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Technical report No. V999

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## **New subroutines for large-scale optimization**

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### Abstract:

We present fourteen basic FORTRAN subroutines for large-scale optimization with simple bounds and large-scale systems of nonlinear equations. Subroutines PLIS and PLIP, intended for dense general optimization problems, are based on limited-memory variable metric methods. Subroutine PNET, also intended for dense general optimization problems, is based on an inexact truncated Newton method. Subroutines PNED and PNEC, intended for sparse general optimization problems, are based on modifications of the discrete Newton method. Subroutines PSED and PSEC, intended for partially separable optimization problems, are based on partitioned variable metric updates. Subroutine PSEN, intended for nonsmooth partially separable optimization problems, is based on partitioned variable metric updates and on an aggregation of subgradients. Subroutines PGAD and PGAC, intended for sparse nonlinear least squares problems, are based on modifications and corrections of the Gauss-Newton method. Subroutine PMAX, intended for minimization of a maximum value (minimax), is based on the primal line-search interior-point method. Subroutine PSUM, intended for minimization of a sum of absolute values, is based on the primal trust-region interior-point method. Subroutines PEQN and PEQL, intended for sparse systems of nonlinear equations, are based on the discrete Newton method and the inverse column-update quasi-Newton method, respectively. Besides the description of methods and codes, we propose computational experiments which demonstrate the efficiency of the proposed algorithms.

### Keywords:

Large-scale optimization, Large-scale nonsmooth optimization, large-scale nonlinear least squares, large-scale nonlinear minimax, large-scale systems of nonlinear equations, sparse problems, partially separable problems, limited-memory methods, discrete Newton methods, quasi-Newton methods, primal interior-point methods.

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<sup>1</sup>This work was supported by the Grant Agency of the Czech Academy of Sciences, project No. IAA1030405, the Grant Agency of the Czech Republic, project No. 201/06/P397, and the institutional research plan No. AV0Z10300504

# 1 Introduction

We propose fourteen basic subroutines which implement selected large-scale optimization algorithms. The double-precision FORTRAN 77 subroutines `PLIS`, `PLIP`, `PNET` are designed to find a close approximation to a local minimum of a general twice continuously differentiable function  $F : R^n \rightarrow R$  with unknown or dense Hessian matrix. Subroutines `PLIS`, `PLIP` are based on limited-memory variable metric updates: `PLIS` uses Strang recurrences [13], [26] and `PLIP` uses shifted limited-memory variable metric updates [38]. Subroutine `PNET` is based on an inexact truncated Newton method [8].

The double-precision FORTRAN 77 subroutines `PNET`, `PNEC` are designed to find a close approximation to a local minimum of a general twice continuously differentiable function  $F : R^n \rightarrow R$  with the sparse Hessian matrix. These subroutines are based on inexact discrete Newton methods [5], [7]: `PNET` uses matrix direct methods (Dennis–Mei [9] or Moré–Sorensen [25]) and `PNEC` uses matrix iterative methods (Steihaug–Toint [31], [32] or shifted Steihaug–Toint [16]) for computing a trust region step.

The double-precision FORTRAN 77 subroutines `PSED`, `PSEC` are designed to find a close approximation to a local minimum of a smooth partially separable objective function

$$F(x) = \sum_{i=1}^{n_a} f_i(x).$$

Here  $x \in R^n$  is a vector of  $n$  variables and  $f_i : R^n \rightarrow R$ ,  $1 \leq i \leq n_a$ , are twice continuously differentiable functions. These subroutines are based on partitioned variable metric updates [12], [19]: `PSED` uses a matrix direct method (Gill–Murray [10]) and `PSEC` uses a matrix iterative method (safeguarded conjugate gradient method) for computing a line-search step.

The double-precision FORTRAN 77 subroutine `PSEN` is designed to find a close approximation to a local minimum of a nonsmooth partially separable objective function

$$F(x) = \sum_{i=1}^{n_a} f_i(x).$$

Here  $x \in R^n$  is a vector of  $n$  variables and  $f_i : R^n \rightarrow R$ ,  $1 \leq i \leq n_a$ , are locally Lipschitz nondifferentiable functions. This subroutine is based on a bundle variable metric method described in [23].

The double-precision FORTRAN 77 subroutines `PGAD`, `PGAC` are designed to find a close approximation to a local minimum of the least-square function

$$F(x) = \frac{1}{2} \sum_{i=1}^{n_a} f_i^2(x).$$

Here  $x \in R^n$  is a vector of  $n$  variables and  $f_i : R^n \rightarrow R$ ,  $1 \leq i \leq n_a$ , are twice continuously differentiable functions. These subroutines are based on hybrid methods that combine the Gauss–Newton method with the Newton or the variable metric corrections [15], [19]: `PGAD` uses matrix direct methods (Dennis–Mei [9] or Moré–Sorensen [25]) and `PGAC` uses matrix iterative methods (Steihaug–Toint [31], [32] or shifted Steihaug–Toint [16]) for computing a trust region step.

The double-precision FORTRAN 77 subroutine **PMAX** is designed to find a close approximation to a local minimum of maximum functions

$$F(x) = \max_{1 \leq i \leq n_a} f_i(x)$$

or

$$F(x) = \max_{1 \leq i \leq n_a} |f_i(x)|.$$

Here  $x \in R^n$  is a vector of  $n$  variables and  $f_i : R^n \rightarrow R$ ,  $1 \leq i \leq n_a$ , are twice continuously differentiable functions. This subroutine is based on primal interior point methods described in [17].

The double-precision FORTRAN 77 subroutine **PSUM** is designed to find a close approximation to a local minimum of a sum of absolute values

$$F(x) = \sum_{i=1}^{n_a} |f_i(x)|.$$

Here  $x \in R^n$  is a vector of  $n$  variables and  $f_i : R^n \rightarrow R$ ,  $1 \leq i \leq n_a$ , are twice continuously differentiable functions. This subroutine is based on primal interior point methods described in [18].

The double-precision FORTRAN 77 subroutines **PEQN**, **PEQL** are designed to find a solution of a system of nonlinear equations

$$f_i(x) = 0, \quad 1 \leq i \leq n.$$

Here  $x \in R^n$  is a vector of  $n$  variables and  $f_i : R^n \rightarrow R$ ,  $1 \leq i \leq n$ , are continuously differentiable functions. Subroutine **PEQN** is based on the inexact discrete Newton method [2], [6], [22] and subroutine **PEQL** is based on the inverse column-update quasi-Newton method [22], [24].

Subroutines **PLIS**, **PLIP**, **PNET**, **PNED**, **PNEC**, **PSED**, **PSEC**, **PGAD**, **PGAC** allow us to work with box constraints in the form

$$\begin{aligned} x_i - \text{unbounded} & , \quad I_i^x = 0, \\ x_i^l \leq x_i & , \quad I_i^x = 1, \\ x_i \leq x_i^u & , \quad I_i^x = 2, \\ x_i^l \leq x_i \leq x_i^u & , \quad I_i^x = 3, \\ x_i - \text{fixed} & , \quad I_i^x = 5, \end{aligned}$$

where  $1 \leq i \leq n$  ( $I^x$  corresponds to array **IX** in Appendix A).

To simplify the user's work, additional easy-to-use subroutines are added. These subroutines, written in FORTRAN 90 (they use a dynamic allocation of working arrays), call general subroutines **PLIS**, **PLIP**, **PNET**, **PNED**, **PNEC**, **PSED**, **PSEC**, **PSEN**, **PGAD**, **PGAC**, **PMAX**, **PSUM**, **PEQN**, **PEQL**. These subroutines can be easily changed to FORTRAN 77 codes by deleting statements **ALLOCATABLE**, **ALLOCATE**, **DEALLOCATE**, adding working arrays **IA**, **RA** into formal parameters and declaring their dimensions in the main program. Table 1 summarizes properties of easy-to-use subroutines.

Each subroutine contains a description of formal parameters and extensive comments. Moreover, text files **PLIS.TXT**, **PLIP.TXT**, **PNET.TXT**, **PNED.TXT**, **PNEC.TXT**, **PSED.TXT**,

| Subroutine | Problem                | Constraints | Strategy     | Matrices | Solver    |
|------------|------------------------|-------------|--------------|----------|-----------|
| PLISU      | general                | no          | line-search  | no       | no        |
| PLISS      | general                | yes         | line-search  | no       | no        |
| PLIPU      | general                | no          | line-search  | no       | no        |
| PLIPS      | general                | yes         | line-search  | no       | no        |
| PNETU      | general                | no          | line-search  | no       | iterative |
| PNETS      | general                | yes         | line-search  | no       | iterative |
| PNEDU      | general                | no          | trust-region | yes      | direct    |
| PNEDS      | general                | yes         | trust-region | yes      | direct    |
| PNECU      | general                | no          | trust-region | yes      | iterative |
| PNECS      | general                | yes         | trust-region | yes      | iterative |
| PSEDU      | partially separable    | no          | line-search  | yes      | direct    |
| PSEDS      | partially separable    | yes         | line-search  | yes      | direct    |
| PSECU      | partially separable    | no          | line-search  | yes      | iterative |
| PSECS      | partially separable    | yes         | line-search  | yes      | iterative |
| PSENU      | nonsmooth              | no          | line-search  | yes      | direct    |
| PGADU      | sum of squares         | no          | trust-region | yes      | direct    |
| PGADS      | sum of squares         | yes         | trust-region | yes      | direct    |
| PGACU      | sum of squares         | no          | trust-region | yes      | iterative |
| PGACS      | sum of squares         | yes         | trust-region | yes      | iterative |
| PMAXU      | minimax and $l_\infty$ | no          | line-search  | yes      | direct    |
| PSUMU      | $l_1$                  | no          | trust-region | yes      | direct    |
| PEQNU      | nonlinear equations    | no          | line-search  | yes      | iterative |
| PEQLU      | nonlinear equations    | no          | line-search  | yes      | iterative |

Table 1: Easy-to-use subroutines

PSEC.TXT, PSEN.TXT, PGAD.TXT, PGAC.TXT, PMAX.TXT, PSUM.TXT, PEQN.TXT, PEQL.TXT containing a detailed description of all important subroutines are added. Finally, test programs TLISU, TLISS, TLIPU, TLIPS, TNETU, TNETS, TNEDU, TNEDS, TNECU, TNECS, TSEDU, TSEDS, TSECU, TSECS, TSENU, TGADU, TGADS, TGACU, TGACS, TMAXU, TSUMU, TEQNU, TEQLU that use extensive collections of test problems are included. These test programs serve as examples for using the subroutines, verify their correctness and demonstrate their efficiency.

Subroutines presented in this report were generated using the UFO system [20]. We selected the most efficient methods from this system to prepare individual problem-oriented subroutines. This point of view gives a reason for our selection of optimization methods and choice of line-search or trust-region strategies (the UFO system contains many additional methods and strategies which were also tested and compared). This also explains the fact that PNET uses line-search while PNED, PNEC use trust-region strategies and the fact that some methods and strategies are implemented in slightly different ways than those described in the original papers (we have carefully tuned them to obtain the best results). Subroutines PLIS, PNET, PNED, PNEC, PSED, PSEC, PGAD, PGAC, PEQN, PEQL implement classic optimization methods and have equivalents, e.g., L-BFGS [40], TNPACK [30], VE08 [33], VE10 [34], NITSOL [28], NLEQ1S [27]. Numerical comparisons with these equivalents are given in Section 9 (we also used HOMPACT90 [39] for a comparison, but this code

was unable to solve a large number of our test problems). Subroutines PLIP, PSEN, PMAX, PSUM are based on new original methods proposed in [38], [23], [17], [18].

All subroutines described in this report are free for academic use and can be downloaded from [www.cs.cas.cz/~luksan/subroutines.html](http://www.cs.cas.cz/~luksan/subroutines.html).

## 2 Matrix-free methods for general problems

Consider a general continuously differentiable function  $F : R^n \rightarrow R$ , where  $n$  is large, and assume that the structure of the Hessian matrix of  $F$  is unknown. In this case, subroutines PLIS, PLIP, and PNET based on matrix-free methods can be used for seeking a local minimum of  $F$ . These methods are realized in the line-search framework so that they generate a sequence of points  $x_k \in R^n$ ,  $k \in N$ , by the simple process

$$x_{k+1} = x_k + \alpha_k d_k, \quad (1)$$

where  $d_k \in R^n$  is a direction vector and  $0 < \alpha_k \leq \bar{\alpha}_k$  is a scalar step-size. The direction vector is determined in such a way that

$$-d_k^T g(x_k) \geq \underline{\varepsilon} \|d_k\| \|g(x_k)\| \quad (2)$$

(the uniform descent condition) holds, where  $0 < \underline{\varepsilon} \leq 1$  (we use the value  $\underline{\varepsilon} = 10^{-4}$  in our subroutines). The step-size is chosen in such a way that

$$F(x_{k+1}) - F(x_k) \leq \varepsilon_1 \alpha_k d_k^T g(x_k), \quad d_k^T g(x_{k+1}) \geq \varepsilon_2 d_k^T g(x_k) \quad (3)$$

(the weak Wolfe conditions) hold, where  $0 < \varepsilon_1 < 1/2$  is a tolerance for the function value decrease and  $\varepsilon_1 < \varepsilon_2 < 1$  is a tolerance for the directional derivative increase (we use the values  $\varepsilon_1 = 0.0001$  and  $\varepsilon_2 = 0.9$  in our subroutines). The maximum step-size  $\bar{\alpha}_k$  is given by the formula  $\bar{\alpha}_k = \bar{\Delta} / \|d_k\|$ , where  $\bar{\Delta}$  is an upper bound for the norm  $\|x_{k+1} - x_k\|$  (parameter **XMAX** in our subroutines). The step-size  $\alpha_k$  is chosen iteratively either by bisection (**MES** = 1), or by quadratic interpolation with two function values (**MES** = 2), or by quadratic interpolation with two directional derivatives (**MES** = 3), or by cubic interpolation (**MES** = 4). We start with the initial estimate  $\alpha_k = 1$  if **IEST** = 0 or the initial estimate is derived by using the lower bound for  $F$  (parameter **FMIN** in our subroutines) if **IEST** = 1.

The direction vector  $d_k$  is usually computed by the formula  $d_k = -H_k g_k$  or by solving the linear system  $B_k d_k = -g_k$ , where  $g_k = g(x_k)$ ,  $B_k$  is an approximation of the Hessian matrix  $G(x_k)$  and  $H_k$  is an approximation of its inverse. Limited-memory variable metric methods use the matrix  $H_k$  implicitly (it is not stored). Similarly, the truncated Newton method uses the matrix  $B_k$ , which is not stored as well. If the direction vector computed by using the above way does not satisfy the uniform descent condition (2), a restart is performed, which implies that the direction vector  $d_k = -g_k$ , satisfying (2), is used.

### 2.1 Limited-memory BFGS method

Subroutine PLIS is an implementation of the limited-memory BFGS method proposed in [13], [26]. This method works with matrices  $H_k = H_k^k$ , where  $H_{k-m}^k = \gamma_k I$ ,  $\gamma_k > 0$  and

$$H_{j+1}^k = V_j^T H_j^k V_j + \frac{1}{b_j} s_j s_j^T, \quad V_j = I - \frac{1}{b_j} y_j s_j^T$$

for  $k - m \leq j \leq k - 1$ . Here  $s_j = x_{j+1} - x_j$ ,  $y_j = g_{j+1} - g_j$ ,  $a_j = y_j^T H_j^k y_j$ ,  $b_j = y_j^T s_j$ . Thus

$$H_{j+1}^k = \frac{b_{k-1}}{a_{k-1}} \left( \prod_{i=k-m}^j V_i \right)^T \left( \prod_{i=k-m}^j V_i \right) + \sum_{l=k-m}^j \frac{1}{b_l} \left( \prod_{i=l+1}^j V_i \right)^T s_l s_l^T \left( \prod_{i=l+1}^j V_i \right)$$

(we use  $\gamma_k = b_{k-1}/a_{k-1}$  in our implementation). The matrix  $H_k = H_k^k$  need not be constructed explicitly since we need only a vector  $d_k = -H_k^k g_k$ , which can be computed by using two recurrences (the Strang formula). First, vectors

$$u_j = - \left( \prod_{i=j}^{k-1} V_i \right) g_k,$$

$k - 1 \geq j \geq k - m$ , are computed by using the backward recurrence

$$\begin{aligned} \sigma_j &= s_j^T u_{j+1} / b_j, \\ u_j &= u_{j+1} - \sigma_j y_j, \end{aligned}$$

where  $u_k = -g_k$ . Then vectors

$$v_{j+1} = \frac{b_{k-1}}{a_{k-1}} \left( \prod_{i=k-m}^j V_i \right)^T u_{k-m} + \sum_{l=k-m}^j \frac{1}{b_l} \left( \prod_{i=l+1}^j V_i \right)^T s_l s_l^T u_{l+1},$$

$k - m \leq j \leq k - 1$ , are computed by using the forward recurrence

$$v_{j+1} = v_j + (\sigma_j - y_j^T v_j / b_j) s_j,$$

where  $v_{k-m} = (b_{k-1}/a_{k-1})u_{k-m}$ . Finally, we set  $d_k = v_k$ . Note that  $2m$  vectors  $s_j$ ,  $y_j$ ,  $k - m \leq j \leq k - 1$  are used and stored. The number of consecutive variable metric updates is defined as  $m = \min(\text{MF}, k - \underline{k})$ , where  $\text{MF}$  is a parameter of the subroutine `PLIS` and  $\underline{k}$  is an index of the iteration corresponding to the last restart.

## 2.2 Shifted limited-memory variable metric methods

Subroutine `PLIP` is an implementation of shifted limited-memory variable metric methods proposed in [38]. These methods work with matrices  $H_k = \zeta_k I + U_k U_k^T$ , where  $n \times m$  matrix  $U_k$  is updated by formula  $U_{k+1} = V_k U_k$  with a low rank matrix  $V_k$  chosen in such a way that the (modified) quasi-Newton condition  $U_{k+1} U_{k+1}^T y_k = \rho_k \tilde{s}_k$  with  $\tilde{s}_k = s_k - \zeta_{k+1} y_k$  is satisfied (we use the same notation, namely  $s_k$ ,  $y_k$ ,  $a_k$ ,  $b_k$  as in Section 2.1). This condition can be replaced by equations

$$U_{k+1}^T y_k = z_k, \quad U_{k+1} z_k = \rho_k \tilde{s}_k, \quad \|z_k\|^2 = \rho_k y_k^T \tilde{s}_k.$$

where  $z_k$  is an optional vector parameter. Note that the last equality, which is a consequence of the first two equalities, is the only restriction laid on the vector  $z_k$ . To simplify the notation, we define vectors  $u_k = U_k^T y_k$  and  $v_k = U_k^T H_k^{-1} s_k = -\alpha_k U_k^T g_k$ .

The choice of a shift parameter  $\zeta_{k+1}$  is a crucial part of shifted limited-memory variable metric methods. The value

$$\zeta_{k+1} = \mu_k \frac{b_k}{\|y_k\|^2}, \quad \mu_k = \frac{\sqrt{1 - \|u_k\|^2/a_k}}{1 + \sqrt{1 - b_k^2/(\|s_k\|^2 \|y_k\|^2)}}$$

is used in subroutine PLIP. The most efficient shifted limited-memory variable metric methods can be derived by a variational principle. Let  $T_k$  be a symmetric positive definite matrix. It can be shown (see [38]) that the Frobenius norm  $\|T_k^{-1/2}(U_{k+1}-U_k)\|_F^2$  is minimal on the set of all matrices satisfying the quasi-Newton condition if and only if

$$U_{k+1} = U_k - \frac{T_k y_k}{y_k^T T_k y_k} y_k^T U_k + \left( \rho_k \tilde{s}_k - U_k z_k + \frac{y_k^T U_k z_k}{y_k^T T_k y_k} T_k y_k \right) \frac{z_k^T}{\|z_k\|^2}.$$

Here  $T_k y_k$  and  $z_k$  are vector parameters defining a class of shifted limited-memory variable metric methods. Using suitable values of these vectors, we obtain particular methods of this class.

Assuming that  $T_k y_k$  and  $\rho_k \tilde{s}_k - U_k z_k$  are linearly dependent and setting

$$z_k = \vartheta_k v_k, \quad \vartheta_k = \pm \sqrt{\rho_k y_k^T \tilde{s}_k / \|v_k\|^2}$$

we obtain rank 1 variationally derived method (VAR1), where

$$U_{k+1} = U_k - \frac{\rho_k \tilde{s}_k - \vartheta_k U_k v_k}{\rho_k y_k^T \tilde{s}_k - \vartheta_k u_k^T v_k} (u_k - \vartheta_k v_k)^T,$$

which gives the best results for the choice  $\text{sgn}(\vartheta_k u_k^T v_k) = -1$ . Method VAR1 is chosen if  $\text{MET} = 1$  in the subroutine PLIP. Using  $z_k$  given above and setting  $T_k y_k = \tilde{s}_k$ , which corresponds to the BFGS method in the full-memory case, we obtain rank 2 variationally derived method (VAR2), where

$$U_{k+1} = U_k - \frac{\tilde{s}_k}{y_k^T \tilde{s}_k} u_k^T + \left( \rho_k \frac{\tilde{s}_k}{\vartheta_k} - U_k v_k + \frac{u_k^T v_k}{y_k^T \tilde{s}_k} \tilde{s}_k \right) \frac{v_k^T}{\|v_k\|^2}.$$

Method VAR2 is chosen if  $\text{MET} = 2$  in the subroutine PLIP. The efficiency of both these methods depends on the value of the correction parameter  $\rho_k$ . This value is determined by the formula  $\rho_k = \sqrt{\nu_k \varepsilon_k}$ . Here  $\nu_k = \mu_k / (1 - \mu_k)$ ,  $\mu_k$  is a relative shift parameter defined above and

$$\varepsilon_k = \sqrt{1 - \|u_k\|^2 / a_k}$$

is a damping factor of  $\mu_k$ . The number of columns of the matrix  $U_k$  is defined as  $m = \min(\text{MF}, k - \underline{k})$ , where  $\text{MF}$  is a parameter of the subroutine PLIP and  $\underline{k}$  is an index of the iteration corresponding to the last restart.

## 2.3 Inexact truncated Newton method

Subroutine PNET is based on a line-search realization of the Newton method, which uses conjugate gradient (CG) iterations for solving a system of linear equations  $G(x)d = -g(x)$  ( $g(x)$  and  $G(x)$  are the gradient and the Hessian matrix of function  $F : R^n \rightarrow R$  at the point  $x$ , respectively). Since the matrix  $G(x)$  can be indefinite, a modification of the (possibly preconditioned) CG method is used, which terminates if a negative curvature is detected. More precisely, we set  $d_1 = 0$ ,  $g_1 = g(x)$ ,  $h_1 = C^{-1}g_1$ ,  $p_1 = -h_1$ ,  $\sigma_1 = g_1^T h_1$  and for  $i = 1, 2, 3, \dots$  we proceed in the following way. If  $\|g_i\| \leq \bar{\omega}(x)\|g(x)\|$ , then set  $d = d_i$  and terminate the computation, otherwise set

$$q_i = G(x)p_i, \quad \tau_i = p_i^T q_i.$$



If  $\tau_i < \underline{\tau}$  then set  $d = -g(x)$  (if  $i = 1$ ) or  $d = d_i$  (if  $i > 1$ ) and terminate the computation, otherwise set  $\alpha_i = \sigma_i/\tau_i$  and compute

$$\begin{aligned} d_{i+1} &= d_i + \alpha_i p_i, \\ g_{i+1} &= g_i + \alpha_i q_i, \\ h_{i+1} &= C^{-1} g_{i+1}, \quad \sigma_{i+1} = g_{i+1}^T h_{i+1} \\ p_{i+1} &= -h_{i+1} + (\sigma_{i+1}/\sigma_i) p_i. \end{aligned}$$

The principal feature of the inexact truncated Newton method is the fact that the Hessian matrix  $G(x)$  is not used explicitly, but the vector  $G(x)p_i$  is computed by numerical differentiation using the formula

$$G(x)p_i \approx \frac{g(x + \delta_i p_i) - g(x)}{\delta_i}, \quad (4)$$

where  $\delta_i = \sqrt{\varepsilon_M}/\|p_i\|$  ( $\varepsilon_M$  is the machine precision). Thus one extra gradient evaluation is needed in every CG iteration.

The CG method is terminated if  $\tau_i < \underline{\tau}$  (a negative curvature is detected) or if  $\|g_i\| \leq \bar{\omega}(x)\|g(x)\|$  (a sufficient precision is achieved). We use the value  $\underline{\tau} = 10^{-60}$  in subroutine PNET. The value  $\bar{\omega}(x)$  is chosen according to the inexact Newton approach [7]. In the  $k$ -th Newton iteration we use the value

$$\bar{\omega}(x_k) = \min \left( \sqrt{\|g(x_k)\|}, 1/k, \bar{\omega} \right), \quad (5)$$

where  $\bar{\omega} = 0.8$  in subroutine PNET

The matrix  $C$  serving as a preconditioner (symmetric and positive definite) cannot be derived from the Hessian matrix, which is not known explicitly. If  $\text{MOS2} = 1$  ( $\text{MOS2}$  is a parameter of the subroutine PNET), the unpreconditioned CG method ( $C = I$ ) is used. If  $\text{MOS2} = 2$ , we use the preconditioner obtained by the limited memory BFGS method. In this case  $C^{-1} = H_k = H_k^k$ , where  $H_k^k$  is a matrix defined in Subsection 2.1. This matrix need not be constructed explicitly, since we need only the vector  $h_i = C^{-1}g_i = H_k^k g_i$  ( $i$  is an inner index of the CG method), which can be computed by using two recurrences (the Strang formula). First, vectors  $u_j$ ,  $k-1 \geq j \geq k-m$ , are computed by using the backward recurrence

$$\begin{aligned} \sigma_j &= s_j^T u_{j+1}/b_j, \\ u_j &= u_{j+1} - \sigma_j y_j, \end{aligned}$$

where  $u_k = g_i$ . Then vectors  $v_{j+1}$ ,  $k-m \leq j \leq k-1$ , are computed by using the forward recurrence

$$v_{j+1} = v_j + (\sigma_j - y_j^T v_j/b_j) s_j,$$

where  $v_{k-m} = (b_{k-1}/a_{k-1})u_{k-m}$ . Finally, we set  $h_i = v_k$ . Note that  $2m$  additional vectors  $s_j = x_{j+1} - x_j$ ,  $y_j = g_{j+1} - g_j$ ,  $k-m \leq j \leq k-1$ , has to be stored if  $\text{MOS2} = 2$ .

## 2.4 Active set strategy for box constraints

If box constraints are considered, then a simple active set strategy is used. To simplify the notation, we omit iteration index  $k$  in the following description. Every iteration is started by the detection of new candidates for active constraints. Thus we set

$$\begin{aligned}
 x_i = x_i^l, \quad I_i^x = -1 & \quad \text{if} \quad I_i^x = 1, \quad x_i \leq x_i^l + \varepsilon_c \max(|x_i^l|, 1), \\
 x_i = x_i^u, \quad I_i^x = -2 & \quad \text{if} \quad I_i^x = 2, \quad x_i \geq x_i^u - \varepsilon_c \max(|x_i^u|, 1), \\
 x_i = x_i^l, \quad I_i^x = -3 & \quad \text{if} \quad I_i^x = 3, \quad x_i \leq x_i^l + \varepsilon_c \max(|x_i^l|, 1), \\
 x_i = x_i^u, \quad I_i^x = -4 & \quad \text{if} \quad I_i^x = 3, \quad x_i \geq x_i^u - \varepsilon_c \max(|x_i^u|, 1), \\
 & \quad I_i^x = -5 \quad \text{if} \quad I_i^x = 5
 \end{aligned}$$

for  $1 \leq i \leq n$ , where  $\varepsilon_c$  is a required precision (we use value  $\varepsilon_c = 10^{-8}$  in our subroutines). After computing gradient  $g = g(x)$ , we determine projected gradient  $g^p$  and chopped gradient  $g^c$  in such a way that

$$\begin{aligned}
 g_i^p = 0, \quad g_i^c = \max(0, g_i) & \quad \text{for} \quad I_i^x = -1 \quad \text{or} \quad I_i^x = -3, \\
 g_i^p = 0, \quad g_i^c = \min(0, g_i) & \quad \text{for} \quad I_i^x = -2 \quad \text{or} \quad I_i^x = -4, \\
 g_i^p = 0, \quad g_i^c = 0 & \quad \text{for} \quad I_i^x = -5, \\
 g_i^p = g_i, \quad g_i^c = 0 & \quad \text{for} \quad I_i^x \geq 0.
 \end{aligned}$$

If  $\|g^c\|_\infty > \|g^p\|_\infty$  and the previous step was successful, we delete redundant active constraints by setting

$$\begin{aligned}
 I_i^x = 1 & \quad \text{if} \quad I_i^x = -1 \quad \text{and} \quad g_i > 0, \\
 I_i^x = 2 & \quad \text{if} \quad I_i^x = -2 \quad \text{and} \quad g_i < 0, \\
 I_i^x = 3 & \quad \text{if} \quad I_i^x = -3 \quad \text{and} \quad g_i > 0, \\
 I_i^x = 3 & \quad \text{if} \quad I_i^x = -4 \quad \text{and} \quad g_i < 0.
 \end{aligned}$$

In this way, we have obtained a current set of active constraints for the direction determination, step-size selection and variable metric update. This active set defines a reduced problem with variables  $x_i$ ,  $I_i^x < 0$ , fixed. If we introduce matrix  $Z$  containing columns  $e_i$ ,  $I_i^x \geq 0$  ( $e_i$  is the  $i$ -th column of the unit matrix), we can define reduced gradient  $g^r = Z^T g$  and reduced matrices  $H^r$  or  $B^r$  to obtain reduced direction vectors  $d^r = -H^r g^r$  or  $B^r d^r = -g^r$ . Finally, we use the direction vector  $d = Z d^r$ . In this way, we can adapt an arbitrary line-search or trust-region method to solve the reduced problem. Since the set of active constraints can change, we have to use a suitable restart strategy (conditions for setting  $B^r = I$ ,  $H_r = I$  or  $d^r = -g^r$ ). To guarantee descent, the restart is always performed when more than one redundant active constraint is deleted. The preconditioned truncated Newton method is restarted after every change of the set of active constraints.

From a practical point of view, it is not advantageous to construct reduced quantities. A better way is to construct projected gradients  $g^p = Z Z^T g$  and projected matrices  $H^p = Z Z^T H Z Z^T + Y Y^T$  or  $B^p = Z Z^T B Z Z^T + Y Y^T$ , where  $Y$  contains columns  $e_i$ ,  $I_i^x < 0$ , to obtain direction vectors  $d = -H^p g^p$  or  $B^p d = -g^p$ . Matrices  $H^p$  or  $B^p$  are block diagonal (with blocks  $H^r$ ,  $I$  or  $B^r$ ,  $I$ ) and they can be updated by using projected vectors  $s^p = Z Z^T s = Z Z^T (x^+ - x)$  and  $y^p = Z Z^T (g^+ - g)$ . Thus it suffices to use projected quantities instead of standard ones. Diagonal blocks of matrices  $H^p$  or  $B^p$  can

be easily derived from their sparsity pattern by considering only the elements  $H_{ij}^p$  or  $B_{ij}^p$  for which  $I_i^x \geq 0$ ,  $I_j^x \geq 0$  hold simultaneously. These blocks are then used in matrix multiplications and matrix decompositions.

Before step-size selection, we have to determine the maximum step-size  $\bar{\alpha}$  to assure the feasibility. This is computed by the formula  $\bar{\alpha} = \min(\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, \bar{\alpha}_4, \bar{\Delta}/\|d\|)$ , where

$$\begin{aligned}\bar{\alpha}_1 &= \min_{I_i^x=1, d_i < 0} \frac{x_i^l - x_i}{d_i}, & \bar{\alpha}_2 &= \min_{I_i^x=2, d_i > 0} \frac{x_i^u - x_i}{d_i}, \\ \bar{\alpha}_3 &= \min_{I_i^x=3, d_i < 0} \frac{x_i^l - x_i}{d_i}, & \bar{\alpha}_4 &= \min_{I_i^x=3, d_i > 0} \frac{x_i^u - x_i}{d_i}\end{aligned}$$

(if a corresponding set is empty we use the value  $\infty$ ).

### 3 Inexact discrete Newton methods for sparse problems

Consider a general twice continuously differentiable function  $F : R^n \rightarrow R$ , where  $n$  is large, and assume that the Hessian matrix  $G(x) = [G_{ij}(x)] = [\partial^2 F(x)/(\partial x_i \partial x_j)]$  is sparse. In this case, discrete versions of the Newton method can be efficiently used for seeking a local minimum of  $F$ . These methods are based on the fact that sufficiently sparse Hessian matrices can be estimated by using a small number of gradient differences [5]. We use the algorithm proposed in [36] in subroutines PNED, PNEC. The sparsity pattern of the Hessian matrix (only the upper part) is stored in the coordinate form (if `ISPAS` = 1) or in the standard compressed row format (if `ISPAS` = 2) using arrays `IH` and `JH`. For example, if the Hessian matrix has the pattern

$$G = \begin{bmatrix} * & * & * & 0 & * \\ * & * & 0 & * & 0 \\ * & 0 & * & 0 & * \\ 0 & * & 0 & * & 0 \\ * & 0 & * & 0 & * \end{bmatrix}$$

(asterisks denote nonzero elements), then arrays `IH` and `JH` contain elements

$$\text{IH} = [ 1 \ 1 \ 1 \ 1 \ 2 \ 2 \ 3 \ 3 \ 4 \ 5 ], \quad \text{JH} = [ 1 \ 2 \ 3 \ 5 \ 2 \ 4 \ 3 \ 5 \ 4 \ 5 ]$$

if `ISPAS` = 1 or

$$\text{IH} = [ 1 \ 5 \ 7 \ 9 \ 10 \ 11 ], \quad \text{JH} = [ 1 \ 2 \ 3 \ 5 \ 2 \ 4 \ 3 \ 5 \ 4 \ 5 ]$$

if `ISPAS` = 2. In the first case, nonzero elements in the upper part of the Hessian matrix can be sorted in an arbitrary order (not only by rows as in the above example) and arrays `IH` and `JH` have to be declared with lengths  $n + m$ , where  $m$  is the number of nonzero elements. In the second case, nonzero elements can be sorted only by rows. Components of `IH` contain addresses of the diagonal elements in this sequence and components of `JH` contain corresponding column indices (note that `IH` has  $n + 1$  elements and the last element is equal to  $m + 1$ ). Arrays `IH` and `JH` have to be declared with lengths  $n + 1$  and  $m$ , respectively.

Since the Hessian matrix can be indefinite, discrete versions of the Newton method are realized in the trust-region framework. Let  $B_k$  be a gradient-difference approximation of the Hessian matrix  $G_k = G(x_k)$ . Denote

$$Q_k(d) = \frac{1}{2}d^T B_k d + g_k^T d$$

the quadratic function which locally approximates the difference  $F(x_k + d) - F(x_k)$ ,

$$\omega_k(d) = (B_k d + g_k) / \|g_k\|$$

the accuracy of the direction determination and

$$\rho_k(d) = \frac{F(x_k + d) - F(x_k)}{Q_k(d)}$$

the ratio of the actual and the predicted decrease of the objective function. Trust-region methods (used in subroutines PNED, PNEC, PGAD, PGAC) generate points  $x_k \in R^n$ ,  $k \in N$ , in such a way that  $x_1$  is arbitrary and

$$x_{k+1} = x_k + \alpha_k d_k, \quad k \in N, \quad (6)$$

where  $d_k \in R^n$  are direction vectors and  $\alpha_k \geq 0$  are step-sizes. Direction vectors  $d_k \in R^n$  are chosen to satisfy conditions

$$\|d_k\| \leq \Delta_k, \quad (7)$$

$$\|d_k\| < \Delta_k \Rightarrow \|\omega_k(d_k)\| \leq \bar{\omega}_k, \quad (8)$$

$$-Q_k(d_k) \geq \underline{\sigma} \|g_k\| \min(\|d_k\|, \|g_k\| / \|B_k\|), \quad (9)$$

where  $0 \leq \bar{\omega}_k \leq \bar{\omega} < 1$  and  $0 < \underline{\sigma} < 1$  (we use value  $\bar{\omega} = 0.9$  in our subroutines;  $\underline{\sigma}$  is a theoretical value given implicitly). Step-sizes  $\alpha_k \geq 0$  are selected so that

$$\rho_k(d_k) \leq 0 \Rightarrow \alpha_k = 0, \quad (10)$$

$$\rho_k(d_k) > 0 \Rightarrow \alpha_k = 1. \quad (11)$$

Trust-region radii  $0 < \Delta_k \leq \bar{\Delta}$  are chosen in such a way that  $0 < \Delta_1 \leq \bar{\Delta}$  ( $\Delta_1$  and  $\bar{\Delta}$  are given by parameters XDEL and XMAX in our subroutines) and

$$\rho_k(d_k) < \underline{\rho} \Rightarrow \underline{\beta} \|d_k\| \leq \Delta_{k+1} \leq \bar{\beta} \|d_k\|, \quad (12)$$

$$\underline{\rho} \leq \rho_k(d_k) \leq \bar{\rho} \Rightarrow \Delta_{k+1} = \Delta_k, \quad (13)$$

$$\bar{\rho} < \rho_k(d_k) \Rightarrow \Delta_{k+1} = \min(\gamma \Delta_{k+1}, \bar{\Delta}), \quad (14)$$

where  $0 < \underline{\beta} \leq \bar{\beta} < 1 < \gamma$  and  $0 < \underline{\rho} < \bar{\rho} < 1$  (we use values  $\underline{\beta} = 0.05$ ,  $\bar{\beta} = 0.75$ ,  $\gamma = 2$ ,  $\underline{\rho} = 0.1$ ,  $\bar{\rho} = 0.9$  in our subroutines). Note that the initial trust-region radius  $\Delta_1$  is computed by a simple formula when XDEL = 0. This formula depends on a gradient norm  $\|g_k\|$  and contains a lower bound for  $F$  (parameter FMIN in our subroutines) if INITS = 1. If INITS = 0, parameter FMIN need not be defined.

The direction vector satisfying (7)–(9) can be computed by four different strategies. Subroutines PNED, PGAD are based on matrix decomposition methods. They use either the Dennis–Mei (double dog-leg) method [9] (if MOS = 1) or Moré–Sorensen method [25] (if MOS = 2). Subroutines PNEC, PGAC are based on matrix iterative methods. They use either the Steihaug–Toint method [31], [32] (if MOS1 = 1) or the shifted Steihaug–Toint method [16] (if MOS1 = 2). To simplify the description of these methods, we omit the outer index  $k$  and denote the inner index by  $i$ .

### 3.1 Matrix decomposition Moré–Sorensen trust region method

The most sophisticated methods are based on a computation of the optimal locally constrained step. A vector  $d \in R^n$  is obtained by solving a subproblem

$$\text{minimize } Q(d) = \frac{1}{2}d^T B d + g^T d \quad \text{subject to } \|d\| \leq \Delta. \quad (15)$$

Necessary and sufficient conditions for this solution are

$$\|d\| \leq \Delta, \quad (B + \lambda I)d + g = 0, \quad B + \lambda I \succeq 0, \quad \lambda \geq 0, \quad \lambda(\Delta - \|d\|) = 0 \quad (16)$$

(we use the symbol  $\succeq$  for ordering by positive semidefiniteness). The Moré–Sorensen method [25] is based on solving a nonlinear equation

$$1/\|d(\lambda)\| = 1/\Delta \quad \text{with} \quad (B + \lambda I)d(\lambda) = -g$$

by the Newton method using a modification of the sparse Choleski decomposition of  $B + \lambda I$  (we use the Gill–Murray decomposition [10]). More precisely, we determine  $\underline{\mu}_1$  as the maximal diagonal element of the matrix  $-B$ , set  $\underline{\lambda}_1 = \max(\underline{\mu}_1, 0)$ ,  $\bar{\lambda}_1 = \|g\|/\Delta + \|B\|$ ,  $\lambda_1 = \underline{\lambda}_1$  and for  $i = 1, 2, 3, \dots$  we proceed in the following way. Carry out the Gill–Murray decomposition  $B + \lambda_i I + E_i = R_i^T R_i$ . If  $E_i \neq 0$ , determine a vector  $v_i \in R^n$  such that  $\|v_i\| = 1$  and  $v_i^T (B + \lambda_i I)v_i < 0$ , set  $\underline{\mu}_i = \lambda_i - v_i^T (B + \lambda_i I)v_i$ ,  $\underline{\lambda}_i = \underline{\mu}_i$ ,  $\lambda_i = \underline{\lambda}_i$  and repeat this process (i.e., carry out the new Gill–Murray decomposition  $B + \lambda_i I + E_i = R_i^T R_i$ ). If  $E_i = 0$ , compute a vector  $d_i \in R^n$  by solving the equation  $R_i^T R_i d_i + g = 0$ . If  $\|d_i\| > \bar{\delta}\Delta$ , set  $\underline{\lambda}_{i+1} = \lambda_i$  and  $\bar{\lambda}_{i+1} = \bar{\lambda}_i$ . If  $\underline{\delta}\Delta \leq \|d_i\| \leq \bar{\delta}\Delta$  or  $\|d_i\| < \underline{\delta}\Delta$  and  $\lambda_i = 0$ , set  $d = d_i$  and terminate the computation. If  $\|d_i\| < \underline{\delta}\Delta$  and  $\lambda_i \neq 0$ , set  $\underline{\lambda}_{i+1} = \underline{\lambda}_i$ ,  $\bar{\lambda}_{i+1} = \lambda_i$ , determine a vector  $v_i \in R^n$  such that  $\|v_i\| = 1$  and  $v_i^T d_i \geq 0$ , which is a good approximation of an eigenvector of the matrix  $B$  corresponding to its minimal eigenvalue, and compute a number  $\alpha_i \geq 0$  such that  $\|d_i + \alpha_i v_i\| = \Delta$ . If

$$\alpha_i^2 \|R_i v_i\|^2 \leq (1 - \underline{\delta}^2)(\|R_i d_i\|^2 + \lambda_i \Delta^2),$$

set  $d = d_i + \alpha_i v_i$  and terminate the computation, otherwise set  $\underline{\mu}_i = \lambda_i - \|R_i v_i\|^2$ . In this case or if  $\|d_i\| > \bar{\delta}\Delta$ , compute a vector  $v_i \in R^n$  by solving the equation  $R_i^T v_i = d_i$  and set

$$\lambda_{i+1} := \lambda_i + \frac{\|d_i\|^2}{\|v_i\|^2} \left( \frac{\|d_i\| - \Delta}{\Delta} \right).$$

If  $\lambda_{i+1} < \underline{\lambda}_{i+1}$ , set  $\lambda_{i+1} = \underline{\lambda}_{i+1}$ . If  $\lambda_{i+1} > \bar{\lambda}_{i+1}$ , set  $\lambda_{i+1} = \bar{\lambda}_{i+1}$ . We use values  $\underline{\delta} = 0.9$  and  $\bar{\delta} = 1.1$  in our subroutines.

### 3.2 Matrix decomposition Dennis–Mei trust region method

The Moré–Sorensen method is very robust but requires 2-3 Choleski-type decompositions per iteration on average. Simpler methods are based on minimization of  $Q(d)$  on a two-dimensional subspace containing the Cauchy step  $d_C = -(g^T g / g^T B g)g$  and the Newton step  $d_N = -B^{-1}g$ . The Dennis–Mei double dog-leg method described in [9] seeks  $d$  as a linear combination of these two steps. This method uses vectors  $d = d_N$  if  $\|d_N\| \leq \Delta$  or

$d = (\Delta/\|d_C\|)d_C$  if  $\|d_C\| \geq \Delta$ . In the remaining case (if  $\|d_C\| < \Delta < \|d_N\|$ ),  $d$  is a convex combination of  $d_C$  and  $\tau d_N$ , where  $\tau = \max(d_C^T d_C / d_C^T d_N, \Delta / \|d_N\|)$ , such that  $\|d\| = \Delta$ .

The Newton step is computed by using the sparse Gill–Murray decomposition [10], which has the form  $B + E = LDL^T = R^T R$ , where  $E$  is a positive semidefinite diagonal matrix (equal to zero when  $B$  is positive definite),  $L$  is a lower triangular matrix,  $D$  is a positive definite diagonal matrix and  $R$  is an upper triangular matrix. The matrix  $LDL^T = R^T R$  then replaces  $B$  in  $Q(d)$ . The Dennis–Mei method requires only one Choleski-type decomposition per iteration.

### 3.3 Matrix iterative Steihaug–Toint trust region method

If  $B$  is not sufficiently sparse, then the sparse Choleski-type decomposition of  $B$  is expensive. In this case, methods based on preconditioned conjugate gradient (CG) iterations are more suitable. Steihaug [31] and Toint [32] proposed a method based on the fact that  $Q(d_{i+1}) < Q(d_i)$  and  $\|d_{i+1}\|_C > \|d_i\|_C$  (where  $\|d_i\|_C^2 = d_i^T C d_i$ ) hold in the preconditioned CG iterations if CG coefficients are positive. We either obtain an unconstrained solution with a sufficient precision or stop on the trust-region boundary if a negative curvature is indicated or if the trust-region is left. More precisely, we set  $d_1 = 0$ ,  $g_1 = g$ ,  $p_1 = -C^{-1}g$  and for  $i = 1, 2, 3, \dots$  we proceed in the following way. If  $\|g_i\| \leq \bar{\omega}\|g\|$ , then set  $d = d_i$  and terminate the computation, otherwise set

$$q_i = Bp_i, \quad \alpha_i = g_i^T C^{-1} g_i / p_i^T q_i.$$

If  $\alpha_i \leq 0$ , determine  $\alpha_i \geq 0$  in such a way that  $\|d_i + \alpha_i p_i\| = \Delta$ , set  $d := d_i + \alpha_i p_i$  and terminate the computation, otherwise compute  $d_{i+1} = d_i + \alpha_i p_i$ . If  $\|d_{i+1}\| \geq \Delta$ , determine  $\alpha_i \geq 0$  in such a way that  $\|d_i + \alpha_i p_i\| = \Delta$ , set  $d := d_i + \alpha_i p_i$  and terminate the computation, otherwise compute

$$\begin{aligned} g_{i+1} &= g_i + \alpha_i q_i, & \beta_i &= g_{i+1}^T C^{-1} g_{i+1} / g_i^T C^{-1} g_i \\ p_{i+1} &= -C^{-1} g_{i+1} + \beta_i p_i. \end{aligned}$$

The matrix  $C$  serves as a preconditioner (symmetric and positive definite). If `MOS2` = 1 (`MOS2` is a parameter of subroutines `PNEC`, `PGAC`), then no preconditioning is performed ( $C = I$ ), if `MOS2` = 2, an incomplete Choleski decomposition of the matrix  $B$  is used, and if `MOS2` = 3, a preliminary solution obtained by the incomplete Choleski decomposition can be accepted. In this case, we first compute  $p_1 = -C^{-1}g$ . If  $\|Bp_1 + g\| \leq \bar{\omega}\|g\|$ , we set  $d = p_1$  and terminate the computation, otherwise we continue by CG iterations as above.

There are two possible ways that the Steihaug–Toint method can be preconditioned. The first way uses norms  $\|d_i\|_{C_i}$  (instead of  $\|d_i\|$ ) in (7)–(14), where  $C_i$  are preconditioners chosen. This possibility has been tested in [11] and showed that such a way is not always efficient. This is caused by the fact that norms  $\|d_i\|_{C_i}$ ,  $i \in N$ , vary considerably in the major iterations and preconditioners  $C_i$ ,  $i \in N$ , can be ill-conditioned. The second way uses Euclidean norms in (7)–(14) even if arbitrary preconditioners  $C_i$ ,  $i \in N$ , are used. In this case the trust region can be left prematurely and the direction vector obtained can be farther from the optimal locally-constrained step than that obtained without preconditioning. This shortcoming is usually compensated by the rapid convergence of the preconditioned CG method. Our computational experiments indicated that the second way is more efficient in general and we use it in our subroutines.

### 3.4 Matrix iterative shifted Steihaug–Toint trust region method

Since the optimal locally constrained step has to satisfy the equation  $(B + \lambda I)d + g = 0$ , where  $\lambda \geq 0$  is the optimal Lagrange multiplier (see (16)), it seems to be advantageous to apply the Steihaug–Toint method to the subproblem

$$\text{minimize } \tilde{Q}(d) = Q_{\tilde{\lambda}}(d) = \frac{1}{2}d^T(B + \tilde{\lambda}I)d + g^T d \quad \text{s.t. } \|d\| \leq \Delta, \quad (17)$$

where  $\tilde{\lambda} \geq 0$  is an approximation of the optimal  $\lambda$ . The number  $\tilde{\lambda} \geq 0$  is found by solving a small-size subproblem

$$\frac{1}{2}\tilde{d}^T T \tilde{d} + \|g\|e_1^T \tilde{d} \quad (18)$$

with the tridiagonal matrix  $T$  obtained by using a small number of Lanczos steps. This method combines good properties of the Moré–Sorensen and the Steihaug–Toint methods and can be successfully preconditioned by the second way described in the previous subsection. The point on the trust-region boundary obtained by this method is usually closer to the optimal solution in comparison with the point obtained by the original Steihaug–Toint method.

The above considerations form a basis for the shifted Steihaug–Toint method proposed in [16]. This method consists of the three steps:

1. Let  $m = \text{MOS1}$  (the default value is  $\text{MOS1} = 5$ ). Determine a tridiagonal matrix  $T$  of order  $m$  by using  $m$  steps of the (unpreconditioned) Lanczos method (described, e.g., in [11], [14]) applied to the matrix  $B$  with the initial vector  $g$ .
2. Solve the subproblem

$$\text{minimize } \frac{1}{2}\tilde{d}^T T \tilde{d} + \|g\|e_1^T \tilde{d} \quad \text{subject to } \|\tilde{d}\| \leq \Delta \quad (19)$$

by using the Moré–Sorensen method described in Section 3.1 to obtain a Lagrange multiplier  $\tilde{\lambda}$ .

3. Apply the (preconditioned) Steihaug–Toint method described in Section 3.3 to the subproblem

$$\text{minimize } \frac{1}{2}d^T(B + \tilde{\lambda}I)d + g^T d \quad \text{subject to } \|d\| \leq \Delta \quad (20)$$

to obtain a direction vector  $d = d(\tilde{\lambda})$ .

Let  $\tilde{\lambda}$  be the Lagrange multiplier of small-size subproblem (19) and  $\lambda$  be the Lagrange multiplier obtained by the Moré–Sorensen method applied to the original trust-region subproblem (15). It can be shown (see [16]) that  $0 \leq \tilde{\lambda} \leq \lambda$ . This inequality assures that  $\lambda = 0$  implies  $\tilde{\lambda} = 0$  so  $\|d\| < \Delta$  implies  $\tilde{\lambda} = 0$ . Thus the shifted Steihaug–Toint method reduces to the standard one in this case. At the same time, if  $B$  is positive definite and  $\tilde{\lambda} > 0$ , then one has  $\Delta \leq \|(B + \tilde{\lambda}I)^{-1}g\| < \|B^{-1}g\|$ . Thus the unconstrained minimizer of the shifted quadratic function (20) is closer to the trust-region boundary than the unconstrained minimizer of the original quadratic function (15) and we can expect that  $d(\tilde{\lambda})$  is closer to the optimal locally constrained step than  $d(0)$ . Finally, if  $\tilde{\lambda} > 0$ , then the matrix  $B + \tilde{\lambda}I$  is better conditioned than  $B$  and we can expect that the shifted Steihaug–Toint method will converge more rapidly than the original one.

## 4 Methods for partially separable problems

Consider a function of the form

$$F(x) = \sum_{i=1}^{n_a} f_i(x), \quad (21)$$

where  $f_i(x)$ ,  $1 \leq i \leq n_a$  ( $n_a$  is usually large), are smooth particular functions depending on a small number of variables ( $n_i$ , say). In this case, the Jacobian matrix  $J(x) = [J_{ij}(x)] = [\partial f_i(x)/\partial x_j]$  is sparse. In subroutines PSED, PSEC, and PSEN, the sparsity pattern of the Jacobian matrix is stored in the coordinate form (if ISPAS = 1) or in the standard compressed row format (if ISPAS = 2) using arrays IAG and JAG. For example, if the Jacobian matrix has the pattern

$$J = \begin{bmatrix} * & * & 0 & * \\ * & * & * & 0 \\ * & 0 & 0 & * \\ 0 & * & * & 0 \\ * & 0 & * & 0 \end{bmatrix}$$

(asterisks denote nonzero elements) then arrays IAG and JAG contain elements

$$\begin{aligned} \text{IAG} &= [1 \ 1 \ 1 \ 2 \ 2 \ 2 \ 3 \ 3 \ 4 \ 4 \ 5 \ 5], \\ \text{JAG} &= [1 \ 2 \ 4 \ 1 \ 2 \ 3 \ 1 \ 4 \ 2 \ 3 \ 1 \ 3], \end{aligned}$$

if ISPAS = 1 or

$$\text{IAG} = [1 \ 4 \ 7 \ 9 \ 11 \ 13], \quad \text{JAG} = [1 \ 2 \ 4 \ 1 \ 2 \ 3 \ 1 \ 4 \ 2 \ 3 \ 1 \ 3],$$

if ISPAS = 2. In the first case, nonzero elements can be sorted in an arbitrary order (not only by rows as in the above example). Arrays IAG and JAG have to be declared with lengths  $n_a + m_a$  and  $m_a$ , respectively, where  $m_a$  is the number of nonzero elements. In the second case, nonzero elements can be sorted only by rows. Components of IAG contain total numbers of nonzero elements in all previous rows increased by 1 and elements of JAG contain corresponding column indices (note that IAG has  $n_a + 1$  elements and the last element is equal to  $m_a + 1$ ). Arrays IAG and JAG have to be declared with lengths  $n_a + 1$  and  $m_a$ , respectively. This representation of sparse Jacobian matrices is also used in subroutines PGAD, PGAC, PMAX, PSUM, PEQN, PEQL described in the subsequent sections.

Using the sparsity pattern of the Jacobian matrix, we can define packed gradients  $\hat{g}_i(x) \in R^{n_i}$  and packed Hessian matrices  $\hat{G}_i(x) \in R^{n_i \times n_i}$  of functions  $f_i(x)$ ,  $1 \leq i \leq n_a$ , as dense but small-size vectors and matrices. Note that  $\hat{g}_i(x) = Z_i^T g_i(x)$ ,  $\hat{G}_i(x) = Z_i^T G_i(x) Z_i$  and  $g_i(x) = Z_i \hat{g}_i(x)$ ,  $G_i(x) = Z_i \hat{G}_i(x) Z_i^T$ ,  $1 \leq i \leq n_a$ , where  $g_i(x)$  and  $G_i(x)$  are original gradients and Hessian matrices of functions  $f_i(x)$ , respectively, and  $Z_i \in R^{n \times n_i}$  are matrices containing columns of the unit matrix corresponding to the variables appearing in  $f_i(x)$ .

Methods for partially separable problems are implemented in the line-search framework mentioned in Section 2. A direction vector  $d_k$  is computed by solving a system of linear equations with a matrix  $B_k$ , which is an approximation of the Hessian matrix computed from approximations of packed Hessian matrices, see (24). Subroutines PSED and PSEN



use the Gill–Murray matrix decomposition. In this case,  $B_k$  is replaced by  $L_k D_k L_k^T = B_k + E_k$ , where  $L_k$  is a lower triangular matrix,  $D_k$  is a positive definite diagonal matrix, and  $E_k$  is a positive semidefinite diagonal matrix chosen in such a way that  $B_k + E_k$  is positive definite (more details are given in [10]). Subroutine PSEC uses the preconditioned conjugate gradient method described in Subsection 2.3, where multiplications by  $B_k$  are explicitly used instead of (4) and  $\bar{\omega} = 0.9$  in (5).

#### 4.1 Partitioned variable metric methods

Subroutines PSED, PSEC are based on partitioned variable metric updates [12], which consider each particular function separately. Thus approximations  $\hat{B}_i$ ,  $1 \leq i \leq n_a$ , of the packed Hessian matrices  $\hat{G}_i(x)$  are updated by using the quasi-Newton conditions  $\hat{B}_i^+ \hat{s}_i = \hat{y}_i$ , where  $\hat{s}_i = Z_i^T s_i$  and  $\hat{y}_i = \hat{g}_i^+ - \hat{g}_i$  (we omit outer index  $k$  and replace index  $k+1$  by  $+$  in this section). Therefore, a variable metric update can be used for each of the particular functions. However, there is a difference between the classic and the partitioned approach, since conditions  $\hat{s}_i^T \hat{y}_i > 0$ , which are necessary for positive definiteness of  $\hat{B}_i^+$ , are not guaranteed for all  $1 \leq i \leq n_a$ . This difficulty is unavoidable and an efficient algorithm has to handle this situation.

Subroutines PSED, PSEC use three strategies. If  $\text{MET} = 1$ , then the safeguarded partitioned BFGS updates

$$\begin{aligned} \hat{B}_i^+ &= \hat{B}_i + \frac{\hat{y}_i \hat{y}_i^T}{\hat{s}_i^T \hat{y}_i} - \frac{\hat{B}_i \hat{s}_i (\hat{B}_i \hat{s}_i)^T}{\hat{s}_i^T \hat{B}_i \hat{s}_i}, & \hat{s}_i^T \hat{y}_i > 0, \\ \hat{B}_i^+ &= \hat{B}_i, & \hat{s}_i^T \hat{y}_i \leq 0 \end{aligned} \quad (22)$$

are used. If  $\text{MET} = 2$ , then the BFGS updates are combined with the rank-one updates

$$\begin{aligned} \hat{B}_i^+ &= \hat{B}_i + \frac{(\hat{y}_i - \hat{B}_i \hat{s}_i)(\hat{y}_i - \hat{B}_i \hat{s}_i)^T}{\hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i)}, & |\hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i)| \geq \varepsilon_M |\hat{s}_i^T \hat{B}_i \hat{s}_i|, \\ \hat{B}_i^+ &= \hat{B}_i, & |\hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i)| < \varepsilon_M |\hat{s}_i^T \hat{B}_i \hat{s}_i|, \end{aligned} \quad (23)$$

where  $\varepsilon_M$  is the machine precision. We use a strategy, which is based on the observation that (22) usually leads to the loss of convergence if too many particular functions have indefinite Hessian matrices. We start with the partitioned BFGS update (22). If  $n_- \geq \theta n_a$ , where  $n_-$  is a number of particular functions with a negative curvature and  $\theta$  is a threshold value, then (23) is used for all particular functions in all subsequent iterations (we use value  $\theta = 1/2$  in the subroutines PSED, PSEC). If  $\text{MET} = 3$ , then packed matrices  $\hat{B}_i \approx \hat{G}_i(x)$  are computed by using gradient differences. This strategy is in fact the partitioned discrete Newton method.

A disadvantage of partitioned variable metric methods ( $\text{MET} = 1$ ,  $\text{MET} = 2$ ) is the fact that approximations of packed Hessian matrices need to be stored. Therefore, the number of stored elements can be much greater than the number of nonzero elements in the sparse Hessian matrix. Moreover, operations with packed Hessian matrices (decomposition, multiplication) are usually unsuitable (time consuming). Thus the sparse approximation of the Hessian matrix

$$B = \sum_{i=1}^{n_a} Z_i \hat{B}_i Z_i^T \quad (24)$$

(stored as in Section 3) is constructed in subroutines PSED, PSEC. Then a direction vector  $d$ , used in line search, is computed by solving the linear system  $Bd = -g$ . The partitioned Newton method (MET = 3) does not store packed matrices  $\hat{B}_i$ ,  $1 \leq i \leq n_a$ , since they are immediately added to matrix (24).

## 4.2 Partitioned variable metric method for nonsmooth functions

Assume that functions  $f_i(x)$ ,  $1 \leq i \leq n_a$ , appearing in (21), are nonsmooth, locally Lipschitz, and we are able to compute (Clarke) subgradients  $g_i \in \partial f_i(x)$ ,  $1 \leq i \leq n_a$ , at any point  $x \in R^n$ . Then also  $F(x)$  is locally Lipschitz and since locally Lipschitz function is differentiable almost everywhere by the Rademacher theorem, usually  $\partial F(x) = \{\nabla F(x)\}$ . A special feature of nonsmooth functions is the fact that the gradient  $\nabla F(x)$  changes discontinuously and is not small in the neighborhood of a local minimum. Thus the standard optimization methods cannot be used efficiently.

The most commonly used approach for solving nonsmooth optimization problems is based on the bundle principle. In this case, values  $F(x_k)$ ,  $g(x_k) \in \partial F(x_k)$  at a single point  $x_k$  are replaced by a bundle of values  $F_j = F(z_j)$ ,  $g_j \in \partial F(z_j)$  obtained at trial points  $z_j$ ,  $j \in \mathcal{J}_k \subset \{1, \dots, k\}$ . This bundle of values serves for defining a piecewise quadratic function (with a quadratic regularizing term), which is used for direction determination by solving a quadratic programming subproblem. Usually, the bundle contains many dense subgradients. Thus a dense quadratic programming subproblem with many constraints has to be solved, which is unsuitable in the large-scale cases. This disadvantage can be overcome by the bundle variable metric method described in [37], which uses a bundle with three subgradients at most for defining a quadratic programming subproblem. Subroutine PSEN is based on the partitioned bundle variable metric method described in [23], which combines ideas from [37] with partitioned variable metric updates.

Using aggregate subgradients  $\tilde{g}_k$  and aggregated subgradient locality measures  $\tilde{\beta}_k$  (where  $\tilde{g}_1 = g_1$  and  $\tilde{\beta}_1 = 0$  in the first iteration), the partitioned bundle variable metric method generates a sequence of basic points  $\{x_k\} \subset R^n$  and a sequence of trial points  $\{z_k\} \subset R^n$  such that

$$x_{k+1} = x_k + \alpha_k^L d_k, \quad z_{k+1} = x_k + \alpha_k^R d_k,$$

where  $d_k = -(B_k^{-1} + \rho I)\tilde{g}_k$  is a direction vector and  $\alpha_k^R > 0$ ,  $\alpha_k^R \geq \alpha_k^L \geq 0$  are appropriately chosen step-sizes. At the same time,  $B_k$  is a matrix obtained by partitioned variable metric updates and  $\rho$  is a correction parameter (parameter ETA3 in subroutine PSEN). Step-sizes  $\alpha_k^R$  and  $\alpha_k^L$  are chosen by a special line-search procedure in such a way that either

$$F(x_k + \alpha_k^L d_k) \leq F(x_k) - \varepsilon_L \alpha_k^R w_k$$

or

$$d_k^T g(x_k + \alpha_k^R d_k) \geq \gamma_{k+1} - \varepsilon_R w_k.$$

Here  $0 < \varepsilon_L < 1/2$ ,  $\varepsilon_L < \varepsilon_R < 1$  are suitable constants (we use values  $\varepsilon_L = 10^{-4}$ ,  $\varepsilon_R = 0.25$  in our subroutine),  $g(x_k + \alpha_k^R d_k) \in \partial F(x_k + \alpha_k^R d_k)$ ,  $w_k = -(\tilde{g}_k)^T d_k + 2\tilde{\beta}_k$  and

$$\gamma_{k+1} = \max(|F(x^k) - F(x_k + \alpha_k^R d_k) + \alpha_k^R d_k^T g(x_k + \alpha_k^R d_k)|, \gamma \|\alpha_k^R d_k\|^2)$$

where  $\gamma$  is a subgradient locality measure parameter (parameter ETA5 in subroutine PSEN). In the first case (descent step) we set  $z_{k+1} = x_{k+1} = x_k + \alpha_k^L d_k$ ,  $\beta_{k+1} = 0$  and substitute

$\tilde{\beta}_{k+1} = 0$ ,  $\tilde{g}_{k+1} = g_{k+1} \in \partial F(z_{k+1})$ . In the second case (null step) we set  $z_{k+1} = x_k + \alpha_k^R d_k$ ,  $x_{k+1} = x_k$ ,  $\beta_{k+1} = \gamma_{k+1}$  and determine  $\tilde{\beta}_{k+1}$ ,  $\tilde{g}_{k+1}$  by the aggregation procedure.

The aggregation procedure is very simple. Denoting by  $l$  the lowest index satisfying  $x_l = x_k$  (index of the iteration after the last descent step) and using the subgradients  $g_l$ ,  $g_{k+1}$ ,  $\tilde{g}_k$  and the subgradient locality measures  $\beta_l = 0$ ,  $\beta_{k+1}$ ,  $\tilde{\beta}_k$ , we determine multipliers

$$\lambda_k^1 \geq 0, \quad \lambda_k^2 \geq 0, \quad \lambda_k^3 \geq 0, \quad \lambda_k^1 + \lambda_k^2 + \lambda_k^3 = 1,$$

which minimize the quadratic function

$$(\lambda^1 g_l + \lambda^2 g_{k+1} + \lambda^3 \tilde{g}_k)^T (B_k^{-1} + \rho I) (\lambda^1 g_l + \lambda^2 g_{k+1} + \lambda^3 \tilde{g}_k) + 2(\lambda^1 \beta_l + \lambda^2 \beta_{k+1} + \lambda^3 \tilde{\beta}_k),$$

and set

$$\tilde{g}_{k+1} = \lambda_k^1 g_l + \lambda_k^2 g_{k+1} + \lambda_k^3 \tilde{g}_k, \quad \tilde{\beta}_{k+1} = \lambda_k^1 \beta_l + \lambda_k^2 \beta_{k+1} + \lambda_k^3 \tilde{\beta}_k.$$

After obtaining points  $x_{k+1}$ ,  $z_{k+1}$  and subgradient  $g_{k+1} \in \partial F(z_{k+1})$ , the matrix  $B_k$  is updated. To satisfy conditions for the global convergence, we use special symmetric rank-one updates after null steps. This guarantees that elements of  $B_k$  do not decrease. After descent steps, the safeguarded BFGS updates can be used. As the function  $F(x)$  is partially separable, the matrix  $B_k$  can be expressed in the form (24) (we omit outer index  $k$  and replace index  $k+1$  by  $+$ ). Thus we set

$$\begin{aligned} \hat{B}_i^+ &= \hat{B}_i + \frac{\hat{y}_i \hat{y}_i^T}{\hat{s}_i^T \hat{y}_i} - \frac{\hat{B}_i \hat{s}_i (\hat{B}_i \hat{s}_i)^T}{\hat{s}_i^T \hat{B}_i \hat{s}_i}, & \hat{s}_i^T \hat{y}_i > 0, \\ \hat{B}_i^+ &= \hat{B}_i, & \hat{s}_i^T \hat{y}_i \leq 0 \end{aligned}$$

after a descent step or

$$\begin{aligned} \hat{B}_i^+ &= \hat{B}_i + \frac{(\hat{y}_i - \hat{B}_i \hat{s}_i)(\hat{y}_i - \hat{B}_i \hat{s}_i)^T}{\hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i)}, & \hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i) \geq \varepsilon_M \hat{s}_i^T \hat{B}_i \hat{s}_i, \\ \hat{B}_i^+ &= \hat{B}_i, & \hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i) < \varepsilon_M \hat{s}_i^T \hat{B}_i \hat{s}_i \end{aligned}$$

after a null step ( $\varepsilon_M$  is the machine precision). Here  $\hat{s}_i = Z_i^T s_i$  and  $\hat{y}_i = \hat{g}_i^+ - \hat{g}_i = Z_i^T (g_i^+ - g_i)$ , where  $g_i^+$  and  $g_i$  are subgradients computed at points  $z^+$  and  $x$ , respectively (aggregated subgradients  $\tilde{g}_i^+$  and  $\tilde{g}_i$  are not used in variable metric updates).

Since the quadratic programming subproblem used in the aggregation procedure is very simple, initial step-size  $\alpha = 1$  need not be a good choice in connection with its solution. Therefore we store and use a bundle of values  $F_j = F(z_j)$ ,  $g_j \in \partial F(z_j)$  obtained at trial points  $z_j$ ,  $j \in \mathcal{J}_k = \{k-m, \dots, k\}$ . Here  $m$  is a size of the bundle (parameter MB of subroutine PSEN). These values are used for the construction of a piecewise linear function which serves for determination of better initial step-size. More details are given in [23].

## 5 Hybrid methods for nonlinear least-squares

Consider a function of the form

$$F(x) = \frac{1}{2} \sum_{i=1}^{n_a} f_i^2(x) = \frac{1}{2} f^T(x) f(x) \quad (25)$$

(sum of squares), where  $f_i(x)$ ,  $1 \leq i \leq n_a$  ( $n_a$  is usually large), are smooth functions depending on a small number of variables ( $n_i$ , say). In this case, the Jacobian matrix  $J(x) = [J_{ij}(x)] = [\partial f_i(x)/\partial x_j]$  is sparse. The sparsity pattern of the Jacobian matrix is stored using arrays **IAG** and **JAG** in the way described in Section 4.

Using the Jacobian matrix, we can express the gradient  $g(x)$  and the Hessian matrix  $G(x)$  in the form

$$\begin{aligned} g(x) &= \sum_{i=1}^{n_a} f_i(x)g_i(x) = J^T(x)f(x), \\ G(x) &= \sum_{i=1}^{n_a} (g_i(x)g_i^T(x) + f_i(x)G_i(x)) = J^T(x)J(x) + C(x) \end{aligned}$$

( $G_i(x)$  are Hessian matrices of  $f_i(x)$ ,  $1 \leq i \leq n_a$ ). The well-known Gauss-Newton method uses the matrix  $J^T(x)J(x)$  instead of the Hessian matrix  $G(x) = J^T(x)J(x) + C(x)$  (i.e., it omits the second order information contained in  $C(x)$ ). We assume that the matrix  $J^T(x)J(x)$  is sparse (then also  $C(x)$  is sparse).

The matrix  $J^T(x)J(x)$  is frequently ill-conditioned (even singular) so that the Gauss-Newton method and its modifications require trust-region realizations. For computing a trust-region step, subroutine **PGAD** uses matrix decomposition methods and subroutine **PGAC** uses matrix iterative methods. These methods and their choices (using variables **MOS** and **MOS1**), are described in Section 3.

If the minimum value  $F(x^*)$  is large (large residual problem), the Gauss-Newton method can be inefficient. Therefore, modifications that use the estimation of the second-order term have been developed. These modifications are based on the fact (proven in [1]) that  $(F_k - F_{k+1})/F_k \rightarrow 1$  if  $F_k \rightarrow 0$   $Q$ -superlinearly and  $(F_k - F_{k+1})/F_k \rightarrow 0$  if  $F_k \rightarrow F^* > 0$ . Thus we can use the following philosophy. Let  $x_{k+1}$  be a vector obtained by the trust-region strategy described in Section 3. If  $x_{k+1} \neq x_k$ , we compute  $F_{k+1} = F(x_{k+1})$ ,  $J_{k+1} = J(x_{k+1})$  and set

$$\begin{aligned} B_{k+1} &= J_{k+1}^T J_{k+1}, & F_k - F_{k+1} &> \underline{\vartheta} F_k, \\ B_{k+1} &= J_{k+1}^T J_{k+1} + C_{k+1}, & F_k - F_{k+1} &\leq \underline{\vartheta} F_k, \end{aligned}$$

where  $C_{k+1}$  is an approximation of the second order term and  $\underline{\vartheta}$  is a suitable value (parameter **ETA** in subroutines **PGAD** and **PGAC**).

Large-scale correction matrix  $C_{k+1}$  cannot be efficiently obtained by dense variable metric updates [1], which are frequently used for medium-size problems. Fortunately, simple corrections utilizing sparsity also increase the efficiency of the Gauss-Newton method. In subroutines **PGAD** and **PGAC** we have implemented three hybrid methods proposed in [15] (specified by the variable **MEC**), which are described in the subsequent subsections. To simplify the notation, we omit outer index  $k$  and replace index  $k + 1$  by  $+$ .

## 5.1 Gauss-Newton method with sparse variable metric corrections

If **MEC** = 1, the sparse variable metric corrections (Marwil updates) are used. In the first iteration (or after a restart) we use the matrix  $B = J^T J$ . In the subsequent iterations we set

$$\begin{aligned} B^+ &= (J^+)^T J^+, & F - F^+ &> \underline{\vartheta} F, \\ B^+ &= \mathcal{P}_S \mathcal{P}_{QG}((J^+)^T J^+), & F - F^+ &\leq \underline{\vartheta} F, \end{aligned}$$

where  $\mathcal{P}_S$  realizes an orthogonal projection into the subspace of symmetric matrices of order  $n$  and  $\mathcal{P}_{QG}$  realizes an orthogonal projection into the intersection of the subspace of matrices having the same sparsity pattern as  $J^T J$  and the linear manifold of matrices satisfying the quasi-Newton condition  $Ws = y$  with  $s = x^+ - x$ ,  $y = g^+ - g$ . Thus

$$\mathcal{P}_S W = (W + W^T)/2,$$

$$\begin{aligned} (\mathcal{P}_G W)_{ij} &= W_{ij}, & (J^T J)_{ij} &\neq 0, \\ (\mathcal{P}_G W)_{ij} &= 0, & (J^T J)_{ij} &= 0, \end{aligned}$$

for a given square matrix  $W$ , and

$$\mathcal{P}_{QG}((J^+)^T J^+) = \mathcal{P}_G((J^+)^T J^+ + us^T),$$

where  $u \in R^n$  is a solution of the linear system  $Du = y - (J^+)^T J^+ s$  with a diagonal matrix  $D$  such that

$$D_{ii} = \sum_{(J^T J)_{ij} \neq 0} (e_j^T s)^2$$

( $e_j$  is the  $j$ -th column of the unit matrix).

## 5.2 Gauss-Newton method with the Newton corrections

If MEC = 2, the Newton corrections are used. In the first iteration (or after a restart) we use the matrix  $B = J^T J$ . In the subsequent iterations we set

$$\begin{aligned} B^+ &= (J^+)^T J^+, & F - F^+ &> \underline{\vartheta}F, \\ B^+ &= (J^+)^T J^+ + \sum_{i=1}^{n_a} f_i^+ G_i^+, & F - F^+ &\leq \underline{\vartheta}F, \end{aligned}$$

where  $G_i^+$ ,  $1 \leq i \leq n_a$ , are approximations of Hessian matrices determined by using gradient differences at the point  $x^+$ .

## 5.3 Gauss-Newton method with partitioned variable metric corrections

If MEC = 3, the partitioned variable metric corrections (symmetric rank-one updates) are used. In the first iteration (or after a restart) we use the matrix  $B = J^T J$ . In the subsequent iterations we set

$$\begin{aligned} B^+ &= (J^+)^T J^+, & F - F^+ &> \underline{\vartheta}F, \\ B^+ &= (J^+)^T J^+ + \sum_{i=1}^{n_a} f_i^+ Z_i \hat{B}_i^+ Z_i^T, & F - F^+ &\leq \underline{\vartheta}F, \end{aligned}$$

where  $Z_i$ ,  $1 \leq i \leq n_a$ , are matrices defined in Section 4 and  $\hat{B}_i^+$ ,  $1 \leq i \leq n_a$ , are packed matrices updated using symmetric rank-one formulas

$$\begin{aligned} \hat{B}_i^+ &= \hat{B}_i + \frac{(\hat{y}_i - \hat{B}_i \hat{s}_i)(\hat{y}_i - \hat{B}_i \hat{s}_i)^T}{\hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i)}, & |\hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i)| &\geq \varepsilon_M |\hat{s}_i^T \hat{B}_i \hat{s}_i|, \\ \hat{B}_i^+ &= \hat{B}_i, & |\hat{s}_i^T (\hat{y}_i - \hat{B}_i \hat{s}_i)| &< \varepsilon_M |\hat{s}_i^T \hat{B}_i \hat{s}_i| \end{aligned}$$

( $\varepsilon_M$  is the machine precision), where  $\hat{B}_i = I$ ,  $1 \leq i \leq n_a$ , in the first iteration (or after a restart). A disadvantage of partitioned variable metric corrections is the fact that approximations of packed Hessian matrices need to be stored. Thus the choice  $\text{MEC} = 3$  is usually less suitable than choices  $\text{MEC} = 1$  and  $\text{MEC} = 2$ .

## 6 Primal interior point methods for minimax optimization

Consider a function of the form

$$F(x) = \max_{1 \leq i \leq n_a} f_i(x) \quad (26)$$

(pointwise maximum), where  $f_i(x)$ ,  $1 \leq i \leq n_a$  ( $n_a$  is usually large), are smooth functions depending on a small number of variables ( $n_i$ , say). In this case, the Jacobian matrix  $J(x) = [J_{ij}(x)] = [\partial f_i(x)/\partial x_j]$  is sparse. The sparsity pattern of the Jacobian matrix is stored using arrays **IAG** and **JAG** in the way described in Section 4.

Primal interior point methods for minimax optimization, proposed in [17], are based on three basic ideas. First, minimization of  $F$  is equivalent to the nonlinear programming problem with  $n + 1$  variables  $x \in R^n$ ,  $z \in R$ :

$$\text{minimize } z \quad \text{subject to } f_i(x) \leq z, \quad 1 \leq i \leq n_a.$$

Secondly, this constrained problem is replaced by a sequence of unconstrained problems

$$\text{minimize } B_\mu(x, z) = z - \mu \sum_{i=1}^{n_a} \log(z - f_i(x)),$$

where  $z > F(x)$  and  $\mu > 0$  (we assume that  $\mu \rightarrow 0$  monotonically). Finally, the extra variable  $z$  is eliminated by solving the scalar nonlinear equation

$$\sum_{i=1}^{n_a} \frac{\mu}{z - f_i(x)} = 1, \quad (27)$$

which follows from the first-order necessary conditions for the barrier function  $B_\mu(x, z)$  with fixed  $x \in R^n$ . The above equation has a unique root  $z_\mu(x)$  such that  $F(x) + \mu \leq z_\mu(x) \leq F(x) + n_a \mu$ . This approach leads to inexact unconstrained minimizations of functions  $B_\mu(x) = B_\mu(x, z_\mu(x))$  for suitable values of  $\mu$  using the fact that

$$\nabla B_\mu(x) = g_\mu(x) = J^T(x)u_\mu(x)$$

and

$$\nabla^2 B_\mu(x) = G_\mu(x) + J^T(x)V_\mu(x)J(x) - \frac{J^T(x)V_\mu(x)ee^T V_\mu(x)J(x)}{e^T V_\mu(x)e},$$

where

$$u_\mu(x) = \begin{bmatrix} \mu/(z_\mu(x) - f_1(x)) \\ \dots \\ \mu/(z_\mu(x) - f_{n_a}(x)) \end{bmatrix}, \quad e = \begin{bmatrix} 1 \\ \dots \\ 1 \end{bmatrix},$$

$$G_\mu(x) = \sum_{i=1}^{n_a} e_i^T u_\mu(x) \nabla^2 f_i(x),$$

$$V_\mu(x) = \text{diag} \left( \mu / (z_\mu(x) - f_1(x))^2, \dots, \mu / (z_\mu(x) - f_{n_a}(x))^2 \right).$$

The Hessian matrix  $\nabla^2 B_\mu(x)$  of the barrier function  $B_\mu(x)$  is positive definite if  $G_\mu(x)$  (the Hessian matrix of the Lagrangian function) is positive definite.

Subroutine **P**MAX is based on a line search realization of the Newton-like methods. Thus  $x^+ = x + \alpha d$ , where  $\nabla^2 B_\mu(x)d = -g_\mu(x)$  and  $\alpha$  is a suitable step-size. In fact, we use an approximation of  $\nabla^2 B_\mu(x)$ , such that  $G_\mu(x)$  is determined either by partitioned variable metric updates described in Section 4 (if **MED** = 1) or by gradient differences as in [5] (if **MED** = 2). In the second case, the matrix  $G_\mu(x)$  is not positive definite in general so a restart strategy guaranteeing descent is used (more details are given in [17]). If **MED** = 1, then we define reduced approximations of the Hessian matrices  $\tilde{G}_i = Z_i^T G_i Z_i$ ,  $1 \leq i \leq n_a$ , as in Section 4. New reduced approximations of the Hessian matrices are computed by the formulas

$$\begin{aligned} \tilde{G}_i^+ &= \frac{1}{\tilde{\gamma}_i} \left( \tilde{G}_i - \frac{\tilde{G}_i \tilde{s}_i \tilde{s}_i^T \tilde{G}_i}{\tilde{s}_i^T \tilde{G}_i \tilde{s}_i} \right) + \frac{\tilde{y}_i \tilde{y}_i^T}{\tilde{s}_i^T \tilde{y}_i}, \quad \tilde{s}_i^T \tilde{y}_i > 0, \\ \tilde{G}_i^+ &= \tilde{G}_i, \quad \tilde{s}_i^T \tilde{y}_i \leq 0, \end{aligned} \quad (28)$$

where

$$\tilde{s}_i = Z_i^T (x^+ - x), \quad \tilde{y}_i = Z_i^T (\nabla f_i(x^+) - \nabla f_i(x)), \quad 1 \leq i \leq n_a,$$

and where either  $\tilde{\gamma}_i = 1$  or  $\tilde{\gamma}_i = \tilde{s}_i^T \tilde{G}_i \tilde{s}_i / \tilde{s}_i^T \tilde{y}_i$ . The particular choice of  $\tilde{\gamma}_i$  is determined by the controlled scaling strategy described in [19]. In the first iteration we set  $\tilde{G}_i = I$ ,  $1 \leq i \leq n_a$ , where  $I$  are unit matrices of suitable orders. Finally,  $G_i^+ = Z_i \tilde{G}_i^+ Z_i^T$ ,  $1 \leq i \leq n_a$ .

A very important part of the primal interior point method is an update of the barrier parameter  $\mu$ . There are two requirements, which play opposite roles. First,  $\mu \rightarrow 0$  should hold, since this is the main property of every interior-point method. On the other hand, round-off errors can cause that  $z_\mu(x) = F(x)$  when  $\mu$  is too small and  $|F(x)|$  is sufficiently large (since  $F(x) + \mu \leq z_\mu(x) \leq F(x) + n_a \mu$ ), which leads to a breakdown (division by  $z_\mu(x) - F(x) = 0$ ). Thus a lower bound  $\underline{\mu}$  for the barrier parameter (parameter **ETA5** in subroutine **P**MAX) is used.

The efficiency of the primal interior point method is also sensitive to the way in which the barrier parameter decreases. Subroutine **P**MAX uses the formula

$$\mu_{k+1} = \max \left( \tilde{\mu}_{k+1}, \underline{\mu}, 10 \varepsilon_M |F(x_{k+1})| \right),$$

where  $F(x_{k+1}) = \max_{1 \leq i \leq m} f_i(x_{k+1})$ ,  $\varepsilon_M$  is the machine precision, and

$$\tilde{\mu}_{k+1} = \min \left[ \max(\lambda \mu_k, \mu_k / (100 \mu_k + 1)), \max(\|g_{\mu_k}(x_k)\|^2, 10^{-2k}) \right],$$

where  $\lambda$  is the rate of the barrier parameter decrease (parameter **ETA4** in subroutine **P**MAX).

Subroutine **P**MAX serves for minimization of three particular functions. If **IEXT** < 0, then function (26) is considered. If **IEXT** = 0, then

$$F(x) = \max_{1 \leq i \leq n_a} |f_i(x)| = \max_{1 \leq i \leq n_a} [\max(f_i(x), -f_i(x))].$$

If **IEXT** > 0, then

$$F(x) = \max_{1 \leq i \leq n_a} (-f_i(x)).$$

## 7 Primal interior point methods for $l_1$ optimization

Consider a function of the form

$$F(x) = \sum_{i=1}^{n_a} |f_i(x)| \quad (29)$$

(a sum of absolute values), where  $f_i(x)$ ,  $1 \leq i \leq n_a$  ( $n_a$  is usually large), are smooth functions depending on a small number of variables ( $n_i$ , say). In this case, the Jacobian matrix  $J(x) = [J_{ij}(x)] = [\partial f_i(x)/\partial x_j]$  is sparse. The sparsity pattern of the Jacobian matrix is stored using arrays **IAG** and **JAG** in the way described in Section 4.

Primal interior point methods for  $l_1$  optimization, proposed in [18], are based on three basic ideas. First, minimization of  $F$  is equivalent to the nonlinear programming problem with  $n + n_a$  variables  $x \in R^n$ ,  $z \in R^{n_a}$ :

$$\text{minimize } \sum_{i=1}^{n_a} z_i \quad \text{subject to } -z_i \leq f_i(x) \leq z_i, \quad 1 \leq i \leq n_a.$$

Secondly, this constrained problem is replaced by a sequence of unconstrained problems

$$\begin{aligned} \text{minimize } B_\mu(x, z) &= \sum_{i=1}^{n_a} z_i - \mu \sum_{i=1}^{n_a} \log(z_i - f_i(x)) - \mu \sum_{i=1}^{n_a} \log(z_i + f_i(x)) \\ &= \sum_{i=1}^{n_a} z_i - \mu \sum_{i=1}^{n_a} \log(z_i^2 - f_i^2(x)) \end{aligned}$$

where  $z_i > |f_i(x)|$ ,  $1 \leq i \leq n_a$ , and  $\mu > 0$  (we assume that  $\mu \rightarrow 0$  monotonically). Finally, the extra variables  $z_i$ ,  $1 \leq i \leq n_a$ , are eliminated by solving the set of quadratic equations

$$\frac{2\mu z_i}{z_i^2 - f_i^2(x)} = 1, \quad 1 \leq i \leq n_a,$$

which follow from the first-order necessary conditions for the barrier function  $B_\mu(x, z)$  with fixed  $x \in R^n$ . Solutions of the above equations define a vector  $z_\mu(x) \in R^{n_a}$ , where

$$z_\mu(x)_i = e_i^T z_\mu(x) = \mu + \sqrt{\mu^2 + f_i^2(x)}, \quad 1 \leq i \leq n_a. \quad (30)$$

This approach leads to inexact unconstrained minimizations of functions  $B_\mu(x) = B_\mu(x, z_\mu(x))$  for suitable values of  $\mu$  using the fact that

$$\nabla B_\mu(x) = g_\mu(x) = J^T(x)u_\mu(x)$$

and

$$\nabla^2 B_\mu(x) = G_\mu(x) + J^T(x)V_\mu(x)J(x),$$

where

$$u_\mu(x) = \begin{bmatrix} 2\mu f_1(x)/(z_\mu(x)_1^2 - f_1^2(x)) \\ \vdots \\ 2\mu f_{n_a}(x)/(z_\mu(x)_{n_a}^2 - f_{n_a}^2(x)) \end{bmatrix},$$



$$G_\mu(x) = \sum_{i=1}^{n_a} e_i^T u_\mu(x) \nabla^2 f_i(x),$$

$$V_\mu(x) = \text{diag} \left( 2\mu/(z_\mu(x)_1^2 + f_1^2(x)), \dots, 2\mu/(z_\mu(x)_{n_a}^2 + f_{n_a}^2(x)) \right).$$

The Hessian matrix  $\nabla^2 B_\mu(x)$  of the barrier function  $B_\mu(x)$  is positive definite if  $G_\mu(x)$  (the Hessian matrix of the Lagrangian function) is positive definite.

Subroutine PSUM is based on a trust-region realization of the Newton-like methods. The Dennis–Mei (dog-leg) method described in Section 3 is used for computation of the trust-region step  $d$  using the quadratic model

$$Q(d) = \frac{1}{2} d^T \nabla^2 B_\mu(x) d + g_\mu^T(x) d$$

(more details are given in [18]). In fact, we use an approximation of  $\nabla^2 B_\mu(x)$ , such that  $G_\mu(x)$  is determined either by partitioned variable metric updates described in Section 4 (if **MED** = 1) or by gradient differences as in [5] (if **MED** = 2). If **MED** = 1, then we define reduced approximations of the Hessian matrices  $\tilde{G}_i = Z_i^T G_i Z_i$ ,  $1 \leq i \leq n_a$ , as in Section 4. New reduced approximations of the Hessian matrices are computed by the formulas (28) described in Section 6.

A very important part of the primal interior point method is an update of the barrier parameter  $\mu$ . There are two requirements, which play opposite roles. First,  $\mu \rightarrow 0$  should hold, since this is the main property of every interior-point method. On the other hand, round-off errors can cause that  $z_\mu(x)_i^2 = f_i^2(x)$  when  $\mu$  is too small and  $|f_i(x)|$  is sufficiently large (see (30)), which leads to a breakdown (division by  $z_\mu(x)_i^2 - f_i^2(x) = 0$ ). Thus a lower bound  $\underline{\mu}$  for the barrier parameter (parameter **ETA5** in subroutine PSUM) is used.

The efficiency of the primal interior point method is also sensitive to the way in which the barrier parameter decreases. Subroutine PSUM uses the formula

$$\mu_{k+1} = \max(\underline{\mu}, \|g_k(x_k)\|^2) \quad \text{if} \quad \rho(d_k) \geq \underline{\rho} \quad \text{and} \quad \|g_k(x_k)\|^2 \leq \mu_k/100,$$

and  $\mu_{k+1} = \mu_k$  otherwise ( $\rho(d_k)$  and  $\underline{\rho}$  are defined in Section 3).

## 8 Methods for sparse systems of nonlinear equations

Consider the system of nonlinear equations

$$f(x) = 0, \tag{31}$$

where  $f : R^n \rightarrow R^n$  is a continuously differentiable mapping and assume that the Jacobian matrix  $J(x) = [J_{ij}(x)] = [\partial f_i(x)/\partial x_j]$  is sparse. The sparsity pattern of the Jacobian matrix is stored using arrays **IAG** and **JAG** in the way described in Section 4 (where  $n_a = n$ ). Let  $A$  be an approximation of the Jacobian matrix  $J = J(x)$  and let  $F = F(x) = (1/2)\|f(x)\|^2$ . Methods considered in this section are realized in the line-search framework. They generate a sequence of points  $x_i \in R^n$ ,  $i \in N$ , such that

$$x_{k+1} = x_k + \alpha_k d_k, \quad k \in N, \tag{32}$$

where  $d_k \in R^n$  is a direction vector determined as an approximate solution of the linear system  $A_k d + f_k = 0$  such that

$$\|A_k d_k + f_k\| \leq \bar{\omega}_k \|f_k\| \tag{33}$$

with the precision  $0 \leq \bar{\omega}_k \leq \bar{\omega} < 1$  and  $\alpha_k$  is the step-size chosen in such a way that it is the first member of the sequence  $\alpha_k^j$ ,  $j \in N$ , where  $\alpha_k^1 = 1$  and  $\underline{\beta}\alpha_k^j \leq \alpha_k^{j+1} \leq \bar{\beta}\alpha_k^j$  with  $0 < \underline{\beta} \leq \bar{\beta} < 1$ , satisfying

$$F_{k+1} - F_k \leq -\varepsilon_1 \alpha_k f_k^T A_k d_k, \quad (34)$$

with the line search parameter  $0 < \varepsilon_1 < 1/2$ . We use the values  $\underline{\beta} = 0.1$ ,  $\bar{\beta} = 0.9$  and  $\varepsilon_1 = 10^{-4}$  in our subroutines. The value  $\alpha_k^{j+1}$  can be determined by a bisection (MES = 1) or by a two-point quadratic interpolation (MES = 2) or by a three-point quadratic interpolation (MES = 3) or by a three-point cubic interpolation (MES = 4).

To obtain a superlinear rate of convergence, the condition  $\bar{\omega}_k \rightarrow 0$  has to be satisfied. Therefore, we set

$$\bar{\omega}_k = \min(\max(\|f_k\|^\nu, \gamma(\|f_k\|/\|f_{k-1}\|)^\alpha), 1/k, \bar{\omega}),$$

where  $\nu = 1/2$ ,  $\gamma = 1$ ,  $\alpha = (1 + \sqrt{5})/2$  and  $\bar{\omega} = 1/2$ .

If  $A_k \neq J_k$ , then a safeguard based on restarts is used. It consists in setting  $A_{k+1} = J_{k+1}$  if  $j > \underline{j}$  or  $A_k = J_k$  (with repeating the  $k$ -th iteration) if  $j > \bar{j}$ , where  $0 < \underline{j} < \bar{j}$ . We use the values  $\underline{j} = 1$  and  $\bar{j} = 5$ . The restart of the form  $A_k = J_k$  is also used whenever

$$-d_k^T J_k^T f_k \leq \underline{\varepsilon} \|d_k\| \|J_k^T f_k\|,$$

where  $0 < \underline{\varepsilon} < 1$  is a restart tolerance (we use the value  $\underline{\varepsilon} = 10^{-12}$  in our subroutines).

The direction vector  $d_k$  (an approximate solution of the linear system  $A_k d + f_k = 0$ ) is determined by using the preconditioned smoothed CGS method described in [35]. To simplify the description of this method, we omit the outer index  $k$  and denote the inner index by  $i$ . Let  $h = A^T f$ . We set  $s_1 = 0$ ,  $\bar{s}_1 = 0$ ,  $r_1 = f$ ,  $\bar{r}_1 = f$ ,  $p_1 = f$ ,  $u_1 = f$  and for  $i = 1, 2, 3, \dots$  we proceed in the following way. If  $\|r_i\| \leq \bar{\omega} \|f\|$ , then set  $d = s_i$  and terminate the process. Otherwise compute

$$\begin{aligned} v_i &= AC^{-1}p_i, & \alpha_i &= h^T \bar{r}_i / h^T v_i, \\ q_i &= u_i - \alpha_i v_i, \\ \bar{s}_{i+1} &= \bar{s}_i + \alpha_i C^{-1}(u_i + q_i), \\ \bar{r}_{i+1} &= \bar{r}_i + \alpha_i AC^{-1}(u_i + q_i), & \beta_i &= h^T \bar{r}_{i+1} / h^T \bar{r}_i, \\ u_{i+1} &= \bar{r}_{i+1} + \beta_i q_i, \\ p_{i+1} &= u_{i+1} + \beta_i (q_i + \beta_i p_i), \\ [\lambda_i, \mu_i]^T &= \arg \min_{[\lambda, \mu]^T \in \mathbb{R}^2} \|\bar{r}_{i+1} + \lambda(r_i - \bar{r}_{i+1}) + \mu v_i\|, \\ s_{i+1} &= \bar{s}_{i+1} + \lambda_i (s_i - \bar{s}_{i+1}) + \mu_i C^{-1} p_i, \\ r_{i+1} &= \bar{r}_{i+1} + \lambda_i (r_i - \bar{r}_{i+1}) + \mu_i v_i. \end{aligned}$$

The matrix  $C$  serves as a preconditioner. The choice  $C = I$  is used if MOS2 = 1 or  $C$  is defined as an incomplete LU decomposition of the matrix  $A$  if MOS2 = 2 (MOS2 is a parameter of the subroutines PEQN and PEQL). If MOS2 = 3, a preliminary solution obtained by the incomplete LU decomposition can be accepted. In this case, we first compute vectors  $d_1 = -C^{-1}f$ ,  $r_1 = Ad_1 + f$ . If  $\|r_1\| \leq \bar{\omega} \|f\|$ , then we set  $d = d_1$  and terminate the process, otherwise we continue by CGS iterations as above.

More details concerning globally convergent line-search methods for systems of nonlinear equations can be found in [22].

## 8.1 Inexact discrete Newton method

Subroutine PEQN is an implementation of the inexact discrete Newton method. This simple method is based on the elementwise differentiation. We always set  $A_k = J(x_k)$ , where

$$J_{ij}(x) = \frac{f_i(x + \delta_j e_j) - f_i(x)}{\delta_j} \quad (35)$$

for all pairs  $(i, j)$  corresponding to structurally nonzero elements of  $J(x)$ . Thus we need  $m$  scalar function evaluations (i.e.  $m/n$  equivalent vector function evaluations), where  $m$  is the number of structurally nonzero elements of  $J(x)$ .

Nonzero elements of sparse Jacobian matrix  $J(x)$  can be also derived by using the groupwise differentiation [4]. Since our comparative tests have shown that the efficiencies of both these approaches are practically the same (see [22]), we use the simpler elementwise differentiation in our subroutines.

## 8.2 Inverse column-update quasi-Newton method

Subroutine PEQL is an implementation of the inverse column update method, which is introduced in [24]. This method uses an approximation  $S_k = A_k^{-1}$  of the inverse Jacobian matrix  $J_k^{-1}$  in (33). Therefore, we simply set  $d_k = -S_k f_k$  instead of using the preconditioned smoothed CGS method if the restart is not used (if  $A_k \neq J_k$ ). Denote by  $s_k = x_{k+1} - x_k$ ,  $s_{k-1} = x_k - x_{k-1}$ ,  $\dots$ ,  $s_{k-m} = x_{k-m+1} - x_{k-m}$  and  $y_k = f_{k+1} - f_k$ ,  $y_{k-1} = f_k - f_{k-1}$ ,  $\dots$ ,  $y_{k-m} = f_{k-m+1} - f_{k-m}$  the last  $m$  differences of points and function vectors, respectively, where the lower index  $k - m$  corresponds to the iteration with the restart. Let  $e_{k-1} = \arg \max_{e_i} |e_i^T y_{k-1}|$ ,  $\dots$ ,  $e_{k-m} = \arg \max_{e_i} |e_i^T y_{k-m}|$  ( $\arg \max$  is taken over all columns  $e_i$ ,  $1 \leq i \leq n$ , of the unit matrix). Then the vector  $S_k f_k$  can be computed by the formula

$$S_k f_k = S_{k-m} f_k + \frac{e_{k-1}^T f_k}{e_{k-1}^T y_{k-1}} v_{k-1} + \dots + \frac{e_{k-m}^T f_k}{e_{k-m}^T y_{k-m}} v_{k-m},$$

where  $v_{k-1} = d_{k-1} - S_{k-1} y_{k-1}$ ,  $\dots$ ,  $v_{k-m} = d_{k-m} - S_{k-m} y_{k-m}$  are vectors computed recursively by the formula

$$v_k = d_k - S_k y_k = d_k - S_{k-m} y_k - \frac{e_{k-1}^T y_k}{e_{k-1}^T y_{k-1}} v_{k-1} - \dots - \frac{e_{k-m}^T y_k}{e_{k-m}^T y_{k-m}} v_{k-m}.$$

In both of these formulae we use the matrix  $S_{k-m} = (L_{k-m} U_{k-m})^{-1}$ , where  $L_{k-m} U_{k-m}$  is the incomplete LU decomposition of the Jacobian matrix  $J(x_{k-m})$  computed by (35). Note that the vectors  $e_{k-1}$ ,  $\dots$ ,  $e_{k-m}$  do not need to be stored. We only use indices of their unique nonzero elements. The limited memory column update method needs to be restarted periodically after  $\bar{m}$  iterations (parameter MF in the subroutine PEQL), since at most  $\bar{m}$  vectors can be stored.

## 9 Comparison of subroutines

In this section, we compare some of our subroutines with the most commonly known subroutines that solve the same problems. The comparison has been performed by using test collections TEST14 (with 1000 variables) for subroutines PLIS, PLIP, PNET, PNED, PNEC, PSED, PSEC, TEST15 (with 1000 variables) for subroutines PGAD, PGAC and TEST18 (with 3000 equations and unknowns) for subroutines PEQN, PEQL. These collections can be downloaded from [www.cs.cas.cz/~luksan/test.html](http://www.cs.cas.cz/~luksan/test.html). Results of tests are listed in six tables. Rows corresponding to individual test problems contain the number of iterations NIT, the number of function evaluations NFV, the number of gradient evaluations NFG, the final value of the objective function F, the value of the termination criterion G, and the cause of termination ITERM. The last row of every table contains the total number of NIT, NFV, NFG, the total computational time in seconds and the number of problems successfully solved.

Table 2 contains the comparison of PLIS and PLIP with the subroutine L-BFGS [40]. Subroutine L-BFGS had to be slightly modified to eliminate overflows. Thus we have added statement  $STPMAX=XMAX/MXVNR(N,S)$  ( $MXVNR(N,S)$  is the Euclidean norm of  $N$  dimensional vector  $S$ ) to the subroutine MCSRCH, realizing the Moré-Thuente line search, and used  $XMAX=1.0D1$  for some problems. The value  $M=10$  (corresponding to  $MF=10$  in PLIS and PLIP) has been used in the subroutine L-BFGS.

Table 3 contains the comparison of PNET with the subroutine TNMIN from TNPACK [30]. As in the previous case, we have added statement  $DELH=MIN(DELH,XMAX/DNORM)$  to the subroutine OURHDP and statement  $STPMAX=XMAX/MXVNR(N,S)$  to the subroutine MLINES. The default values of parameters in OPTLIST have been used in the subroutine TNMIN.

Table 4 contains the comparison of PSED and PSEC with the Harwell subroutine VE08AD [33]. The values  $DIFGRD=10^{-8}$ ,  $FKNOWN='FALSE'$ ,  $RESTRT='FALSE'$ ,  $TESTGX='FALSE'$ ,  $HESDIF='FALSE'$ ,  $STEPL(1)=-1$  and  $STMAX=XMAX$  have been used in the subroutine VE08AD ( $XMAX$ , which has the same meaning as in PSED, PSEC, was sometimes tuned).

Table 5 contains the comparison of PGAD and PGAC with the Harwell subroutine VE10AD [34]. The values  $DIFGRD=10^{-8}$ ,  $FKNOWN='FALSE'$ ,  $RESTRT='FALSE'$ ,  $TESTGX='FALSE'$ ,  $HESDIF='FALSE'$ ,  $STEPL(1)=-1$  and  $STMAX=XMAX$  have been used in the subroutine VE10AD ( $XMAX$ , which has the same meaning as in PGAD, PGAC, was sometimes tuned).

Table 6 contains the comparison of PEQN and PEQL (using only function values) with the subroutine NITSOL [28]. Since NITSOL does not contain an internal preconditioner, the less efficient unpreconditioned iterative method was used.

Table 7 contains the comparison of PEQN and PEQL (using function values and the first derivatives) with the subroutine NLEQ1S [27]. Subroutine NLEQ1S frequently required very large working arrays and a complete LU decomposition was sometimes very time-consuming.

The results introduced in Table 2–Table 7 demonstrate that PLIS and PLIP are comparable with L-BFGS. Other our subroutines tested are more efficient than their equivalents.

| Method   | TLISU |       |       | TLIPU |       |       | LBFGS |       |       |
|----------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Problem  | NIT   | NFV   | NFG   | NIT   | NFV   | NFG   | NIT   | NFV   | NFG   |
| 1        | 4988  | 5554  | 5554  | 5383  | 5417  | 5417  | 4935  | 5821  | 5821  |
| 2        | 425   | 454   | 454   | 530   | 557   | 557   | 4048  | 4375  | 4375  |
| 3        | 74    | 78    | 78    | 125   | 128   | 128   | 88    | 96    | 96    |
| 4        | 103   | 112   | 112   | 109   | 114   | 114   | 113   | 120   | 120   |
| 5        | 24    | 26    | 26    | 26    | 27    | 27    | 23    | 24    | 24    |
| 6        | 30    | 31    | 31    | 35    | 36    | 36    | 36    | 38    | 38    |
| 7        | 38    | 43    | 43    | 36    | 41    | 41    | 29    | 50    | 50    |
| 8        | 29    | 33    | 33    | 33    | 36    | 36    | 32    | 55    | 55    |
| 9        | 13    | 16    | 16    | 15    | 18    | 18    | 11    | 15    | 15    |
| 10       | 1540  | 1582  | 1582  | 2003  | 2030  | 2030  | 1367  | 1403  | 1403  |
| 11       | 114   | 138   | 138   | 157   | 175   | 175   | 174   | 213   | 213   |
| 12       | 248   | 267   | 267   | 337   | 350   | 350   | 278   | 297   | 297   |
| 13       | 7     | 8     | 8     | 9     | 10    | 10    | 12    | 13    | 13    |
| 14       | 10    | 12    | 12    | 8     | 10    | 10    | 1     | 3     | 3     |
| 15       | 2830  | 2929  | 2929  | 1226  | 1256  | 1256  | 2773  | 2861  | 2861  |
| 16       | 196   | 210   | 210   | 237   | 246   | 246   | 229   | 240   | 240   |
| 17       | 1007  | 1032  | 1032  | 598   | 604   | 604   | 968   | 998   | 998   |
| 18       | 1449  | 1474  | 1474  | 989   | 998   | 998   | 1685  | 1732  | 1732  |
| 19       | 1393  | 1431  | 1431  | 1261  | 1272  | 1272  | 1703  | 1759  | 1759  |
| 20       | 2129  | 2191  | 2191  | 2045  | 2058  | 2058  | 2379  | 2433  | 2433  |
| 21       | 2120  | 2169  | 2169  | 2175  | 2196  | 2196  | 1945  | 1998  | 1998  |
| 22       | 1305  | 1346  | 1346  | 1261  | 1292  | 1292  | 1652  | 1706  | 1706  |
| $\Sigma$ | 20072 | 21136 | 21136 | 18598 | 18871 | 18871 | 24481 | 26250 | 26250 |

| Method   | TLISU       |      |       | TLIPU       |      |       | LBFGS       |      |       |
|----------|-------------|------|-------|-------------|------|-------|-------------|------|-------|
| Problem  | F           | G    | ITERM | F           | G    | ITERM | F           | G    | IFLAG |
| 1        | 9.6E-15     | E-06 | 4     | 6.0E-14     | E-06 | 4     | 6.1E-13     | E-04 | 0     |
| 2        | 14.9945     | E-05 | 2     | 3.57277     | E-05 | 2     | 276.253     | E-04 | 0     |
| 3        | 6.6E-10     | E-06 | 4     | 3.4E-13     | E-06 | 4     | 8.1E-11     | E-06 | 0     |
| 4        | 269.500     | E-06 | 4     | 269.500     | E-06 | 4     | 269.500     | E-04 | 0     |
| 5        | 1.3E-12     | E-06 | 4     | 7.1E-12     | E-06 | 4     | 4.5E-11     | E-04 | 0     |
| 6        | 2.2E-11     | E-06 | 4     | 1.4E-11     | E-06 | 4     | 1.3E-11     | E-05 | 0     |
| 7        | 335.137     | E-06 | 4     | 336.937     | E-06 | 4     | 336.937     | E-04 | -1    |
| 8        | 761775.     | E-03 | 2     | 761775.     | E-02 | 2     | 761775.     | E-03 | -1    |
| 9        | 316.436     | E-06 | 4     | 316.436     | E-06 | 4     | 316.436     | E-04 | 0     |
| 10       | -124.630    | E-04 | 2     | -124.950    | E-04 | 2     | -131.810    | E-04 | 0     |
| 11       | 10.7766     | E-06 | 4     | 10.7766     | E-06 | 4     | 10.7766     | E-04 | 0     |
| 12       | 982.274     | E-04 | 2     | 982.274     | E-04 | 2     | 982.274     | E-04 | 0     |
| 13       | 1.7E-13     | E-06 | 4     | 2.3E-15     | E-07 | 4     | 1.6E-20     | E-09 | 0     |
| 14       | 1.3E-09     | E-06 | 4     | 1.3E-09     | E-06 | 4     | 1.3E-09     | E-05 | 0     |
| 15       | 1.92402     | E-06 | 4     | 1.92402     | E-06 | 4     | 1.92402     | E-04 | -1    |
| 16       | -427.404    | E-05 | 2     | -427.404    | E-04 | 2     | -427.404    | E-05 | 0     |
| 17       | -3.8E-02    | E-06 | 4     | -3.8E-02    | E-06 | 4     | -3.8E-02    | E-05 | 0     |
| 18       | -2.5E-02    | E-06 | 4     | -2.5E-02    | E-06 | 4     | -2.5E-02    | E-05 | 0     |
| 19       | 59.5986     | E-05 | 2     | 59.5986     | E-05 | 2     | 59.5986     | E-04 | 0     |
| 20       | -1.00014    | E-06 | 4     | -1.00014    | E-06 | 4     | -1.00014    | E-06 | 0     |
| 21       | 2.13867     | E-06 | 4     | 2.13866     | E-06 | 4     | 2.13866     | E-04 | 0     |
| 22       | 1.00000     | E-06 | 4     | 1.00000     | E-06 | 4     | 1.00000     | E-06 | 0     |
| $\Sigma$ | TIME = 8.90 |      | 22    | TIME = 8.82 |      | 22    | TIME = 9.34 |      | 22    |

Table 2: Comparison of TLISU, TLIPU and LBFGS

| Method   | TNETU |      |       |             |      |       | TNMIN |      |       |              |      |        |
|----------|-------|------|-------|-------------|------|-------|-------|------|-------|--------------|------|--------|
|          | NIT   | NFV  | NFG   | F           | G    | ITERM | NIT   | NFV  | NFG   | F            | G    | INFORM |
| 1        | 1481  | 1656 | 26037 | 1.2E-16     | E-06 | 4     | 1756  | 2597 | 34032 | 4.1E-20      | E-08 | 1      |
| 2        | 132   | 387  | 7945  | 1.5E-16     | E-08 | 4     | 70    | 144  | 4166  | 7.0E-17      | E-07 | 1      |
| 3        | 19    | 20   | 110   | 4.2E-10     | E-06 | 4     | 19    | 20   | 145   | 5.2E-10      | E-06 | 1      |
| 4        | 19    | 20   | 230   | 269.500     | E-07 | 4     | 18    | 19   | 261   | 269.500      | E-07 | 1      |
| 5        | 12    | 13   | 49    | 4.7E-12     | E-06 | 4     | 11    | 12   | 60    | 1.0E-10      | E-05 | 1      |
| 6        | 13    | 14   | 76    | 3.7E-12     | E-06 | 4     | 12    | 13   | 99    | 2.8E-11      | E-05 | 1      |
| 7        | 9     | 10   | 37    | 336.937     | E-06 | 4     | 8     | 9    | 42    | 336.937      | E-07 | 1      |
| 8        | 11    | 12   | 58    | 761775.     | E-07 | 4     | 6     | 7    | 30    | 761775.      | E-01 | 1      |
| 9        | 7     | 11   | 28    | 316.436     | E-07 | 4     | 7     | 14   | 27    | 316.436      | E-04 | 1      |
| 10       | 75    | 153  | 3213  | -133.610    | E-08 | 4     | 72    | 152  | 4936  | -126.610     | E-07 | 1      |
| 11       | 33    | 45   | 181   | 10.7766     | E-07 | 4     | 30    | 41   | 188   | 10.7766      | E-10 | 1      |
| 12       | 23    | 30   | 457   | 982.274     | E-08 | 4     | 26    | 30   | 467   | 982.274      | E-04 | 1      |
| 13       | 7     | 8    | 16    | 5.3E-16     | E-07 | 4     | 7     | 8    | 17    | 8.9E-31      | E-14 | 1      |
| 14       | 1     | 2    | 1005  | 1.2E-09     | E-07 | 4     | 1     | 2    | 1002  | 1.2E-09      | E-06 | 1      |
| 15       | 14    | 15   | 4033  | 1.92402     | E-07 | 4     | 8     | 9    | 2765  | 1.92402      | E-04 | 1      |
| 16       | 13    | 17   | 295   | -427.404    | E-08 | 4     | 13    | 18   | 473   | -427.404     | E-06 | 1      |
| 17       | 4     | 5    | 810   | -3.8E-02    | E-06 | 4     | 3     | 4    | 996   | -3.8E-02     | E-09 | 1      |
| 18       | 4     | 5    | 1146  | -2.5E-02    | E-06 | 4     | 3     | 4    | 1156  | -2.5E-02     | E-10 | 1      |
| 19       | 10    | 11   | 1986  | 59.5986     | E-06 | 4     | 7     | 8    | 1532  | 59.5986      | E-04 | 1      |
| 20       | 18    | 39   | 3051  | -1.00014    | E-07 | 4     | 14    | 35   | 4009  | -1.00014     | E-06 | 1      |
| 21       | 7     | 8    | 4901  | 2.13866     | E-08 | 4     | 7     | 8    | 5610  | 2.13866      | E-09 | 1      |
| 22       | 55    | 145  | 4760  | 1.00000     | E-08 | 4     | 37    | 94   | 13588 | 1.00000      | E-06 | 1      |
| $\Sigma$ | 1967  | 2626 | 60424 | TIME = 6.95 |      | 22    | 2135  | 3248 | 75601 | TIME = 17.20 |      | 22     |

Table 3: Comparison of TNETU and TNMIN

| Method   | TSEDU |      |      | TSECU |      |      | VE08AD |      |      |
|----------|-------|------|------|-------|------|------|--------|------|------|
| Problem  | NIT   | NFV  | NFG  | NIT   | NFV  | NFG  | NIT    | NFV  | NFG  |
| 1        | 2654  | 3627 | 3627 | 2606  | 3566 | 3566 | 4669   | 686  | 686  |
| 2        | 105   | 179  | 179  | 108   | 177  | 177  | 152    | 193  | 193  |
| 3        | 40    | 45   | 45   | 40    | 45   | 45   | 44     | 51   | 51   |
| 4        | 37    | 45   | 45   | 37    | 45   | 45   | 65     | 75   | 75   |
| 5        | 16    | 17   | 17   | 16    | 17   | 17   | 272    | 416  | 416  |
| 6        | 38    | 40   | 40   | 38    | 40   | 40   | 62     | 76   | 76   |
| 7        | 22    | 26   | 26   | 26    | 31   | 31   | 249    | 463  | 463  |
| 8        | 26    | 40   | 40   | 25    | 39   | 39   | 10     | 19   | 19   |
| 9        | 193   | 202  | 202  | 191   | 210  | 210  | 44     | 64   | 64   |
| 10       | 227   | 258  | 258  | 233   | 264  | 264  | 74     | 123  | 123  |
| 11       | 100   | 127  | 127  | 113   | 144  | 144  | 108    | 166  | 166  |
| 12       | 28    | 29   | 29   | 28    | 29   | 29   | 72     | 108  | 108  |
| 13       | 1     | 2    | 2    | 1     | 2    | 2    | 7      | 10   | 10   |
| 14       | 25    | 28   | 28   | 25    | 28   | 28   | 20     | 28   | 28   |
| 15       | 8     | 15   | 15   | 27    | 41   | 41   | 65     | 87   | 87   |
| 16       | 25    | 35   | 35   | 25    | 35   | 35   | 19     | 26   | 26   |
| 17       | 15    | 17   | 17   | 15    | 17   | 17   | 23     | 31   | 31   |
| 18       | 5     | 11   | 11   | 8     | 12   | 12   | 29     | 40   | 40   |
| 19       | 19    | 23   | 23   | 19    | 23   | 23   | 24     | 29   | 29   |
| 20       | 37    | 97   | 97   | 42    | 74   | 74   | 40     | 57   | 57   |
| 21       | 37    | 40   | 40   | 37    | 40   | 40   | 28     | 38   | 38   |
| 22       | 55    | 211  | 211  | 48    | 192  | 192  | 114    | 231  | 231  |
| $\Sigma$ | 3713  | 5114 | 5114 | 3708  | 5071 | 5071 | 6190   | 3017 | 3017 |

| Method   | TSEDU       |       |       | TSECU       |       |       | VE08AD       |      |       |
|----------|-------------|-------|-------|-------------|-------|-------|--------------|------|-------|
| Problem  | F           | G     | ITERM | F           | G     | ITERM | F            | G    | IFLAG |
| 1        | 7.9E-17     | E-06  | 3     | 6.5E-18     | E-07  | 3     | 4.9E-17      | E-06 | 1     |
| 2        | 83.3161     | E-06  | 4     | 1111.36     | E-05  | 2     | 5.0E-17      | E-06 | 1     |
| 3        | 2.6E-13     | E-06  | 4     | 2.7E-13     | E-06  | 4     | 1.4E-13      | E-06 | 1     |
| 4        | 269.500     | E-06  | 4     | 269.500     | E-06  | 4     | 269.500      | E-06 | 1     |
| 5        | 1.1E-12     | E-06  | 4     | 1.1E-12     | E-06  | 4     | 1.1E-11      | E-06 | 1     |
| 6        | 5.5E-12     | E-06  | 4     | 5.5E-12     | E-06  | 4     | 6.8E-13      | E-06 | 1     |
| 7        | 335.253     | E-06  | 4     | 335.253     | E-06  | 4     | 316.783      | E-07 | 1     |
| 8        | 761775.     | E-04  | 2     | 761775.     | E-03  | 2     | 761775.      | E-05 | 29    |
| 9        | 316.436     | E-05  | 2     | 316.436     | E-05  | 2     | 316.436      | E-06 | 1     |
| 10       | -125.810    | E-04  | 2     | -121.692    | E-04  | 2     | -125.790     | E-05 | 29    |
| 11       | 10.7766     | E-06  | 4     | 10.7766     | E-07  | 4     | 10.7766      | E-07 | 1     |
| 12       | 982.274     | E-06  | 4     | 982.274     | E-06  | 4     | 982.274      | E-06 | 1     |
| 13       | 0.00000     | 0.000 | 4     | 0.00000     | 0.000 | 3     | 6.5E-21      | E-09 | 1     |
| 14       | 1.0E-09     | E-06  | 4     | 1.0E-09     | E-06  | 4     | 1.2E-09      | E-06 | 1     |
| 15       | 1.92402     | E-07  | 4     | 1.92402     | E-07  | 4     | 1.92402      | E-06 | 1     |
| 16       | -427.404    | E-06  | 4     | -427.404    | E-06  | 4     | -427.404     | E-06 | 1     |
| 17       | -3.8E-02    | E-06  | 4     | -3.8E-02    | E-06  | 4     | -3.8E-02     | E-07 | 1     |
| 18       | -2.5E-02    | E-07  | 4     | -0.5E-02    | E-11  | 4     | -2.5E-02     | E-06 | 1     |
| 19       | 59.5986     | E-06  | 4     | 59.5986     | E-06  | 4     | 59.5986      | E-06 | 1     |
| 20       | -1.00014    | E-08  | 4     | -1.00014    | E-09  | 4     | -1.00014     | E-06 | 1     |
| 21       | 2.13866     | E-06  | 4     | 2.13866     | E-06  | 4     | 2.13866      | E-06 | 1     |
| 22       | 1.00000     | E-07  | 4     | 1.00000     | E-08  | 4     | 1.00000      | E-06 | 1     |
| $\Sigma$ | TIME = 4.27 |       | 22    | TIME = 7.63 |       | 22    | TIME = 19.40 |      | 22    |

Table 4: Comparison of TSEDU, TSECU and VE08AD

| Method   | TGADU |      |      | TGACU |      |      | VE10AD |      |      |
|----------|-------|------|------|-------|------|------|--------|------|------|
| Problem  | NIT   | NFV  | NFG  | NIT   | NFV  | NFG  | NIT    | NFV  | NFG  |
| 1        | 1377  | 1379 | 1379 | 1108  | 1110 | 1110 | 1456   | 180  | 180  |
| 2        | 41    | 46   | 46   | 624   | 640  | 649  | 348    | 509  | 509  |
| 3        | 11    | 12   | 14   | 11    | 12   | 14   | 17     | 18   | 18   |
| 4        | 13    | 16   | 21   | 11    | 13   | 17   | 23     | 24   | 24   |
| 5        | 4     | 5    | 7    | 4     | 5    | 7    | 6      | 7    | 7    |
| 6        | 6     | 7    | 13   | 6     | 7    | 13   | 7      | 8    | 8    |
| 7        | 10    | 12   | 23   | 17    | 40   | 29   | 8      | 9    | 9    |
| 8        | 21    | 26   | 24   | 22    | 25   | 25   | 96     | 267  | 267  |
| 9        | 15    | 16   | 36   | 13    | 15   | 38   | 48     | 50   | 50   |
| 10       | 12    | 18   | 21   | 129   | 147  | 176  | 9      | 10   | 10   |
| 11       | 2587  | 2593 | 2649 | 3010  | 3016 | 3012 | 3233   | 404  | 404  |
| 12       | 16    | 20   | 23   | 205   | 226  | 236  | 18     | 34   | 34   |
| 13       | 17    | 21   | 28   | 123   | 132  | 152  | 19     | 26   | 26   |
| 14       | 5     | 8    | 18   | 7     | 8    | 32   | 6      | 7    | 7    |
| 15       | 6     | 7    | 15   | 13    | 20   | 42   | 8      | 9    | 9    |
| 16       | 15    | 21   | 40   | 14    | 15   | 35   | 13     | 14   | 14   |
| 17       | 15    | 20   | 19   | 29    | 34   | 33   | 18     | 26   | 26   |
| 18       | 42    | 44   | 45   | 49    | 53   | 52   | 922    | 2397 | 2397 |
| 19       | 15    | 16   | 23   | 15    | 16   | 23   | 18     | 25   | 25   |
| 20       | 26    | 27   | 29   | 17    | 18   | 32   | 18     | 33   | 33   |
| 21       | 10    | 11   | 17   | 15    | 18   | 23   | 26     | 28   | 28   |
| 22       | 26    | 32   | 45   | 47    | 59   | 98   | 24     | 30   | 30   |
| $\Sigma$ | 4290  | 4357 | 4535 | 5489  | 5629 | 5848 | 6341   | 4115 | 4115 |

| Method   | TGADU       |      |       | TGACU       |      |       | VE10AD       |      |       |
|----------|-------------|------|-------|-------------|------|-------|--------------|------|-------|
| Problem  | F           | G    | ITERM | F           | G    | ITERM | F            | G    | IFLAG |
| 1        | 7.0E-23     | E-09 | 3     | 0.00000     | E+00 | 3     | 2.6E-16      | E-06 | 1     |
| 2        | 2.2E-17     | E-06 | 3     | 66.4089     | E-07 | 4     | 4.7E-16      | E-07 | 1     |
| 3        | 1.4E-10     | E-06 | 4     | 2.0E-10     | E-06 | 4     | 1.3E-10      | E-06 | 1     |
| 4        | 134.750     | E-06 | 4     | 134.750     | E-07 | 4     | 134.750      | E-06 | 1     |
| 5        | 1.1E-11     | E-06 | 4     | 1.2E-11     | E-06 | 4     | 7.9E-19      | E-08 | 1     |
| 6        | 7.4E-27     | E-12 | 3     | 7.9E-27     | E-12 | 3     | 2.3E-17      | E-07 | 1     |
| 7        | 60734.9     | E-07 | 4     | 60734.9     | E-05 | 6     | 60734.9      | E-06 | 1     |
| 8        | 2.5E-09     | E-06 | 4     | 1.3E-08     | E-06 | 4     | 1.1E-09      | E-07 | 1     |
| 9        | 2216.46     | E-10 | 4     | 2216.46     | E-06 | 4     | 2216.46      | E-05 | 29    |
| 10       | 191.511     | E-07 | 4     | 191.511     | E-07 | 4     | 191.511      | E-06 | 1     |
| 11       | 6.5E-28     | E-12 | 3     | 4.0E-25     | E-11 | 3     | 1.0E-16      | E-07 | 1     |
| 12       | 19264.6     | E-10 | 4     | 22287.9     | E-08 | 4     | 22287.9      | E-08 | 1     |
| 13       | 131234.     | E-08 | 4     | 131234.     | E-09 | 4     | 131234.      | E-07 | 1     |
| 14       | 108.518     | E-08 | 4     | 108.518     | E-07 | 4     | 108.518      | E-07 | 1     |
| 15       | 18.1763     | E-06 | 4     | 18.1763     | E-05 | 2     | 18.1763      | E-09 | 1     |
| 16       | 2.51110     | E-06 | 4     | 2.51110     | E-09 | 4     | 2.51110      | E-06 | 1     |
| 17       | 2.6E-17     | E-08 | 3     | 1.4E-10     | E-06 | 4     | 1.2E-12      | E-06 | 1     |
| 18       | 1.5E-25     | E-10 | 3     | 1.2E-22     | E-09 | 3     | 8.4E-14      | E-05 | 1     |
| 19       | 3.5E-15     | E-06 | 4     | 3.4E-14     | E-06 | 4     | 8.3E-17      | E-06 | 1     |
| 20       | 3.8E-11     | E-07 | 4     | 3.4E-12     | E-07 | 4     | 1.1E-17      | E-08 | 1     |
| 21       | 647.829     | E-11 | 4     | 647.696     | E-06 | 4     | 647.696      | E-05 | 29    |
| 22       | 4486.97     | E-07 | 4     | 4486.97     | E-08 | 4     | 4486.97      | E-06 | 1     |
| $\Sigma$ | TIME = 4.56 |      | 22    | TIME = 5.01 |      | 22    | TIME = 27.31 |      | 22    |

Table 5: Comparison of TGADU, TGACU and VE10AD



| Method<br>Problem | TEQNU |      |     |             |       | TEQLU |      |     |             |       | NITSOL |        |     |              |       |
|-------------------|-------|------|-----|-------------|-------|-------|------|-----|-------------|-------|--------|--------|-----|--------------|-------|
|                   | NIT   | NFV  | NFG | F           | ITERM | NIT   | NFV  | NFG | F           | ITERM | NIT    | NFV    | NFG | F            | ITERM |
| 1                 | 10    | 41   | 0   | 2.2E-23     | 3     | 30    | 64   | 0   | 3.3E-19     | 3     | 37     | 14095  | 0   | 1.1E-15      | 0     |
| 2                 | 9     | 46   | 0   | 1.1E-23     | 3     | 17    | 57   | 0   | 7.2E-20     | 3     | 14     | 967    | 0   | 0.16900      | 5     |
| 3                 | 3     | 19   | 0   | 3.3E-20     | 3     | 5     | 11   | 0   | 8.6E-17     | 3     | 4      | 9      | 0   | 0.00000      | 0     |
| 4                 | 7     | 23   | 0   | 3.5E-18     | 3     | 11    | 19   | 0   | 1.2E-19     | 3     | 10     | 44     | 0   | 0.00000      | 0     |
| 5                 | 12    | 63   | 0   | 1.2E-17     | 3     | 20    | 56   | 0   | 3.4E-17     | 3     | 9      | 2548   | 0   | 142.883      | 5     |
| 6                 | 17    | 52   | 0   | 1.1E-17     | 3     | 22    | 31   | 0   | 1.7E-17     | 3     | 41     | 207    | 0   | 3.2E-14      | 6     |
| 7                 | 13    | 41   | 0   | 3.4E-20     | 3     | 25    | 42   | 0   | 1.4E-21     | 3     | 183    | 570    | 0   | 0.00000      | 0     |
| 8                 | 13    | 73   | 0   | 1.3E-26     | 3     | 21    | 60   | 0   | 5.0E-29     | 3     | 31     | 187    | 0   | 2.0E-15      | 6     |
| 9                 | 13    | 99   | 0   | 4.3E-22     | 3     | 32    | 71   | 0   | 2.2E-22     | 3     | 22     | 136    | 0   | 8.9E-15      | 6     |
| 10                | 5     | 41   | 0   | 8.0E-26     | 3     | 9     | 24   | 0   | 2.0E-21     | 3     | 9      | 80     | 0   | 2.8E-15      | 6     |
| 11                | 12    | 37   | 0   | 1.9E-26     | 3     | 16    | 23   | 0   | 1.2E-22     | 3     | 14     | 37     | 0   | 0.00000      | 0     |
| 12                | 18    | 55   | 0   | 1.3E-17     | 3     | 23    | 40   | 0   | 8.6E-17     | 3     | 31     | 152    | 0   | 7.3E-17      | 0     |
| 13                | 18    | 39   | 0   | 1.1E-17     | 3     | 24    | 32   | 0   | 2.3E-17     | 3     | 55     | 198    | 0   | 1.4E-14      | 6     |
| 14                | 4     | 13   | 0   | 7.7E-21     | 3     | 8     | 13   | 0   | 6.0E-22     | 3     | 10     | 92     | 0   | 3.2E-15      | 6     |
| 15                | 5     | 36   | 0   | 1.8E-18     | 3     | 12    | 28   | 0   | 1.2E-18     | 3     | 8      | 96     | 0   | 4.6E-15      | 6     |
| 16                | 53    | 319  | 0   | 4.6E-18     | 3     | 22    | 78   | 0   | 9.8E-21     | 3     | 243    | 706    | 0   | 0.00000      | 0     |
| 17                | 14    | 48   | 0   | 4.5E-23     | 3     | 17    | 43   | 0   | 1.3E-21     | 3     | 112    | 444    | 0   | 6.0E-13      | 6     |
| 18                | 26    | 79   | 0   | 2.5E-21     | 3     | 46    | 61   | 0   | 2.2E-18     | 3     | 24     | 1925   | 0   | 37.8584      | 5     |
| 19                | 2     | 7    | 0   | 3.1E-22     | 3     | 2     | 5    | 0   | 7.0E-19     | 3     | 30     | 15000  | 0   | -            | 3     |
| 20                | 13    | 43   | 0   | 4.3E-21     | 3     | 18    | 30   | 0   | 1.6E-17     | 3     | 24     | 15000  | 0   | -            | 3     |
| 21                | 12    | 37   | 0   | 2.0E-21     | 3     | 25    | 34   | 0   | 2.3E-17     | 3     | 23     | 15000  | 0   | -            | 3     |
| 22                | 7     | 50   | 0   | 2.0E-20     | 3     | 14    | 45   | 0   | 1.9E-18     | 3     | 12     | 3582   | 0   | 2.3E-02      | 5     |
| 23                | 29    | 262  | 0   | 3.9E-18     | 3     | 23    | 106  | 0   | 1.9E-19     | 3     | 20     | 15000  | 0   | -            | 3     |
| 24                | 6     | 31   | 0   | 8.2E-24     | 3     | 20    | 53   | 0   | 7.4E-18     | 3     | 16     | 4187   | 0   | 8.3E-15      | 6     |
| 25                | 9     | 46   | 0   | 1.5E-24     | 3     | 29    | 50   | 0   | 2.1E-18     | 3     | 15     | 1053   | 0   | 8.7E-15      | 6     |
| 26                | 12    | 61   | 0   | 6.1E-18     | 3     | 36    | 67   | 0   | 1.3E-18     | 3     | 25     | 1326   | 0   | 1.3E-12      | 6     |
| 27                | 10    | 51   | 0   | 2.8E-21     | 3     | 40    | 75   | 0   | 6.6E-18     | 3     | 19     | 3434   | 0   | 8.4E-15      | 6     |
| 28                | 10    | 60   | 0   | 2.3E-17     | 3     | 27    | 83   | 0   | 4.6E-19     | 3     | 24     | 658    | 0   | 1.2E-14      | 6     |
| 29                | 4     | 53   | 0   | 1.2E-20     | 3     | 12    | 95   | 0   | 2.1E-17     | 3     | 15     | 15000  | 0   | -            | 3     |
| 30                | 12    | 162  | 0   | 2.2E-22     | 3     | 18    | 145  | 0   | 7.4E-17     | 3     | 33     | 15000  | 0   | -            | 3     |
| $\Sigma$          | 378   | 1987 | 0   | TIME = 3.81 | 30    | 624   | 1541 | 0   | TIME = 3.22 | 30    | 1113   | 126733 | 0   | TIME = 84.28 | 20    |

Table 6: Comparison of TEQNU, TEQLU and NITSOL

| Method   | TEQNU |     |     |             |       | TEQLU |     |     |             |       | NLEQ1S |     |     |               |      |
|----------|-------|-----|-----|-------------|-------|-------|-----|-----|-------------|-------|--------|-----|-----|---------------|------|
|          | NIT   | NFV | NFG | F           | ITERM | NIT   | NFV | NFG | F           | ITERM | NIT    | NFV | NFG | F             | IERR |
| 1        | 10    | 11  | 10  | 2.2E-23     | 3     | 30    | 43  | 7   | 3.3E-19     | 3     | 14     | 16  | 14  | 6.0E-12       | 0    |
| 2        | 9     | 10  | 9   | 1.1E-23     | 3     | 17    | 34  | 6   | 1.4E-17     | 3     | 6      | 8   | 6   | 1.55409       | 3    |
| 3        | 3     | 4   | 3   | 2.4E-20     | 3     | 5     | 6   | 1   | 8.6E-17     | 3     | 4      | 5   | 4   | 2.4E-14       | 0    |
| 4        | 6     | 15  | 6   | 4.1E-17     | 3     | 10    | 19  | 4   | 1.3E-17     | 3     | 7      | 10  | 7   | 0.00000       | 0    |
| 5        | 6     | 12  | 6   | 9.6E-18     | 3     | 9     | 15  | 3   | 8.4E-18     | 3     | 1      | 1   | 1   | 148.879       | 80   |
| 6        | 17    | 18  | 17  | 1.0E-17     | 3     | 22    | 23  | 4   | 1.6E-17     | 3     | 24     | 25  | 24  | 6.1E-13       | 5    |
| 7        | 13    | 15  | 13  | 3.2E-20     | 3     | 25    | 32  | 5   | 2.0E-21     | 3     | 44     | 73  | 44  | 7.7E-11       | 0    |
| 8        | 13    | 21  | 13  | 5.6E-27     | 3     | 21    | 32  | 7   | 1.5E-30     | 3     | 29     | 35  | 29  | 4.3E-10       | 0    |
| 9        | 13    | 21  | 13  | 4.0E-22     | 3     | 32    | 35  | 6   | 2.5E-22     | 3     | 25     | 26  | 25  | 9.4E-15       | 0    |
| 10       | 5     | 6   | 5   | 1.4E-26     | 3     | 9     | 10  | 2   | 2.0E-21     | 3     | 6      | 7   | 6   | 1.8E-14       | 0    |
| 11       | 12    | 13  | 12  | 0.00000     | 3     | 16    | 17  | 3   | 1.2E-22     | 3     | 13     | 14  | 13  | 0.00000       | 0    |
| 12       | 18    | 19  | 18  | 1.3E-17     | 3     | 23    | 30  | 5   | 9.9E-17     | 3     | 25     | 26  | 25  | 6.9E-13       | 5    |
| 13       | 21    | 24  | 21  | 9.2E-17     | 3     | 27    | 30  | 6   | 4.5E-17     | 3     | 1      | 1   | 1   | 30.8162       | 80   |
| 14       | 4     | 5   | 4   | 7.5E-21     | 3     | 8     | 9   | 2   | 6.1E-22     | 3     | 5      | 6   | 5   | 2.4E-14       | 0    |
| 15       | 5     | 6   | 5   | 1.8E-18     | 3     | 12    | 16  | 2   | 1.2E-18     | 3     | 6      | 7   | 6   | 3.7E-14       | 0    |
| 16       | 34    | 35  | 34  | 2.1E-21     | 3     | 22    | 46  | 16  | 9.8E-21     | 3     | 16     | 17  | 16  | 0.00000       | 0    |
| 17       | 14    | 20  | 14  | 1.1E-24     | 3     | 17    | 31  | 6   | 2.4E-21     | 3     | 16     | 18  | 16  | 5.2E-13       | 0    |
| 18       | 32    | 33  | 32  | 1.1E-17     | 3     | 37    | 39  | 6   | 3.6E-21     | 3     | 19     | 23  | 19  | 6.4E-11       | 0    |
| 19       | 2     | 3   | 2   | 3.8E-17     | 3     | 2     | 3   | 1   | 7.0E-19     | 3     | 4      | 5   | 4   | 8.0E-16       | 0    |
| 20       | 13    | 17  | 13  | 8.6E-24     | 3     | 18    | 22  | 4   | 1.6E-17     | 3     | 15     | 16  | 15  | 4.1E-12       | 0    |
| 21       | 12    | 13  | 12  | 2.0E-21     | 3     | 25    | 26  | 4   | 2.4E-17     | 3     | 17     | 18  | 17  | 1.3E-15       | 0    |
| 22       | 7     | 22  | 7   | 2.1E-20     | 3     | 14    | 29  | 4   | 2.0E-18     | 3     | 9      | 11  | 9   | 3.3E-14       | 0    |
| 23       | 10    | 11  | 10  | 1.7E-18     | 3     | 21    | 38  | 7   | 8.0E-21     | 3     | 5      | 7   | 5   | 1.29373       | 3    |
| 24       | 6     | 7   | 6   | 8.0E-24     | 3     | 20    | 33  | 5   | 7.3E-18     | 3     | 7      | 8   | 7   | 1.3E-14       | 0    |
| 25       | 9     | 10  | 9   | 1.5E-24     | 3     | 29    | 30  | 5   | 2.1E-18     | 3     | 5      | 6   | 5   | 1.9E-14       | 0    |
| 26       | 12    | 13  | 12  | 1.8E-20     | 3     | 41    | 42  | 6   | 9.8E-17     | 3     | 8      | 9   | 8   | 5.4E-11       | 0    |
| 27       | 10    | 11  | 10  | 1.1E-20     | 3     | 40    | 43  | 8   | 2.6E-18     | 3     | 9      | 10  | 9   | 3.2E-12       | 0    |
| 28       | 10    | 20  | 10  | 2.3E-17     | 3     | 27    | 47  | 9   | 4.6E-19     | 3     | 8      | 9   | 8   | 1.7E-14       | 0    |
| 29       | 7     | 8   | 7   | 6.3E-17     | 3     | 14    | 43  | 7   | 1.3E-17     | 3     | 14     | 15  | 14  | 3.6E-11       | 5    |
| 30       | 11    | 16  | 11  | 2.3E-17     | 3     | 23    | 40  | 9   | 9.8E-19     | 3     | 9      | 10  | 9   | 1.1E-14       | 0    |
| $\Sigma$ | 344   | 439 | 344 | TIME = 3.31 | 30    | 616   | 863 | 160 | TIME = 3.50 | 30    | 371    | 442 | 371 | TIME = 254.25 | 26   |

Table 7: Comparison of TEQNU, TEQLU and NLEQ1S

# Appendix

## A Description of subroutines

In this section we describe easy-to-use subroutines PLISU, PLISS, PLIPU, PLIPS, PNETU, PNETS, PNEDU, PNEDS, PNECU, PNECS, PSEDU, PSEDS, PSECU, PSECS, PSENU, PGADU, PGADS, PGACU, PGACS, PMAXU, PSUMU, PEQNU, PEQLU, which can be called from the user's program. In the description of formal parameters we introduce a type of the argument denoted by two letters. The first letter is either I for integer arguments or R for double-precision real arguments. The second letter specifies whether the argument must have a value defined on the entry to the subroutine (I), whether it is a value which will be returned (O), or both (U), or whether it is an auxiliary value (A). Beside the formal parameters, we use a COMMON /STAT/ block containing statistical information. This block, used in each subroutine, has the form

```
COMMON /STAT/ NRES,NDEC,NIN,NIT,NFV,NFG,NFH
```

whose elements have the following meanings:

| Element | Type | Significance |
|---------|------|--------------|
|---------|------|--------------|

---

|      |    |  |
|------|----|--|
| NRES | IO | Number of restarts.                                      |
| NDEC | IO | Number of matrix decompositions.                         |
| NIN  | IO | Number of inner iterations (for solving linear systems). |
| NIT  | IO | Number of iterations.                                    |
| NFV  | IO | Number of function evaluations.                          |
| NFG  | IO | Number of gradient evaluations.                          |
| NFH  | IO | Number of Hessian evaluations.                           |

Easy-to-use subroutines are called by the following statements:

```
CALL PLISU(NF,X,IPAR,RPAR,F,GMAX,IPRNT,ITERM)
CALL PLISS(NF,X,IX,XL,XU,IPAR,RPAR,F,GMAX,IPRNT,ITERM)
CALL PLIPU(NF,X,IPAR,RPAR,F,GMAX,IPRNT,ITERM)
CALL PLIPS(NF,X,IX,XL,XU,IPAR,RPAR,F,GMAX,IPRNT,ITERM)
CALL PNETU(NF,X,IPAR,RPAR,F,GMAX,IPRNT,ITERM)
CALL PNETS(NF,X,IX,XL,XU,IPAR,RPAR,F,GMAX,IPRNT,ITERM)
CALL PNEDU(NF,MH,X,IH,JH,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PNEDS(NF,MH,X,IX,XL,XU,IH,JH,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PNECU(NF,MH,X,IH,JH,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PNECS(NF,MH,X,IX,XL,XU,IH,JH,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PSEDU(NF,NA,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PSEDS(NF,NA,MA,X,IX,XL,XU,AF,IAG,JAG,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PSECU(NF,NA,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PSECS(NF,NA,MA,X,IX,XL,XU,AF,IAG,JAG,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PSENU(NF,NA,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PGADU(NF,NA,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,IDER,ISPAS,IPRNT,ITERM)
```

```

CALL PGADS(NF,NA,MA,X,IX,XL,XU,AF,IAG,JAG,IPAR,RPAR,F,GMAX,IDER,ISPAS,IPRNT,ITERM)
CALL PGACU(NF,NA,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,IDER,ISPAS,IPRNT,ITERM)
CALL PGACS(NF,NA,MA,X,IX,XL,XU,AF,IAG,JAG,IPAR,RPAR,F,GMAX,IDER,ISPAS,IPRNT,ITERM)
CALL PMAXU(NF,NA,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,IEXT,ISPAS,IPRNT,ITERM)
CALL PSUMU(NF,NA,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,ISPAS,IPRNT,ITERM)
CALL PEQNU(N,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,IDER,ISPAS,IPRNT,ITERM)
CALL PEQLU(N,MA,X,AF,IAG,JAG,IPAR,RPAR,F,GMAX,IDER,ISPAS,IPRNT,ITERM)

```

Their arguments have the following meanings:

Argument Type Significance

---

|           |    |  |
|-----------|----|--|
| NF        | II | Number of variables of the objective function.   |
| NA        | II | Number of partial functions.   |
| N         | II | Number of nonlinear equations and unknowns.  |
| MH        | II | Number of nonzero elements in the upper part of the Hessian matrix. This parameter is used as input only if $ISPAS = 1$ (it defines dimensions of arrays IH and JH in this case).  |
| MA        | II | Number of nonzero elements in the Jacobian matrix. This parameter is used as input only if $ISPAS = 1$ (it defines dimensions of arrays IAG and JAG in this case).   |
| X(NF)     | RU | On input, vector with the initial estimate to the solution. On output, the approximation to the minimum.   |
| IX(NF)    | II | Vector containing the box constraint types (significant only if box constraints are considered):<br>IX(I) = 0: the variable X(I) is unbounded,<br>IX(I) = 1: the lower bound $X(I) \geq XL(I)$ ,<br>IX(I) = 2: the upper bound $X(I) \leq XU(I)$ ,<br>IX(I) = 3: the two-side bound $XL(I) \leq X(I) \leq XU(I)$ ,<br>IX(I) = 5: the variable X(I) is fixed (given by its initial estimate). |
| XL(NF)    | RI | Vector with lower bounds for variables (significant only if box constraints are considered).   |
| XU(NF)    | RI | Vector with upper bounds for variables (significant only if box constraints are considered).   |
| IH(NIH)   | IU | Row indices of the nonzero elements in the upper part of the Hessian matrix ( $NIH = NF + MH$ ) if $ISPAS = 1$ . Indices in array JH of the diagonal elements of the Hessian matrix ( $NIH = NF + 1$ ) if $ISPAS = 2$ .  |
| JH(NJH)   | IU | Column indices of the nonzero elements in the upper part of the Hessian matrix ( $NJH = NF + MH$ if $ISPAS = 1$ or $NJH = MH$ if $ISPAS = 2$ ).  |
| AF(NA)    | RO | Vector which contains values of partial functions.   |
| IAG(NIAG) | IU | Row indices of nonzero elements of the Jacobian matrix ( $NIAG = NA + MA$ ) if $ISPAS = 1$ . Indices in array JAG of the first elements in the rows of the Jacobian matrix ( $NIAG = NA + 1$ ) if $ISPAS = 2$ .  |
| JAG(NJAG) | IU | Column indices of nonzero elements of the Jacobian matrix ( $NJAG = NA + MA$ if $ISPAS = 1$ or $NJAG = MA$ if $ISPAS = 2$ ).   |
| IPAR(7)   | IU | Integer parameters (see Table 8).  |

|         |    |   |
|---------|----|---|
| RPAR(9) | RU | Real parameters (see Table 8).  |
| F       | RO | Value of the objective function at the solution $\mathbf{X}$ .  |
| GMAX    | RO | Maximum absolute value ( $l_\infty$ norm) of the gradient of the Lagrangian function.   |
| IEXT    | II | The type of minimax:<br>IEXT < 0: minimization of the maximum positive value,<br>IEXT = 0: minimization of the maximum absolute value,<br>IEXT > 0: minimization of the maximum negative value.   |
| IDER    | II | Degree of analytically computed derivatives (0 or 1).   |
| ISPAS   | II | Sparse structure of the Hessian or Jacobian matrix:<br>ISPAS = 1: the coordinate form is used,<br>ISPAS = 2: the standard row compressed format is used.  |
| IPRNT   | II | Print specification:<br>IPRNT = 0: print is suppressed,<br>IPRNT = 1: basic print of final results,<br>IPRNT = -1: extended print of final results,<br>IPRNT = 2: basic print of intermediate and final results,<br>IPRNT = -2: extended print of intermediate and final results.   |
| ITERM   | IO | Variable that indicates the cause of termination:<br>ITERM = 1: if $\ \mathbf{X} - \mathbf{X}_0\ $ was less than or equal to TOLX in two subsequent iterations ( $\mathbf{X}_0$ is the vector of variables in the previous iteration),<br>ITERM = 2: if $ \mathbf{F} - \mathbf{F}_0 $ was less than or equal to TOLF in two subsequent iterations ( $\mathbf{F}_0$ is the function value in the previous iteration),<br>ITERM = 3: if $\mathbf{F}$ is less than or equal to TOLB,<br>ITERM = 4: if GMAX is less than or equal to TOLG,<br>ITERM = 6: if termination criterion was not satisfied, but the solution is probably acceptable,<br>ITERM = 11: if NIT exceeded MIT,<br>ITERM = 12: if NFV exceeded MFV,<br>ITERM = 13: if NFG exceeded MFG,<br>ITERM < 0: if the method failed. |

Integer and real parameters **IPAR** and **RPAR** need not be defined by the user who is not familiar with details of optimization methods. If we assign zeroes to these parameters, the suitable default values are assumed. An advanced user can change these default values by his knowledge-based options. The individual parameters, presented in Table 8, have the following meanings:

Argument Type Significance

---

|     |    |   |
|-----|----|---|
| MIT | II | Maximum number of iterations; the choice MIT = 0 causes that the default value (see Table 9) will be taken.           |
| MFV | II | Maximum number of function evaluations; the choice MFV = 0 causes that the default value (see Table 9) will be taken. |
| MFG | II | Maximum number of gradient evaluations; the choice MFG = 0 causes that the default value (see Table 9) will be taken. |

| Parameter | PLIS | PLIP | PNET | PNED | PNEC | PSED | PSEC | PSEN | PGAD | PGAC | PMAX | PSUM | PEQN | PEQL |
|-----------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| IPAR(1)   | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  | MIT  |
| IPAR(2)   | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  | MFV  |
| IPAR(3)   | -    | -    | MFG  | MFG  | MFG  | MFG  | MFG  | -    | MFG  | MFG  | MFG  | MFG  | -    | -    |
| IPAR(4)   | IENT | IENT | IENT | IENT | IENT | IENT | IENT | IENT | MEC  | MEC  | IENT | IENT | -    | -    |
| IPAR(5)   | -    | MET  | MOS1 | MOS  | MOS1 | MET  | MET  | -    | MOS  | MOS1 | MED  | MED  | MOS1 | MOS1 |
| IPAR(6)   | -    | -    | MOS2 | -    | MOS2 | -    | MOS2 | MB   | -    | MOS2 | -    | -    | MOS2 | MOS2 |
| IPAR(7)   | MF   | MF   | MF   | IFIL | IFIL | IFIL | IFIL | IFIL | IFIL | IFIL | IFIL | IFIL | -    | MF   |
| RPAR(1)   | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX | XMAX |
| RPAR(2)   | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX | TOLX |
| RPAR(3)   | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF | TOLF |
| RPAR(4)   | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB | TOLB |
| RPAR(5)   | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG | TOLG |
| RPAR(6)   | FMIN | FMIN | FMIN | FMIN | FMIN | FMIN | FMIN | FMIN | FMIN | FMIN | FMIN | FMIN | -    | -    |
| RPAR(7)   | -    | -    | -    | XDEL | XDEL | -    | -    | -    | XDEL | XDEL | -    | XDEL | -    | -    |
| RPAR(8)   | -    | -    | -    | -    | -    | -    | -    | ETA3 | ETA  | ETA  | ETA4 | -    | ETA2 | ETA2 |
| RPAR(9)   | -    | -    | -    | -    | -    | -    | -    | ETA5 | -    | -    | ETA5 | ETA5 | -    | -    |

Table 8: Integer and real parameters

|      |    |   |
|------|----|---|
| IENT | II | <p>Estimation of the minimum function value for the line search:</p> <p>IENT = 0: estimation is not used,<br/> IENT = 1: lower bound FMIN is used as an estimation for the minimum function value.</p>  |
| MEC  | II | <p>Variable that determines the method of a second order correction:</p> <p>MEC = 1: correction by the Marwil sparse variable metric update,<br/> MEC = 2: correction by differences of gradients (discrete Newton correction),<br/> MEC = 3: correction by the Griewank–Toint partitioned variable metric update (symmetric rank-one).</p> <p>The choice MEC = 0 causes that the default value MEC = 2 will be taken.</p>                          |
| MED  | II | <p>Variable that specifies the method used:</p> <p>MED = 1: partitioned variable metric method,<br/> MED = 2: safeguarded discrete Newton method.</p> <p>The choice MED = 0 causes that the default value MED = 1 will be taken.</p>  |
| MET  | II | <p>In PLIP: Variable that specifies the limited-memory method:</p> <p>MET = 1: rank-one method,<br/> MET = 2: rank-two method.</p> <p>The choice MET = 0 causes that the default value MET = 2 will be taken.</p> <p>In PSED, PSEC: Variable that specifies the variable metric update:</p> <p>MET = 1: safeguarded BFGS method,<br/> MET = 2: combination of the BFGS and the symmetric rank-one method,<br/> MET = 3: discrete Newton method.</p> |

|      |    |  |
|------|----|--|
|      |    | The choice $MET = 0$ causes that the default value $MET = 2$ will be taken.  |
| MOS  | II | Method for computing the trust-region step:<br>MOS = 1: double dog-leg method of Dennis and Mei,<br>MOS = 2: method of More and Sorensen for obtaining optimum locally constrained step.<br>The choice $MOS = 0$ causes that the default value $MOS = 2$ will be taken.  |
| MOS1 | II | In PNET: Choice of restarts after constraint change:<br>MOS1 = 1: restarts are suppressed,<br>MOS1 = 2: restarts with steepest descent directions are used.<br>The choice $MOS1 = 0$ causes that the default value $MOS1 = 1$ will be taken.<br>In PNEC, PGAC: Method for computing trust-region step:<br>MOS1 = 1: Steihaug–Toint conjugate gradient method,<br>MOS1 = 2: shifted Steihaug–Toint method with five Lanczos steps,<br>MOS1 > 2: shifted Steihaug–Toint method with MOS1 Lanczos steps.<br>The choice $MOS1 = 0$ causes that the default value $MOS1 = 2$ will be taken.<br>In PEQN, PEQL: Variable that specifies the smoothing strategy for the CGS method:<br>MOS1 = 1: smoothing is not used,<br>MOS1 = 2: single smoothing strategy is used,<br>MOS1 = 3: double smoothing strategy is used.<br>The choice $MOS1 = 0$ causes that the default value $MOS1 = 3$ will be taken. |
| MOS2 | II | Choice of preconditioning strategy:<br>MOS2 = 1: preconditioning is not used,<br>MOS2 = 2: preconditioning by the incomplete Gill-Murray decomposition (in PNET, PNEC, PSEC, PGAC) or incomplete LU decomposition in PEQN, PEQL),<br>MOS2 = 3: preconditioning as in case MOS2; the preliminary solution of the preconditioned system is accepted if it satisfies the termination criteria.<br>The choice $MOS2 = 0$ causes that the default values $MOS2 = 1$ in PNET, $MOS2 = 2$ in PNEC, PSEC, PGAC or $MOS2 = 3$ in PEQN, PEQL will be taken.  |
| MB   | II | Dimension of a bundle used in the line search; the choice $MB = 0$ causes that the default value $MB = 20$ will be taken.  |
| MF   | II | The number of limited-memory variable metric updates in every iteration; the choice $MF = 0$ causes that the default values $MF = 10$ in PLIS, PLIP, PNET or $MF = 6$ in PEQL will be taken.   |
| IFIL | II | Variable that specifies a relative size of the space reserved for fill-in; the choice $IFIL = 0$ causes that the default value $IFIL = 1$ will be taken.   |
| XMAX | RI | Maximum stepsize; the choice $XMAX = 0$ causes that the default value (see Table 9) will be taken.   |
| TOLX | RI | Tolerance for the change of the coordinate vector $\mathbf{X}$ ; the choice $TOLX = 0$ causes that the default value (see Table 9) will be taken.  |
| TOLF | RI | Tolerance for the change of function values; the choice $TOLF = 0$ causes that the default value (see Table 9) will be taken.  |
| TOLB | RI | Minimum acceptable function value; the choice $TOLB = 0$ causes that the default value (see Table 9) will be taken.  |

|      |    |  |
|------|----|--|
| TOLG | RI | Tolerance for the Lagrangian function gradient; the choice $TOLG = 0$ causes that the default value (see Table 9) will be taken.   |
| FMIN | RI | Lower bound for the minimum function value. This value is not used if $IEST=0$ .   |
| XDEL | RI | Trust region step-size; the choice $XDEL = 0$ causes that a suitable default value will be computed.   |
| ETA  | RI | Parameter for switch between the Gauss-Newton method and variable metric correction; the choice $ETA = 0$ causes that the default value $ETA = 1.5 \cdot 10^{-4}$ will be taken.   |
| ETA2 | RI | Damping parameter for an incomplete LU preconditioner; the choice $ETA2 = 0$ causes that the default value $ETA2 = 0$ will be taken.   |
| ETA3 | RI | Correction parameter; the choice $ETA3 = 0$ causes that the default value $ETA3 = 10^{-12}$ will be taken.   |
| ETA4 | RI | Coefficient for the barrier parameter decrease; the choice $ETA4 = 0$ causes that the default value $ETA4 = 0.85$ will be taken.   |
| ETA5 | RI | In PSEN: Parameter for subgradient locality measure; the choice $ETA5 = 0$ causes that the default value $ETA5 = 10^{-12}$ will be taken.<br>In PMAX,PSUM: Minimum permitted value of the barrier parameter; the choice $ETA5 = 0$ causes that the default value $ETA5 = 10^{-10}$ in PMAX and $ETA5 = 10^{-8}$ in PSUM will be taken. |

| Value | PLIS<br>PLIP | PNET       | PNET<br>PNEC | PSED<br>PSEC | PSEN       | PGAD<br>PGAC | PMAX       | PSUM       | PEQL<br>PEQN |
|-------|--------------|------------|--------------|--------------|------------|--------------|------------|------------|--------------|
| MIT   | 9000         | 5000       | 5000         | 9000         | 20000      | 5000         | 10000      | 10000      | 1000         |
| MFV   | 9000         | 5000       | 5000         | 9000         | 20000      | 5000         | 10000      | 10000      | 1000         |
| MFG   | 9000         | 30000      | 10000        | 9000         | 20000      | 10000        | 20000      | 20000      | 10000        |
| XMAX  | $10^{16}$    | $10^{16}$  | $10^{16}$    | $10^{16}$    | $10^{16}$  | $10^{16}$    | $10^{16}$  | $10^{16}$  | $10^{16}$    |
| TOLX  | $10^{-16}$   | $10^{-16}$ | $10^{-16}$   | $10^{-16}$   | $10^{-16}$ | $10^{-16}$   | $10^{-16}$ | $10^{-16}$ | $10^{-16}$   |
| TOLF  | $10^{-14}$   | $10^{-14}$ | $10^{-14}$   | $10^{-14}$   | $10^{-12}$ | $10^{-14}$   | $10^{-14}$ | $10^{-12}$ | $10^{-16}$   |
| TOLB  | $10^{-16}$   | $10^{-16}$ | $10^{-16}$   | $10^{-16}$   | $10^{-12}$ | $10^{-16}$   | $10^{-16}$ | $10^{-12}$ | $10^{-16}$   |
| TOLG  | $10^{-6}$    | $10^{-6}$  | $10^{-6}$    | $10^{-6}$    | $10^{-8}$  | $10^{-6}$    | $10^{-6}$  | $10^{-6}$  | $10^{-6}$    |

Table 9: Default values

The subroutines PLISU, PLISS, PLIPU, PLIPS, PNETU, PNETS, PNEDU, PNEDS, PNECU, PNECS require the user supplied subroutines OBJ,DOBJ that define the objective function and its gradient and have the form

```

SUBROUTINE OBJ(NF,X,F)
SUBROUTINE DOBJ(NF,X,G)

```

The subroutines PSEDU, PSEDS, PSECU, PSECS, PSENU, PGADU, PGADS, PGACU, PGACS, PMAXU, PSUMU, PEQNU, PEQLU require the user supplied subroutines FUN,DFUN that define particular functions and their gradients and have the form

```

SUBROUTINE FUN(NF,KA,X,FA)
SUBROUTINE DFUN(NF,KA,X,GA)

```



If  $IDER = 0$ , the subroutine `DFUN` can be empty. The arguments of the user supplied subroutines have the following meanings:

Argument    Type    Significance

---

|                     |    |  |
|---------------------|----|--|
| <code>NF</code>     | II | Number of variables, equations and unknowns.   |
| <code>KA</code>     | II | Index of the partial function.   |
| <code>X(NF)</code>  | RI | An estimate to the solution.   |
| <code>F</code>      | RO | Value of the objective function at the point $X$ .   |
| <code>FA</code>     | RO | Value of the $KA$ -th partial function at the point $X$ .  |
| <code>G(NF)</code>  | RO | Gradient of the objective function at the point $X$ .  |
| <code>GA(NF)</code> | RO | Gradient of the $KA$ -th smooth partial function (or an arbitrary subgradient of the $KA$ -th nonsmooth partial function) at the point $X$ . |

## B Verification of subroutines

In this section we report the results obtained by using test programs `TLISU`, `TLISS`, `TLIPU`, `TLIPS`, `TNETU`, `TNETS`, `TNEDU`, `TNEDS`, `TNECU`, `TNECS`, `TSEDU`, `TSEDS`, `TSECU`, `TSECS`, `TSENU`, `TGADU`, `TGADS`, `TGACU`, `TGACS`, `TMAXU`, `TSUMU`, `TEQNU`, `TEQLU`, which serve for demonstration, verification and testing of subroutines `PLISU`, `PLISS`, `PLIPU`, `PLIPS`, `PNETU`, `PNETS`, `PNEDU`, `PNEDS`, `PNECU`, `PNECS`, `PSEDU`, `PSEDS`, `PSECU`, `PSECS`, `PSENU`, `PGADU`, `PGADS`, `PGACU`, `PGACS`, `PMAXU`, `PSUMU`, `PEQNU`, `PEQLU`. These results are listed in the following tables (rows corresponding to individual test problems contain the number of iterations `NIT`, the number of function evaluations `NFV`, the number of gradient evaluations `NFG`, the final value of the objective function `F`, the value of the termination criterion `G`, and the cause of termination `ITERM`). The last row of every table contains the total number of `NIT`, `NFV`, `NFG`, and, moreover, for programs `TNECU`, `TNECS`, `TSECU`, `TSECS`, `TGACU`, `TGACS`, `TEQNU`, `TEQLU` also the total number of conjugate gradient iterations `NCG`. The total computational time in seconds is included. All computations reported were performed on a Pentium PC computer, under the Windows XP system using the Digital Visual Fortran (Version 6) compiler, in double-precision arithmetic.

The above test programs are based on test collections `TEST14`, `TEST15`, `TEST18` described in [21], which can be downloaded from [www.cs.cas.cz/~luksan/test.html](http://www.cs.cas.cz/~luksan/test.html). The box constraints are assumed in the form  $-1 \leq x_i \leq 1$ ,  $1 \leq i \leq n$ . Subroutines for nonlinear equations were tested by problems with 3000 equations and unknowns. Subroutines for nonsmooth unconstrained optimization were tested by problems with 200 variables. The remaining subroutines were tested by problems with 1000 variables.

| Problem  | NIT   | NFV   | NFG   | F                | G           | ITERM |
|----------|-------|-------|-------|------------------|-------------|-------|
| 1        | 4988  | 5554  | 5554  | 0.963780013E-14  | 0.891E-06   | 4     |
| 2        | 425   | 454   | 454   | 14.9944763       | 0.773E-05   | 2     |
| 3        | 74    | 78    | 78    | 0.655101686E-09  | 0.539E-06   | 4     |
| 4        | 103   | 112   | 112   | 269.499543       | 0.899E-06   | 4     |
| 5        | 24    | 26    | 26    | 0.130639280E-11  | 0.671E-06   | 4     |
| 6        | 30    | 31    | 31    | 0.216102227E-10  | 0.946E-06   | 4     |
| 7        | 38    | 43    | 43    | 335.137433       | 0.730E-06   | 4     |
| 8        | 29    | 33    | 33    | 761774.954       | 0.432E-03   | 2     |
| 9        | 13    | 16    | 16    | 316.436141       | 0.369E-06   | 4     |
| 10       | 1540  | 1582  | 1582  | -124.630000      | 0.124E-04   | 2     |
| 11       | 114   | 138   | 138   | 10.7765879       | 0.380E-06   | 4     |
| 12       | 248   | 267   | 267   | 982.273617       | 0.123E-04   | 2     |
| 13       | 7     | 8     | 8     | 0.165734137E-12  | 0.453E-06   | 4     |
| 14       | 10    | 12    | 12    | 0.128729169E-08  | 0.916E-06   | 4     |
| 15       | 2830  | 2929  | 2929  | 1.92401599       | 0.936E-06   | 4     |
| 16       | 196   | 210   | 210   | -427.404476      | 0.991E-05   | 2     |
| 17       | 1007  | 1032  | 1032  | -0.379921091E-01 | 0.876E-06   | 4     |
| 18       | 1449  | 1474  | 1474  | -0.245741193E-01 | 0.862E-06   | 4     |
| 19       | 1393  | 1431  | 1431  | 59.5986241       | 0.259E-05   | 2     |
| 20       | 2129  | 2191  | 2191  | -1.00013520      | 0.908E-06   | 4     |
| 21       | 2120  | 2169  | 2169  | 2.13866377       | 0.927E-06   | 4     |
| 22       | 1305  | 1346  | 1346  | 1.00000000       | 0.982E-06   | 4     |
| $\Sigma$ | 20072 | 21136 | 21136 |                  | TIME = 8.90 |       |

Table 10: Results obtained by program TLISU

| Problem  | NIT   | NFV   | NFG   | F                | G            | ITERM |
|----------|-------|-------|-------|------------------|--------------|-------|
| 1        | 5055  | 5595  | 5595  | 0.00000000       | 0.000E+00    | 3     |
| 2        | 2016  | 2289  | 2289  | 3926.45961       | 0.304E-04    | 2     |
| 3        | 95    | 106   | 106   | 0.217616100E-12  | 0.780E-06    | 4     |
| 4        | 58    | 64    | 64    | 269.522686       | 0.124E-05    | 2     |
| 5        | 24    | 26    | 26    | 0.130639280E-11  | 0.671E-06    | 4     |
| 6        | 30    | 31    | 31    | 0.216102227E-10  | 0.946E-06    | 4     |
| 7        | 31    | 35    | 35    | 337.722479       | 0.776E-06    | 4     |
| 8        | 50    | 58    | 58    | 761925.725       | 0.257E-03    | 2     |
| 9        | 504   | 506   | 506   | 428.056916       | 0.940E-07    | 4     |
| 10       | 1152  | 1211  | 1211  | -82.0207503      | 0.176E-04    | 2     |
| 11       | 13    | 23    | 23    | 96517.2947       | 0.126E-08    | 4     |
| 12       | 79    | 88    | 88    | 4994.21410       | 0.325E-06    | 4     |
| 13       | 7     | 8     | 8     | 0.165734137E-12  | 0.453E-06    | 4     |
| 14       | 10    | 12    | 12    | 0.128729169E-08  | 0.916E-06    | 4     |
| 15       | 2830  | 2929  | 2929  | 1.92401599       | 0.936E-06    | 4     |
| 16       | 176   | 184   | 184   | -427.391653      | 0.348E-04    | 2     |
| 17       | 1007  | 1032  | 1032  | -0.379921091E-01 | 0.876E-06    | 4     |
| 18       | 1449  | 1474  | 1474  | -0.245741193E-01 | 0.862E-06    | 4     |
| 19       | 1150  | 1183  | 1183  | 1654.94525       | 0.908E-05    | 2     |
| 20       | 2211  | 2274  | 2274  | -1.00013520      | 0.886E-06    | 4     |
| 21       | 1280  | 1303  | 1303  | 2.41354873       | 0.997E-06    | 4     |
| 22       | 1562  | 1598  | 1598  | 1.00000000       | 0.786E-06    | 4     |
| $\Sigma$ | 20789 | 22029 | 22029 |                  | TIME = 11.37 |       |

Table 11: Results obtained by program TLISS

| Problem  | NIT   | NFV   | NFG   | F                | G           | ITERM |
|----------|-------|-------|-------|------------------|-------------|-------|
| 1        | 5383  | 5417  | 5417  | 0.601022658E-13  | 0.599E-06   | 4     |
| 2        | 530   | 557   | 557   | 3.57276719       | 0.124E-05   | 2     |
| 3        | 125   | 128   | 128   | 0.338270284E-12  | 0.518E-06   | 4     |
| 4        | 109   | 114   | 114   | 269.499543       | 0.669E-06   | 4     |
| 5        | 26    | 27    | 27    | 0.710072396E-11  | 0.951E-06   | 4     |
| 6        | 35    | 36    | 36    | 0.142942272E-10  | 0.737E-06   | 4     |
| 7        | 36    | 41    | 41    | 336.937181       | 0.956E-06   | 4     |
| 8        | 33    | 36    | 36    | 761774.954       | 0.192E-02   | 2     |
| 9        | 15    | 18    | 18    | 316.436141       | 0.264E-06   | 4     |
| 10       | 2003  | 2030  | 2030  | -124.950000      | 0.116E-04   | 2     |
| 11       | 157   | 175   | 175   | 10.7765879       | 0.299E-06   | 4     |
| 12       | 337   | 350   | 350   | 982.273617       | 0.145E-04   | 2     |
| 13       | 9     | 10    | 10    | 0.230414406E-14  | 0.642E-07   | 4     |
| 14       | 8     | 10    | 10    | 0.128834241E-08  | 0.977E-06   | 4     |
| 15       | 1226  | 1256  | 1256  | 1.92401599       | 0.970E-06   | 4     |
| 16       | 237   | 246   | 246   | -427.404476      | 0.501E-04   | 2     |
| 17       | 598   | 604   | 604   | -0.379921091E-01 | 0.908E-06   | 4     |
| 18       | 989   | 998   | 998   | -0.245741193E-01 | 0.975E-06   | 4     |
| 19       | 1261  | 1272  | 1272  | 59.5986241       | 0.410E-05   | 2     |
| 20       | 2045  | 2058  | 2058  | -1.00013520      | 0.911E-06   | 4     |
| 21       | 2175  | 2196  | 2196  | 2.13866377       | 0.996E-06   | 4     |
| 22       | 1261  | 1292  | 1292  | 1.00000000       | 0.927E-06   | 4     |
| $\Sigma$ | 18598 | 18871 | 18871 |                  | TIME = 8.82 |       |

Table 12: Results obtained by program TLIPU

| Problem  | NIT   | NFV   | NFG   | F                | G           | ITERM |
|----------|-------|-------|-------|------------------|-------------|-------|
| 1        | 5263  | 5321  | 5321  | 0.530131995E-13  | 0.370E-05   | 2     |
| 2        | 2293  | 2447  | 2447  | 3930.43962       | 0.251E-04   | 2     |
| 3        | 127   | 132   | 132   | 0.210550150E-12  | 0.437E-06   | 4     |
| 4        | 70    | 72    | 72    | 269.522686       | 0.794E-06   | 4     |
| 5        | 26    | 27    | 27    | 0.710072396E-11  | 0.951E-06   | 4     |
| 6        | 35    | 36    | 36    | 0.142942272E-10  | 0.737E-06   | 4     |
| 7        | 37    | 43    | 43    | 336.937181       | 0.133E-05   | 2     |
| 8        | 59    | 65    | 65    | 761925.725       | 0.399E-03   | 2     |
| 9        | 508   | 510   | 510   | 428.056916       | 0.776E-06   | 4     |
| 10       | 1253  | 1277  | 1277  | -82.5400568      | 0.120E-04   | 2     |
| 11       | 13    | 19    | 19    | 96517.2947       | 0.150E-04   | 2     |
| 12       | 95    | 102   | 102   | 4994.21410       | 0.790E-04   | 2     |
| 13       | 9     | 10    | 10    | 0.230414406E-14  | 0.642E-07   | 4     |
| 14       | 8     | 10    | 10    | 0.128834241E-08  | 0.977E-06   | 4     |
| 15       | 1226  | 1256  | 1256  | 1.92401599       | 0.970E-06   | 4     |
| 16       | 227   | 228   | 228   | -427.391653      | 0.952E-05   | 2     |
| 17       | 598   | 604   | 604   | -0.379921091E-01 | 0.908E-06   | 4     |
| 18       | 989   | 998   | 998   | -0.245741193E-01 | 0.975E-06   | 4     |
| 19       | 1367  | 1383  | 1383  | 1654.94525       | 0.105E-04   | 2     |
| 20       | 2274  | 2303  | 2303  | -1.00013520      | 0.798E-06   | 4     |
| 21       | 1196  | 1211  | 1211  | 2.41354873       | 0.975E-06   | 4     |
| 22       | 1361  | 1381  | 1381  | 1.00000000       | 0.962E-06   | 4     |
| $\Sigma$ | 19034 | 19435 | 19435 |                  | TIME = 9.42 |       |

Table 13: Results obtained by program TLIPS

| Problem  | NIT  | NFV  | NFG   | F                | G           | ITERM |
|----------|------|------|-------|------------------|-------------|-------|
| 1        | 1481 | 1656 | 26037 | 0.117631766E-15  | 0.354E-06   | 4     |
| 2        | 132  | 387  | 7945  | 0.153382199E-15  | 0.988E-08   | 4     |
| 3        | 19   | 20   | 110   | 0.421204156E-09  | 0.353E-06   | 4     |
| 4        | 19   | 20   | 230   | 269.499543       | 0.779E-07   | 4     |
| 5        | 12   | 13   | 49    | 0.465606821E-11  | 0.364E-06   | 4     |
| 6        | 13   | 14   | 76    | 0.366783327E-11  | 0.404E-06   | 4     |
| 7        | 9    | 10   | 37    | 336.937181       | 0.248E-06   | 4     |
| 8        | 11   | 12   | 58    | 761774.954       | 0.155E-07   | 4     |
| 9        | 7    | 11   | 28    | 316.436141       | 0.158E-07   | 4     |
| 10       | 75   | 153  | 3213  | -133.610000      | 0.777E-08   | 4     |
| 11       | 33   | 45   | 181   | 10.7765879       | 0.414E-07   | 4     |
| 12       | 23   | 30   | 457   | 982.273617       | 0.591E-08   | 4     |
| 13       | 7    | 8    | 16    | 0.533593908E-15  | 0.327E-07   | 4     |
| 14       | 1    | 2    | 1005  | 0.120245125E-08  | 0.879E-07   | 4     |
| 15       | 14   | 15   | 4033  | 1.92401599       | 0.468E-07   | 4     |
| 16       | 13   | 17   | 295   | -427.404476      | 0.800E-08   | 4     |
| 17       | 4    | 5    | 810   | -0.379921091E-01 | 0.537E-06   | 4     |
| 18       | 4    | 5    | 1146  | -0.245741193E-01 | 0.425E-06   | 4     |
| 19       | 10   | 11   | 1986  | 59.5986241       | 0.423E-06   | 4     |
| 20       | 18   | 39   | 3051  | -1.00013520      | 0.712E-07   | 4     |
| 21       | 7    | 8    | 4901  | 2.13866377       | 0.120E-08   | 4     |
| 22       | 55   | 145  | 4760  | 1.00000000       | 0.206E-08   | 4     |
| $\Sigma$ | 1967 | 2626 | 60424 |                  | TIME = 6.95 |       |

Table 14: Results obtained by program TNETU

| Problem  | NIT  | NFV  | NFG   | F                | G           | ITERM |
|----------|------|------|-------|------------------|-------------|-------|
| 1        | 1611 | 1793 | 28524 | 0.00000000       | 0.000E+00   | 3     |
| 2        | 259  | 259  | 4418  | 3930.43956       | 0.230E-07   | 4     |
| 3        | 17   | 18   | 98    | 0.158634811E-08  | 0.954E-06   | 4     |
| 4        | 12   | 13   | 105   | 269.522686       | 0.103E-07   | 4     |
| 5        | 12   | 13   | 49    | 0.465606821E-11  | 0.364E-06   | 4     |
| 6        | 13   | 14   | 76    | 0.366783327E-11  | 0.404E-06   | 4     |
| 7        | 9    | 10   | 37    | 336.937181       | 0.248E-06   | 4     |
| 8        | 40   | 41   | 248   | 761925.725       | 0.281E-06   | 4     |
| 9        | 553  | 555  | 2056  | 428.056916       | 0.850E-07   | 4     |
| 10       | 112  | 137  | 2109  | -84.1426617      | 0.732E-06   | 4     |
| 11       | 7    | 8    | 17    | 96517.2947       | 0.112E-11   | 4     |
| 12       | 133  | 136  | 2689  | 4994.21410       | 0.180E-06   | 4     |
| 13       | 7    | 8    | 16    | 0.533593908E-15  | 0.327E-07   | 4     |
| 14       | 1    | 2    | 1005  | 0.120245125E-08  | 0.879E-07   | 4     |
| 15       | 14   | 15   | 4033  | 1.92401599       | 0.468E-07   | 4     |
| 16       | 12   | 13   | 294   | -427.391653      | 0.594E-06   | 4     |
| 17       | 4    | 5    | 810   | -0.379921091E-01 | 0.537E-06   | 4     |
| 18       | 4    | 5    | 1146  | -0.245741193E-01 | 0.425E-06   | 4     |
| 19       | 8    | 9    | 1902  | 1654.94525       | 0.690E-07   | 4     |
| 20       | 16   | 25   | 3254  | -1.00013520      | 0.836E-08   | 4     |
| 21       | 4    | 5    | 1211  | 2.41354873       | 0.135E-06   | 4     |
| 22       | 52   | 137  | 4843  | 1.00000000       | 0.657E-06   | 4     |
| $\Sigma$ | 2900 | 3221 | 58940 |                  | TIME = 8.56 |       |

Table 15: Results obtained by program TNETS

| Problem  | NIT  | NFV  | NFG  | F                | G           | ITERM |
|----------|------|------|------|------------------|-------------|-------|
| 1        | 1421 | 1425 | 5688 | 0.465831486E-25  | 0.418E-12   | 3     |
| 2        | 39   | 45   | 200  | 0.231406390E-14  | 0.350E-06   | 4     |
| 3        | 17   | 18   | 108  | 0.839782900E-09  | 0.933E-06   | 4     |
| 4        | 24   | 25   | 100  | 269.499543       | 0.666E-10   | 4     |
| 5        | 11   | 12   | 72   | 0.795109456E-10  | 0.473E-06   | 4     |
| 6        | 13   | 16   | 196  | 0.125944855E-10  | 0.815E-06   | 4     |
| 7        | 12   | 13   | 78   | 336.937181       | 0.300E-06   | 4     |
| 8        | 4    | 5    | 90   | 761774.954       | 0.216E-06   | 4     |
| 9        | 7    | 9    | 16   | 316.436141       | 0.146E-06   | 4     |
| 10       | 69   | 75   | 630  | -135.290000      | 0.291E-11   | 4     |
| 11       | 67   | 68   | 408  | 10.7765879       | 0.199E-06   | 4     |
| 12       | 127  | 128  | 512  | 982.273617       | 0.495E-09   | 4     |
| 13       | 6    | 7    | 28   | 0.598998674E-10  | 0.693E-06   | 4     |
| 14       | 2    | 3    | 18   | 0.129013604E-08  | 0.792E-06   | 4     |
| 15       | 9    | 10   | 40   | 1.92401599       | 0.414E-06   | 4     |
| 16       | 7    | 8    | 48   | -427.404476      | 0.565E-07   | 4     |
| 17       | 8    | 9    | 54   | -0.379921091E-01 | 0.314E-10   | 4     |
| 18       | 7    | 8    | 48   | -0.245741193E-01 | 0.218E-09   | 4     |
| 19       | 6    | 7    | 42   | 59.5986241       | 0.952E-08   | 4     |
| 20       | 14   | 15   | 90   | -1.00013520      | 0.139E-08   | 4     |
| 21       | 11   | 12   | 72   | 2.13866377       | 0.331E-08   | 4     |
| 22       | 30   | 34   | 186  | 1.00000000       | 0.164E-08   | 4     |
| $\Sigma$ | 1911 | 1952 | 8724 |                  | TIME = 3.00 |       |

Table 16: Results obtained by program TNEDU

| Problem  | NIT  | NFV  | NFG   | F                | G           | ITERM |
|----------|------|------|-------|------------------|-------------|-------|
| 1        | 1420 | 1424 | 5680  | 0.00000000       | 0.000E+00   | 3     |
| 2        | 128  | 130  | 640   | 1980.05047       | 0.911E-10   | 4     |
| 3        | 17   | 19   | 108   | 0.189355864E-09  | 0.340E-06   | 4     |
| 4        | 10   | 12   | 44    | 269.522686       | 0.328E-09   | 4     |
| 5        | 13   | 15   | 84    | 0.391905635E-12  | 0.536E-06   | 4     |
| 6        | 13   | 14   | 196   | 0.136396633E-11  | 0.901E-06   | 4     |
| 7        | 30   | 32   | 186   | 336.920046       | 0.151E-05   | 2     |
| 8        | 37   | 38   | 684   | 761925.725       | 0.119E-06   | 4     |
| 9        | 507  | 508  | 1016  | 428.056916       | 0.347E-13   | 4     |
| 10       | 109  | 127  | 990   | -80.4518214      | 0.639E-06   | 4     |
| 11       | 6    | 8    | 42    | 72291.4951       | 0.178E-08   | 4     |
| 12       | 519  | 520  | 2080  | 4994.21410       | 0.236E-06   | 4     |
| 13       | 3    | 4    | 16    | 0.660542076E-23  | 0.363E-11   | 3     |
| 14       | 2    | 3    | 18    | 0.129013604E-08  | 0.792E-06   | 4     |
| 15       | 9    | 10   | 40    | 1.92401599       | 0.414E-06   | 4     |
| 16       | 15   | 18   | 96    | -427.391653      | 0.342E-06   | 4     |
| 17       | 8    | 9    | 54    | -0.379921091E-01 | 0.314E-10   | 4     |
| 18       | 7    | 8    | 48    | -0.245741193E-01 | 0.218E-09   | 4     |
| 19       | 13   | 16   | 84    | 1654.94525       | 0.174E-08   | 4     |
| 20       | 14   | 15   | 90    | -1.00013520      | 0.139E-08   | 4     |
| 21       | 9    | 10   | 60    | 2.41354873       | 0.388E-08   | 4     |
| 22       | 30   | 34   | 186   | 1.00000000       | 0.164E-08   | 4     |
| $\Sigma$ | 2919 | 2974 | 12442 |                  | TIME = 6.56 |       |

Table 17: Results obtained by program TNEDS

| Problem  | NIT  | NFV  | NFG  | F                | G           | ITERM |
|----------|------|------|------|------------------|-------------|-------|
| 1        | 1447 | 1450 | 5792 | 0.173249493E-16  | 0.138E-06   | 3     |
| 2        | 79   | 89   | 400  | 0.169144088E-20  | 0.382E-09   | 3     |
| 3        | 18   | 19   | 114  | 0.180692317E-09  | 0.316E-06   | 4     |
| 4        | 24   | 25   | 100  | 269.499543       | 0.136E-08   | 4     |
| 5        | 11   | 12   | 72   | 0.990922474E-10  | 0.511E-06   | 4     |
| 6        | 17   | 21   | 252  | 0.166904871E-10  | 0.898E-06   | 4     |
| 7        | 11   | 12   | 72   | 336.937181       | 0.629E-06   | 4     |
| 8        | 6    | 11   | 126  | 761774.954       | 0.237E-05   | 2     |
| 9        | 7    | 8    | 16   | 316.436141       | 0.362E-08   | 4     |
| 10       | 70   | 74   | 639  | -133.630000      | 0.221E-07   | 4     |
| 11       | 71   | 72   | 432  | 10.7765879       | 0.237E-10   | 4     |
| 12       | 133  | 134  | 536  | 982.273617       | 0.203E-07   | 4     |
| 13       | 7    | 8    | 32   | 0.402530175E-26  | 0.153E-13   | 3     |
| 14       | 2    | 3    | 18   | 0.129028794E-08  | 0.820E-06   | 4     |
| 15       | 10   | 11   | 44   | 1.92401599       | 0.217E-06   | 4     |
| 16       | 12   | 15   | 78   | -427.404476      | 0.894E-09   | 4     |
| 17       | 8    | 9    | 54   | -0.379921091E-01 | 0.391E-09   | 4     |
| 18       | 8    | 9    | 54   | -0.245741193E-01 | 0.705E-10   | 4     |
| 19       | 7    | 8    | 48   | 59.5986241       | 0.106E-08   | 4     |
| 20       | 10   | 11   | 66   | -1.00013520      | 0.277E-11   | 4     |
| 21       | 11   | 12   | 72   | 2.13866377       | 0.154E-06   | 4     |
| 22       | 46   | 51   | 282  | 1.00000000       | 0.376E-08   | 4     |
| $\Sigma$ | 2015 | 2064 | 9299 | NCG = 1182       | TIME = 2.92 |       |

Table 18: Results obtained by program TNECU

| Problem  | NIT  | NFV  | NFG   | F                | G           | ITERM |
|----------|------|------|-------|------------------|-------------|-------|
| 1        | 1433 | 1438 | 5736  | 0.000000000      | 0.000E-00   | 3     |
| 2        | 218  | 241  | 1085  | 3918.57298       | 0.377E+01   | 4     |
| 3        | 17   | 19   | 108   | 0.191263604E-09  | 0.349E-06   | 4     |
| 4        | 10   | 12   | 44    | 269.522686       | 0.733E-08   | 4     |
| 5        | 13   | 15   | 84    | 0.309044401E-13  | 0.194E-06   | 4     |
| 6        | 13   | 14   | 196   | 0.328095928E-12  | 0.411E-06   | 4     |
| 7        | 19   | 27   | 120   | 337.413070       | 0.438E-06   | 4     |
| 8        | 37   | 38   | 684   | 761925.725       | 0.536E-06   | 2     |
| 9        | 643  | 644  | 1288  | 428.056916       | 0.432E-13   | 4     |
| 10       | 124  | 151  | 1125  | -79.4726101      | 0.531E-07   | 4     |
| 11       | 6    | 8    | 42    | 72291.4951       | 0.188E-08   | 4     |
| 12       | 199  | 200  | 800   | 4994.21410       | 0.238E-06   | 4     |
| 13       | 4    | 5    | 20    | 0.650986116E-23  | 0.504E-11   | 3     |
| 14       | 2    | 3    | 18    | 0.129028794E-08  | 0.820E-06   | 4     |
| 15       | 10   | 11   | 44    | 1.92401599       | 0.217E-06   | 4     |
| 16       | 14   | 17   | 90    | -427.391653      | 0.114E-12   | 4     |
| 17       | 8    | 9    | 54    | -0.379921091E-01 | 0.391E-09   | 4     |
| 18       | 8    | 9    | 54    | -0.245741193E-01 | 0.705E-10   | 4     |
| 19       | 13   | 16   | 84    | 1654.94525       | 0.155E-08   | 4     |
| 20       | 10   | 11   | 66    | -1.00013520      | 0.277E-11   | 4     |
| 21       | 9    | 10   | 60    | 2.41354873       | 0.517E-06   | 4     |
| 22       | 46   | 51   | 282   | 1.00000000       | 0.376E-08   | 4     |
| $\Sigma$ | 2900 | 2989 | 12304 | NCG = 1877       | TIME = 6.17 |       |

Table 19: Results obtained by program TNECS

| Problem  | NIT  | NFV  | NFG  | F                | G           | ITERM |
|----------|------|------|------|------------------|-------------|-------|
| 1        | 2654 | 3627 | 3627 | 0.794789730E-16  | 0.213E-06   | 3     |
| 2        | 105  | 179  | 179  | 83.3161404       | 0.498E-06   | 4     |
| 3        | 40   | 45   | 45   | 0.267007684E-12  | 0.823E-06   | 4     |
| 4        | 37   | 45   | 45   | 269.499543       | 0.605E-06   | 4     |
| 5        | 16   | 17   | 17   | 0.106026711E-11  | 0.728E-06   | 4     |
| 6        | 38   | 40   | 40   | 0.546961387E-11  | 0.882E-06   | 4     |
| 7        | 22   | 26   | 26   | 335.252624       | 0.105E-06   | 4     |
| 8        | 26   | 40   | 40   | 761774.954       | 0.295E-04   | 2     |
| 9        | 193  | 202  | 202  | 316.436141       | 0.155E-05   | 2     |
| 10       | 227  | 258  | 258  | -125.810000      | 0.351E-04   | 2     |
| 11       | 100  | 127  | 127  | 10.7765879       | 0.566E-06   | 4     |
| 12       | 28   | 29   | 29   | 982.273617       | 0.102E-06   | 4     |
| 13       | 1    | 2    | 2    | 0.00000000       | 0.000E+00   | 3     |
| 14       | 25   | 28   | 28   | 0.104289352E-08  | 0.927E-06   | 4     |
| 15       | 8    | 15   | 15   | 1.92401599       | 0.482E-07   | 4     |
| 16       | 25   | 35   | 35   | -427.404476      | 0.130E-06   | 4     |
| 17       | 15   | 17   | 17   | -0.379921091E-01 | 0.141E-06   | 4     |
| 18       | 5    | 11   | 11   | -0.245741193E-01 | 0.311E-07   | 4     |
| 19       | 19   | 23   | 23   | 59.5986241       | 0.466E-06   | 4     |
| 20       | 37   | 97   | 97   | -1.00013520      | 0.212E-08   | 4     |
| 21       | 37   | 40   | 40   | 2.13866377       | 0.767E-06   | 4     |
| 22       | 55   | 211  | 211  | 1.00000000       | 0.610E-07   | 4     |
| $\Sigma$ | 3713 | 5114 | 5114 |                  | TIME = 4.27 |       |

Table 20: Results obtained by program TSEDU

| Problem  | NIT  | NFV  | NFG  | F                | G           | ITERM |
|----------|------|------|------|------------------|-------------|-------|
| 1        | 2591 | 3322 | 3322 | 0.00000000       | 0.000E+00   | 3     |
| 2        | 344  | 347  | 347  | 35.1211309       | 0.107E-06   | 4     |
| 3        | 39   | 43   | 43   | 0.441691821E-12  | 0.425E-06   | 4     |
| 4        | 21   | 22   | 22   | 269.522686       | 0.105E-06   | 4     |
| 5        | 16   | 17   | 17   | 0.783032535E-11  | 0.279E-06   | 4     |
| 6        | 32   | 33   | 33   | 0.959526458E-11  | 0.801E-06   | 4     |
| 7        | 19   | 21   | 21   | 337.722479       | 0.247E-06   | 4     |
| 8        | 52   | 56   | 56   | 761925.725       | 0.780E-04   | 2     |
| 9        | 1001 | 1003 | 1003 | 428.056916       | 0.192E-06   | 4     |
| 10       | 191  | 222  | 222  | -86.7038382      | 0.225E-05   | 2     |
| 11       | 13   | 18   | 18   | 72291.4951       | 0.285E-08   | 4     |
| 12       | 228  | 235  | 235  | 4994.21410       | 0.304E-06   | 4     |
| 13       | 1    | 2    | 2    | 0.00000000       | 0.000E+00   | 3     |
| 14       | 25   | 28   | 28   | 0.104289352E-08  | 0.927E-06   | 4     |
| 15       | 8    | 15   | 15   | 1.92401599       | 0.534E-07   | 4     |
| 16       | 21   | 22   | 22   | -427.391653      | 0.759E-06   | 4     |
| 17       | 15   | 17   | 17   | -0.379921091E-01 | 0.299E-06   | 4     |
| 18       | 5    | 10   | 10   | -0.245741193E-01 | 0.193E-07   | 4     |
| 19       | 20   | 25   | 25   | 1654.94525       | 0.351E-06   | 4     |
| 20       | 78   | 130  | 130  | -1.00013520      | 0.196E-06   | 4     |
| 21       | 27   | 31   | 31   | 2.41354873       | 0.202E-06   | 4     |
| 22       | 52   | 190  | 190  | 1.00000000       | 0.418E-06   | 4     |
| $\Sigma$ | 4799 | 5809 | 5809 |                  | TIME = 7.68 |       |

Table 21: Results obtained by program TSEDS

| Problem  | NIT  | NFV  | NFG  | F                | G           | ITERM |
|----------|------|------|------|------------------|-------------|-------|
| 1        | 2606 | 3566 | 3566 | 0.650526028E-17  | 0.969E-07   | 3     |
| 2        | 108  | 177  | 177  | 111.363179       | 0.853E-05   | 2     |
| 3        | 40   | 45   | 45   | 0.267007684E-12  | 0.823E-06   | 4     |
| 4        | 37   | 45   | 45   | 269.499543       | 0.605E-06   | 4     |
| 5        | 16   | 17   | 17   | 0.106026711E-11  | 0.728E-06   | 4     |
| 6        | 38   | 40   | 40   | 0.546961387E-11  | 0.882E-06   | 4     |
| 7        | 26   | 31   | 31   | 335.252624       | 0.315E-06   | 4     |
| 8        | 25   | 39   | 39   | 761774.954       | 0.149E-03   | 2     |
| 9        | 191  | 210  | 210  | 316.436141       | 0.115E-05   | 2     |
| 10       | 233  | 264  | 264  | -121.691827      | 0.190E-04   | 2     |
| 11       | 113  | 144  | 144  | 10.7765879       | 0.649E-07   | 4     |
| 12       | 28   | 29   | 29   | 982.273617       | 0.103E-06   | 4     |
| 13       | 1    | 2    | 2    | 0.00000000       | 0.000E+00   | 3     |
| 14       | 25   | 28   | 28   | 0.104289348E-08  | 0.927E-06   | 4     |
| 15       | 27   | 41   | 41   | 1.92401599       | 0.668E-07   | 4     |
| 16       | 25   | 35   | 35   | -427.404476      | 0.263E-06   | 4     |
| 17       | 15   | 17   | 17   | -0.379921091E-01 | 0.141E-06   | 4     |
| 18       | 8    | 12   | 12   | -0.245741193E-01 | 0.358E-11   | 4     |
| 19       | 19   | 23   | 23   | 59.5986241       | 0.466E-06   | 4     |
| 20       | 42   | 74   | 74   | -1.00013520      | 0.965E-09   | 4     |
| 21       | 37   | 40   | 40   | 2.13866377       | 0.767E-06   | 4     |
| 22       | 48   | 192  | 192  | 1.00000000       | 0.107E-06   | 4     |
| $\Sigma$ | 3708 | 5071 | 5071 | NCG = 48642      | TIME = 7.63 |       |

Table 22: Results obtained by program TSECU

| Problem  | NIT  | NFV  | NFG  | F                | G           | ITERM |
|----------|------|------|------|------------------|-------------|-------|
| 1        | 2598 | 3347 | 3347 | 0.00000000       | 0.000E+00   | 3     |
| 2        | 352  | 361  | 361  | 35.1211309       | 0.853E-05   | 2     |
| 3        | 39   | 43   | 43   | 0.441691822E-12  | 0.425E-06   | 4     |
| 4        | 21   | 22   | 22   | 269.522686       | 0.105E-06   | 4     |
| 5        | 16   | 17   | 17   | 0.783032535E-11  | 0.279E-06   | 4     |
| 6        | 32   | 33   | 33   | 0.959526458E-11  | 0.801E-06   | 4     |
| 7        | 19   | 21   | 21   | 337.722479       | 0.162E-05   | 2     |
| 8        | 46   | 49   | 49   | 761925.725       | 0.792E-04   | 2     |
| 9        | 1001 | 1003 | 1003 | 428.056916       | 0.348E-08   | 4     |
| 10       | 203  | 233  | 233  | -86.7188428      | 0.288E-04   | 2     |
| 11       | 21   | 38   | 38   | 72291.4951       | 0.135E-10   | 4     |
| 12       | 223  | 230  | 230  | 4994.21410       | 0.303E-06   | 4     |
| 13       | 1    | 2    | 2    | 0.00000000       | 0.000E+00   | 3     |
| 14       | 25   | 28   | 28   | 0.104289348E-08  | 0.927E-06   | 4     |
| 15       | 17   | 27   | 27   | 1.92401599       | 0.553E-07   | 4     |
| 16       | 21   | 22   | 22   | -427.391653      | 0.759E-06   | 4     |
| 17       | 15   | 17   | 17   | -0.379921091E-01 | 0.299E-06   | 4     |
| 18       | 8    | 12   | 12   | -0.245741193E-01 | 0.358E-11   | 4     |
| 19       | 20   | 25   | 25   | 1654.94525       | 0.351E-06   | 4     |
| 20       | 33   | 46   | 46   | -1.00013520      | 0.959E-10   | 4     |
| 21       | 27   | 31   | 31   | 2.41354873       | 0.202E-06   | 4     |
| 22       | 51   | 185  | 185  | 1.00000000       | 0.834E-06   | 4     |
| $\Sigma$ | 4789 | 5792 | 5792 | NCG = 15187      | TIME = 6.32 |       |

Table 23: Results obtained by program TSECS



| Problem  | NIT   | NFV   | NFG   | F               | G            | ITERM |
|----------|-------|-------|-------|-----------------|--------------|-------|
| 1        | 3124  | 3134  | 3134  | 0.287703261E-08 | 0.582E-08    | 4     |
| 2        | 286   | 287   | 287   | 0.379499216E-08 | 0.203E-06    | 2     |
| 3        | 71    | 71    | 71    | 0.233196848E-09 | 0.100E-07    | 4     |
| 4        | 40    | 40    | 40    | 126.863549      | 0.699E-08    | 4     |
| 5        | 282   | 282   | 282   | 0.732927514E-07 | 0.400E-08    | 4     |
| 6        | 344   | 344   | 344   | 0.836329152E-08 | 0.326E-08    | 4     |
| 7        | 286   | 287   | 287   | 2391.16999      | 0.673E-04    | 2     |
| 8        | 610   | 611   | 611   | 0.317244739E-05 | 0.548E-08    | 4     |
| 9        | 2514  | 2516  | 2516  | 552.380551      | 0.448E-08    | 4     |
| 10       | 907   | 907   | 907   | 131.888476      | 0.579E-08    | 4     |
| 11       | 269   | 271   | 271   | 0.173668302E-09 | 0.266E-08    | 4     |
| 12       | 1805  | 1810  | 1810  | 621.128947      | 0.906E-02    | 2     |
| 13       | 680   | 681   | 681   | 2940.50943      | 0.140E-03    | 2     |
| 14       | 370   | 370   | 370   | 112.314954      | 0.622E-08    | 4     |
| 15       | 364   | 364   | 364   | 36.0935676      | 0.986E-08    | 4     |
| 16       | 1004  | 1004  | 1004  | 13.2000000      | 0.904E-08    | 4     |
| 17       | 380   | 380   | 380   | 0.268534232E-01 | 0.871E-09    | 4     |
| 18       | 15319 | 15321 | 15321 | 0.589970806E-08 | 0.925E-08    | 4     |
| 19       | 3972  | 4056  | 4056  | 0.565862690E-08 | 0.887E-08    | 4     |
| 20       | 774   | 988   | 988   | 0.406495193E-08 | 0.468E-08    | 4     |
| 21       | 247   | 248   | 248   | 264.000000      | 0.364E-03    | 2     |
| 22       | 1191  | 1192  | 1192  | 593.360762      | 0.145E-03    | 2     |
| $\Sigma$ | 34839 | 35164 | 35164 |                 | TIME = 13.49 |       |

Table 24: Results obtained by program TSENU

| Problem  | NIT  | NFV  | NFG  | F               | G           | ITERM |
|----------|------|------|------|-----------------|-------------|-------|
| 1        | 1377 | 1379 | 1379 | 0.697391982E-22 | 0.130E-09   | 3     |
| 2        | 41   | 46   | 46   | 0.216572157E-16 | 0.154E-06   | 3     |
| 3        | 11   | 12   | 14   | 0.136731713E-09 | 0.233E-06   | 4     |
| 4        | 13   | 16   | 21   | 134.749772      | 0.279E-06   | 4     |
| 5        | 4    | 5    | 7    | 0.111058357E-10 | 0.887E-06   | 4     |
| 6        | 6    | 7    | 13   | 0.742148235E-26 | 0.303E-12   | 3     |
| 7        | 10   | 12   | 23   | 60734.8551      | 0.648E-07   | 4     |
| 8        | 21   | 26   | 24   | 0.253357740E-08 | 0.800E-06   | 4     |
| 9        | 15   | 16   | 36   | 2216.45871      | 0.104E-10   | 4     |
| 10       | 12   | 18   | 21   | 191.511336      | 0.524E-07   | 4     |
| 11       | 2587 | 2593 | 2649 | 0.647358980E-27 | 0.359E-12   | 3     |
| 12       | 16   | 20   | 23   | 19264.6341      | 0.513E-10   | 4     |
| 13       | 17   | 21   | 28   | 131234.018      | 0.784E-08   | 4     |
| 14       | 5    | 8    | 18   | 108.517888      | 0.227E-08   | 4     |
| 15       | 6    | 7    | 15   | 18.1763146      | 0.290E-06   | 4     |
| 16       | 15   | 21   | 40   | 2.51109677      | 0.724E-06   | 4     |
| 17       | 15   | 20   | 19   | 0.257973699E-16 | 0.275E-08   | 3     |
| 18       | 42   | 44   | 45   | 0.151517993E-24 | 0.122E-10   | 3     |
| 19       | 15   | 16   | 23   | 0.354943701E-14 | 0.255E-06   | 4     |
| 20       | 26   | 27   | 29   | 0.378161520E-10 | 0.407E-07   | 4     |
| 21       | 10   | 11   | 17   | 647.828517      | 0.773E-11   | 4     |
| 22       | 26   | 32   | 45   | 4486.97024      | 0.602E-07   | 4     |
| $\Sigma$ | 4290 | 4357 | 4535 |                 | TIME = 4.56 |       |

Table 25: Results obtained by program TGADU

| Problem  | NIT  | NFV  | NFG  | F               | G           | ITERM |
|----------|------|------|------|-----------------|-------------|-------|
| 1        | 1011 | 1013 | 1013 | 0.00000000      | 0.000E+00   | 3     |
| 2        | 260  | 273  | 508  | 1959.28649      | 0.439E-12   | 4     |
| 3        | 10   | 12   | 13   | 0.784354965E-09 | 0.868E-06   | 4     |
| 4        | 14   | 18   | 19   | 134.761343      | 0.827E-08   | 4     |
| 5        | 4    | 5    | 7    | 0.438081882E-11 | 0.697E-06   | 4     |
| 6        | 6    | 7    | 13   | 0.791460684E-17 | 0.934E-08   | 3     |
| 7        | 22   | 23   | 61   | 145814.000      | 0.000E+00   | 4     |
| 8        | 25   | 32   | 28   | 0.978141069E-06 | 0.782E-06   | 4     |
| 9        | 44   | 45   | 153  | 2220.17880      | 0.181E-09   | 4     |
| 10       | 12   | 19   | 21   | 191.511336      | 0.301E-07   | 4     |
| 11       | 3977 | 2992 | 2990 | 0.00000000      | 0.000E+00   | 3     |
| 12       | 29   | 30   | 50   | 67887.2385      | 0.438E-12   | 4     |
| 13       | 19   | 20   | 36   | 147906.000      | 0.000E+00   | 4     |
| 14       | 1    | 2    | 6    | 126.690556      | 0.000E+00   | 4     |
| 15       | 24   | 27   | 81   | 18.1763146      | 0.203E-10   | 4     |
| 16       | 46   | 50   | 135  | 3.59074140      | 0.470E-10   | 4     |
| 17       | 11   | 12   | 15   | 0.969524252E-21 | 0.171E-10   | 3     |
| 18       | 0    | 1    | 3    | 0.00000000      | 0.000E+00   | 3     |
| 19       | 26   | 30   | 34   | 0.202602070E-14 | 0.193E-06   | 4     |
| 20       | 929  | 930  | 2780 | 498.800124      | 0.359E-05   | 2     |
| 21       | 20   | 21   | 33   | 649.598077      | 0.280E-08   | 4     |
| 22       | 24   | 31   | 55   | 4488.96148      | 0.242E-07   | 4     |
| $\Sigma$ | 6514 | 5593 | 8054 |                 | TIME = 7.77 |       |

Table 26: Results obtained by program TGADS

| Problem  | NIT  | NFV  | NFG  | F               | G           | ITERM |
|----------|------|------|------|-----------------|-------------|-------|
| 1        | 1108 | 1110 | 1110 | 0.00000000      | 0.000E+00   | 3     |
| 2        | 624  | 640  | 649  | 66.4089431      | 0.283E-07   | 4     |
| 3        | 11   | 12   | 14   | 0.202412411E-09 | 0.210E-06   | 4     |
| 4        | 11   | 13   | 17   | 134.749772      | 0.592E-07   | 4     |
| 5        | 4    | 5    | 7    | 0.116836300E-10 | 0.908E-06   | 4     |
| 6        | 6    | 7    | 13   | 0.787821743E-26 | 0.311E-12   | 3     |
| 7        | 17   | 40   | 29   | 60734.8551      | 0.428E-05   | 6     |
| 8        | 22   | 25   | 25   | 0.127726626E-07 | 0.160E-06   | 4     |
| 9        | 13   | 15   | 38   | 2216.45871      | 0.846E-06   | 4     |
| 10       | 129  | 147  | 176  | 191.511336      | 0.104E-07   | 4     |
| 11       | 3010 | 3016 | 3012 | 0.402368464E-24 | 0.902E-11   | 3     |
| 12       | 205  | 226  | 236  | 22287.9069      | 0.449E-08   | 4     |
| 13       | 123  | 132  | 152  | 131234.018      | 0.743E-09   | 4     |
| 14       | 7    | 8    | 32   | 108.517888      | 0.148E-07   | 4     |
| 15       | 13   | 20   | 42   | 18.1763146      | 0.445E-05   | 2     |
| 16       | 14   | 15   | 35   | 2.51109677      | 0.103E-09   | 4     |
| 17       | 29   | 34   | 33   | 0.139780007E-09 | 0.238E-06   | 4     |
| 18       | 49   | 53   | 52   | 0.119511868E-21 | 0.344E-09   | 3     |
| 19       | 15   | 16   | 23   | 0.339085307E-13 | 0.788E-06   | 4     |
| 20       | 17   | 18   | 32   | 0.336618309E-11 | 0.137E-07   | 4     |
| 21       | 15   | 18   | 23   | 647.696136      | 0.262E-06   | 4     |
| 22       | 47   | 59   | 98   | 4486.97024      | 0.663E-08   | 4     |
| $\Sigma$ | 5489 | 5629 | 5848 | NCG = 8282      | TIME = 5.01 |       |

Table 27: Results obtained by program TGACU

| Problem  | NIT  | NFV  | NFG  | F               | G           | ITERM |
|----------|------|------|------|-----------------|-------------|-------|
| 1        | 1028 | 1031 | 1030 | 0.00000000      | 0.000E+00   | 3     |
| 2        | 263  | 262  | 511  | 1959.28649      | 0.819E-10   | 4     |
| 3        | 10   | 12   | 13   | 0.814133878E-09 | 0.897E-06   | 4     |
| 4        | 11   | 14   | 17   | 134.761343      | 0.206E-10   | 4     |
| 5        | 4    | 5    | 7    | 0.438081882E-11 | 0.697E-06   | 4     |
| 6        | 6    | 7    | 13   | 0.791460667E-17 | 0.934E-08   | 3     |
| 7        | 15   | 16   | 42   | 145814.000      | 0.000E+00   | 4     |
| 8        | 17   | 18   | 20   | 0.201167216E-07 | 0.162E-06   | 4     |
| 9        | 54   | 55   | 203  | 2220.17880      | 0.614E-10   | 4     |
| 10       | 95   | 105  | 126  | 191.511336      | 0.527E-06   | 4     |
| 11       | 4577 | 3591 | 3587 | 0.00000000      | 0.000E+00   | 3     |
| 12       | 49   | 50   | 84   | 67887.2385      | 0.351E-07   | 4     |
| 13       | 18   | 19   | 41   | 147906.000      | 0.000E+00   | 4     |
| 14       | 1    | 2    | 6    | 126.690556      | 0.000E+00   | 4     |
| 15       | 33   | 72   | 85   | 18.1763146      | 0.182E-04   | 6     |
| 16       | 8    | 12   | 29   | 3.59074140      | 0.542E-06   | 4     |
| 17       | 25   | 29   | 29   | 0.716457302E-10 | 0.922E-07   | 4     |
| 18       | 0    | 1    | 3    | 0.00000000      | 0.000E+00   | 3     |
| 19       | 28   | 32   | 36   | 0.209831733E-13 | 0.620E-06   | 4     |
| 20       | 937  | 938  | 2806 | 498.800124      | 0.572E-12   | 4     |
| 21       | 21   | 22   | 34   | 649.598077      | 0.324E-08   | 4     |
| 22       | 44   | 51   | 89   | 4488.96148      | 0.645E-10   | 4     |
| $\Sigma$ | 7244 | 6344 | 8811 | NCG = 11206     | TIME = 6.56 |       |

Table 28: Results obtained by program TGACS

| Problem  | NIT  | NFV  | NFG  | C                | G           | ITERM |
|----------|------|------|------|------------------|-------------|-------|
| 1        | 53   | 66   | 54   | 0.260681654E-14  | 0.120E-07   | 4     |
| 2        | 107  | 160  | 108  | 0.502441303E-12  | 0.262E-06   | 4     |
| 3        | 33   | 41   | 34   | 0.535439934E-08  | 0.814E-06   | 4     |
| 4        | 51   | 93   | 52   | 0.540217976      | 0.383E-06   | 4     |
| 5        | 23   | 24   | 24   | 0.132910215E-08  | 0.482E-06   | 4     |
| 6        | 46   | 52   | 47   | 0.216701250E-08  | 0.436E-06   | 4     |
| 7        | 48   | 113  | 49   | 0.260162540      | 0.430E-06   | 4     |
| 8        | 21   | 58   | 22   | 282.380956       | 0.806E-06   | 4     |
| 9        | 59   | 146  | 60   | 0.185849706      | 0.287E-06   | 4     |
| 10       | 159  | 215  | 160  | -0.251638288     | 0.250E-06   | 4     |
| 11       | 70   | 96   | 71   | 0.538829394E-01  | 0.139E-07   | 4     |
| 12       | 136  | 245  | 137  | 0.941962422      | 0.207E-06   | 4     |
| 13       | 2    | 4    | 3    | 0.456380111E-19  | 0.304E-11   | 3     |
| 14       | 5    | 6    | 6    | 0.162409086E-08  | 0.671E-06   | 4     |
| 15       | 116  | 120  | 117  | 0.199003538E-01  | 0.436E-06   | 4     |
| 16       | 110  | 214  | 111  | -0.388943896E-02 | 0.518E-05   | 2     |
| 17       | 33   | 49   | 34   | -0.110417781E-06 | 0.764E-06   | 4     |
| 18       | 62   | 77   | 63   | 0.744234285E-09  | 0.611E-07   | 4     |
| 19       | 9    | 23   | 10   | 42.6746811       | 0.373E-09   | 4     |
| 20       | 25   | 32   | 26   | -0.497512435E-02 | 0.422E-06   | 4     |
| 21       | 16   | 23   | 17   | 0.298487756E-01  | 0.595E-06   | 4     |
| 22       | 32   | 82   | 33   | 0.577532726E-02  | 0.972E-07   | 4     |
| $\Sigma$ | 1216 | 1939 | 1238 |                  | TIME = 0.75 |       |

Table 29: Results obtained by program TMAXU

| Problem  | NIT  | NFV  | NFG  | C               | G           | ITERM |
|----------|------|------|------|-----------------|-------------|-------|
| 1        | 337  | 355  | 338  | 0.193178806E-13 | 0.254E-05   | 3     |
| 2        | 127  | 151  | 128  | 0.120336380E-12 | 0.424E-05   | 3     |
| 3        | 25   | 28   | 26   | 0.383710546E-09 | 0.331E-06   | 4     |
| 4        | 67   | 77   | 68   | 126.863549      | 0.358E-02   | 2     |
| 5        | 6    | 7    | 7    | 0.494049246E-14 | 0.666E-07   | 3     |
| 6        | 13   | 17   | 14   | 0.663150090E-13 | 0.141E-06   | 3     |
| 7        | 73   | 108  | 74   | 2391.16999      | 0.209E+00   | 2     |
| 8        | 241  | 243  | 242  | 0.383133726E-07 | 0.708E-06   | 4     |
| 9        | 209  | 251  | 209  | 552.682636      | 0.267E+01   | -6    |
| 10       | 84   | 106  | 85   | 131.888475      | 0.242E-05   | 2     |
| 11       | 732  | 751  | 733  | 0.799693645E-12 | 0.581E-05   | 3     |
| 12       | 203  | 237  | 204  | 612.723020      | 0.601E-04   | 2     |
| 13       | 90   | 111  | 91   | 2940.50941      | 0.245E-03   | 2     |
| 14       | 84   | 107  | 85   | 112.314955      | 0.480E-05   | 2     |
| 15       | 39   | 64   | 40   | 36.0935678      | 0.163E-01   | 2     |
| 16       | 67   | 108  | 67   | 13.2000005      | 0.139E-03   | 6     |
| 17       | 337  | 344  | 338  | 0.100472795E-13 | 0.167E-06   | 3     |
| 18       | 3637 | 3794 | 3638 | 0.199840144E-14 | 0.419E-09   | 3     |
| 19       | 23   | 24   | 24   | 0.938360500E-12 | 0.217E-04   | 3     |
| 20       | 22   | 44   | 22   | 0.121058719E-11 | 0.398E-05   | 6     |
| 21       | 65   | 90   | 66   | 262.921649      | 0.108E-05   | 2     |
| 22       | 608  | 627  | 609  | 593.367735      | 0.525E-02   | 2     |
| $\Sigma$ | 7089 | 7644 | 7108 |                 | TIME = 2.80 |       |

Table 30: Results obtained by program TSUMU

| Problem  | NIT | NFV  | NFG | F            | G            | ITERM |
|----------|-----|------|-----|--------------|--------------|-------|
| 1        | 10  | 41   | 0   | 0.224531E-22 | 0.168207E-07 | 3     |
| 2        | 9   | 46   | 0   | 0.106897E-22 | 0.163517E-06 | 3     |
| 3        | 3   | 19   | 0   | 0.333989E-19 | 0.223053E-06 | 3     |
| 4        | 7   | 23   | 0   | 0.348196E-17 | 0.177085E-02 | 3     |
| 5        | 12  | 63   | 0   | 0.117206E-16 | 0.694210E-06 | 3     |
| 6        | 17  | 52   | 0   | 0.110919E-16 | 0.167579E-11 | 3     |
| 7        | 13  | 41   | 0   | 0.339913E-19 | 0.457009E-03 | 3     |
| 8        | 13  | 73   | 0   | 0.125748E-25 | 0.193922E-04 | 3     |
| 9        | 13  | 99   | 0   | 0.432936E-21 | 0.201706E-03 | 3     |
| 10       | 5   | 41   | 0   | 0.803846E-25 | 0.415983E-03 | 3     |
| 11       | 12  | 37   | 0   | 0.189327E-25 | 0.423583E-05 | 3     |
| 12       | 18  | 55   | 0   | 0.129272E-16 | 0.713317E-13 | 3     |
| 13       | 18  | 39   | 0   | 0.105290E-16 | 0.341327E-13 | 3     |
| 14       | 4   | 13   | 0   | 0.774783E-20 | 0.441968E-05 | 3     |
| 15       | 5   | 36   | 0   | 0.182567E-17 | 0.471251E-03 | 3     |
| 16       | 53  | 319  | 0   | 0.462169E-17 | 0.153957     | 3     |
| 17       | 14  | 48   | 0   | 0.449140E-22 | 0.105525E-03 | 3     |
| 18       | 26  | 79   | 0   | 0.977445E-16 | 0.245792E-01 | 3     |
| 19       | 2   | 7    | 0   | 0.309324E-21 | 0.370062E-09 | 3     |
| 20       | 13  | 43   | 0   | 0.428279E-20 | 0.203421E-07 | 3     |
| 21       | 12  | 37   | 0   | 0.200623E-20 | 0.255404E-10 | 3     |
| 22       | 7   | 50   | 0   | 0.195350E-19 | 0.106707E-05 | 3     |
| 23       | 29  | 262  | 0   | 0.390327E-17 | 0.200697E-10 | 3     |
| 24       | 6   | 31   | 0   | 0.822526E-23 | 0.812457E-09 | 3     |
| 25       | 9   | 46   | 0   | 0.147127E-23 | 0.395357E-09 | 3     |
| 26       | 12  | 61   | 0   | 0.608837E-17 | 0.420862E-07 | 3     |
| 27       | 10  | 51   | 0   | 0.275078E-20 | 0.121824E-06 | 3     |
| 28       | 10  | 60   | 0   | 0.229532E-16 | 0.213811E-05 | 3     |
| 29       | 4   | 53   | 0   | 0.124549E-19 | 0.130673E-05 | 3     |
| 30       | 12  | 162  | 0   | 0.222959E-21 | 0.107876E-07 | 3     |
| $\Sigma$ | 378 | 1987 | 0   | NCG = 1543   | TIME = 3.81  |       |

Table 31: Results obtained by program TEQNU

| Problem  | NIT | NFV  | NFG | F            | G            | ITERM |
|----------|-----|------|-----|--------------|--------------|-------|
| 1        | 30  | 64   | 0   | 0.326079E-18 | 0.154142E-03 | 3     |
| 2        | 17  | 57   | 0   | 0.720058E-19 | 0.261551E-07 | 3     |
| 3        | 5   | 11   | 0   | 0.861220E-16 | 0.366389E-03 | 3     |
| 4        | 11  | 19   | 0   | 0.115060E-18 | 0.358897E-01 | 3     |
| 5        | 20  | 56   | 0   | 0.335602E-16 | 0.121910E-06 | 3     |
| 6        | 22  | 31   | 0   | 0.167377E-16 | 0.898624E-08 | 3     |
| 7        | 25  | 42   | 0   | 0.137004E-20 | 0.185851E-05 | 3     |
| 8        | 21  | 60   | 0   | 0.496243E-28 | 0.183782E-07 | 3     |
| 9        | 32  | 71   | 0   | 0.220876E-21 | 0.800603E-05 | 3     |
| 10       | 9   | 24   | 0   | 0.202316E-20 | 0.162996E-03 | 3     |
| 11       | 16  | 23   | 0   | 0.116022E-21 | 0.130018E-02 | 3     |
| 12       | 23  | 40   | 0   | 0.861690E-16 | 0.190460E-08 | 3     |
| 13       | 24  | 32   | 0   | 0.234892E-16 | 0.204525E-08 | 3     |
| 14       | 8   | 13   | 0   | 0.596974E-21 | 0.811563E-05 | 3     |
| 15       | 12  | 28   | 0   | 0.124901E-17 | 0.305897     | 3     |
| 16       | 22  | 78   | 0   | 0.984840E-20 | 0.125407E-03 | 3     |
| 17       | 17  | 43   | 0   | 0.130235E-20 | 0.154659E-04 | 3     |
| 18       | 46  | 61   | 0   | 0.224793E-17 | 0.116353E-01 | 3     |
| 19       | 2   | 5    | 0   | 0.704403E-18 | 0.221630E-06 | 3     |
| 20       | 18  | 30   | 0   | 0.158787E-16 | 0.312477E-03 | 3     |
| 21       | 25  | 34   | 0   | 0.233925E-16 | 0.135133E-05 | 3     |
| 22       | 14  | 45   | 0   | 0.189862E-17 | 0.128826E-01 | 3     |
| 23       | 23  | 106  | 0   | 0.194742E-18 | 0.550497E-08 | 3     |
| 24       | 20  | 53   | 0   | 0.737500E-17 | 0.611156E-08 | 3     |
| 25       | 29  | 50   | 0   | 0.208794E-17 | 0.413643E-08 | 3     |
| 26       | 36  | 67   | 0   | 0.132055E-17 | 0.481013E-08 | 3     |
| 27       | 40  | 75   | 0   | 0.659356E-17 | 0.862034E-08 | 3     |
| 28       | 27  | 83   | 0   | 0.461856E-18 | 0.268680E-08 | 3     |
| 29       | 12  | 95   | 0   | 0.206962E-16 | 0.754042E-08 | 3     |
| 30       | 18  | 145  | 0   | 0.740533E-16 | 0.167985E-07 | 3     |
| $\Sigma$ | 624 | 1541 | 0   | NCG = 1332   | TIME = 3.22  |       |

Table 32: Results obtained by program TEQLU

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