} \geq \frac{1}{C_{3,2}} \frac{\varepsilon_{j+1}^2}{\varepsilon_j^4},$$

for a constant $C_{3,2}$. With $C_6 = \max\{C_{3,1}, C_{3,2}\}$, we have in any case, that

$$\det(M_{i+1}) \geq \det(M_n) \prod_{j=n}^i \frac{1}{C_6 j} \frac{\varepsilon_{j+1}^2}{\varepsilon_j^4} = \det(M_n) \frac{\varepsilon_{i+1}^2}{\varepsilon_n^2} \prod_{j=n}^i \frac{1}{C_6 j} \frac{1}{\varepsilon_j^2}. \quad (8)$$

To bound $\det(M_{i+1})$ above, we fix the index i and split M_{i+1} into

$$M_{i+1} = \underbrace{\sum_{k=0}^{n-1} \frac{\tilde{s}_{i-k} \tilde{s}_{i-k}^T}{\varepsilon_{i-k}^2}}_{SDS^T} + M_{i-n+1}.$$

Here $S = [\tilde{s}_i, \dots, \tilde{s}_{i-n+1}]$, $D = \text{diag}(1/\varepsilon_i^2, \dots, 1/\varepsilon_{i-n+1}^2)$, and SDS^T as well as M_{i-n+1} are positive semidefinite. Thus with [Ber05, C.s 8.4.2 and 8.4.10]

$$\det(M_{i+1}) \leq \det(SDS^T + \|M_{i-n+1}\|I) \leq \det(SDS^T + \text{trace}(M_{i-n+1})I).$$

With the element-wise representation of the normalized quasi-Newton directions $\tilde{s}_j = (\tilde{s}_j^1, \dots, \tilde{s}_j^n)^T$, we have for variable but fixed i

$$\text{trace}(M_{i+1}) = \sum_{k=1}^n \sum_{j=0}^i \frac{[\tilde{s}_j^k]^2}{\varepsilon_j^2} = \sum_{j=0}^i \frac{1}{\varepsilon_j^2} \sum_{k=1}^n [\tilde{s}_j^k]^2 = \sum_{j=0}^i \frac{1}{\varepsilon_j^2} \|\tilde{s}_j\|^2 = \sum_{j=0}^i \frac{1}{\varepsilon_j^2}.$$

Since we assume q -linear convergence, this gives that

$$\sum_{j=0}^i \frac{1}{\varepsilon_j^2} = \frac{1}{\varepsilon_i^2} \sum_{j=0}^i \frac{\varepsilon_i^2}{\varepsilon_j^2} = \frac{1}{\varepsilon_i^2} \sum_{j=0}^i r^{2j} \leq \frac{1}{1-r^2} \frac{1}{\varepsilon_i^2}.$$

This yields

$$\det(M_{i+1}) \leq \det\left(SDS^T + \frac{1}{(1-r^2)\varepsilon_{i-n}^2} I\right).$$

Applying the result (7) of Part 2 gives

$$\det(M_{i+1}) \leq \prod_{k=0}^{n-1} \frac{n}{\varepsilon_{i-k}^2} + \frac{1}{(1-r^2)\varepsilon_{i-n}^2} \leq \prod_{k=0}^{n-1} \frac{1}{\varepsilon_{i-k}^2} \left(n + \frac{\varepsilon_{i-k}^2}{(1-r^2)\varepsilon_{i-n}^2} \right)$$

and thus

$$\det(M_{i+1}) \leq \left(n + \frac{r^2}{(1-r^2)} \right)^n \cdot \prod_{k=0}^{n-1} \frac{1}{\varepsilon_{i-k}^2} \quad (9)$$

Combining now the results of (8) and (9) yields that

$$\det(M_n) \frac{\varepsilon_{i+1}^2}{\varepsilon_n^2} \prod_{j=n}^i \frac{1}{C_6 j} \frac{1}{\varepsilon_j^2} \leq \det(M_{i+1}) \leq \left(n + \frac{r^2}{(1-r^2)} \right)^n \cdot \prod_{k=0}^{n-1} \frac{1}{\varepsilon_{i-k}^2}.$$

This means, there is a positive constant C_7 , so that

$$\varepsilon_{i+1}^2 \prod_{k=0}^{n-1} \varepsilon_{i-k}^2 \leq C_7 \prod_{j=n}^i C_6 j \varepsilon_j^2$$

and dividing both sides of the inequality by $\prod_{k=0}^{n-1} \varepsilon_{i-k}^2$, gives

$$\varepsilon_{i+1}^2 \leq C_7 \prod_{j=n}^{i-n} C_6 j \varepsilon_j^2 \cdot \underbrace{\prod_{j=i-n+1}^i C_6 j}_{\leq C_6^n i^n}$$

From this, we get that for sufficiently large i

$$\varepsilon_{i+1} \leq \sqrt{C_7 C_6^n i^n} \prod_{j=n}^{i-n} \sqrt{C_6} \sqrt{j} \varepsilon_j \leq \frac{\sqrt{C_7 C_6^{i-n+1} i^n \cdot \sqrt{(n-1)!}}}{\sqrt{(i-n)!}} \prod_{j=n}^{i-n} j \varepsilon_j.$$

Multiplying both sides by $(i+1)$ yields

$$(i+1)\varepsilon_{i+1} \leq \underbrace{\frac{(i+1)\sqrt{C_7 C_6^{i-n+1} i^n \cdot \sqrt{(n-1)!}}}{\sqrt{(i-n)!}}}_{f_i} \prod_{j=n}^{i-n} j \varepsilon_j.$$

Since $\sqrt{i!}$ grows more than exponentially, the factor f_i tends towards zero and for sufficiently large i , we have $f_i \leq 1$. Thus we get for $i \geq i_0$

$$(i+1)\varepsilon_{i+1} \leq \prod_{j=n}^{i-n} j \varepsilon_j \tag{10}$$

Part 4 From inequality (10) we may conclude, that for sufficiently large indices i and for any fixed integer $m \in \{n, \dots, i-n\}$,

$$-\log((i+1)\varepsilon_{i+1}) \geq \sum_{j=n}^{i-n} -\log(j\varepsilon_j) \geq \sum_{j=i-m}^{i-n} -\log(j\varepsilon_j).$$

Considering the family of difference equations

$$\tilde{\varepsilon}_{i+1} = \sum_{j=i-m}^{i-n} \tilde{\varepsilon}_j$$

with initial conditions $\tilde{\varepsilon}_j = -\log(j\varepsilon_j)$ for $j = 0, \dots, m$, yields that (for variable but fixed m)

$$-\log(j\varepsilon_j) \geq \tilde{\varepsilon}_j > 0.$$

The ansatz $\tilde{\varepsilon}_j = c_m \rho_m^j$ with $\rho_m > 1$ gives that

$$c_m \rho_m^{i+1} = \sum_{j=i-m}^{i-n} c_m \rho_m^j = c_m \rho_m^{i-n} \left(1 + \frac{1}{\rho_m} + \dots + \frac{1}{\rho_m^{m-n}} \right)$$

and thus

$$\rho_m^{n+1} = \sum_{j=0}^{m-n} \frac{1}{\rho_m^j} = \frac{1 - \frac{1}{\rho_m^{m-n+1}}}{1 - \frac{1}{\rho_m}}.$$

For $m \rightarrow \infty$, we get that

$$\rho^{n+1} = \frac{\rho}{\rho - 1} \quad \text{or} \quad \rho^n(\rho - 1) = 1.$$

By substituting back, we get that

$$\varepsilon_i \leq i \varepsilon_i \leq e^{-\tilde{\varepsilon}} = e^{-c_m(\rho_m^i)}$$

and thus

$$\liminf_{i \rightarrow \infty} \sqrt[i]{|\log(\varepsilon_i)|} \geq \liminf_{i \rightarrow \infty} \rho_m = \liminf_{i \rightarrow \infty} \lim_{m \rightarrow \infty} \rho_m = \rho.$$

□

With this result, we have an r -order of convergence, which equals the r -order of convergence of a sequence with $\varepsilon_{i+1} = \varepsilon_i \cdot \varepsilon_{i-n}$. Moreover, we get that for any $a > 1$ there is an $n_a \in \mathbb{N}$, so that for $n \geq n_a$ always $a^{1/n} < 1 + \frac{1}{a}$. Hence

$$1 > a(a^{1/n} - 1) = \left(a^{1/n}\right)^n (a^{1/n} - 1).$$

Since $\rho^n(\rho - 1)$ is monotonically increasing for $\rho > 1$, we get that $\rho^n(\rho - 1) = 1$ implies, that $\rho > a^{1/n}$ for n sufficiently large. Hence, in particular for $a = 2$, we have $\rho > \sqrt[n]{2}$ for $n > 1$.

This rate of convergence is optimal in the sense that it is the same as for general secant methods [OR00, Theorem 11.3.5]. In this work Ortega and Rheinbold showed, that a general secant method that uses values of F at previous iterates to approximate the system Jacobian may have an r -order of at least ρ with $\rho^n(\rho - 1) = 1$. Hence, a quasi-Newton method based on rank-1 updates and approximations of the Jacobian in the range of previous steps can not be expected to be better in the general case.

3 Conclusions

In this paper we showed for quasi-Newton methods, that the combination of heredity and least change property implies an r -order of convergence at least equal to ρ , where

$$\rho^n(\rho - 1) = 1.$$

This rate of convergence is the same as for general secant methods in [OR00] and is therefore considered to be optimal. Here, neither uniform linear independent quasi-Newton steps nor line searches are required. The assumptions are satisfied by ATR1 update formulas presented in [SGW06].

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