

NLPQL

NLPQL

Introduction

Overview

Welcome to the TOMLAB /NLPQL User's Guide. TOMLAB /NLPQL includes the NLPQLP, NLPJOB and DFNLP solvers from Klaus Schittkowski and an interface to The MathWorks' MATLAB.

TOMLAB /NLPQL solves general nonlinear mathematical programming problems with equality and inequality constraints. It is assumed that all problem functions are continuously differentiable.

The internal algorithm is a sequential quadratic programming (SQP) method. Proceeding from a quadratic approximation of the Lagrangian function and a linearization of the constraints, a quadratic subproblem is formulated and solved by dual code. Subsequently a line search is performed with respect to two alternative merit functions and the Hessian approximation is updated by the modified BFGS-formula.

TOMLAB /NLPJOB solves multicriteria optimization problems. NLPJOB offers a total of 15 different possibilities to transform the objective function vector into a scalar function. An SQP method is also used to solve the problem in this case.

TOMLAB /DFNLP is a sequential quadratic programming method for solving nonlinear data fitting problems. The algorithm introduces new decision variables as well as constraints to formulate a smooth nonlinear programming problem, which is solved by SQP.

Contents of this Manual

- #Introduction provides a basic overview of the TOMLAB /NLPQL solver package.
- #Using the Matlab Interface provides an overview of the Matlab interface to NLPQL.
- #Setting NLPQL Options describes how to set NLPQL solver options from Matlab.
- #NLPQL Solver Reference gives detailed information about the interface routine *nlpqlTL*.
- #NLPJOB Solver Reference gives detailed information about the interface routine *nlpjobTL*.
- #DFNLP Solver Reference gives detailed information about the interface routine *dfnlpTL*.

More information

Please visit the following links for more information:

- <http://tomopt.com/tomlab/products/nlpql/> ^[1]
- <http://www.uni-bayreuth.de/departments/math/~kschittkowski/nlpql.htm> ^[2]

Prerequisites

In this manual we assume that the user is familiar with global optimization and nonlinear programming, setting up problems in TOMLAB (in particular constrained nonlinear (**con**) problems) and the Matlab language in general.

Using the Matlab Interface

The NLPQL solver is accessed via the *tomRun* driver routine, which calls the *nlpqITL* interface routine. The solver itself is located in the MEX file *nlpql*. The same applies for the other two solvers.

Observe that *clsAssign* should be used when defining the problem for NLPJOB and DFNLP, as the problem solved is multi criteria, i.e. has several objective functions.

| Function | Description |
|------------------|---|
| <i>nlpqITL</i> | The interface routine called by the TOMLAB driver routine <i>tomRun</i> . This routine then calls the MEX file <i>nlpql</i> |
| <i>nlpjobITL</i> | The interface routine called by the TOMLAB driver routine <i>tomRun</i> . This routine then calls the MEX file <i>nlpjob</i> |
| <i>dfnlpITL</i> | The interface routine called by the TOMLAB driver routine <i>tomRun</i> . This routine then calls the MEX file <i>dfnlp</i> |

Setting NLPQL Options

All NLPQL control parameters are possible to set from Matlab.

Setting options using the Prob.NLPQL structure

The parameters can be set as subfields in the *Prob.NLPQL* structure. The following example shows how to set a limit on the maximum number of iterations.

```
Prob = conAssign(...) % Setup problem, see help conAssign for more information
Prob.NLPQL.maxit = 2000; % Setting maximum number of iterations
```

The maximum number of iterations can also be done through the TOMLAB parameter *MaxIter*:

```
Prob.optParam.MaxIter = 200;
```

In the cases where a solver specific parameter has a corresponding TOMLAB general parameter, the latter is used only if the user has not given the solver specific parameter.

A complete description of the available NLPQL parameters can be found in *#nlpqITL*.

NLPQL Solver Reference

A detailed description of the TOMLAB /NLPQL solver interface is given below. Also see the M-file help for *nlpqITL.m*.

nlpqITL

Purpose

Solves constrained nonlinear programming problems.

NLPQL solves problems of the form

$$\min_x f(x)$$

$$s/t \quad \begin{array}{l} x_L \leq x \leq x_U \\ b_L \leq Ax \leq b_U \\ c_L \leq c(x) \leq c_U \end{array}$$

where $x, x_L, x_U \in R^n$, $A \in R^{m_1 \times n}$, $b_L, b_U \in R^{m_1}$ and $c(x), c_L, c_U \in R^{m_2}$.

Calling Syntax

```
Prob = conAssign( ... );
Result = tomRun('nlpql', Prob, ...);
```

Description of Inputs

Prob Problem description structure. The following fields are used:

| Input | Description |
|------------------|--|
| <i>A</i> | Linear constraints coefficient matrix. |
| <i>x_L, x_U</i> | Bounds on variables. |
| <i>b_L, b_U</i> | Bounds on linear constraints. |
| <i>c_L, c_U</i> | Bounds on nonlinear constraints. For equality constraints (or fixed variables), set e.g. $b_L(k) == b_U(k)$. |
| <i>PriLevOpt</i> | Print level in MEX interface. |
| <i>WarmStart</i> | If true, use warm start, otherwise cold start. When using WarmStart the following parameters are required: <i>NLPQL.u</i> Contains the multipliers with respect to the actual iterate stored in the first column of X. The first M locations contain the multipliers of the M nonlinear constraints, the subsequent N locations the multipliers of the lower bounds, and the final N locations the multipliers of the upper bounds. At an optimal solution, all multipliers with respect to inequality constraints should be nonnegative. |
| <i>NLPQL.c</i> | On return, C contains the last computed approximation of the Hessian matrix of the Lagrangian function stored in form of an LDL decomposition. C contains the lower triangular factor of an LDL factorization of the final quasi-Newton matrix (without diagonal elements, which are always one). In the driving program, the row dimension of C has to be equal to NMAX. |
| <i>NLPQL.d</i> | The elements of the diagonal matrix of the LDL decomposition of the quasi-Newton matrix are stored in the one-dimensional array D. |
| <i>NLPQL</i> | Structure with special fields for the NLPQL solver: |
| <i>maxfun</i> | The integer variable defines an upper bound for the number of function calls during the line search. |
| <i>maxit</i> | Maximum number of outer iterations, where one iteration corresponds to one formulation and solution of the quadratic programming subproblem, or, alternatively, one evaluation of gradients. |
| <i>acc</i> | The user has to specify the desired final accuracy (e.g. 1.0e-7). The termination accuracy should not be smaller than the accuracy by which gradients are computed. |
| <i>accqp</i> | The tolerance is needed for the QP solver to perform several tests, for example whether optimality conditions are satisfied or whether a number is considered as zero or not. If ACCQP is less or equal to zero, then the machine precision is computed by NLPQL and subsequently multiplied by 1.0e+4. |
| <i>PrintFile</i> | Name of NLPQL Print file. Amount and type of printing determined by PriLevOpt. |

Description of Outputs

Result Structure with result from optimization. The following fields are set:

| Output | Description |
|-------------------|---|
| f_k | Function value at optimum. |
| g_k | Gradient of the function. |
| x_k | Solution vector. |
| x_0 | Initial solution vector. |
| c_k | Nonlinear constraint residuals. |
| $cJac$ | Nonlinear constraint gradients. |
| $xState$ | State of variables. Free == 0; On lower == 1; On upper == 2; Fixed == 3; |
| $bState$ | State of linear constraints. Free == 0; Lower == 1; Upper == 2; Equality == 3; |
| $cState$ | State of nonlinear constraints. Free == 0; Lower == 1; Upper == 2; Equality == 3; |
| $ExitFlag$ | Exit status from NLPQL MEX. |
| $ExitText$ | Exit text from NLPQL MEX. |
| $Inform$ | NLPQL information parameter. |
| $FuncEv$ | Number of function evaluations. |
| $GradEv$ | Number of gradient evaluations. |
| $ConstrEv$ | Number of constraint evaluations. |
| $QP.B$ | Basis vector in TOMLAB QP standard. |
| $Solver$ | Name of the solver (NLPQL). |
| $SolverAlgorithm$ | Description of the solver. |
| $NLPQL.act$ | The logical array indicates constraints, which NLPQL considers to be active at the last computed iterate. |
| $NLPQL.u$ | See inputs. |
| $NLPQL.c$ | See inputs. |
| $NLPQL.d$ | See inputs. |

NLPJOB Solver Reference

A detailed description of the TOMLAB /NLPJOB solver interface is given below. Also see the M-file help for *nlpjobTL.m*. The 15 different possibilities for the scalar objective function are listed below.

nlpjobTL

Purpose

Solves multicriteria nonlinear programming problems.

NLPJOB solves problems of the form

$$\min_x f(1, x), \dots, f(L, x)$$

$$s/t \quad \begin{array}{l} x_L \leq x \leq x_U \\ b_L \leq Ax \leq b_U \\ c_L \leq c(x) \leq c_U \end{array}$$

where $x, x_L, x_U \in R^n$, $A \in R^{m_1 \times n}$, $b_L, b_U \in R^{m_1}$ and $c(x), c_L, c_U \in R^{m_2}$.

L is the number of objective functions. For details on the objective function see that different methods below.

Calling Syntax

```
Prob = clsAssign( ... );
Result = tomRun('nlpjob', Prob, ...);
```

Description of Inputs

Prob Problem description structure. The following fields are used:

| Input | Description |
|------------------|--|
| <i>A</i> | Linear constraints coefficient matrix. |
| <i>x_L, x_U</i> | Bounds on variables. |
| <i>b_L, b_U</i> | Bounds on linear constraints. |
| <i>c_L, c_U</i> | Bounds on nonlinear constraints. For equality constraints (or fixed variables), set e.g. $b_L(k) == b_U(k)$. |
| <i>PriLevOpt</i> | Print level in MEX interface. |
| <i>NLPJOB</i> | <p>Structure with special fields for the NLPJOB solver:</p> <p><i>model</i> Desired scalar transformation as indicated below.</p> <p>1 Weighted sum: The scalar objective function is the weighted sum of individual objectives, i.e., $F(X) := W_1 * F_1(X) + W_2 * F_2(X) + \dots + W_L * F_L(X)$, where W_1, \dots, W_L are non-negative weights given by the user.</p> <p>2 Hierarchical optimization method: The idea is to formulate a sequence of L scalar optimization problems with respect to the individual objective functions subject to bounds on previously computed optimal values, i.e., we minimize $F(X) := F_I(X)$, $I = 1, \dots, L$ subject to the original and the additional constraints $F_J(X) \leq (1 + EJ/100) * F_J$, $J = 1, \dots, I-1$, where EJ is the given coefficient of relative function increment as defined by the user and where F_J is the individual minimum. It is assumed that the objective functions are ordered with respect to their importance.</p> <p>3 Trade-off method: One objective is selected by the user and the other ones are considered as constraints with respect to individual minima, i.e., $F(X) := F_I(X)$ is minimized subject to the original and some additional constraints of the form $F_J(X) \leq EJ$, $J = 1, \dots, L, J \neq I$, where EJ is a bound value of the J-th objective function.</p> <p>4 Method of distance functions in L1-norm: A sum of absolute values of the differences of objective functions from predetermined goals Y_1, \dots, Y_L is minimized, i.e., $F(X) := F_1(X) - Y_1 + \dots + F_L(X) - Y_L$. The goals are given by the user and their choice requires some knowledge about the ideal solution vector.</p> <p>5 Method of distance functions in L2-norm: A sum of squared values of the differences of objective functions from predetermined goals Y_1, \dots, Y_L is minimized, $F(X) := (F_1(X) - Y_1)^2 + \dots + (F_L(X) - Y_L)^2$. Again the goals are provided by the user.</p> <p>6 Global criterion method: The scalar function to be minimized, is the sum of relative distances of individual objectives from their known minimal values, i.e., $F(X) := (F_1(X) - F_1)/ F_1 + \dots + (F_L(X) - F_L)/ F_L$ where F_1, \dots, F_L are the optimal function values obtained by minimizing $F_1(x), \dots, F_L(x)$ subject to original constraints.</p> <p>7 Global criterion method in L2-norm: The scalar function to be minimized, is the sum of squared distances of individual objectives from their known optimal values, i.e., $F(X) := ((F_1 - F_1(X))/ F_1)^2 + \dots + ((F_L - F_L(X))/ F_L)^2$ where F_1, \dots, F_L are the individual optimal function values.</p> <p>8 Min-max method no. 1: The maximum of absolute values of all objectives is minimized, i.e., $F(X) := \text{MAX}(F_I(X) , I = 1, \dots, L)$</p> <p>9 Min-max method no. 2: The maximum of all objectives is minimized, i.e., $F(X) := \text{MAX}(F_I(X), I = 1, \dots, L)$</p> |

| | |
|------------------|---|
| | <p>10 Min-max method no. 3: The maximum of absolute distances of objective function values from given goals Y_1, \dots, Y_L is minimized, i.e., $F(X) := \text{MAX}(F_I(X) - Y_I , I = 1, \dots, L)$. The goals must be determined by the user.</p> <p>11 Min-max method no. 4: The maximum of relative distances of objective function values from ideal values is minimized, i.e., $F(X) := \text{MAX}((F_I(X) - F_I)/F_I, I = 1, \dots, L)$</p> <p>12 Min-max method no. 5: The maximum of weighted relative distances of objective function values from individual minimal values is minimized, $F(X) := \text{MAX}(W_I * (F_I(X) - F_I)/F_I, I = 1, \dots, L)$. Weights must be provided by the user.</p> <p>13 Min-max method no. 6: The maximum of weighted objective function values is minimized, i.e., $F(X) := \text{MAX}(W_I * F_I(X), I = 1, \dots, L)$ Weights must be provided by the user.</p> <p>14 Weighted global criterion method: The scalar function to be minimized, is the weighted sum of relative distances of individual objectives from their goals, i.e., $F(X) := (F_1(X) - Y_1)/Y_1 + \dots + (F_L(X) - Y_L)/Y_L$ The weights W_1, \dots, W_L and the goals Y_1, \dots, Y_L must be set by the user.</p> <p>15 Weighted global criterion method in L2-norm: The scalar function to be minimized, is the weighted sum of squared relative distances of individual objectives from their goals, i.e., $F(X) := ((F_1(X) - Y_1)/Y_1)^2 + \dots + ((F_L(X) - Y_L)/Y_L)^2$ The weights W_1, \dots, W_L and the goals Y_1, \dots, Y_L must be set by the user.</p> |
| <i>imin</i> | If necessary (model = 2 or 3), <i>imin</i> defines the index of the objective function to be taken into account for the desired scalar transformation. |
| <i>maxf</i> | The integer variable defines an upper bound for the number of function calls during the line search (e.g. 20). |
| <i>maxit</i> | Maximum number of iterations, where one iteration corresponds to one formulation and solution of the quadratic programming subproblem, or, alternatively, one evaluation of gradients (e.g. 100). |
| <i>acc</i> | The user has to specify the desired final accuracy (e.g. 1.0e-7). The termination accuracy should not be much smaller than the accuracy by which gradients are computed. |
| <i>scbou</i> | The real variable allows an automatic scaling of the problem functions. If at the starting point x_0 , a function value is greater than SCBOU (e.g. E+3), then the function is divided by the square root. If SCBOU is set to any negative number, then the objective function will be multiplied by the value stored in WA(MMAX+1) and the J th constraint function by the value stored in WA(J), $J=1, \dots, M$. |
| <i>w</i> | Weight vector of dimension L , to be filled with suitable values when calling NLPJOB depending on the transformation model: MODEL=1,10,12,13,14,15 - weights, MODEL=2 - bounds, MODEL=3 - bounds for objective functions, MODEL=4,5 - goal values. |
| <i>fk</i> | For MODEL=2,6,7,11,12,14,15, FK has to contain the optimal values of the individual scalar subproblems when calling NLPJOB. |
| <i>PrintFile</i> | Name of NLPJOB Print file. Amount and type of printing determined by PriLevOpt. |

Description of Outputs

Result Structure with result from optimization. The following fields are set:

| Output | Description |
|-----------------|---|
| <i>f_k</i> | Function value at optimum. |
| <i>g_k</i> | Gradient of the function. |
| <i>x_k</i> | Solution vector. |
| <i>x_0</i> | Initial solution vector. |
| <i>c_k</i> | Nonlinear constraint residuals. |
| <i>cJac</i> | Nonlinear constraint gradients. |
| <i>xState</i> | State of variables. Free == 0; On lower == 1; On upper == 2; Fixed == 3; |
| <i>bState</i> | State of linear constraints. Free == 0; Lower == 1; Upper == 2; Equality == 3; |
| <i>cState</i> | State of nonlinear constraints. Free == 0; Lower == 1; Upper == 2; Equality == 3; |
| <i>ExitFlag</i> | Exit status from NLPJOB MEX. |
| <i>ExitText</i> | Exit text from NLPJOB MEX. |
| <i>Inform</i> | NLPJOB information parameter. |
| <i>FuncEv</i> | Number of function evaluations. |

| | |
|------------------------|---|
| <i>GradEv</i> | Number of gradient evaluations. |
| <i>ConstrEv</i> | Number of constraint evaluations. |
| <i>QP.B</i> | Basis vector in TOMLAB QP standard. |
| <i>Solver</i> | Name of the solver (NLPJOB). |
| <i>SolverAlgorithm</i> | Description of the solver. |
| <i>NLPJOB.u</i> | Contains the multipliers with respect to the actual iterate stored in X. The first M locations contain the multipliers of the nonlinear constraints, the subsequent N locations the multipliers of the lower bounds, and the final N locations the multipliers of the upper bounds subject to the scalar subproblem chosen. At an optimal solution, all multipliers with respect to inequality constraints should be nonnegative. |
| <i>NLPJOB.act</i> | The logical array indicates constraints, which NLPJOB considers to be active at the last computed iterate. |

DFNLP Solver Reference

A detailed description of the TOMLAB /DFNLP solver interface is given below. Also see the M-file help for *dfnlpTL.m*.

dfnlpTL

Purpose

Solves nonlinear data fitting problems.

DFNLP solves problems of the form

$$\min_x f(1, x), \dots, f(L, x)$$

$$\begin{array}{l} s/t \\ x_L \leq x \leq x_U \\ b_L \leq Ax \leq b_U \\ c_L \leq c(x) \leq c_U \end{array}$$

where $x, x_L, x_U \in R^n$, $A \in R^{m_1 \times n}$, $b_L, b_U \in R^{m_1}$ and $c(x), c_L, c_U \in R^{m_2}$.

L is the number of objective functions. For details on the objective function see that different methods below.

Calling Syntax

```
Prob = clsAssign( ... );
Result = tomRun('dfnlp', Prob, ...);
```

Description of Inputs

Prob Problem description structure. The following fields are used:

| Input | Description |
|------------------|--|
| <i>A</i> | Linear constraints coefficient matrix. |
| <i>x_L, x_U</i> | Bounds on variables. |
| <i>b_L, b_U</i> | Bounds on linear constraints. |
| <i>c_L, c_U</i> | Bounds on nonlinear constraints. For equality constraints (or fixed variables), set e.g. $b_L(k) == b_U(k)$. |
| <i>PriLevOpt</i> | Print level in MEX interface. |
| <i>DFNLP</i> | Structure with special fields for the DFNLP solver: |
| <i>model</i> | Desired scalar transformation as indicated below. 1 L1 - DATA FITTING: Minimize $ F(1, X) + \dots + F(L, X) $ by introducing L additional variables $Z(1), \dots, Z(L)$ and L + L additional inequality constraints, the above problem is transformed into a smooth nonlinear programming problem, that is then solved by a sequential quadratic programming algorithm. |
| <i>Prob</i> | Problem description structure. The following fields are used:, continued 2 L2 - OR LEAST SQUARES DATA FITTING: Minimize $F(1, X)^2 + \dots + F(L, X)^2$ The algorithm transform the above problem into an equivalent nonlinear programming problem by introducing L additional variables $Z(1), \dots, Z(L)$. The new objective function is $H(X, Z) = 0.5 * (Z(1)^2 + \dots + Z(L)^2)$ and L equality constraints of the form $F(J, X) - Z(J) = 0$ are formulated, $J = 1, \dots, L$. 3 MAXIMUM-NORM DATA FITTING: Minimize Maximum $-F(I, X)$: $I=1, \dots, L$ The problem is transformed into a smooth nonlinear programming problem by introducing one additional variable Z yielding the objective function $H(X, Z) = Z$ and L + L additional inequality constraints of the form $-F(J, X) + Z \geq 0, J = 1, \dots, L, F(J, X) + Z \geq 0, J = 1, \dots, L$. 4 MAXIMUM FUNCTION: Minimize Maximum $F(I, X)$: $I=1, \dots, L$ Similar to the model above, one additional variable X is introduced to get a simple objective function of the type $H(X, Z) = Z$ and L additional restrictions $-F(J, X) + Z \geq 0, J=1, \dots, L$. |
| <i>maxfun</i> | The integer variable defines an upper bound for the number of function calls during the line search. |
| <i>maxit</i> | Maximum number of outer iterations, where one iteration corresponds to one formulation and solution of the quadratic programming subproblem, or, alternatively, one evaluation of gradients. |
| <i>acc</i> | The user has to specify the desired final accuracy (e.g. $1.0e-7$). The termination accuracy should not be smaller than the accuracy by which gradients are computed. |
| <i>ressiz</i> | The user must indicate a guess for the approximate size of the least squares residual, i.e. a low positive real number if the residual is supposed to be small, and a large one in the order of 1 if the residual is supposed to be large. If model is not equal to 2, ressiz must not be set by the user. |
| <i>PrintFile</i> | Name of DFNLP Print file. Amount and type of printing determined by PriLevOpt. |

Description of Outputs

Result Structure with result from optimization. The following fields are set:

| Output | Description |
|---------------|---|
| <i>f_k</i> | Function value at optimum. |
| <i>g_k</i> | Gradient of the function. |
| <i>x_k</i> | Solution vector. |
| <i>x_0</i> | Initial solution vector. |
| <i>c_k</i> | Nonlinear constraint residuals. |
| <i>cJac</i> | Nonlinear constraint gradients. |
| <i>xState</i> | State of variables. Free == 0; On lower == 1; On upper == 2; Fixed == 3; |
| <i>bState</i> | State of linear constraints. Free == 0; Lower == 1; Upper == 2; Equality == 3; |
| <i>cState</i> | State of nonlinear constraints. Free == 0; Lower == 1; Upper == 2; Equality == 3; |

| | |
|------------------------|---|
| <i>ExitFlag</i> | Exit status from DFNLP MEX. |
| <i>ExitText</i> | Exit text from DFNLP MEX. |
| <i>Inform</i> | DFNLP information parameter. |
| <i>FuncEv</i> | Number of function evaluations. |
| <i>GradEv</i> | Number of gradient evaluations. |
| <i>ConstrEv</i> | Number of constraint evaluations. |
| <i>QP.B</i> | Basis vector in TOMLAB QP standard. |
| <i>Solver</i> | Name of the solver (DFNLP). |
| <i>SolverAlgorithm</i> | Description of the solver. |
| <i>DFNLP.u</i> | Contains the multipliers with respect to the actual iterate stored in X. The first M locations contain the multipliers of the nonlinear constraints, the subsequent N locations the multipliers of the lower bounds, and the final N locations the multipliers of the upper bounds subject to the scalar subproblem chosen. At an optimal solution, all multipliers with respect to inequality constraints should be nonnegative. |
| <i>DFNLP.act</i> | The logical array indicates constraints, which DFNLP considers to be active at the last computed iterate. |

References

- [1] <http://tomopt.com/tomlab/products/nlpql/>
- [2] <http://www.uni-bayreuth.de/departments/math/~kschittkowski/nlpql.htm>

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