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ON THE SEPARABLE NONLINEAR LEAST SQUARES PROBLEMS*

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Dedicated to the 70th birthday of Professor Junzhi Cui

Abstract

Separable nonlinear least squares problems are a special class of nonlinear least squares problems, where the objective functions are linear and nonlinear on different parts of variables. Such problems have broad applications in practice. Most existing algorithms for this kind of problems are derived from the variable projection method proposed by Golub and Pereyra, which utilizes the separability under a separate framework. However, the methods based on variable projection strategy would be invalid if there exist some constraints to the variables, as the real problems always do, even if the constraint is simply the ball constraint. We present a new algorithm which is based on a special approximation to the Hessian by noticing the fact that certain terms of the Hessian can be derived from the gradient. Our method maintains all the advantages of variable projection based methods, and moreover it can be combined with trust region methods easily and can be applied to general constrained separable nonlinear problems. Convergence analysis of our method is presented and numerical results are also reported.

Mathematics subject classification: 65K05, 65H10.
Key words: Separable nonlinear least squares problem, Variable projection method, Gauss-Newton method, Levenberg-Marquardt method, Trust region method, Asymptotical convergence rate, Data fitting.

1. Introduction

In this paper, we consider the separable nonlinear least squares problem, which is derived from the following special nonlinear data fitting problem

$$y_i = \sum_{j=1}^{p} a_j \phi_j(b, t_i), \quad (i = 1, 2, \cdots, m), \tag{1.1}$$

where $\phi_j(b,t)(j = 1, \cdots, p)$ are real functions defined on $\Re^{q+1}$, t_i and y_i $(i = 1, \cdots, m)$ are given data, $a \in \Re^p$ and $b \in \Re^q$ are parameters to be decided, and p and q are two positive

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integers satisfying $p+q=n$. In practice, it is usual to have $m>n$, which is also assumed in this paper. Data fitting problem (1.1) can be written as general nonlinear equations as follows

$$f_i(a,b)=0, \quad i=1,2,\cdots,m, \tag{1.2}$$

where

$$f_i(a,b)=y_i-\sum_{j=1}^{p}a_j\phi_j(b,t_i), \quad i=1,2,\cdots,m. \tag{1.3}$$

It is easy to see that the nonlinear equations (1.2) are linear to variable set a. Models of this type are very common and have a variety of applications in different fields, such as inverse problems, signal analysis, medical and biological imaging, neural networks, robotics and vision, telecommunications, electrical and electronics engineering, environmental sciences and time series analysis, differential equations and dynamical systems, etc. (see, e.g., [4, 5]). It is natural to consider the nonlinear least squares formulation

$$\min_{a\in R^p, b\in R^q}\frac{1}{2}\sum_{i=1}^{m}(f_i(a,b))^2, \tag{1.4}$$

because (1.4) is equivalent to (1.2) when the latter has solutions and numerical methods for (1.4) can be used for solving (1.2) (see, e.g., [2, 12, 16, 19]).

If y_i $(i=1,\cdots,m)$ depend on b, the data fitting problem (1.1) is generalized to the standard form of separable nonlinear least squares problems

$$\min_{a\in R^p, b\in R^q}\psi(a,b)=\frac{1}{2}||\ y(b)-\Phi(b)a||_2^2, \tag{1.5}$$

where $y: R^q\mapsto R^m$; $\Phi: R^q\mapsto R^{m\times p}$, with $(\Phi(b))_{ij}=\phi_j(b,t_i)$, $1\le i\le m$, $1\le j\le p$.

Golub and Pereyra [4] proposed the variable projection method for (1.4), which is (1.5) with $y(b)=y_0$. The main idea of their variable projection method is as follows. For any fixed $b\in R^q$, (1.5) reduces to a linear least squares problem and we can obtain the least-norm solution

$$\hat{a}(b)=\Phi^+(b)y_0, \tag{1.6}$$

where $\Phi^+(b)$ is the Moore-Penrose inverse of $\Phi(b)$. Substituting (1.6) into (1.4), we have

$$\min_{a\in R^p, b\in R^q}\psi(a,b)=\min_{b\in R^q}\frac{1}{2}||\ y_0-\Phi(b)\Phi^+(b)y_0||_2^2=\min_{b\in R^q}\frac{1}{2}||P_{\Phi(b)}^{\perp}y_0||_2^2. \tag{1.7}$$

Here, $P_{\Phi(b)}^{\perp}$ is the orthogonal projector from R^m to the null space of $\Phi(b)^T$. Thus, we derive a reduced problem (1.7). A solution $\hat{b}$ of (1.7) can be obtained by applying any nonlinear least squares algorithm, and consequently $\hat{a}(\hat{b})$ can be defined by (1.6). In Golub and Pereyra [5], the computing and storage methods for the Fréchet derivative of the orthogonal projector are also developed, and it is proved that the separating variables approach led to the same solution set as that of the original problem when $\Phi(b)$ has a constant rank. The main feature of the variable projection methods is the elimination of the linear variables, which leads to three main advantages over the standard Gauss-Newton method: less iteration steps to convergence; less initial guess; decreasingly ill-conditioned if the whole problem is.

Kaufman[6] simplified the Jacobian formula of the orthogonal projector in Golub and Pereyra's method. It has extensively demonstrated that savings of up to 25% are achieved

by this simplification, making the variable projection method as cost efficient per iteration as working with the full functional.

Ruhe and Wedin [14] extended the variable projection idea to the general nonlinear case. They considered and developed the implicit reduction methods for the separable nonlinear least squares problem (1.5) by adopting alternate iteration between the two sets of the variables. Consider the minimization problem

$$\min_{a\in R^p} \psi(a,b), \tag{1.8}$$

where $\psi(a,b)$ is a general nonlinear function. Assume that (1.8) is easy to solve numerically for every fixed b in the domain under consideration. Of course, such an assumption is satisfied for the separable nonlinear least squares problem, when the objective function $\psi(a,b)$ is of the form in (1.5). Let $a(b)$ denote a solution of (1.8). It is easy to see that $(a(\hat{b}),\hat{b})$ solves (1.5) if $\hat{b}$ solves

$$\min_{b\in R^q} \psi(a(b),b). \tag{1.9}$$

Inexact Newton's method is used by Ruhe and Wedin[14] to solve the above problem (1.9). It is important is to obtain a good approximation to the Hessian of $\psi(a(b),b)$ without evaluating any second order derivatives, by using the special structure of the problem. For example, when problem (1.8) is the special problem (1.5), we can define

$$\varphi(a,b) = y(b) - \Phi(b)a. \tag{1.10}$$

Direct calculations show that

$$\varphi_a(a,b) = \Phi(b), \quad \varphi_b(a,b) = y'(b) - \Phi'(b)a, \tag{1.11}$$

$$\varphi_{ab}(a,b) = \Phi'(b)^T, \quad \varphi_{ba}(a,b) = \Phi'(b), \quad \varphi_{aa}(a,b) = 0. \tag{1.12}$$

Hence only $\varphi_{bb}(a,b)$ is not available if we do not compute any second order derivatives.

The implicit reduction algorithm for separable nonlinear least squares problems (1.5) can be described as follows.

Algorithm 1.1. (Implicit Reduction Algorithm)

Step 1 *Given* b_0, $a_0 = 0$; $\epsilon > 0$ *sufficiently small,* $k := 0$.

Step 2 *Compute* $\varphi^{(k)} = \varphi(a_k, b_k)$, *and* $\varphi_a^{(k)} = \Phi(b_k)$,

$$a_{k+1} = a_k - (\varphi_a^{(k)})^+ \varphi^{(k)}. \tag{1.13}$$

Step 3 *Compute* $\varphi_b^{(k)} = y'(b_k) - \Phi'(b_k)a_k$,
set b_{k+1} *either by Kaufman's step*

$$b_{k+1} = b_k - (P^{\perp}_{\varphi_a^{(k)}}\varphi_b^{(k)})^+[I - \varphi_a^{(k)}(\varphi_a^{(k)})^+]\varphi^{(k)} = b_k - (P^{\perp}_{\varphi_a^{(k)}}\varphi_b^{(k)})^+\varphi^{(k)}, \tag{1.14}$$

or by Golub and Pereyra's step

$$b_{k+1} = b_k - (P^{\perp}_{\varphi_a^{(k)}}\varphi_b^{(k)} + P_{\varphi_a^{(k)}}{\varphi_a^{(k)}}^+ \Phi'(b_k)\varphi)^+\varphi^{(k)}. \tag{1.15}$$

Step 4 $k := k+1$, *If* $||{\varphi_a^{(k)}}^T\varphi^{(k)} + {\varphi_b^{(k)}}^T\varphi^{(k)}|| < \epsilon$ *then stop, else go to* Step 2.

According to the analysis in [14], the steps defined by the above algorithm are equivalent to Golub and Pereyra's step and Kaufman's step respectively, and the calculation of the steps can be more concise. It is also found that the variable projection methods require almost the same arithmetical operations per iteration as the unseparated Gauss-Newton method, while their asymptotical convergence properties are better than the unseparated Gauss-Newton method.

Some other modifications of the variable projection method and extensions to separable nonlinear least squares problems are mentioned in [1, 7, 8] etc.. For instance, Böckmann [1] introduces a finite-difference approximation with function evaluation for the reduced problem (1.7), and uses a trust-region method to solve it. Kaufman and Pereyra [7] extends separable nonlinear least squares problems to the cases with separate nonlinear equality constraints.

However, in practice, the separable nonlinear least squares problems normally do not have separate equality constraints. For example, box constraints or ball constraints are very common. In these cases, the variable projection method can not be easily applied. In fact, it is rather difficult to extend the variable projection method to solve a nonlinear constrained least squares problem if there exists a constraint which does not have the same separable pattern as the objective function. To overcome these difficulties, we propose an unseparated framework for the separable nonlinear least squares problems.

The rest of this paper is organized as follows. Our new unseparated framework will be introduced in the next section. We will analyze the convergence properties of the unseparated framework in Section 3. In Section 4, results of some numerical experiments will be showed. Finally, conclusions and discussions are given in the last section.

2. A New Unseparated Framework

Before we present our new unseparated framework, the motivation will be clarified. To achieve it, we give a brief review on general methods for nonlinear least squares problems.

2.1. General methods for nonlinear least squares problems

The general nonlinear least squares problem can be described as

$$\min_{x\in R^n} F(x) = \frac{1}{2}||f(x)||_2^2, \tag{2.1}$$

where

$$f : R^n \mapsto R^m, \quad \text{with} \quad (f(x))_i = f_i(x).$$

There are quite a few kinds of iterative methods proposed for solving (2.1). Most of these methods for nonlinear least squares problems are based on the linear approximation of f in each iteration, which is derived from Gauss-Newton method. The main idea of Gauss-Newton method is as follows [2, 12]. Suppose our current iterative point is x_k, then we obtain the next point $x_{k+1} = x_k + d_k$ by solving the following linear least squares problem

$$\min_{d\in R^n} \frac{1}{2}||f(x_k) + J(x_k)d||_2^2, \tag{2.2}$$

where $J(x)$ is the Jacobian of $f(x)$. A solution of problem (2.2) is

$$d_k = -(J(x_k))^+ f(x_k) = -(J(x_k)^T J(x_k))^{-1} J(x_k)^T f(x_k). \tag{2.3}$$

If we compare (2.3) with the Newton step of (2.1), we can find that Gauss-Newton method use $J(x_k)^T J(x_k)$, which consists of only the first-order information of f, to substitute the actual Hessian of $F(x)$

$$\nabla^2 F(x) = J(x)^T J(x) + \sum_{i=1}^{m} \nabla^2 f_i(x) f_i(x), \tag{2.4}$$

by omitting the second term in (2.4). It can be proved easily that Gauss-Newton method has good local convergence properties when the second term is significantly small, which is normally true if the least squares has a zero minimum.

Most efficient methods for nonlinear least squares problems, such as Levenberg-Marquardt method and structured quasi-Newton methods, can be regarded as some kinds of modifications or extensions of the Gauss-Newton method. To guarantee the global convergence without losing nice local convergence properties, Levenberg-Marquardt method tries to control the step length at each iteration by replacing the last term by a positive definite scalar matrix [3]. Modern versions of the Levenberg-Marquardt method restrict the step length directly by posing a trust region constraint [9, 11, 16]. Structured quasi-Newton methods reserve the first-order information $J(x_k)^T J(x_k)$ of $\nabla^2 F(x)$ and apply quasi-Newton techniques to approximate the last term in (2.4) (for example, see [18]).

2.2. Motivation of our approach

Using the special structure of the separable nonlinear least squares problem, variable projection methods eliminate the linear part of variables in order to reduce the objective function to a function depending on only the nonlinear part of variables. Then, standard methods for general nonlinear least squares problems can be applied to the reduced problem. Both theoretical analysis and numerical results show that the variable projection based methods need less iteration steps than the corresponding unseparated methods (for example, see [5]). A comprehensible reason is that the general unseparated frame neglects the speciality of separable nonlinear least squares problem.

However, when we add some general constraints on (1.5), the variable projection methods will be invalid. Since their successes rely too much on the explicit expression of the optimum when the nonlinear part of variables is fixed.

Due to the low efficiency of general unseparated methods and the low compatibility of the variable projection methods, we want to design an unseparated framework which can utilize the separable information. Consequently, the derived algorithms can easily be extended to constrained problems.

Consider problem (1.5). Define φ by (1.10), we can write the Hessian of $\psi(a, b)$ as follows:

$$\nabla^2 \psi = \begin{pmatrix} \varphi_a^T \varphi_a + \varphi_{aa}^T \varphi & \varphi_a^T \varphi_b + \varphi_{ab}^T \varphi \\ \varphi_b^T \varphi_a + \varphi_{ba}^T \varphi & \varphi_b^T \varphi_b + \varphi_{bb}^T \varphi \end{pmatrix}. \tag{2.5}$$

Due to the special structure of the problem, using (1.12), we have that

$$\nabla^2 \psi = \begin{pmatrix} \varphi_a^T \varphi_a & \varphi_a^T \varphi_b + \Phi'(b)\varphi \\ \varphi_b^T \varphi_a + (\Phi'(b)\varphi)^T & \varphi_b^T \varphi_b + \varphi_{bb}^T \varphi \end{pmatrix}. \tag{2.6}$$

Because Newton's method converges quadratically, an efficient method for (1.5) should use a good approximation to the Hessian matrix (2.6). Under the general unseparated scheme, the

Gauss-Newton method approximates the Hessian by the first order term of φ as

$$H^{GN} = \begin{pmatrix} \varphi_a^T\varphi_a & \varphi_a^T\varphi_b \\ \varphi_b^T\varphi_a & \varphi_b^T\varphi_b \end{pmatrix}. \tag{2.7}$$

However, comparing (2.7) and (2.6) we can easily find that there is a term $\Phi'(b)\varphi$, neglected by (2.7), which can be obtained without computing any second order derivatives. Therefore, it seems that it is more natural to approximate the Hessian matrix (2.6) by

$$H^{(0)} = \begin{pmatrix} \varphi_a^T\varphi_a & \varphi_a^T\varphi_b + \Phi'(b)\varphi \\ \varphi_b^T\varphi_a + (\Phi'(b)\varphi)^T & \varphi_b^T\varphi_b \end{pmatrix}. \tag{2.8}$$

Unfortunately, it is not a good idea, because $H^{(0)}$ may not be positive semi-definite, even when the real Hessian $\nabla^2\psi$ is positive definite. In the next section, we can show that $H^{(0)}$ based scheme is not as good as Gauss-Newton method in most cases.

Now we try to modify (2.8) so that positive definite condition is satisfied. First, we define

$$\varphi_C = (\varphi_a^+)^T\Phi'(b)\varphi$$

and replace $\varphi_a^T\varphi_b + \Phi'(b)\varphi$ by $\varphi_a^T(\varphi_b + \varphi_C)$. Furthermore, if the lower right block term $\varphi_b^T\varphi_b$ is replaced by $(\varphi_b + \varphi_c)^T(\varphi_b + \varphi_c)$, we would have the following approximation formula:

$$H^{(1)} = \begin{pmatrix} \varphi_a^T\varphi_a & \varphi_a^T(\varphi_b + \varphi_c) \\ (\varphi_b + \varphi_c)^T\varphi_a & (\varphi_b + \varphi_C)^T(\varphi_b + \varphi_C) \end{pmatrix}. \tag{2.9}$$

Now, we can see $H^{(1)}$ is always positive semi-definite and has more second-order information than H^{GN}. If $\Phi(b)$ has rank p, we can show that

$$\varphi_a^T\varphi_b + \Phi'(b)\varphi = \varphi_a^T(\varphi_b + \varphi_C). \tag{2.10}$$

In this case, we have

$$H^{(1)} = \nabla^2\psi + \begin{pmatrix} 0 & 0 \\ 0 & \varphi_b^T\varphi_C + \varphi_C^T\varphi_b + \varphi_C^T\varphi_C - \varphi_{bb}^T\varphi \end{pmatrix}. \tag{2.11}$$

Hence the error matrix $H^{(1)}$–$\nabla^2\psi$ is a rank q matrix. We will prove in the next section that (2.9) is really a better approximation to $\nabla^2\psi$ than H^{GN}. Now we add $\varphi_C^T\varphi_C$ to the bottom-right part of (2.9) and have

$$H^{(2)} = \begin{pmatrix} \varphi_a^T\varphi_a & \varphi_a^T(\varphi_b + \varphi_c) \\ (\varphi_b + \varphi_c)^T\varphi_a & (\varphi_b + \varphi_C)^T(\varphi_b + \varphi_C) + \varphi_C^T\varphi_C \end{pmatrix}. \tag{2.12}$$

$H^{(2)}$ can be proved to be another better approximation to $\nabla^2\psi$. We call methods based on approximate Hessian (2.9) or (2.12) structured unseparated methods for separable nonlinear least squares problem.

2.3. Methods Based on Our New Scheme

Using the approximation Hessian (2.9) and (2.12), we can give three algorithms which apply line search, Levenberg-Marquardt technique and trust region approach respectively. The descriptions of the algorithms are given as follows.

Algorithm 2.1. (Structured Unseparated Method: Line Search Version)

Step 1 *Given* $x_0 = (a_0^T, b_0^T)^T$*; given* $\rho \in (0, 0.5)$ *and* $\epsilon > 0$ *sufficiently small.*
$k := 0$.

Step 2 *If* $||\nabla\psi(x_k)|| < \epsilon$*, then stop;*

Step 3 *Compute* H_k *by either* (2.9) *or* (2.12)*, set*

$$d_k = -(H_k)^{-1}\nabla\psi(x_k). \tag{2.13}$$

Step 4 *Find* $\alpha > 0$ *satisfying:*

$$\psi(x_k + \alpha d_k) \le \psi(x_k) + \rho\alpha\nabla\psi(x_k)^T d_k, \tag{2.14}$$
$$\psi(x_k + \alpha d_k) \ge \psi(x_k) + (1-\rho)\alpha\nabla\psi(x_k)^T d_k. \tag{2.15}$$

Step 5 $x_{k+1} = x_k + \alpha d_k$*, k:=k+1, goto* Step 2.

Line search type algorithms normally will have numerical difficulties when the approximate Hessian matrix H_k is nearly singular. To overcome this, we can employ either the Levenberg-Marquardt technique or the trust region approach.

Algorithm 2.2. (Structured Unseparated Method: Levenberg-Marquardt Version)

Step 1 *Given* x_0*, given* $c_1 > 1$*,* $c_2 > 1$*,* $0 < p_1 < p_2 < 1$ *and* $\epsilon > 0$ *sufficiently small.*
Let $\lambda_0 = ||\psi(x_0)||$*,* $k := 0$.

Step 2 *If* $||\nabla\psi(x_k)|| < \epsilon$*, then stop;*

Step 3 *Compute* H_k *by either* (2.9) *or* (2.12)*, let*

$$d_k = -(H_k + \lambda_k I)^{-1}\nabla\psi(x_k). \tag{2.16}$$

Step 4 *Compute the ratio*

$$r_k = \frac{\psi(x_k) - \psi(x_k + d_k)}{-\nabla\psi(x_k)^T d_k - \frac{1}{2}d_k^T H_k d_k}, \tag{2.17}$$

Generate λ_{k+1} *and* x_{k+1}*:*

$$\lambda_{k+1} = \begin{cases} c_1\lambda_k & \text{if } r_k \le p_1, \\ \frac{1}{c_2}\lambda_k & \text{if } r_k \ge p_2, \\ \lambda_k & \text{otherwise}; \end{cases} \tag{2.18}$$

$$x_{k+1} = \begin{cases} x_k + d_k & \text{if } r_k > 0, \\ x_k & \text{otherwise.} \end{cases} \tag{2.19}$$

Step 5 $k := k + 1$*, goto* Step 2.

Algorithm 2.3. (Structured Unseparated Method: Trust Region Version)

Step 1 *Given* x_0, $\Delta_0 > 0$, $c_1 > 1$, $c_2 > 1$, $0 < p_1 < p_2 < 1$; *and* $\epsilon > 0$ *sufficiently small.* *k=0;*

Step 2 *If* $||\nabla\psi(x_k)|| < \epsilon$, *then stop;*

Step 3 *Compute* H_k *by either* (2.9) *or* (2.12), *solve*

$$\min_{d\in\Re^n} \quad m_k(d) = \nabla\psi(x_k)^T d + \frac{1}{2} d^T H_k d, \tag{2.20}$$

$$\text{s.t.} \quad ||d||_2 \le \Delta_k, \tag{2.21}$$

obtaining d_k.

Step 4 *Compute the ratio*

$$r_k = \frac{\psi(x_k) - \psi(x_k + d_k)}{m(0) - m(d_k)}, \tag{2.22}$$

Generate Δ_{k+1} *and* x_{k+1}*:*

$$\Delta_{k+1} = \begin{cases} \frac{1}{c_1}\|d_k\|_2 & \text{if } r_k \le p_1, \\ \max[c_2\|d_k\|_2,\ \Delta_k] & \text{if } r_k \ge p_2, \\ \Delta_k & \text{otherwise}; \end{cases} \tag{2.23}$$

$$x_{k+1} = \begin{cases} x_k + d_k & \text{if } r_k > 0, \\ x_k & \text{otherwise.} \end{cases} \tag{2.24}$$

Step 5 $k := k + 1$, *goto* Step 2.

In Step 3 of the above algorithm, d_k can be either an exact solution [10] or an approximation solution of subproblem (2.20)-(2.21) obtained by the truncated conjugate gradient method [15, 17]. The step d_k computed by the truncated conjugate gradient method has the nice property that it reduces the objective function by at least half of the reduction of the exact solution [20]. When we apply the truncated conjugate gradient method, we also use the post process suggested by Powell [13].

3. Convergence Analysis

In this section, we study the convergence properties of our algorithms. Due to the fact that the differences between our methods and the unseparated Gauss-Newton method are different second order terms used in the approximation model, it is straightforward for us to extend the global convergence results of the Gauss-Newton method to all our three algorithms. Therefore, in this section we only study the local convergence properties of our algorithms. First, we show that both the approximate Hessians (2.9) or (2.12) are accurate approximations so that fast local convergence rate is ensured.

3.1. Local convergence rate

First, Similar to Gauss-Newton method, our algorithms are also quadratically convergent for zero-residual problems. Without loss of generality, we only prove the local quadratic convergence result for the step computed by Algorithm 2.1.

Theorem 3.1. *We denote x^* as a local minimum of (1.5) at which $\varphi(x^*) = 0$. If we assume $H^{(i)}(x^*)$, $i = 1, 2$ in (2.9), (2.12) respectively is positive definite, $\nabla^2\psi(x)$ and $H^{(i)}(x)^{-1}$ are Lipschitz continuous in a domain of x^*, then there exists a $\epsilon > 0$, for any $x_k \in \mathrm{N}(x^*, \epsilon)$, we have that*

$$\|x_k + d_k - x^*\| = \mathcal{O}(\|x_k - x^*\|^2). \tag{3.1}$$

Proof. Without loss of generality, we consider the case that H_k is defined by (2.9). Denote $S_k = \nabla^2\psi(x_k) - H_k$. From the definition of φ_C, (2.11), and our assumptions, it follows that

$$\|S_k\| = \mathcal{O}(\|\varphi(x_k)\|) = \mathcal{O}(\|x_k - x^*\|). \tag{3.2}$$

Let

$$d_k^N = -\nabla^2\psi(x_k)\nabla\psi(x_k) \tag{3.3}$$

be the Newton's step. It is well known that

$$x_k + d_k^N - x^* = \mathcal{O}(\|x_k - x^*\|^2), \tag{3.4}$$

which gives

$$\|d_k^N\| = \mathcal{O}(\|x_k - x^*\|). \tag{3.5}$$

Therefore, we have

$$\begin{aligned} \|d_k - d_k^N\| &= \|(\nabla^2\psi(x_k)^{-1} - H_k^{-1})\nabla\psi(x_k)\| \\ &= \|(I - H_k^{-1}\nabla^2\psi(x_k))d_k^N\| \\ &\le \|I - H_k^{-1}\nabla^2\psi(x_k)\|\|d_k^N\| \\ &= \|H_k^{-1}(H_k - \nabla^2\psi(x_k))\|\|d_k^N\| \\ &\le \|H_k^{-1}\|\|S_k\|\|d_k^N\| = \mathcal{O}(\|x_k - x^*\|^2). \end{aligned} \tag{3.6}$$

Now, (3.1) follows from relations (3.4) and (3.6). □

3.2. Asymptotical convergence rate

Now we concentrate on the asymptotical convergence properties among Golub and Pereyra's step, Kaufman's step, unseparated Gauss-Newton step, and our new unseparated step (2.13). Here, our analysis is motivated by the work of Ruhe and Wedin [14], where they compare the asymptotical convergence of the variable projection method with the Gauss-Newton method for the first time. Their comparison testified that the former one needs less iteration steps to convergence.

For any iterative method

$$x_{k+1} = h(x_k), \qquad \lim_{k\to\infty} x_k = x^*, \tag{3.7}$$

we define asymptotical convergence rate

$$R = -\ln \rho(h^{'}(x^*)). \tag{3.8}$$

We know the smaller the spectral radius $\rho(h^{'}(z^*))$ is, the faster the method converges. Here, $\rho(h^{'}(x^*)) = \max(-\alpha, \beta)$, where α and β denote the smallest and largest eigenvalues of generalized symmetrical eigenvalue problem

$$(H - \nabla^2\psi)z = \lambda H z, \tag{3.9}$$

respectively. Since the eigenvalues of (3.9) are the stationary values of the Rayleigh quotient

$$\mu(z) = \frac{z^T(H - \nabla^2\psi)z}{z^T H z}, \tag{3.10}$$

We can estimate the spectral radius by evaluating the extreme values of (3.10).

The theoretical analysis reported in Ruhe and Wedin [14] shows that the following theorem is true.

Lemma 3.1. *The convergence quotients $\mu^{(G.\&P.)}(z)$, $\mu^{(K.)}$, and μ^{GN} of variable projection methods with Golub and Pereyra's step* (1.15) *or Kaufman's step* (1.14) *and unseparated Gauss-Newton step are given by the extreme values of the following functional respectively:*

$$\mu^{(G.\&P.)}(z) = q(z); \qquad \mu^{(K.)} = \frac{q(z) - c(z)}{1 - c(z)};$$
$$\mu^{GN}(z) = \{\textit{solution to } r(\mu, z) = q(z) - \mu + (\mu + \mu^{-1} - 2)c(z) = 0\};$$

where the homogenous parameter independent functionals q, b, and c are defined by

$$q(z) = -||\varphi||_2 \lambda_{max}(K_2),$$

and K_2 is the curvature matrix of φ restricted to $\Im$;

$$c(z) = \frac{||\varphi_a^+ \Phi'(b)\varphi z||_2^2}{||P_{\varphi_a}^{\perp}\varphi_b z||_2^2 + ||\varphi_a^+ \Phi'(b)\varphi z||_2^2}.$$

According to Lemma 3.1, we have the following proposition:

Proposition 3.1. *If we denote α^M, β^M are the smallest and largest eigenvalues of problem* (3.9) *respectively, when $H = H^M$, here M means Gauss-Newton method, variable projection method with Golub and Pereyra's step or Kaufman's step.*

$$\alpha^{GN} \le \alpha^{(K.)} \le \alpha^{(G.\&P.)}, \quad \beta^{(K.)} \le \beta^{(G.\&P.)} \le \beta^{GN}. \tag{3.11}$$

We can see that the spectral radius of unseparated Gauss-Newton method are larger than the two variable projection methods. Therefore, it is very likely that the unseparated Gauss-Newton method is the slowest one among these three methods.

Using the results in Lemma 3.1, we can prove the following theorem.

Theorem 3.2. *If we denote $\alpha^{(i)}$, $\beta^{(i)}$ as the smallest and largest eigenvalues of problem* (3.9), *when $H = H^{(i)}$, $i = 1, 2$, respectively. Here $H^{(1)}$, and $H^{(2)}$ are decided by* (2.9) *and* (2.12). *Then the following results hold:*

$$\alpha^{(1)} = \alpha^{(K.)}, \quad \beta^{(1)} = \beta^{(K.)}; \quad \alpha^{(2)} = \alpha^{(G.\&P.)}, \quad \beta^{(2)} = \beta^{(G.\&P.)}. \tag{3.12}$$

Proof. Firstly, we consider the case $H = H^{(2)}$. Since the extreme values $\mu^{(2)}$ should be the extreme eigenvalues of the generalized eigenvalue problem $(H^{(2)} - \nabla^2\psi)z = \lambda H^{(2)}z$, it should be a zero point of

$$\det[H^{(2)} - \nabla^2\psi - \mu^{(2)}H^{(2)}] = 0.$$

Since we have

$$\det\begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} = \det[X_{11}] \cdot \det[X_{22} - X_{21}X_{11}^{-1}X_{12}]$$

if X_{11} is nonsingular. We have

$$\begin{aligned} & \det[H^{(2)} - \nabla^2\psi - \mu^{(2)}H^{(2)}] \\ = & \det\begin{bmatrix} -\mu^{(2)}\varphi_a^T\varphi_a & -\mu^{(2)}\varphi_a^T\varphi_b + \varphi_{ab}^T\varphi \\ -\mu^{(2)}\varphi_b^T\varphi_a + \varphi_{ba}^T\varphi & (1-\mu^{(2)})(\varphi_b^T\varphi_C + \varphi_C^T\varphi_b + 2\varphi_C^T\varphi_C) - \varphi_{bb}^T\varphi - \mu^{(2)}\varphi_b^T\varphi_b \end{bmatrix} \\ = & (-\mu^{(2)})^{p+q}\det[\varphi_a^T\varphi_a]\det[(H^{(G.\&P.)} - \psi_{\Im}^{''}) - \mu^{(2)}H^{(G.\&P.)}], \end{aligned}$$

where

$$H^{(G.\&P.)} = \varphi_b^T P_{\varphi_a}^{\perp}\varphi_b + (\varphi_a{}^{+}\Phi'(b)\varphi)^T P_{\varphi_a}\varphi_a{}^{+}\Phi'(b)\varphi \tag{3.13}$$

is the iterative matrix of variable projection method with Golub and Pereyra's step, and

$$\psi_{\Im}^{''} = \varphi_{bb} - \varphi_{ba}\varphi_{aa}^{-1}\varphi_{ab} \tag{3.14}$$

is the Hessian of the objective function ψ restricted to $\Im$. The last equation is due to the fact that

$$\varphi_C = \varphi_a^T(\varphi_b + \Phi'(b)\varphi).$$

A nonzero eigenvalue is now a zero point of

$$\det[(H^{(G.\&P.)} - \psi_{\Im}^{''} - \mu^{(2)}H^{(G.\&P.)}].$$

Therefore we proved that $\mu^{(2)}(z)$ is of the same extreme values as $\mu^{(G.\&P.)}(z)$'s.

The proof can be easily generated to the case that $H = H^{(1)}$ and $H^{(K.)} = \varphi_b^T P_{\varphi_a}^{\perp}\varphi_b$ is the iterative matrix of variable projection method with Kaufman's step. □

Theorem 3.2 tells us that our new unseparated framework is of the same asymptotical convergence rate as the two classical variable projection methods given by Golub and Pereyra [4] and Kaufman [6].

Similarly, we can evaluate the asymptotical convergence rate in the case of $H = H^{(0)}$. $\alpha^{(0)}$ and $\beta^{(0)}$ are given by the extreme values of the following functional

$$\mu(z) = \frac{p(z)}{1 + p(z) - q(z)}, \tag{3.15}$$

where

$$p(z) = z^T\varphi_{bb}^T\varphi z/(||P_{\varphi_a}^{\perp}\varphi_b z||_2^2 + ||\varphi_C z||_2^2), \tag{3.16}$$

and $q(z)$ is the Rayleigh quotient of (3.8) in the case of $H = H^{(G.\&P.)}$. (3.15) shows that we can benefit from using $H^{(0)}$ when the second-order term $\varphi_{bb}^T\varphi$ is significantly small. On the other hand, this method has poor asymptotical convergence property when $\varphi_{bb}^T\varphi$ is relatively large comparing to $\varphi_b^T\varphi_C$.

4. Numerical Results

In this section, we will show numerical results of the new methods based on our new separated framework. We compare our methods with the algorithms based on variable projection framework and general unseparated framework. We choose the above two typical test problems from Golub and Pereyra [4] and Ruhe and Wedin [14].

Problem 1. (Exponential data fitting)

$$\phi(a,b;t) = a_1 + a_2 e^{-b_1 t} + a_3 e^{-b_2 t},$$

with $m = 33$ and the optimal solution is $a_1^* = 0.37531$, $a_2^* = 1.9305$, $a_3^* = -1.4592$, $b_1^* = 0.012867$, $b_2^* = 0.022123$.

Test problem is generated by setting $t_i = i$, $y_i = (1 + nf \cdot randn(1))\phi(a^*, b^*; t_i)$, where nf is the noise parameter. Initial point is

$$\begin{aligned} a_i &= (1 + rd \cdot (2rand(1) - 1))a_i^*, \quad i = 1, 2, 3; \\ b_j &= (1 + rd \cdot (2rand(1) - 1))b_j^*, \quad j = 1, 2, \end{aligned}$$

where rd is the initial parameter.

Problem 2. (Fractional data fitting)

$$\phi(a,b;t) = a_1 + a_2 t + a_3 t^2 - a_4 \left[\frac{1}{1 + ((b_1 + 0.5b_2 - t)/b_3)^2} + \frac{1}{1 + ((b_1 - 0.5b_2 - t)/b_3)^2} \right]$$

$$-a_5 \left[\frac{1}{1 + ((b_4 + 0.5b_5 - t)/b_6)^2} + \frac{1}{1 + ((b_4 - 0.5b_5 - t)/b_6)^2} \right] - a_6 \left[\frac{1}{1 + ((b_7 - t)/b_8)^2} \right],$$

with $m = 188$ and the optimal solution is $a_1^* = 1.0$, $a_2^* = 0.2$, $a_3^* = 0.1$, $a_4^* = 0.9$, $a_5^* = 0.7$, $a_6^* = 0.3$, $b_1^* = 0.2$, $b_2^* = 0.8$, $b_3^* = 3.0$, $b_4^* = 0.3$, $b_5^* = 0.7$, $b_6^* = 3.0$, $b_7^* = 0.5$, $b_8^* = 2.0$.

Test problem is generated by setting $t_i = i/m$, $y_i = (1 + nf \cdot randn(1))\phi(a^*, b^*; t_i)$, where nf is the noise parameter. Initial point is

$$\begin{aligned} a_i &= (1 + rd \cdot (2rand(1) - 1))a_i^*, \quad i = 1, 2, \cdots, 6; \\ b_j &= (1 + rd \cdot (2rand(1) - 1))b_j^*, \quad j = 1, 2, \cdots, 8, \end{aligned}$$

where rd is the initial parameter.

We applied our algorithms to the above two problems for two different cases: one without noise ($nf = 0$) and one with nose ($nf = 0.1$). For all the runs, we set $\epsilon = 10^{-10}$ and the approximate Hessian (2.9) is used in all our algorithms.

The results for the case there is no noise are reported in Table 4.1, where the number of iterations and running time in seconds of the standard (unseparated) Gauss-Newton method, the variable projection method with Kaufman's step and our Algorithm 2.1 (with $\rho = 0.01$) are listed.

From Table 4.1, we can see that Algorithm 2.1 performs similarly to the variable projection method, and it is better than the standard Gauss-Newton method.

We also tested our algorithms when there are noise in the data. We compared four algorithms: the standard (unseparated) Levenberg-Marquadt method(L-M), the variable projection

Table 4.1: Test Results for noise-free data.

Problem	Gauss-Newton	Variable Projection	Algorithm 2.1
P1, $rd = 0.01$	6/0.0160	4/0.0140	4/0.0160
P2, $rd = 0.01$	16/0.7540	9/0.4400	10/0.4970

Table 4.2: Test Results for noise data ($nf = 0.1$).

Problem	L-M	Variable Projection	Algorithm 2.2	Algorithm 2.3
P1, $rd = 0.1$	19/0.0310	13/0.0250	14/0.0340	17/0.0410
P1, $rd = 0.2$	21/0.0340	14/0.0270	16/0.0370	18/0.0430
P1, $rd = 0.5$	25/0.0410	16/0.0310	19/0.0430	20/0.0470
P2, $rd = 0.1$	162/0.7660	142/0.7410	154/1.0160	62/0.4370
P2, $rd = 0.2$	169/0.8030	144/0.7880	160/1.0790	72/0.5000
P2, $rd = 0.5$	195/0.9540	158/0.9370	182/1.2910	76/0.5310

method with Kaufman's step and L-M modification, Algorithm 2.2 and Algorithm 2.3. For Algorithms 2.2 and 2.3, the following parameters are chosen: $c_1 = c_2 = 2$, $p_1 = 0.1$, and $p_2 = 0.4$. The results are reported in Table 4.2.

From the above results, it can be seen that our Algorithm 2.2 behaves very similarly to the variable projection method. Both are better than the standard Levenberg-Marquardt method. Our Algorithm 2.3 performs better than the variable projection method for Problem 2, but slightly worse for Problem 1.

5. Discussions

In this paper, we propose a new unseparated framework for the separable nonlinear least squares problem, by using special approximation formulae to the Hessian of the separable problems. Algorithms based on this framework are more efficient than general unseparated methods, and moreover they can be extended to constrained problems easily. Convergence analysis shows, that our new methods have the nice properties of variable projection methods. Numerical results also indicate that our algorithms are comparable to the famous variable projection method with Kaufman's step. The algorithms we presented can be improved if the arithmetical operations for computing the approximate Hessians $H^{(1)}$ and $H^{(2)}$ can be reduced.

Our approach offers a possibility to construct efficient algorithms for general constrained nonlinear least squares problems, particularly the constraints do not have the same separability structure as that of the objective function. However, how to implement such kinds of algorithms need careful studies, for example, attention has to be given to how to use the two different separable properties (those of the objective function and the constraints) properly. Moreover, large scale problems require us to exploit the structure with more sophistication.

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