WHY BROYDEN'S NONSYMMETRIC METHOD TERMINATES ON LINEAR EQUATIONS

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Abstract. The family of algorithms introduced by Broyden in 1965 for solving systems of nonlinear equations has been used quite effectively on a variety of problems. In 1979, Gay proved the then surprising result that the algorithms terminate in at most $2n$ steps on linear problems with n variables. His very clever proof gives no insight into properties of the intermediate iterates, however. In this work we show that Broyden's methods are projection methods, forcing the residuals to lie in a nested set of subspaces of decreasing dimension. The results apply to linear systems as well as linear least squares problems.

Key words. Broyden's method, nonlinear equations, quasi-Newton methods.

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1. Introduction. In 1965, Broyden introduced a method for solving systems of nonlinear equations $g(x^*) = 0$, where $g : \mathcal{R}^n \rightarrow \mathcal{R}^n$ is differentiable [2]. He named it a *quasi-Newton method.* Methods in this class mimic the Newton iteration

$$x_{k+1} = x_k - \{\nabla g(x_k)\}^{-1} g(x_k), \quad k = 0, 1, ...,$$

by substituting an approximation H_k for $\{\nabla g(x_k)\}^{-1}$, the inverse of the Jacobian matrix. This matrix approximation is built up step by step, and the correction to H_k is fashioned so that the *secant condition*

$$H_{k+1} y_k = s_k,$$

is satisfied, where

$$y_k = g(x_{k+1}) - g(x_k) \equiv g_{k+1} - g_k,$$

and

$$s_k = x_{k+1} - x_k.$$

This condition is satisfied if $H_{k+1} = \{\nabla g(x_{k+1})\}^{-1}$ and g is linear, and this is the motivation for choosing the correction to H_k so that H_{k+1} satisfies this condition but so that H_{k+1}^{-1} behaves as H_k^{-1} in all directions orthogonal to s_k. This reasoning led Broyden to the formula

$$H_{k+1} = H_k + (s_k - H_k y_k) v_k^T,$$

where v_k is chosen so that $v_k^T y_k = 1$. Specific choices of v_k lead to different algorithms in Broyden's family.

Although certain members of the family proved to be very effective algorithms (specifically, the so called Broyden "good" method that takes v_k in the same direction as s_k), the algorithms were little understood, to the extent that Broyden himself in

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1972 said, "The algorithm does not enjoy the property of quadratic termination even when used for function minimization with exact line searches." [3, p.97].

This misconception, common to the entire optimization community, was disproved in 1979 by David Gay in a surprising and clever construction [4]. He showed that if

$$g(x) = Ax - b$$

where $A \in \mathcal{R}^{n \times n}$ is nonsingular, then the following result holds.

LEMMA 1.1. *(Gay) If g_k and y_{k-1} are linearly independent, then for $1 \leq j \leq \lfloor (k+1)/2 \rfloor$, the vectors $\{(AH_{k-2j+1})^i g_{k-2j+1}\}$ are linearly independent for $0 \leq i \leq j$.*

This result implies that for some $k \leq 2n$, g_{k-1} and y_{k-2} must be linearly dependent, and Gay showed that in this case $g_k = 0$ and termination occurs.

Gay's construction leads to a proof of a $2n$-step Q-quadratic rate of convergence for Broyden's good method. It yields little insight, though, into how the intermediate iterates in Broyden's method are behaving in the case of linear systems, and the purpose of this work is to develop that understanding.

2. The Character of the Broyden Iterates. First we establish some useful relations. The change in the x vector is given by

$$s_k = -H_k g_k,$$

and the change in the residual g is

$$y_k = A s_k = -A H_k g_k,$$

so we can express the new residual as

$$g_{k+1} = g_k + y_k = (I - AH_k) g_k.$$

For convenience, we denote the matrix in this expression as

$$F_k = I - AH_k,$$

and denote the product of such factors as

$$P_k = F_k F_{k-1} \ldots F_0 = F_k P_{k-1}.$$

Then a simple induction-style argument gives us a useful formula for g_{k+1} and thus for y_k and s_k.

LEMMA 2.1.

$$\begin{aligned} g_{k+1} &= P_k g_0, \\ y_k &= -AH_k P_{k-1} g_0, \\ s_k &= -H_k P_{k-1} g_0. \end{aligned}$$

Thus, the character of the product matrices P_k determines the behavior of the residuals g_k in the course of the iteration. The key to this behavior is the nature of the left null vectors of P_k, the vectors z for which $z^T P_k = 0$. We will prove in the next section that these vectors have a very special form. In particular, the factor matrices

F_k are quite *defective*, having a zero eigenvalue with a Jordan block of size $\lceil k/2 \rceil$. The linearly independent left *principal vectors* of F_k, vectors z_i satisfying

$$\begin{aligned} z_1^T F_k &= 0, \\ z_3^T F_k &= z_1^T, \\ z_i^T F_k &= z_{i-2}^T, \end{aligned}$$

do not depend on k, and in fact are left *eigenvectors* of P_k corresponding to a zero eigenvalue. Thus the vector g_{k+1} is orthogonal to the expanding subspace spanned by the vectors $\{z_i\}$ (i odd and $i \leq k$) and, after at most $2n$ steps, is forced to be zero.

3. The Behavior of the Broyden Iterates. David Gay proved an important fact about the rank of the factor matrices F_k, and the following result is essentially his.

LEMMA 3.1. *(Gay) For $k \geq 1$, if $y_k \neq 0$, $v_k^T y_{k-1} \neq 0$, and $\mathrm{rank}(F_k) = n-1$, then $\mathrm{rank}(F_{k+1}) = n-1$, and y_k spans the null space of F_{k+1}.*

Proof. For $k \geq 0$,

$$\begin{aligned} F_{k+1} &= I - AH_{k+1} \\ &= I - AH_k - (As_k - AH_k y_k)v_k^T \\ &= I - AH_k - (y_k - AH_k y_k)v_k^T \\ &= (I - AH_k)(I - y_k v_k^T) \\ &= F_k(I - y_k v_k^T). \end{aligned}$$

Since $v_k^T y_k = 1$, we see that $F_{k+1} y_k = 0$. Similarly, y_{k-1} spans the null space of F_k ($k \geq 1$). Any other right null vector y of F_{k+1} must (after scaling) satisfy $(I - y_k v_k^T)y = y_{k-1}$. But v_k^T spans the null space of $(I - y_k v_k^T)^T$, and because, by assumption, $v_k^T y_{k-1} \neq 0$, y_{k-1} is not in the range of $(I - y_k v_k^T)$, and thus y_k spans the null space of F_{k+1}. $\square$

This lemma leads to the important observation that the sequence of matrices H_k does not terminate with the inverse of the matrix A, at least in the *usual* case in which all $v_k^T y_{k-1} \neq 0$. In fact, each matrix H_k and A^{-1} agree only on a subspace of dimension 1.

We will make several assumptions on the iteration:

1. $v_j^T y_{j-1} \neq 0$, $j = 1, 2, ..., k$, and $y_k \neq 0$.
2. v_0 is in the range of F_0^T.
3. $k \leq 2n-1$ is odd. (This is for notational convenience.)

We can now show that the matrix F_k is defective and exhibit the left null vectors of P_k (which are the same as the left null vectors of P_{k+1}).

LEMMA 3.2. *Define the sequence of vectors*

$$z_1^T F_1 = 0, \;\; z_i^T F_i = z_{i-2}^T \;\; i = 3, 5, ..., k.$$

These vectors exist and are linearly independent, and z_i^T is a left null vector of P_j for $j = i, i+1, ..., k$. Further, $z_i^T g_j = 0$, $j = i+1, i+2, ..., k$.

Proof. Define z_1 by $z_1^T F_0 = v_0^T$. This nonzero vector exists by Assumption 2, and since

$$F_j = F_0(1 - y_0 v_0^T)...(1 - y_{j-1} v_{j-1}^T),$$

it is easy to see that, for $j = 1, 2, ..., k$, $z_1^T F_j = 0$, and therefore $z_1^T P_j = 0$ as well. In order to continue the construction, we need an orthogonality result: for $j = 2, 3, ..., k$,

$$z_1^T y_j = z_1^T g_{j+1} - z_1^T g_j = z_1^T P_j g_0 - z_1^T P_{j-1} g_0 = 0.$$

For the "induction step", assume that linearly independent vectors $z_1, ..., z_{i-2}$ have been constructed for $i \leq k$, that each of these vectors satisfies $z_m^T F_j = z_{m-2}^T$ ($z_1^T F_j = 0$) and $z_m^T P_j = 0$ for $j = m, ..., k$, and that $z_{i-2}^T y_j = 0$ for $j = i-1, ..., k$. (Linear independence follows from the fact that they are principal vectors for F_{i-2}.) Let $z_i^T F_i = z_{i-2}^T$. Note that z_i exists since $z_{i-2}^T y_{i-1} = 0$, and y_{i-1} spans the null space of F_i. We have that, for $j = i, ..., k$, $z_i^T F_j = z_{i-2}^T$, and therefore $z_i^T P_j = z_{i-2}^T P_{j-1} = 0$ as well. Then for $j = i+1, ..., k$, we have

$$z_i^T y_j = z_i^T g_{j+1} - z_i^T g_j = z_i^T P_j g_0 - z_i^T P_{j-1} g_0 = 0.$$

□

In the course of this proof, we have established the following result.

THEOREM 3.3. *Under the above three assumptions, and if A is nonsingular, then after $k+1$ steps of Broyden's method, the residual $g(x_{k+1})$ is orthogonal to the linearly independent vectors $z_1, z_3, ..., z_k$, and thus the algorithm must terminate with the exact solution vector after at most $2n$ iterations.*

4. Overdetermined or Rank Deficient Linear Systems. Gerber and Luk [5] gave a nice generalization of Gay's results to overdetermined or rank deficient linear systems, and the results in this paper can be generalized this way as well. The matrices F_k have dimensions $m \times m$, where $m \geq n$ is the number of equations. The two lemmas and their proofs are unchanged, but the theorem has a slightly different statement. Let $\mathbf{R}$ denote the range of a matrix, and $\mathbf{N}$ denote the null space.

THEOREM 4.1. *Under the above three assumptions, and if $A \in \mathcal{R}^{m \times n}$ has rank p, and if $\mathbf{N}(H_k) = \mathbf{N}(A^T)$, then after $k+1$ steps of Broyden's method, the residual $g(x_{k+1})$ is orthogonal to the linearly independent vectors $z_1, z_3, ..., z_k$, which are contained in the range of A, and thus the algorithm must terminate with the least squares solution vector after at most $2p$ iterations.*

Proof. The fact that z_i is in the range of A is established by induction. □

Gerber and Luk give sufficient conditions guaranteeing that $\mathbf{N}(H_k) = \mathbf{N}(A^T)$:

1. $\mathbf{R}(H_0) = \mathbf{R}(A^T)$,
2. $\mathbf{N}(H_0) = \mathbf{N}(A^T)$,

3a. $v_k = H_k^T u_k$ for some vector u_k, with $u_k^T s_k \neq 0$.

Condition 3a is satisfied by Broyden's "good" method (v_k parallel to s_k) but not the "bad" method (v_k parallel to y_k). It is easy to show by induction that the condition $\mathbf{N}(H_k) = \mathbf{N}(A^T)$ also holds under the following assumption, valid for the "bad" method:

3b. $v_k = A u_k$ for some vector u_k, with $u_k^T s_k \neq 0$.

First, assume that $z \in \mathbf{N}(H_k)$ and that $\mathbf{N}(H_k) = \mathbf{N}(A^T)$. Then

$$H_{k+1} z = H_k z + (s_k - H_k y_k) v_k^T z,$$

and this is zero if and only if $v_k^T z = 0$, which is assured if either $v_k^T = u_k^T H_k$ or $v_k^T = u_k^T A^T$. Thus, $\mathbf{N}(H_k) \subseteq \mathbf{N}(H_{k+1})$. Now, by writing v_k as $H_k^T u_k$, valid under either 3a or 3b, we can show [5] that $H_{k+1} = (I - H_k g_{k+1} u_k^T) H_k$, and that the determinant of the first factor is $u_k^T s_k$, nonzero by condition 3. Thus $\mathbf{N}(H_{k+1}) = \mathbf{N}(H_k)$.

5. Concluding Notes. Since the vectors v_k are arbitrary except for a normalization, it is easy to ensure that Assumptions 1 and 2 of §3 are are satisfied. But if not, termination actually occurs earlier: if F_k has rank $n-1$ and $v_k^T y_{k-1} = 0$, then F_{k+1} has rank $n-2$ with right null vectors y_k and y_{k-1}. Similarly, P_{k+1} has one extra zero eigenvalue.

The conclusions in this work apply to the Broyden family of methods, whether they are implemented by updating an approximation to the Hessian, its inverse, or its factors. The inverse approximation was only used for notational convenience; other implementations are preferred in numerical computation.

The conclusions depend critically on the assumption that the step length parameter is 1 (i.e., if $s_k = -\alpha H_k g_k$, then $\alpha = 1$).

As noted by a referee, the conclusions depend on only two properties of Broyden's method, consequences of Lemma 2.1:

$$\begin{aligned} F_{k+1} &= F_k(I - (F_k - I)g_k v_k^T), \\ g_{k+1} &= F_k g_k, \end{aligned}$$

where g_0 and F_0 are given, and the v_k are (almost) arbitrary. Thus the results can be applied to a broader class of methods, in the same spirit as the work by Boggs and Tolle [1].

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