# Nonlinear Programming Software

## for Members and Students of Academic Institutions

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The subsequent pages contain brief summaries of mathematical programming codes, numerical analysis software and related interactive systems that were developed by the author. More detailed reports describing the mathematical algorithms, convergence properties, and numerical test results can be provided on request. All numerical routines are implemented in Fortran, as close as necessary to F77, without global variables (COMMON) or 'tricky' Fortran constructs like EQUIVALENCE or ENTRY. Transfer to C by f2c is possible. Nonlinear functions and, if required, partial derivatives must be provided by reverse communication, the most flexible and the most user-friendly way. All codes come with full documentation and demo programs, which show in particular how partial derivatives can be approximated by forward differences.

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# Contents

# 1 NLPQLP - Nonlinear Constrained Optimization

**Purpose:**

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

**Method:**

NLPQLP is a new implementation of a sequential quadratic programming (SQP) method. Proceeding from a quadratic approximation of the Lagrangian function and a linearization of constraints, a quadratic programming subproblem is formulated and solved by QL (see below). The Hessian approximation is updated by the modified BFGS-formula. Depending on the number of nodes of the distributed system, objective and constraint functions can be evaluated simultaneously at predetermined test points along the search direction. Serial and parallel line search is performed with respect to an augmented Lagrangian merit function. In case of an error situation in the line search, a non-monotone line search is started. It can be shown that especially for very noisy objective or constraint functions, the robustness of the code is drastically improved.

**Program Organization:**

NLPQLP is written in double precision Fortran and is organized in form of a subroutine. Nonlinear problem functions and corresponding gradients must be provided by the user within the calling program by reverse communication. Depending on a flag, either new function values (IFAIL=-1) or new gradient values (IFAIL=-2) must be computed and NLPQLP must be started again. If NLPQLP is implemented under a distributed environment, each iteration of NLPQLP requires one simultaneous function evaluation for the line search and another one for approximation of gradients, if the number of parallel processors is sufficiently big. The quadratic programming solver can be exchanged by any other one, e.g., to exploit sparsity patterns.

**Special Features:**

- distributed computation of step-length possible
- upper and lower bounds on the variables handled separately
- initial multiplier and Hessian estimates allowed
- bounds and linear constraints remain satisfied
- step-size reduction in case of non-computable function values

- fast final convergence speed
- robust even in case of very noisy function values
- alternative QP solvers
- full documentation and example codes
- Fortran source code

**Applications:**

NLPQLP and its previous versions are part of commercial redistributed optimization systems, e.g.,

- IMSL Library (Visual Numerics Inc., Houston), Version 1.0 of 1981,
- ANSYS/POPT (CAD-FEM, Grafing) for structural optimization,
- DesignXplorer (ANSYS Inc., Canonsburg) for structural design optimization,
- STRUREL (RCP, Munich) for reliability analysis,
- Microwave Office Suit (Applied Wave Research, El Segundo) for electronic design,
- MOOROPT (Marintek, Trondheim) for the design of mooring systems,
- iSIGHT (Enginious Software, Cary, North Carolina) for multi-disciplinary CAE,
- POINTER (Synaps, Atlanta) for design automation,
- EXCITE (AVL, Graz) for non-linear dynamics of power units,
- FRONTIER (ESTECO, Trieste) for integrated multi-objective and multi-disciplinary design optimization,
- MathCad (MathSoft, Boston) for constrained least squares optimization,
- TOMLAB/MathLab (Tomlab Optimization, Västeras, Sweden) for general nonlinear programming, least squares optimization, data fitting in dynamical systems,
- OptiSLang (DYNARDO, Weimar), for structural design optimization,
- AMESim (IMAGINE, Roanne), for multidisciplinary system design,
- OPTIMUS (NOESIS, Leuven, Belgium) for multi-disciplinary CAE,
- RADIOSS/M-OPT (MECALOG, Antony, France) for multi-disciplinary CAE,
- CHEMASIM (BASF, Ludwigshafen) for the design of chemical reactors.

Customers include AMD, Applied Research Corp., Aramco, Aware, Astrium, Axiva, BASF, Bastra, Bayer, Bell Labs, BMW, CEA, Chevron, DLR, Dornier Systems Dow Chemical, DuPont, EADS, EMCOSS, ENSIGC, EPCOS, ESOC, Eurocopter, Fantoft Prosess, Fernmeldetechnisches Zentralamt, General Electric, GLM Lasertechnik, Hidroelectrica Espanola, Hoechst, IABG, IBM, INRIA, INRS-Telecommunications, KFZ Karlsruhe, Kongsberg Maritime, Lockheed Martin, Markov Processes, Mathematical Systems Institute Honcho, Micronic Laser Systems, MTU, NASA Langley, Nevesbu, National

Airspace Laboratory, Norsk Hydro Research, Norwegian Computing Center, Numerola, OECD Halden, Peaktime, Philips, Polysar, ProSim, Research Triangle Institute, Rolls-Royce, SAQ Kontroll, Shell, Siemens, Solar Turbines, Space Systems/Loral, Statoil, TNO, Transpower, USAF Research Lab, VTT Chemical Technology, Wright R & D Center, and in addition dozens of academic research institutions all over the world.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 2 NLPQLY - Easy-To-Use Nonlinear Constrained Optimization

**Purpose:**

NLPQLY is the easy-to-use version of NLPQLP for solving general nonlinear programming problems with equality and inequality constraints. It is assumed that all problem functions are continuously differentiable.

**Method:**

After setting some default tolerances, NLPQLP is executed. Derivatives are internally approximated by forward differences.

**Program Organization:**

NLPQLY is written in double precision Fortran and is organized in form of a subroutine. Nonlinear objective and constraint function values must be provided by the user within the calling program by reverse communication. Depending on a flag, either new function values (IFAIL<0) must be computed and NLPQLY has to be started again, an error occurred (IFLAG>0), or the optimality conditions are satisfied (IFAIL=0).

**Special Features:**

- upper and lower bounds on the variables handled separately
- bounds and linear constraints remain satisfied
- fast final convergence speed
- robust even in case of very noisy function values
- full documentation and example codes
- Fortran source code

**Applications:**

NLPQLY has the same applications as NLPQLP, as long as forward difference approximations for derivatives are used.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 3 NLPQLB - Nonlinear Programming with Very Many Constraints

**Purpose:**

NLPQLB is an extension of the general nonlinear programming code NLPQLP with the intention to solve also problems with very many constraints, even when the Jacobian matrix of the constraints does not possess any special sparsity structures.

**Method:**

The user defines the maximum number of lines in the matrix of the linearized constraints that can be stored in core. Constraint function values are investigated to update this working set, which must contain at least all violated constraints. The algorithm stops, if too many constraints are violated.

**Program Organization:**

NLPQLB is a double precision Fortran subroutine where all parameters are passed through subroutine arguments. The program organization is very similar to that of NLPQLP.

**Special Features:**

- solves problems with up to 200,000,000 nonlinear constraints
- NLPQLB executes NLPQLP in reverse communication
- full documentation by initial comments
- Fortran source code

**Applications:**

NLPQLB is implemented as part the structural mechanical optimization system LAGRANGE of EADS to solve large design optimization problems by means of finite element technique.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 4 NLPQLG - Nonlinear Global Optimization

**Purpose:**

NLPQLG is an extension of the general nonlinear programming code NLPQLP with the goal to improve local minima successively.

**Method:**

Successively, local minima are cut off by introducing additional restrictions. Moreover, artificial constraints prevent approximation of known local minima. These constraints are relaxed to prevent infeasible domains.

**Program Organization:**

NLPQLG is a double precision Fortran subroutine where all parameters are passed through subroutine arguments. The program organization is very similar to that of NLPQLP.

**Special Features:**

- NLPQLB executes NLPQLP in reverse communication
- full documentation by initial comments
- Fortran source code

**Applications:**

Used, e.g., at EPCOS AG for computing optimal designs of electronic components.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 5 NLPJOB - Multicriteria Optimization

**Purpose:**

NLPJOB solves multicriteria problems interactively, i.e. problems with more than one objective function.

**Method:**

By using a suitable transformation, a scalar nonlinear problem is created and solved by NLPQLP. There are 15 different options available for formulating the scalar subproblem.

**Program Organization:**

NLPJOB is a double precision Fortran subroutine where all parameters are passed through subroutine arguments. Problem functions and gradients must be provided by the user in form of subroutines.

**Special Features:**

- reverse communication
- Fortran source code

**Applications:**

NLPJOB is implemented within the structural mechanical optimization system LAGRANGE of EADS.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 6 NLPLSQ - Constrained Nonlinear Least Squares Optimization

**Purpose:**

NLPLSQ solves constrained nonlinear least squares problems, i.e., nonlinear optimization problems, where the objective function is the sum of squares of function. In addition, there may be any set of equality or inequality constraints. It is assumed that all individual problem functions are continuously differentiable. The most important application is data fitting, where the distance of experimental data from a model function evaluated at given experimental times is to be minimized by the $L_2$ or sum of squares norm.

**Method:**

By introducing additional variables and constraints, the problem is transformed into a general smooth nonlinear programming problem which is then solved by the sequential quadratic programming (SQP) code NLPQLP. It can be shown that typical features of special purpose algorithms are retained, i.e., a combination of a Gauss-Newton and a quasi-Newton search direction. The additionally introduced variables are eliminated in the quadratic programming subproblem, so that calculation time is not increased significantly.

**Program Organization:**

NLPLSQ is a double precision Fortran subroutine and parameters are passed through arguments.

**Special Features:**

- reverse communication
- bounds and linear constraints remain satisfied
- Fortran source code

**Applications:**

The code is in practical use to solve parameter estimation problems, e.g., in chemical and pharmaceutical applications, see EASY-FIT.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 7 NLPLSX - Constrained Nonlinear Least Squares Optimization with Very Many Experimental Data

**Purpose:**

NLPLSX solves constrained nonlinear least squares problems, i.e., nonlinear optimization problems, where the objective function is the sum of squares of function. In addition, there may be any set of equality or inequality constraints. It is assumed that all individual problem functions are continuously differentiable. The most important application is data fitting, where the distance of experimental data from a model function evaluated at given experimental times is to be minimized by the $L_2$ or sum of squares norm.

**Method:**

By assuming now that the transformation technique for NLPLSQ is not applicable because of a too large number of objective functions or measurements, respectively, the sum of squared functions is directly minimized by NLPQLP. Constraints, if available, are passed to NLPQLP.

**Program Organization:**

NLPLSX is a double precision Fortran subroutine and parameters are passed through arguments.

**Special Features:**

- reverse communication
- bounds and linear constraints remain satisfied
- Fortran source code

**Applications:**

The code is in practical use to solve parameter estimation problems, e.g., in chemical and pharmaceutical applications, as part of EASY-FIT.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 8 NLPINF - Constrained Nonlinear Maximum-Norm Optimization

**Purpose:**

NLPINF solves constrained nonlinear $L_\infty$ problems, i.e., nonlinear optimization problems, where the objective function is the maximum of absolute function values. In addition there may be any set of equality or inequality constraints. It is assumed that all individual problem functions are continuously differentiable. The most important application is data fitting, where the distance of experimental data from a model function evaluated at given experimental times is to be minimized by the $L_\infty$ or maximum norm, respectively.

**Method:**

By introducing one additional variable and additional inequality constraints, the problem is transformed into a general smooth nonlinear programming problem which is then solved by the sequential quadratic programming (SQP) code NLPQLP.

**Program Organization:**

NLPINF is a double precision Fortran subroutine and parameters are passed through arguments.

**Special Features:**

- reverse communication
- bounds and linear constraints remain satisfied
- Fortran source code

**Applications:**

The code is part of the data fitting software EASY-FIT.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 9 NLPMMX - Constrained Nonlinear Min-Max Optimization

**Purpose:**

NLPMMX solves constrained nonlinear min-max problems, i.e., nonlinear optimization problems, where the objective function is the maximum of absolute function values. In addition there may be any set of equality or inequality constraints. It is assumed that all individual problem functions are continuously differentiable.

**Method:**

By introducing one additional variable and additional constraints, the problem is transformed into a general smooth nonlinear programming problem which is then solved by the sequential quadratic programming code NLPQLP.

**Program Organization:**

NLPMMX is a double precision Fortran subroutine and parameters are passed through arguments.

**Special Features:**

- reverse communication
- bounds and linear constraints remain satisfied
- Fortran source code

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 10 NLPL1 - Constrained Optimization of Sums of Absolute Function Values

**Purpose:**

NLPL1 solves constrained nonlinear $L_1$ problems, i.e., nonlinear optimization problems, where the objective function is the sum of absolute function values. In addition there may be any set of equality or inequality constraints. It is assumed that all individual problem functions are continuously differentiable. The most important application is data fitting, where the distance of experimental data from a model function evaluated at given experimental times is to be minimized by the $L_1$ norm.

**Method:**

By introducing additional variables and constraints, the problem is transformed into a general smooth nonlinear programming problem which is then solved by the sequential quadratic programming code NLPQLP.

**Program Organization:**

NLPL1 is a double precision Fortran subroutine and parameters are passed through arguments.

**Special Features:**

- reverse communication
- bounds and linear constraints remain satisfied
- Fortran source code

**Applications:**

The code is part of the data fitting software EASY-FIT.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained. The software is free for individuals of academic institutions, see below for details.

# 11 NLPQLF - Feasible Nonlinear Constrained Optimization

**Purpose:**

NLPQLF solves smooth nonlinear programming problems and is an extension of the code NLPQLP. It is assumed that objective function or constraints can be evaluated only at argument values from a convex set described by some other inequality constraints, the so-called feasibility constraints. The numerical method performs a two-stage process. Starting from a point feasible subject to these 'simple' constraints, a new search direction is computed by solving a quadratic program expanded by the nonlinear feasibility constraints. Thus, the new iterate is feasible subject to these constraints and objective function as well as the remaining constraint function values can be evaluated.

**Method:**

NLPQLF is a modification of a sequential quadratic programming (SQP) method by adding the feasibility constraints to the quadratic programming subproblem. The resulting nonlinear program is solved by NLPQLP. Subsequently, the algorithm proceeds like a standard SQP method, i.e., applies a line search and updates the Hessian approximation by the modified BFGS-formula.

**Program Organization:**

NLPQLF is written in double precision Fortran and is organized in form of a subroutine. Nonlinear problem functions and corresponding gradients must be provided by the user within the calling program by reverse communication. Depending on a flag, either new function values or new gradient values are to be computed and NLPQLF must be started again.

**Special Features:**

- starting point must satisfy the feasibility constraints
- upper and lower bounds on the variables handled separately
- objective function and subset of constraints evaluated only at feasible variable values
- full documentation and example codes
- Fortran source code

**Applications:**

Not yet available, new implementation.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the SQP code NLPQLP and the quadratic programming solver QL must be obtained.

# 12 QL - Quadratic Programming

**Purpose:**

QL solves quadratic programming problems with a positive definite objective function matrix and linear equality and inequality constraints.

**Method:**

The algorithm is an implementation of the dual method of Goldfarb and Idnani and a modification of the original implementation of Powell. Initially, the algorithm computes a solution of the unconstrained problem by performing a Cholesky decomposition and by solving the triangular system. In an iterative manner violated constraints are added to a working set and a minimum with respect to the new subsystem with one additional constraint is calculated. Whenever necessary, a constraint is dropped from the working set. The internal matrix transformations are performed in numerically stable way.

**Program Organization:**

QL is a double precision Fortran subroutine where all data are passed by subroutine arguments.

**Special Features:**

- separate handling of upper and lower bounds
- initially given Cholesky decomposition can be exploited
- full documentation by initial comments
- Fortran source code

**Applications:**

As an essential part of the nonlinear programming routine NLPQLP, QL solves the internal quadratic programming subproblem of the SQP method and has therefore the same domain of application as NLPQLP.

**License:**

Contact the author for getting the Fortran source code. The software is free for individuals of academic institutions, see below for details.

# 13 MIQL - Mixed-Integer Quadratic Programming

**Purpose:**

The Fortran subroutine MIQL solves strictly convex mixed-integer quadratic programming problems subject to linear equality and inequality constraints by a branch-and-cut method. At the root node of the branch-and-bound search tree, disjunctive and complemented mixed-integer rounding cuts are generated. The continuous subproblem solutions are obtained by the primal-dual method of Goldfarb and Idnani. The code is designed for solving small to medium size mixed-integer programs. .

**Method:**

A branch-and-cut strategy is implemented where different options are available for selecting a branching variable and a free node:

1. *maximal fractional branching*: We select an integer variable from the solution of the relaxed subproblem with largest distance from next integer value.

2. *minimal fractional branching*: We select an integer variable from the solution of the relaxed subproblem with smallest distance from next integer value.

Then we search for a free node from where branching, i.e., the generation of two new subproblems, is started:

1. *best of two*: The optimal objective function values of the two child nodes are compared and the node with a lower value is chosen. If both are leafs, i.e., if the corresponding solution is integral, or if the corresponding problem is infeasible or if there is already a better integral solution, strategy *best of all* is started.

2. *best of all*: All free nodes are compared and a node with lowest objective function value is selected.

3. *depth first*: This search strategy selects a child node whenever possible. If the node is a leaf the *best of all* strategy is applied.

Moreover, there are complemented mixed-integer rounding cutting planes and disjunctive programming cuts to reduce the search space and to cut-off non-optimal integer points. The corresponding continuous relaxed problems are solved by the Fortran code QL.

**Program Organization:**

MIQL is a double precision Fortran subroutine where all data are passed by subroutine arguments.

**Special Features:**

- separate handling of upper and lower bounds
- full documentation by initial comments
- exploiting dual information for early branching
- warm starts
- Fortran source code

**Applications:**

As an essential part of the mixed-integer nonlinear programming routine MISQP, MIQL solves the internal mixed-integer quadratic programming subproblem of the SQP-trust-region method.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the quadratic programming solver QL must be obtained.

# 14 MISQP - Mixed-Integer Sequential Quadratic Programming

**Purpose:**

The Fortran subroutine MISQP solves mixed-integer nonlinear programming problems by a modified sequential quadratic programming (SQP) method. Under the assumption that integer variables have a *smooth* influence on the model functions, i.e., that function values do not change drastically when in- or decrementing an integer variable, successive quadratic approximations are applied. It is not assumed that integer variables are relaxable, i.e., problem functions are evaluated only at integer points. The code is applicable also to nonconvex optimization problems.

**Method:**

The algorithm is stabilized by a trust region method including Yuan's second order corrections. The Hessian of the Lagrangian function is approximated by BFGS updates subject to the continuous and integer variables. Successively, mixed-integer quadratic programs must be solved.

**Program Organization:**

MISQP is a Fortran subroutine where all data are passed by subroutine arguments. Function and gradient values must be submitted through reverse communication. Partial derivatives subject to integer variables are approximated internally at grid points. The generated mixed-integer quadratic programming subproblems must be solved by the code MIQL.

**Special Features:**

- boolean, integer, and continuous variables
- separate handling of upper and lower bounds
- full documentation by initial comments
- integer, real and logical option arrays
- separate handling of linear constraints
- exploiting known partial derivatives subject to integer variables
- Fortran source code

**Applications:**

The development of MISQP was supported by the Shell GameChanger program, and MISQP is in daily use as part of Shell's simulation packages. In addition, MISQP is in use at General Electric, Dassault/Simulia (iSight), Epcos, BASF (Chemasim), ANSYS (DesignExplorer) and at several other companies and research institutes.

**License:**

Contact the author for getting the Fortran source code. Note that also a license for the mixed-integer quadratic programming solver MIQL must be obtained.

# 15 NLPIP - Large-Scale Nonlinear Constrained Optimization

**Purpose:**

NLPIP solves large nonlinear programming problems with equality and inequality constraints, i.e., problems with a large number of variables. It is implicitly assumed that the Jacobian matrix of the constraints is sparse. Problem functions must be continuously differentiable.

**Method:**

NLPIP applies a combined SQP-IPM strategy. Depending on the preferences of the user, either a standard SQP method is used where the quadratic programming subproblem is solved by an interior point method, or a nonlinear interior point method is executed. Moreover, any combination in between is possible. BFGS updates use the limited memory method, and three different merit functions are available. In any case, the primal-dual system of linear equations possesses the same structure and must be solved by a user-provided routine depending on the sparsity patterns of the Jacobian matrix of the constraints.

**Program Organization:**

NLPIP is written in double precision Fortran and is organized in form of a subroutine. Nonlinear problem functions and corresponding gradients must be provided by the user within the calling program by reverse communication. Depending on a flag, either new function values (IFAIL=-1) or new gradient values (IFAIL=-2) must be computed and NLPIP is restarted. For solving the internal system of linear equations, the so-called primal-dual system, a special subroutine with name LINSLV must be implemented. LINSLV is called from NLPIP with different flags for factorization, matrix times vector products, or retrieving solution vectors with different right-hand sides.

**Special Features:**

- upper and lower bounds on the variables an handled separately
- interfaces (LINSLV) for PARDISO, MUMPS and LAPACK are included
- complex active-set strategy analogously to the one implemented in NLPQLB
- full documentation and example codes
- Fortran source code

**Applications:**

The development of NLPIP was supported by EADS and NLPIP became part of the in-house FE-based structural optimization system LAGRANGE.

**License:**

Contact the author for getting the Fortran source code. Note again that a suitable sparse linear equation solver is not included.

# 16 MIDACO - Ant Colony Optimization Code for General Optimization

**Purpose:**

MIDACO is a black-box optimizer, specially developed for mixed integer nonlinear programs (MINLPs). As the class of MINLPs covers purely continuous and purely combinatorial optimization problems, MIDACO can be employed on a wide range of optimization problems. Its usage is particularly intended for global optimization problems, where the problem formulation is unknown (true black-box) or invokes critical properties like non-convexity, discontinuities, flat spots or stochastic distortions.

**Method:**

The underlying algorithm is based on a stochastic Gauss approximation technique (also known as Ant Colony Optimization) and its combination with the oracle penalty method. It's development was focused especially on constrained mixed integer nonlinear programming (MINLP) problems, but due to the generality of this problem class, the software is well applicable on many different kind of optimization problems. MIDACO is constructed as a derivative free black-box solver, handling all its parameter by itself.

**Program Organization:**

MIDACO has been used for example on various space applications (interplanetary missions, vehicle launch maneuvers, heat shield protection systems) and distillation column sequencing.

**Special Features:**

- applicable to a large class of optimization problems
- Matlab, Fortran, C/C++ versions available
- full documentation
- autopilot mode for parameter selections and automatic internal restarts to escape from local solutions

**Applications:**

MIDACO has been used to compute interplanetary space missions from earth to Jupiter and for distillation column sequencing.

**License:**

Contact the author for getting the Fortran source code.

# 17 BFOUR - A Branch-And-Bound Code for Integer Optimization

**Purpose:**

BFOUR is a black-box method for mixed integer nonlinear programming.

**Method:**

A branch-and-bound strategy is implemented where different options are available for selecting a fractional branching variable:

- *maximal branching* Select an integer variable from the solution of the relaxed subproblem with largest distance from next integer value.
- *minimal branching* Select an integer variable from the solution of the relaxed subproblem with smallest distance from next integer value.

Then we search for a free node from where branching, i.e., the generation of two new subproblems, is started:

- *best of two* The optimal objective function values of the two child nodes are compared and the node with a lower value is chosen. If both are leafs, i.e., if the corresponding solution is integral, or if the corresponding problem is infeasible or if there is already a better integral solution, strategy *best of all* is started.
- *best of all* Select an integer variable from the solution of the relaxed subproblem with smallest distance from next integer value.
- *depth first* Selects a child node whenever possible. If the node is a leaf the *best of all* strategy is applied.

The corresponding continuous relaxed optimization problems are solved by any available external solver.

**Program Organization:**

BFOUR is written in double precision Fortran and is organized in form of a subroutine. Nonlinear problem functions and corresponding gradients must be provided by the user within the calling program by reverse communication.

**Special Features:**

- applicable to a large class of integer optimization problems
- full documentation
- Fortran source code

**Applications:**

As part of MIQL, BFOUR is in practical use since many years. See MIQL or MISQP for applications.

**License:**

Contact the author for getting the Fortran source code. The software is free for individuals of academic institutions, see below for details.

# 18 PCOMP - Automatic Differentiation

**Purpose:**

PCOMP reads symbolically defined nonlinear functions that are composed of standard elementary functions, and precompiles them. Subsequently function and, in particular, derivative values up to order two can be computed directly, i.e. without numerical approximation. Alternatively Fortran code for function and gradient evaluation can be generated automatically by PCOMP.

**Method:**

The underlying syntax of the proposed language is described by means of a formal grammar and is similar to the Fortran language with respect to the input format and arithmetic expressions. In case of successful syntax check, an intermediate code is stored in an integer and a real working array and is passed to the subroutines that evaluate function and gradient values. Gradient evaluation is performed either by forward or backward evaluation.

**Program Organization:**

PCOMP consists of three precision Fortran subroutines for parser, function and gradient evaluation, and code generation. Data must be passed on working arrays or files between these subroutines .

**Special Features:**

- arbitrary index sets
- constants
- names for variables
- SUM- and PROD-statements
- indexed functions, data and variables
- IF, ELSE, ENDIF statements, nested
- interface to user provided functions
- full documentation by separate report
- Fortran source code

**Applications:**

PCOMP is used to develop executable codes for nonlinear optimization which allow symbolic input of nonlinear problem functions, and is implemented, e.g., in EASY-FIT.

**License:**

Contact the author for getting the Fortran source code. The software is free for individuals of academic institutions, see below for details.

# 19 EASY-FIT ModelDesign - Data Fitting and Experimental Design of Dynamical Systems

**Purpose:**

EASY-FIT ModelDesign is an interactive user interface running under Windows, to facilitate the formulation and numerical solution of data fitting problems, where the underlying model is either an explicit function, a Laplace transform, a steady-state system of equations, an ordinary differential equation, a differential algebraic differential equation or a one-dimensional, time-dependent partial differential equation with or without algebraic equations. In addition to data fitting, also optimal experimental designs can be determined.

**Method:**

EASY-FIT ModelDesign is a user interface implemented in form of a database, to execute the parameter estimation codes MODFIT and PDEFIT in form of external programs. Nonlinear functions can be provided by the PCOMP modeling language or in Fortran. EASY-FIT ModelDesign creates input files to execute the numerical codes, and stores results in the database. EASY-FIT comes with statistical analysis utilities, i.e., confidence intervals, significance levels of parameters, experimental design, and optimal location of time values.

**Program Organization:**

EASY-FIT ModelDesign is a complex software system running under MS-Windows XP or Vista. A version for Windows 2K or earlier can be provided on request. The GUI is implemented in form of an MS Access 2–7 database, the numerical codes in Fortran. Interfaces for the INTEL Visual Fortran, WATCOM F77, Salford FTN77, Microsoft Fortran Powerstation, Digital Visual Fortran, Absoft Pro Fortran, and the Lahey F77L3 compiler are available.

**Special Features:**

- embedded modeling language with automatic differentiation (PCOMP),
- declaration of model type and solution parameters by pick-lists, combo boxes etc.
- import and export of data and functions (text, Excel)
- restarts with previously computed variable values

- interactive, context sensitive help
- distributed with run-time version of MS-Access 2007
- 1,300 test problems
- interactive plot facilities for model functions, measurements, residuals and 3D contours based on internal or external graphics systems
- report generator
- comprehensive documentation (about 380 pages)
- trial version (download from home page http://www.klaus-schittkowski.de/, activation by license key)

**Applications:**

EASY-FIT ModelDesign is applied in chemical engineering, pharmaceutics, mechanical engineering, and in natural sciences like biology, geology, ecology. Customers include ACA, BASF, Battery Design, Bayer, Boehringer Ingelheim, Envirogain, Eurocopter, Knoll, Oxeno, Novartis, Prodisc, Springborn Laboratories, and in addition more than 40 academic research institutions.

**License:**

Download trial version from home page and contact the author for license key. The software is free for individuals of academic institutions, see below for details.

# 20 EASY-FIT Express - Interactive Data Fitting

**Purpose:**

EASY-FIT Express is a subset of EASY-FIT ModelDesign to solve data fitting problems, where the underlying model is given by explicit analytical function. Nonlinear equality or inequality constraints are permitted.

**Method:**

Data must be defined through input masks, where nonlinear functions are provided by the modeling language PCOMP. EASY-FIT Express creates input files to call an executable nonlinear programming program EXPFIT, that can be used also independently from the interface. Functions are evaluated directly during run time and gradients are computed automatically by PCOMP.

**Program Organization:**
EASY-FIT Express is a user interface implemented in form of a database, to execute the parameter estimation code EXPFIT in form of an external program. Nonlinear functions are provided in the PCOMP language. EASY-FIT Express creates input files to execute the numerical codes, and stores results in the database. EASY-FIT Express comes with statistical analysis utilities, i.e., confidence intervals, significance levels of parameters, experimental design, and optimal location of time values.

**Special Features:**

- embedded modeling language with automatic differentiation (PCOMP),
- import and export of data and functions (text, Excel)
- restarts with previously computed variable values
- interactive, context sensitive help
- distributed with run-time version of MS-Access 2007
- 240 test problems
- interactive plots for model functions, measurements, residuals and 3D contours
- report generator
- comprehensive documentation (about 380 pages)

**Applications:**

To be used for academic purposes and data fitting applications based on analytical functions.

**License:**

Free, download from home page.

# 21 EASY-OPT Express - Interactive Optimization

**Purpose:**

EASY-OPT Express is an interactive user interface running under Windows, to facilitate the formulation of nonlinear programming models, their implementation and numerical solution. It is possible to solve general constrained nonlinear programming problems interactively, i.e., to minimize a nonlinear objective function subject to nonlinear equality or inequality constraints.

**Method:**

Nonlinear functions are defined in the PCOMP modeling language. EASY-OPT Express creates input files to call an executable program, that can be used also independently from the interface. Functions are evaluated during run time and gradients are computed automatically by PCOMP. The SQP code NLPQLP is internally implemented to solve optimization problems efficiently.

**Program Organization:**
The user interface is implemented in form of a database under MS-Access 2007, the numerical algorithms in Fortran. A distribution-free runtime version of Microsoft Access 2007 is included. EASY-OPT Express runs under Windows XP and Vista and can be downloaded from the home page of the author. A version for Windows 2K or earlier can be provided on request. Since nonlinear functions are interpreted by the modeling language PCOMP, it is not necessary to compile or link any subroutines.

**Special Features:**

- up to 200 variables and 1,000 nonlinear equality and inequality constraints
- interactive, context-sensitive help (F1)
- extensive documentation (pdf)
- internal editor for PCOMP-code
- large set of test problems
- optimization history plot
- report generator

**Applications:**

To be used for academic purposes and smaller optimization applications.

**License:**

Free, download from home page.

# 22 How to Get Software

EASY-FIT ModelDesign, EASY-FIT Express, and EASY-OPT Express can be downloaded from the home page of the author. To activate EASY-FIT ModelDesign, a license key is requested. To get the license key for EASY-FIT ModelDesign or to get any of the Fortran codes, contact the author under klaus@schittkowski.de or klaus.schittkowski@uni-bayreuth.de.
The code MIDACO has been developed by Martin Schlueter and is available under its home page (http://midaco-solver.com/).
The remaining software is free for members and students of academic institutions. An academic institution is defined by its ability to provide academic degrees, e.g., Bachelor, Master, Diploma, or Ph.D. degrees. If you are a member or a student of an academic institution, please outline your application in a few lines and prepare a letter confirming that

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3. to delete the code after finishing your research project or your thesis, respectively,

4. not to pass the code to any other person or organization, neither in form of the source code nor in form of object code or part of another piece of software,

5. to add a reference in related publications, and to send a copy to the author.

Note that especially nobody else in your department is allowed to use the software. Use your full institutional or, in case of a student, private address and sign it. Then scan the letter and attach it to an e-mail. If you are a student, add a letter of your supervisor confirming that you conduct a thesis (Bachelor, Master, Diploma, Ph.D.) under his supervision.
After receiving the agreement, you will get the license key for activating EASY-FIT ModelDesign or the requested Fortran codes by e-mail. Please let me know the operating system and your compiler.

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