A METHOD FOR SEPARABLE NONLINEAR LEAST SQUARES PROBLEMS WITH SEPARABLE NONLINEAR EQUALITY CONSTRAINTS*

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Abstract. Recently several algorithms have been proposed for solving separable nonlinear least squares problems which use the explicit coupling between the linear and nonlinear variables to define a new nonlinear least squares problem in the nonlinear variables only whose solution is the solution to the original problem. In this paper we extend these techniques to the separable nonlinear least squares problem subject to separable nonlinear equality constraints.

1. Introduction. In this paper we will consider the nonlinear least squares problem of finding a and α which minimize

$$||\mathbf{y} - \Phi(\mathbf{\alpha})\mathbf{a}||_2^2,$$

subject to nonlinear equality constraints of the form

(1.2)
$$H(\alpha)\mathbf{a} = \mathbf{g}(\alpha).$$

The abbreviated notation of (1.1) has the following meaning:

$$\Phi_{ij}(\boldsymbol{\alpha}) = (\phi_j(\boldsymbol{\alpha}; t_i)), \qquad i = 1, \dots, m, \quad j = 1, \dots, n,$$

$$\mathbf{a} = (a_1, \dots, a_n)^T, \quad \mathbf{y} = (y_1, \dots, y_m)^T, \quad \boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_k)^T.$$

In (1.2) we have p nonlinear constraints, i.e. $\mathbf{g}(\alpha) = (g_1(\alpha), \dots, g_p(\alpha))^T$, and $H(\alpha)$ is a $p \times n$ nonlinear matrix function $(p \le n + k)$. All the functions involved are assumed to be at least twice continuously differentiable, though somewhat weaker hypotheses could be employed.

In [2], Golub and Pereyra have discussed unconstrained problems of the form (1.1) which they have denoted as "separable nonlinear least squares problems".

Krogh [7] has extended those results to the more general models

(1.3)
$$\|\mathbf{y} - \mathbf{\Psi}(\mathbf{\alpha}) - \mathbf{\Phi}(\mathbf{\alpha})\mathbf{a}\|_{2}^{2}.$$

We do not need to introduce $\Psi(\alpha)$ explicitly in our present formulation, since it can be included in $\Phi(\alpha)$ **a** as $a_{n+1}\Psi(\alpha)$ provided we add the constraint $a_{n+1} = 1$. In [5] one of the authors has introduced more substantial modifications which simplify even further the algorithm.

Constraints of the form (1.2) appear in the applications [6] and they are considered here because of their similarity with (1.1). These problems can be reduced to unconstrained separable problems with a somewhat more complex structure. This is developed in detail in § 2. Once the reduction is performed, one could use any program available for unconstrained separable problems. However, it turns out to be considerably more efficient to devise a completely new algorithm,

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taking into account the structure of the problem, as we have done in § 3 of this paper.

It has been shown in practice [2], [7] and there are some theoretical indications [10], that the separation of the linear variables **a** from the nonlinear variables α by means of the variable projection method [2], [3], [5], [8] speeds up the convergence of iterative methods used to solve problem (1.1).

We extend in this paper the range of applicability of the variable projection method to constrained problems.

The reduction to an unconstrained problem at the beginning of § 2 was anticipated in [3].

2. The reduction to an unconstrained separable problem. In this section we consider the problem of finding vectors $\hat{\mathbf{a}}$ and $\hat{\boldsymbol{\alpha}}$ which minimize

(2.1a)
$$r(\mathbf{a}, \boldsymbol{\alpha}) = \|\mathbf{y} - \boldsymbol{\Phi}(\boldsymbol{\alpha})\mathbf{a}\|_{2}^{2},$$

subject to the nonlinear equality constraints

$$(2.1b) H(\alpha)\mathbf{a} = \mathbf{g}(\alpha),$$

where all the vectors and matrices are as in § 1. In what follows, an upper superscript ⁺ on a matrix will denote its Moore-Penrose generalized inverse (see [9]).

In order to guarantee the existence of feasible points we assume that there are vectors α for which the resulting linear systems (2.1b) is compatible; i.e. $\mathbf{g}(\alpha) \in \text{range } (H(\alpha))$, or equivalently, $\mathbf{g}(\alpha) = H(\alpha)H^+(\alpha)\mathbf{g}(\alpha)$. The set of all such vectors α will be denoted by A.

For each fixed $\alpha \in A$, the general solution of the resulting system of linear equations (2.1b) is given by [8]

(2.2)
$$\mathbf{a} = H^{+}(\alpha)\mathbf{g}(\alpha) + Y(\alpha)\mathbf{z},$$

with $H^+(\alpha)^T Y(\alpha) = 0$, and z varying over all R^{n-r} where r is the rank of H. In other words, the columns of $Y(\alpha)$ are a basis for the null space of $H(\alpha)$. The set of all pairs (a, α) , where $\alpha \in A$, and a is defined in (2.2), is the feasible set for problem (2.1). Therefore, this problem is equivalent to minimizing in z and α ,

(2.3)
$$s(\mathbf{z}, \boldsymbol{\alpha}) = \|\mathbf{y} - \Phi(\boldsymbol{\alpha}) H(\boldsymbol{\alpha})^{+} \mathbf{g}(\boldsymbol{\alpha}) - \Phi(\boldsymbol{\alpha}) Y(\boldsymbol{\alpha}) \mathbf{z}\|_{2}^{2}$$
$$\equiv \|\mathbf{y} - \boldsymbol{\zeta}(\boldsymbol{\alpha}) - G(\boldsymbol{\alpha}) \mathbf{z}\|_{2}^{2}.$$

where

$$\zeta(\alpha) = \Phi(\alpha)H(\alpha)^{+}g(\alpha)$$
 and $G(\alpha) = \Phi(\alpha)Y(\alpha)$.

If the dimension (n-r) of **z** is nonzero, then we would have a separable problem of the form (1.3). Since we want to apply the variable projection technique we will assume that r < n.

This problem could then be solved with any program for unconstrained separable problems by simply giving it the appropriate information. Once z is computed in the standard fashion, a is found by an application of formula (2.2). However, we would like to develop a completely new and more efficient algorithm, avoiding all redundant computation.

Let

(2.4)
$$\mathbf{f}(\alpha) = V(\alpha)^{T}(\mathbf{y} - \zeta(\alpha))$$

where $V(\alpha)$ is an orthogonal basis for the null space of $G(\alpha)$. Using a proof similar to Theorem 2.1 of [2], one can show that an α which minimizes $t(\alpha) = \|\mathbf{f}(\alpha)\|_2^2$ also minimizes $s(\mathbf{z}, \alpha)$. Except for the terms involving $\zeta(\alpha)$, the function $t(\alpha)$ is similar to $r_3(\alpha)$ of equation (4.1) in Kaufman [5]. The Marquardt-Levenberg algorithm applied to $t(\alpha)$ using the derivative formula for $r_3(\alpha)$ in [3] modified to account for $\zeta(\alpha)$, gives the following scheme for generating the required α : one starts with an arbitrary $\alpha^{(0)}$ and, until convergence is attained, generates the vectors $\alpha^{(f)}$ by the rule

(2.5)
$$\boldsymbol{\alpha}^{(j+1)} = \boldsymbol{\alpha}^{(j)} - \left(\frac{B}{\nu I}\right)^{+} \left(\frac{\mathbf{f}(\boldsymbol{\alpha}^{(j)})}{\mathbf{0}}\right)_{k},$$

where ν_i is large enough so that

$$\|\mathbf{f}(\boldsymbol{\alpha}^{(j+1)})\|_2 \leq \|\mathbf{f}(\boldsymbol{\alpha}^{(j)})\|_2$$

and $B = V^T[-D(\zeta) - D(G)G^-(y-\zeta)]$. The operator D represents the Fréchet derivative with respect to α , and G^- is any matrix satisfying $GG^-G = G$ and $(GG^-)^T = GG^-$.

Once B and $f(\alpha^{(i)})$ have been computed, one may efficiently obtain trial values of $\alpha^{(i+1)}$ for various values of ν_i using the algorithm of [2].

A vector \mathbf{z} which minimizes $s(\mathbf{z}, \boldsymbol{\alpha})$ for fixed $\boldsymbol{\alpha}$ is then given by $G^{-}(\boldsymbol{\alpha})(\mathbf{y}-\boldsymbol{\zeta}(\boldsymbol{\alpha}))$.

The compact formula for B in (2.5) is in terms of $D(\zeta)$ and D(G). A more convenient expression for B for the implementation of the algorithm is given in the following theorem:

THEOREM.

(2.6)
$$B = -V^{T} \{ \Phi H^{+} [-D(H)\mathbf{b} + H^{+T}D(H^{T})P_{H}^{\perp}\mathbf{g} + D(\mathbf{g})] + D(\Phi)\mathbf{b} \}$$
where $\mathbf{b} = YG^{-1}(\mathbf{y} - \zeta) + H^{+}\mathbf{g}$.

Proof. By (2.3),

$$(2.7) D(G) = \Phi D(Y) + D(\Phi)Y$$

and

(2.8)
$$D(\zeta) = D(\Phi)H^{\dagger}\mathbf{g} + \Phi D(H^{\dagger})\mathbf{g} + \Phi H^{\dagger}D(\mathbf{g}).$$

Thus, to obtain an expression for B, we need expressions for $D(H^+)$ and D(Y). Golub and Pereyra [2] have proved that

(2.9)
$$D(H^{+}) = -H^{+}D(H)H^{+} + H^{+}H^{+T}D(H)^{T}P_{H}^{\perp} + {}_{H}P^{\perp}D(H)^{T}H^{+T}H^{T}$$

where

$$P_H^{\perp} = I - HH^+$$

and

$$_{H}P^{\perp} = I - H^{+}H = YY^{T}$$

When this formula is inserted into (2.8) and then into (2.5), the last term of (2.9) is canceled since

$$V^T \Phi_H P^{\perp} = V^T \Phi Y Y^T = V^T G Y^T = 0.$$

To obtain a formula for D(Y) we'll use the orthogonal decomposition of H given by

$$(2.10) H = Q^T \left(\frac{T \mid 0}{0 \mid 0}\right) Z^T$$

where Q and Z are orthogonal matrices and T is an $r \times r$ nonsingular upper triangular matrix where H has rank r. It is easy to verify that

$$H^+ = Z \left(\frac{T^{-1} \mid 0}{0 \mid 0} \right) Q$$

and that if Z is partitioned as

$$Z^T = \left[-\frac{Z_1^T}{Z_2^T} - \right]_{n-r}^{r},$$

then $H^{+T}Z_2 = 0$. Thus one may set $Y = Z_2$.

A formula for D(Y) can be derived using the ideas of § 4 of [5]. From (2.10) we have

$$Z^T H^T Q^T = \left(\frac{T^T \mid 0}{0 \mid 0} \right),$$

which, according to $\S 4$ of [5], implies that there exists a matrix M such that

(2.11)
$$\frac{\partial Z_2^T}{\partial \alpha_i} = -Z_2^T \frac{\partial H^T}{\partial \alpha_i} H^{T+} + M Z_2^T.$$

This means that

$$D(Y) = -H^+D(H)Z_2 + Z_2M^T$$
.

The matrix Z_2 is not unique and M depends on which Z_2 is computed. Fortunately, when (2.11) is inserted into (2.7) and then into (2.5) the term with Z_2M^T is canceled since

$$V^T \Phi Z_2 M^T = V^T \Phi Y M^T = V^T G M^T = 0.$$

Thus one does not have to be concerned about M.

Combining (2.5), (2.7), (2.8), (2.9) and (2.10) we have

$$\begin{split} B &= -V^T \{D(\Phi)H^+\mathbf{g} + \Phi H^+[-D(H)H^+\mathbf{g} + H^{+T}D(H)^T P_H^\perp \mathbf{g} + D(\mathbf{g})] \\ &\qquad \qquad + [-\Phi H^+D(H)Y + D(\Phi)Y]G^-(\mathbf{y} - \boldsymbol{\zeta})\} \\ &= -V^T \{\Phi H^+[-D(H)\mathbf{b} + H^{+T}D(H^T)P_H^\perp \mathbf{g} + D(\mathbf{g})] + D(\Phi)\mathbf{b}\} \end{split}$$

where $\mathbf{b} = YG^{-}(\mathbf{y} - \boldsymbol{\zeta}) + H^{+}\mathbf{g}$. \square

The matrix V in (2.4) and (2.6) and the matrix G^- in (2.6) can be computed using the orthogonal decomposition of G given by

$$G = U\left(\frac{R \mid S}{0 \mid 0}\right)P$$

where U is an orthogonal matrix, P is a permutation matrix and R is a $q \times q$ nonsingular upper triangular matrix. If U is partitioned into

$$U=(\underbrace{U_1}_{q} : U_2),$$

then $G^TU_2 = 0$ so V can be U_2 . V can be generated using a sequence of Householder transformations as in [1]. The matrix G^- can be represented as

$$P^T \left(\frac{R^{-1} \mid 0}{0 \mid 0} \right) U^T.$$

- 3. Computational procedure. For a fixed value of α , the vector $\mathbf{f}(\alpha)$ of (2.4) may be constructed as follows:
 - 1) Determine $\Phi(\alpha)$, $H(\alpha)$.
- 2) Determine a complete orthogonal decomposition of $H(\alpha)$ by finding orthogonal matrices H and Z such that

$$QHZ = \left(\frac{T \mid 0}{0 \mid 0}\right)$$

where T is an $r \times r$ nonsingular upper triangular matrix. As in Golub [1] Q and Z may be the products of Householder transformations designed to reduce H to T. The matrices Q and Z need not be explicitly formed. Only the information required to generate the Householder transformations need be saved.

- 3) Form the matrix $C = \Phi Z$ by applying the Householder transformations which form Z to the matrix Φ . The last n-r columns of C form the matrix G in (2.3).
- 4) Determine the orthogonal matrix U and the permutation matrix P such that

$$UC\left(\frac{I \mid 0}{0 \mid P}\right) = \left(\frac{M \mid R \mid S}{N \mid 0 \mid 0}\right)$$

where R is a $q \times q$ nonsingular upper triangular matrix. Again U may be the product of Householder transformations and need not be explicitly formed.

5) Compute $\mathbf{d} = \mathbf{H}^{+}\mathbf{g}$ as follows:

(a) Set
$$\mathbf{a} = Q\mathbf{g} = \left(-\frac{\mathbf{a}_1}{\mathbf{a}_2}\right)^r$$
.

(b) Solve $T\mathbf{c} = \mathbf{a}_1$.

(c) Set
$$\mathbf{d} = Z\left(-\frac{\mathbf{c}}{0}\right)$$
.

6) Compute $f(\alpha)$ by setting

$$\mathbf{p} = U(\mathbf{y} - \Phi \mathbf{d}) = \left(\frac{\mathbf{p}_1}{\mathbf{p}_2}\right)_{m-q}^q.$$

The vector $\mathbf{f}(\boldsymbol{\alpha})$ is contained in \mathbf{p}_2 and hence $\|\mathbf{f}(\boldsymbol{\alpha})\|_2$ is simply $\|\mathbf{p}_2\|_2$.

When B of (2.5) is also required, one should continue the procedure as follows:

7) Compute $D(\Phi(\alpha))$, $D(H(\alpha))$, and $D(\mathbf{g})$.

Usually $D(\Phi)$ and D(H) are tensors with many columns that are zero. Golub and Pereyra [2] describe a scheme for storing only the nonzero columns and determining tensor by vector products using this compact storage arrangement.

- 8) Compute **b** of (2.6) as follows:
 - (a) Solve $Re = \mathbf{p}_1$ where R was formed in step 4) and \mathbf{p}_1 in step 6).
 - (b) Set $\mathbf{h} = P \begin{pmatrix} \mathbf{e} \\ 0 \end{pmatrix}$.
 - (c) Set $\mathbf{b} = Z \begin{pmatrix} 0 \\ \mathbf{h} \end{pmatrix} + \mathbf{d}$.
- 9) Set R = QD(H) by applying the Householder transformations which form Q to the nonzero columns of the tensor D(H).
 - 10) Form $J = Q(D(H)\mathbf{b} H^{+T}(DH)^T P_H^{\perp} \mathbf{g} \mathbf{D}(\mathbf{g})).$
 - (a) Form $(DH)^T P_H^{\perp} g$ by setting

$$E = R^T \binom{0}{\mathbf{a}_2}.$$

(b) Set
$$F = Z^T E = \left(\frac{F_1}{F_2}\right)^r$$

(c) Solve the $k r \times r$ systems

$$T^TG = F_1$$

(d) Set
$$J = R\mathbf{b} - \begin{bmatrix} G \\ 0 \end{bmatrix} - QD(\mathbf{g}) = \left(-\frac{J_1}{J_2}\right)^r$$
.

- 11) The matrix B is finally obtained as follows:
 - (a) Solve the $k r \times r$ systems

$$TK = J_1$$
.

(b) Set
$$L = UD(\Phi)\mathbf{b} = \left(\frac{L_1}{L_2}\right)_{m-q}^q$$

(c)
$$B = -(NK + L_2)$$

4. Algorithm implementation and numerical results for linear constraints. Considerable simplifications arise in the aglorithm of § 3 when $H(\alpha)$ is a constant matrix. Since this is the case we have actually implemented as a computer code and for which currently we have practical applications we would like to indicate these simplifications.

Naturally $H(\alpha)$ is not evaluated in 1) each time, since H does not depend upon α . For the same reason 2) is done once and for all at the beginning of the process. Steps 3)-6) remain the same, while in step 7) $DH(\alpha)$ need not be calculated. Step 8) is the same, while 9) is eliminated. In 10) J simply becomes $-QD(\mathbf{g})$, so parts (a)-(d) are eliminated. Step (11) remains.

The algorithm was implemented in FORTRAN and tested on two examples, in both of which H and g were constant.

The first problem considered was fitting Gaussians with an expoential background, i.e., the model

$$a_1 e^{-\alpha_1 t} + a_2 e^{-\alpha_2 (t-\alpha_3)^2} + a_3 e^{-\alpha_4 (t-\alpha_5)^2} + a_4 e^{-\alpha_6 (t-\alpha_7)^2}$$

is fitted to 65 data points. See [11] for a listing of the data and starting values for α . The a's were constrained to the hyperplanes

$$a_1 + 2a_2 + 3a_3 + 4a_4 = 6.27006284,$$

 $a_1 + a_3 = 1.74158318.$

This problem was chosen in order to verify the correctness of the formulas and the corresponding code.

With these constraints the solution to the problem coincides with the solution to the unconstrained problem which is available in [2], [11].

With 9 function evaluations, 8 derivative evaluations and 3.23 seconds of computing time on a CDC 6400 computer (Run compiler) the residual $r(\mathbf{a}, \alpha)$ was reduced to .04013774.

The second problem was supplied by Peter Kirkegaard of the Atomic Energy Commission, Risö, Denmark. Kirkegaard and Eldrup [6] had devised a method for solving separable nonlinear least squares problems with linear constraints on the linear variables which arose in the analysis of positron lifetime spectra. Their algorithm used Marquardt's algorithm based on the fact that for a fixed α , the optimal arc could be obtained via the symmetric indefinite system

$$\begin{bmatrix} \Phi^T \Phi & H^T \\ H & 0 \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} \Phi^T \mathbf{y} \\ \mathbf{g} \end{bmatrix}.$$

Kirkegaard gave the authors an example in which the Φ matrix was given by

$$\Phi_{ij} = x_i^{1/2} \sum_{p=1}^2 w_p (z_{ijp} - z_{i+1,jp} - \operatorname{erf} \{ (t_i - \alpha_4 - d_p) / \sigma_p \} + \operatorname{erf} \{ (t_{i+1} - \alpha_4 - d_p) / \sigma_p \}).$$

where

$$z_{ijp} = e^{-\alpha_j (t_i - \alpha_4 - d_p - 1/4\alpha_j \sigma_p^2)} (1 - \operatorname{erf} \{\alpha_j \sigma_p / 2 - (t_i - \alpha_4 - d_p) / \sigma_p \}) \quad \text{for } j = 1, 2, 3,$$

$$z_{ijp} = e^{-\lambda (t_i - \alpha_4 - d_p - 1/4\lambda \sigma_p^2)} (1 - \operatorname{erf} \{\lambda \sigma_p / 2 - t_i - \alpha_4 - d_p) / \sigma_p \})),$$

and

$$w_1 = 6$$
, $w_2 = 4$, $d_1 = 25/70$, $d_2 = 0$, $\lambda = \frac{.07}{1.7}$,
 $\sigma_1 = \frac{.38}{.14 [\ln{(2)}]^{1/2}}$ and $\sigma_2 = \frac{.485}{.14 [\ln{(2)}]^{1/2}}$

and the values of x_i are given in the Table 1 below. Thus n = 4 and k = 4. The vector \mathbf{t} was given by

$$t_i = i + 121$$
 for $i = 1, 2, \dots, 379$

and the vector y was given by

$$y_i = \frac{(x_i - 85)}{x_i^{1/2}}$$
 for $i = 1, 2, \dots, 379$.

TABLE 1 (x values)

107	74	100	104	106	99	88	84	101	
419	195	141	112	84	90	99	105	109	105
28,497	29,418	27,804	24,154	18,596	12,952	7,947	4,352	2,099	919
8,115	9,088	10,007	11,264	12,727	14,495	17,241	19,579	22,837	25,948
3,461	3,677	4,136	4,324	4,691	5,192	5,626	6,131	6,642	7,473
1,656	1,697	1,967	1,997	2,105	2,394	2,589	2,628	2,977	3,219
891	910	1,003	1,029	1,144	1,199	1,264	1,346	1,481	1,511
465	509	548	600	644	644	695	751	737	847
292	318	315	320	346	357	371	411	454	447
195	190	212	204	205	204	252	264	263	252
152	162	147	159	157	168	171	183	169	198
129	122	112	106	133	124	157	132	120	153
86	121	105	105	101	127	102	116	133	104
87	82	98	89	112	94	99	97	100	84
104	96	95	88	113	92	95	100	87	82
91	107	95	84	85	77	80	87	103	102
84	97	90	88	80	80	88	100	94	80
106	82	88	63	108	86	77	94	72	75
91	89	85	90	67	72	79	87	79	77
87	80	90	97	91	93	102	87	89	86
90	92	93	76	77	83	82	68	93	82
78	72	76	87	93	75	77	102	90	68
84	90	88	89	84	83	93	84	79	84
70	101	75	89	82	96	93	71	88	91
85	92	88	83	81	72	70	72	88	78
97	77	76	88	80	84	82	86	84	91
85	89	87	91	64	89	92	96	83	85
81	82	77	79	88	75	100	80	103	79
91	81	88	78	81	92	98	77	104	81
88	78	84	77	72	92	95	72	90	78
81	75	76	80	83	79	91	76	80	83
93	93	79	92	88	102	77	94	80	105
90	77	82	78	99	86	87	82	82	82
92	84	83	70	94	89	95	85	104	83
90	84	98	76	86	99	97	85	99	89
78	75	79	78	73	82	98	79	69	86
87	90	86	88	103	77	97	75	76	95
71	81	99	107	98	85	91	72	76	93
80	75	89	93	91	63	80	78	82	90
80	96	90	83	90	103	86	82	83	72

There was only 1 linear constraint for this particular problem:

$$.54a_1 + .54a_2 + .46a_3 + .54a_4 = 0.$$

Initially α was $(.54, .2, .07, 127.4)^T$ which gave a residual of 1,353.036. The residuals at successive iterations were

426.9649 359.8339 359.1253 359.0751 335.0720

Initially ν_i in (2.5) was set to $(\|B\|_2^2/(m \cdot k))$. On successive iterations ν was half of its previous value. The final α was (.53777671, .211172, .073373458, 126.92371)^T while the final α was (32,783.984, 52,140.2229, 108,630.17, 7,612.5942)^T.

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