

Solving Applied Optimization Problems Using TOMLAB

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Abstract

TOMLAB is a Matlab 5 development environment for research and teaching in optimization, running on both Unix and PC systems. One motivation for TOMLAB is to simplify research on practical optimization problems, giving easy access to all types of solvers; at the same time having full access to the power of Matlab. In this paper we discuss the design and contents of TOMLAB, as well as some applications where TOMLAB has been successfully applied.

TOMLAB includes routines for linear, integer and nonlinear programming, nonlinear parameter estimation and global optimization. More than 65 algorithms are implemented, together with graphical and computational utilities, menu systems and a graphical user interface. It is possible to call solvers in the Math Works Optimization Toolbox and, using MEX-file interfaces, general-purpose solvers implemented in Fortran or C.

TOMLAB implements powerful and robust state-of-the-art routines for nonlinear parameter estimation and global optimization; areas of special interest in applied research. Results on practical applications in these areas will be discussed. Our new algorithms for constrained nonlinear least squares algorithms are out-performing the state-of-the-art commercial solvers on classical test problems. For exponential sum model fitting on real-life data from radiotherapy planning our new separable nonlinear least squares algorithm is converging > 35% faster than other solvers.

1 Introduction

Many scientists and engineers are using Matlab as a modeling and analysis tool, but for the solution of optimization problems, the support is weak. That was one strong motivation for the development of TOMLAB [11]. Another motivation was to provide powerful tools for the research on the hard-to-solve applied problems our research group are working on, by systematic development of a large set of usable optimization tools.

The paper is organized as follows. In Section 2 the optimization environment TOMLAB is described. Global optimization is the topic of Section 3, with emphasis on the current tools available in TOMLAB. An example of global optimization in finance is given in Section 4, the aim being optimal stock market trading performance. Nonlinear parameter estimation and the tools in TOMLAB are discussed in Section 5. TOMLAB includes special treatment and efficient algorithms for model fitting in exponential models, which are presented in Section 6. Results on a real-life example from cancer treatment in radiotherapy is given. Two more applications are shortly discussed in Section 7. Some conclusions are given in Section 8.

2 The Optimization Environment TOMLAB

TOMLAB is a Matlab 5 based development environment for research and teaching in optimization, running on both Unix and PC systems. One motivation for TOMLAB is to simplify research on practical optimization problems, giving easy access to all types of solvers; at the same time having full access to the power of Matlab. The design principle is: *define your problem once, optimize using any suitable solver*. This is possible using general gateway and interface routines, global variables, string evaluations and structure arrays. When solving advanced applied problems, the design principle is of special importance, as it might be a huge task to rewrite the function, constraint and derivative specifications. The aim of TOMLAB is to provide access to most state-of-the-art numerical optimization software in an integrated and easy-to-use way. TOMLAB could be used as a stand-alone tool or as part of a more general algorithm.

For the optimization algorithm developer and the applied researcher in need of optimization tools it is very easy to compare different solvers or do test runs on thousands of problems. TOMLAB should be seen as a proposal for a standard for optimization in Matlab.

In TOMLAB itself about 65 numerical optimization algorithms are implemented, and using different types of pre-defined interfaces, many more solvers are directly possible to use, like *SNOPT*, *MINOS*, *XPRESS/MP*, *NPSOL*, *NPOPT*, *NLSSOL*, *LPOPT*, *QPOPT*, *LSSOL*, *FSQP*, *LSQR*, *SYMMLQ* and solvers in the Math Works Optimization Toolbox. Most areas of optimization are covered. There are solvers for linear programming, mixed-integer programming, quadratic programming, unconstrained optimization, general nonlinear programming, constrained linear and nonlinear least squares, box-bounded global optimization and global mixed-integer nonlinear programming.

A number of routines for special problems are implemented, e.g. partially separable functions, separable nonlinear least squares, dual linear programming, approximation of parameters in exponential models, transportation simplex programming, network simplex programming and binary mixed-integer programming.

A stack strategy for the global variables makes recursive calls possible, in e.g. separable nonlinear least squares algorithms. One structure holds all information about the problem and one holds the results. There are several ways to solve optimization problems in TOMLAB. Either by a direct call to a solver or to a general multi-solver driver routine, or interactively, using the Graphical User Interface (GUI) [6] or a menu system. Yet another way to solve an optimization problem in TOMLAB is to use the call-compatible interfaces simulating the behaviour of the Math Works Optimization Toolbox 2.0, which is especially useful for users that previously used that toolbox. The GUI may also be used as a preprocessor to generate Matlab code for stand-alone runs.

If analytical derivatives are not available, automatic differentiation is easy using an interface to ADMAT/ADMIT TB, free for academic use. Furthermore, five methods for numerical differentiation are implemented. A large set of standard test problems are included, as well as example and demonstration files. New user-defined problems are easily added.

Using MEX-file interfaces, problems in the CUTE test problem data base and problems defined in the AMPL [8] modeling language can be solved. The Constrained and Unconstrained Testing Environment (CUTE) [4, 5] is a well-known software environment for nonlinear programming. The distribution of CUTE includes a test problem data base of nearly 1000 optimization problems, both academic and real-life applications. This data base is often used as a benchmark test in the development of general optimization software. Using the TOMLAB CUTE interface it is possible to run the huge set of CUTE test problems using any solver.

TOMLAB v1.0 handles small and medium size dense problems, is free for academic use and is possible to download at the home page of the Applied Optimization and Modeling (TOM) group, URL: <http://www.ima.mdh.se/tom>. No support is given. TOMLAB 1.0 is based on NLPLIB TB, a Matlab toolbox for nonlinear programming and parameter estimation [15], and OPERA TB, a Matlab toolbox for linear and discrete optimization [16]. A User's Guide for TOMLAB v1.0 is available [17].

The new TOMLAB v2.0 system, first presented in Holmström [12], also handles large, sparse problems and the code is possible to automatically convert to C++ and compile and run much faster than in Matlab using the Mideva system. Both TOMLAB v2.0 and Mideva are available from the web site of MathTools Inc, URL:

<http://www.mathtools.com>. A User's Guide for TOMLAB v2.0, by Holmström [13], is possible to download at the URL: <http://www.ima.mdh.se/tom>.

3 Global Optimization

Consider the following the following bounded unconstrained problem

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & x_L \leq x \leq x_U, \end{aligned} \tag{1}$$

where $x, x_L, x_U \in \mathbb{R}^n$ and $f(x) \in \mathbb{R}$. With the additional assumption that the elements in x_L, x_U all take finite values, and $f(x)$ might have several local minima, the problem is that of **box-bounded global optimization**.

The TOMLAB routine *glbSolve* implements the DIRECT algorithm by Jones, Perttunen and Stuckman [19] that solves the box-bounded global optimization problem using no derivative information. The algorithm is a modification of the standard Lipschitzian approach that eliminates the need to specify a Lipschitz constant. The idea is to carry out simultaneous searches using all possible constants from zero to infinity. Jones et al. introduce a different way of

looking at the Lipschitz constant. Really, the Lipschitz constant is viewed as a weighting parameter that indicate how much emphasis to place on global versus local search. In standard Lipschitzian methods, this constant is usually large because it must be equal to or exceed the maximum rate of change of the objective function. As a result, these methods place a high emphasis on global search, which leads to slow convergence. In contrast, the DIRECT algorithm carries out simultaneous searches using all possible constants, and therefore operates on both the global and local level. The algorithm implemented in TOMLAB is fully described in [3].

The DIRECT algorithm is guaranteed to converge to the global optimal function value, if the objective function f is continuous or at least continuous in the neighborhood of a global optimum. This could be guaranteed since, as the number of iterations goes to infinity, the set of points sampled by DIRECT form a dense subset of the unit hypercube. In other words, given any point x in the unit hypercube and any $\delta > 0$, DIRECT will eventually sample a point (compute the objective function) within a distance δ of x .

Adding integer, linear and nonlinear constraints to the model, formulate the **global mixed-integer nonlinear programming (GMINLP)** problem as

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & x_L \leq x \leq x_U, \\ & b_L \leq Ax \leq b_U \\ & c_L \leq c(x) \leq c_U \\ & x_i \text{ integer } \forall i \in I \end{aligned} \tag{2}$$

where $x, x_L, x_U \in \mathbb{R}^n$ and $f(x) \in \mathbb{R}$. $A \in \mathbb{R}^{m_1 \times n}$, $b_L, b_U \in \mathbb{R}^{m_1}$ and $c_L, c(x), c_U \in \mathbb{R}^{m_2}$. The index set I is a arbitrarily subset of the n variables. Assume that the elements in x_L, x_U all take finite values, and that $f(x)$ might have several local minima.

The TOMLAB routine *glcSolve* implements an extended version of DIRECT by Jones [20] that handles GMINLP problems.

The very general GMINLP problem formulation covers most problems in the field of optimization and it is evident that only a small sub-class of these problems can be solved in a reasonable time frame with our solver. The number of variables should not be too high.

When simulating complex systems, as in finance, one simulation is often very costly and derivatives are difficult to obtain. To find the global optimum for adjustable parameters in such models in a reasonable time frame, possibly also including integer and nonlinear constraints, it is evident that the information from each simulation, i.e. cost function evaluation, must be efficiently used.

A new technique by Jones, Schonlau and Welch [21] called Efficient Global Optimization (EGO), has been developed for problems where the function is costly to compute. EGO tries to exploit all function evaluations efficiently. The idea of the EGO algorithm is to first fit a response surface to data collected by evaluating the objective function at a few points. Then, EGO balances between finding the minimum of the surface and improving the approximation by sampling where the prediction error may be high. building a response surface doing parameter estimation, and then applying global optimization techniques on the response surface to find new sample points. The TOMLAB routine *ego* implements a variation of this algorithm, where the unconstrained TOMLAB solver is used for the parameter estimation problem of finding the response surface and *glbSolve*, previously discussed, is used to find the global optimum on the response surface.

In our most current research a new algorithm with a similar approach as EGO is developed. This algorithm is using approximation with radial basis functions to build the response surface and seems very promising. Preliminary results show better results than the previously discussed solvers, and this routine is soon to be included in TOMLAB.

In the next section an application of global optimization in computational finance is discussed.

4 Global Optimization of Stock Market Trading

In our research on prediction methods in computational finance, we study the prediction of various kinds of quantities related to stock markets, like stock prices, stock volatility and ranking measures. In one project we instead of the classical time series approach used the more realistic prediction problem of building a multi-stock artificial trader (ASTA). The behavior of the trader is controlled by a parameter vector which is tuned for best performance. Here, one of our global optimization routines in TOMLAB, *glbSolve*, is used to find the optimal parameters for the noisy functions obtained, when running on a large database of Swedish stock market data. The ASTA system and this

problem are discussed in more detail in [9].

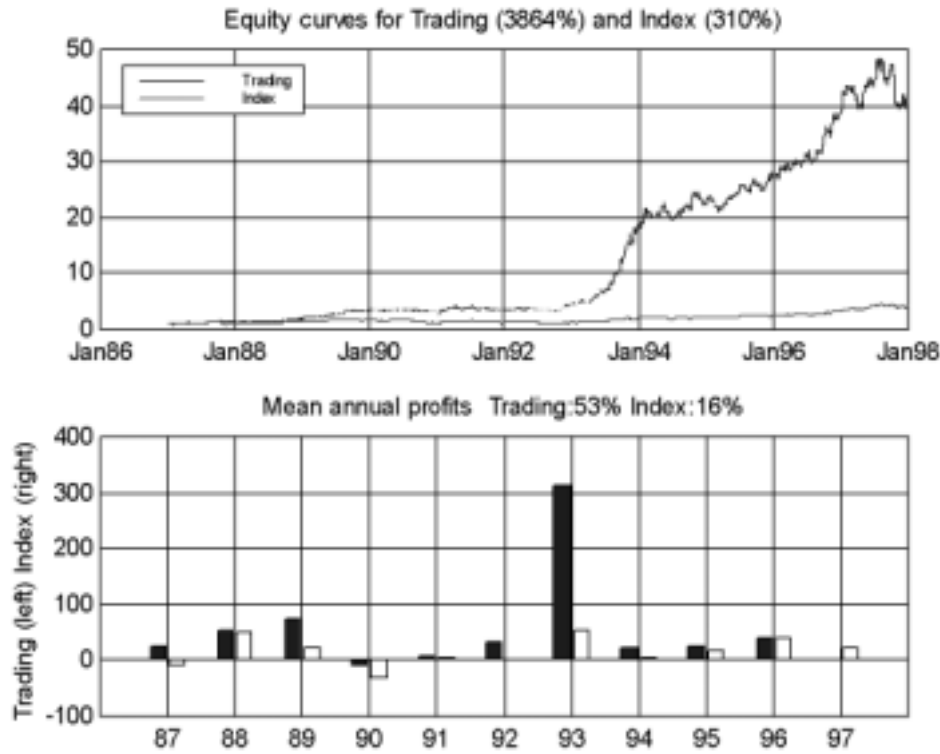


Figure 1: Performance of the trading function $Stoch(30, 3, 3, 20, 80)$ based on the Stochastics indicator.

The Stochastics Indicator is a classical technical trading rule. We have obtained very good results in ASTA using this rule to select buy and sell rules in a multi-stock trading algorithm, see Figure 1 for a performance diagram that compares the trading results with the stock market index. We tried to tune two of the parameters in this trading rule. In Figure 2 we see the points sampled when trying to find the optimal buy and sell rules in the Stochastics Indicator. They cluster around $(40, 78)$, which seems to be the global optimum. In Figure 3 one-dimensional views of the *Net profit* (with reversed sign) versus the *Buylevel* and the *Sellelevel* are shown. The optimum is more well-determined and distinct in the *Buylevel*. The global optimum is in fact very close to the standard values used in technical analysis. Further testing and analysis are needed to establish robustness properties of the parameters found.

5 Nonlinear Parameter Estimation

Nonlinear parameter estimation problems, especially of exponential type, are often ill-conditioned. Practical numerical tests on real applications show that solvers often return erroneous results, claiming success when not having converged to a true local minimum. Or the solvers simply fail to converge.

The TOMLAB nonlinear least squares solver, *clsSolve*, is designed to be robust for ill-conditioned problems and has in tests showed to be more robust than other available software. It also converges faster (with less function evaluations) than other solvers. It is often the case in model approximation that there are bounds on the variables, like nonnegativity constraints. Some solvers do not handle such bounds. Furthermore, the model might include linear constraints on the variables. The TOMLAB *clsSolve* solver has special treatment of both simple bounds and linear constraints, and tests show that it performs very robust on all these types of problems, see

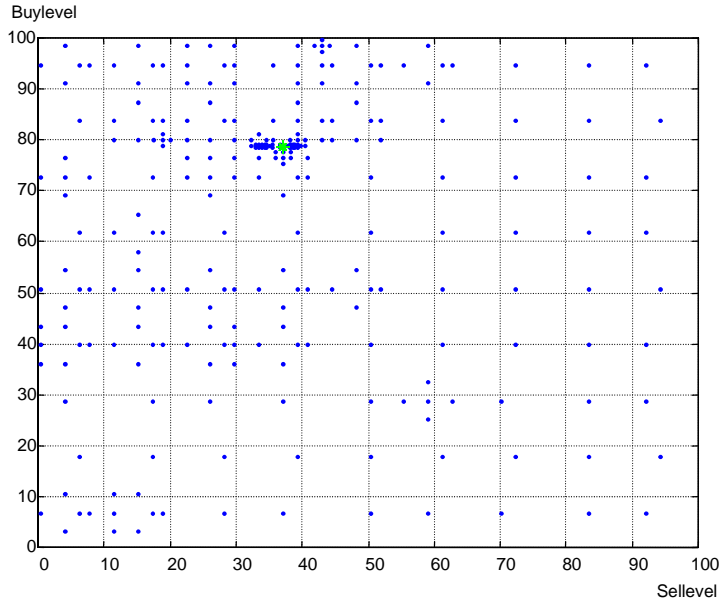


Figure 2: Sampled points by *glbSolve* in the parameter space when optimizing the buy and sell levels for the trading function $Stoch(30, 3, 3, Sellevel, Buylevel)$.

The **constrained nonlinear least squares problem (cls)** is defined as

$$\begin{aligned}
 \min_x \quad & f(x) = \frac{1}{2}r(x)^T r(x) \\
 \text{s.t.} \quad & x_L \leq x \leq x_U, \\
 & b_L \leq Ax \leq b_U
 \end{aligned} \tag{3}$$

where $x, x_L, x_U \in \mathbb{R}^n$, $r(x) \in \mathbb{R}^N$, $A \in \mathbb{R}^{m \times n}$, $b_L, b_U \in \mathbb{R}^m$.

The routine *clsSolve* implements four methods for nonlinear least squares problems: the Gauss-Newton method, the Al-Baali and Fletcher hybrid method [1], the Fletcher and Xu hybrid method [7], and the Huschens TSSM method [18]. If rank problems occur, the algorithm is using subspace minimization. The line search algorithm is a modification of an algorithm by Fletcher. Linear equality and inequality constraint are treated using an active-set strategy.

The *clsSolve* solver is used in several of our applied research projects, e.g. estimation of formation constants in chemical equilibrium analysis, analysis of plasmid stability in fermentation processes and fitting of exponential sums to empirical data in radiotherapy planning. The radiotherapy planning problem is discussed in Section 6.

Another case where special treatment of linear constraints gives numerical advantages is in the solution of nonlinear equation systems. If some of equations are linear in the variables it is better to solve the problem as a linearly constrained nonlinear least squares problem. More formally, define the nonlinear systems of equations $g(x) = 0$, $g \in \mathbb{R}^m$. If partitioning into two parts the nonlinear and linear equations, i.e. $g(x) = [r(x), Ax - b]$, then the solution is obtained solving the following linearly constrained nonlinear least squares problem

$$\begin{aligned}
 \min_x \quad & f(x) = \frac{1}{2}r(x)^T r(x) \\
 \text{s.t.} \quad & Ax = b
 \end{aligned} \tag{4}$$

Additional constraints, like bounds, are easy to add to the problem formulation.

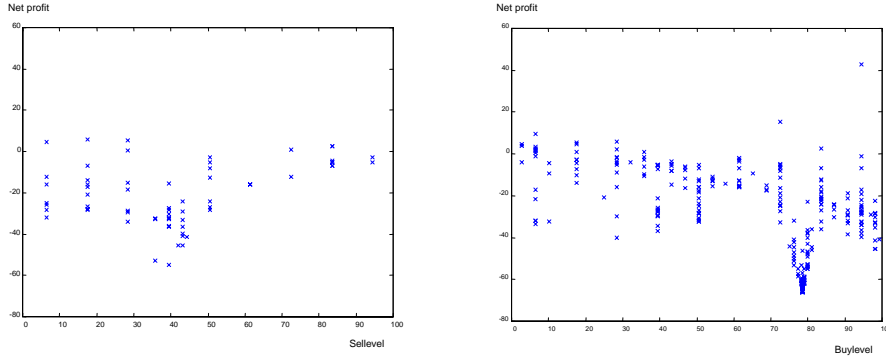


Figure 3: One-dimensional views of the global optimization of the parameters in the trading function $Stoch(30, 3, 3, Sellevel, Buylevel)$. The left graph shows the *Net profit* versus the *Buylevel* for an equidistant grid of values of the *Sellevel*. The right graph shows the *Net profit* versus the *Sellevel* for an equidistant grid of values of the *Buylevel*.

6 Parameter Estimation in Exponential Models

In TOMLAB the problem of fitting sums of positively weighted exponential functions to empirical data may be formulated either as a nonlinear least squares problem or a separable nonlinear least squares problem. Several empirical data series are predefined and artificial data series may also be generated. Algorithms to find starting values for different number of exponential terms are implemented.

There are five different types of exponential models with special treatment in TOMLAB, shown in Table 1. In current research in cooperation with Todd Walton, Vicksburg, USA, TOMLAB has been used to estimate parameters using maximum likelihood in simulated Weibull distributions, and Gumbel and Gamma distributions with real data. TOMLAB has also been useful for parameter estimation in stochastic hydrology using real-life data.

Table 1: Exponential models treated in TOMLAB.

$f(t) = \sum_i^p \alpha_i e^{-\beta_i t},$	$\alpha_i \geq 0,$	$0 \leq \beta_1 < \beta_2 < \dots < \beta_p.$
$f(t) = \sum_i^p \alpha_i (1 - e^{-\beta_i t}),$	$\alpha_i \geq 0,$	$0 \leq \beta_1 < \beta_2 < \dots < \beta_p.$
$f(t) = \sum_i^p t \alpha_i e^{-\beta_i t},$	$\alpha_i \geq 0,$	$0 \leq \beta_1 < \beta_2 < \dots < \beta_p.$
$f(t) = \sum_i^p (t \alpha_i - \gamma_i) e^{-\beta_i t},$	$\alpha_i, \gamma_i \geq 0,$	$0 \leq \beta_1 < \beta_2 < \dots < \beta_p.$
$f(t) = \sum_i^p t \alpha_i e^{-\beta_i (t - \gamma_i)},$	$\alpha_i \geq 0,$	$0 \leq \beta_1 < \beta_2 < \dots < \beta_p.$

In [14] algorithms for fitting exponential sums $D(r) = \sum_{i=1}^p a_i (1 - \exp(-b_i r))$ to numerical data are presented and compared for efficiency and robustness. The numerical examples stem from parameter estimation in dose calculation for radiotherapy planning. The doses are simulated by emitting an ionizing photon beam into water and at different depths d and different radius r from the beam center measuring the absorption. The absorbed dose is normally distinguished into primary dose from particles excited by the photon beam and scattered dose from the following particle interactions.

In Table 2. results are presented from a comparison of different nonlinear solvers for the Helax problems described above. The tested solvers are:

- TOMLAB v1.0 clsSolve, Gauss-Newton with subspace minimization.
- TOMLAB v1.0 clsSolve, Fletcher-Xu Hybrid algorithm. Problems solved using a separable nonlinear least

squares algorithm.

- MathWorks Optimization Toolbox 2.0, Matlab solver lsqnonlin, a Levenberg-Marquardt algorithm.
- MathWorks Optimization Toolbox 2.0, Matlab solver lsqnonlin, a large-scale trust-region algorithm.
- Systems Optimization Laboratory, Stanford. The constrained nonlinear least squares solver NLSSOL, run through TOMLAB v1.0 MEX-file interface.
- Systems Optimization Laboratory, Stanford. The general nonlinear solver NPSOL, run through TOMLAB v1.0 MEX-file interface.

The table entries for each solver consists of three integers which give the numbers of iterations, residual evaluations and Jacobian evaluations required to solve the problem. We restrict to present detailed information for the first fifteen and the last two problems but the average values and the number of failures are based on all the 334 problems. The † indicates that the separable nonlinear least squares algorithm II from [23] is run. Note that the lsqnonlin LS algorithm has convergence problems, giving many failures. The efficiency of the *clsSolve* Fletcher-Xu method with the separable algorithm is obvious, less than 65 percent of the number of iterations, residual evaluations and Jacobian evaluations for the best of the other solvers are required to solve the problems.

Worth mentioning is that TOMLAB includes routines for computing (initial) parameter estimates for exponential sum model fitting problems that are very close to the true solution for equidistant problems and fairly good for non-equidistant problems, see the thesis by Petersson [22]. This is extremely important when solving problems in real life applications, and these good initial values are used in the radiotherapy example.

7 Other Applications of TOMLAB

To find unknown species formation constants and other unknown parameters in multi-phase chemical equilibrium analysis, we have formulated a separable nonlinear least squares algorithm. The separation aims at using the structure of a large, ill-conditioned parameter estimation problem, to obtain a solvable set of optimization problems. Each iteration in the separable algorithm consists of a major problem and the solution of hundreds or thousands of minor ill-conditioned problems. To obtain a practically useful tool, a combination of approximation algorithms to find initial values for the unknown parameters are needed, together with robust constrained nonlinear least squares solvers [10]. As we are using the weighted L_2 -norm, sensitive to outliers, all the minor problems must be solved with high accuracy and no failures. Here the TOMLAB constrained nonlinear least squares solver *clsSolve* is used in our new Matlab toolbox LAKE TB. Results so far are excellent and *clsSolve* converges fast and the parameters are determined with high accuracy [10]. As TOMLAB handles recursive calls in a proper way, it is possible to use *clsSolve* for both the major and minor optimization problems.

In a joint project with Prof. Jordan M. Berg, Texas Tech University, Lubbock, TX, the aim is to find accurate low-order phenomenological models of thin film etching and deposition processes. These processes are central to the manufacture of micro-electronic devices. We have developed algorithms and software for parameter estimation using level sets. i.e. the problem of selecting the member of a parameterized family of curves that best matches a given curve. Level set methods offer several attractive features for treating such problems. The method is completely geometric; there is no need to introduce an arbitrary coordinate system for the curves. We have derived analytic results necessary for the application of gradient descent algorithms, and made numerical computations using TOMLAB[2].

8 Conclusions and Future work

We have discussed a new and useful tool in applied mathematical computations, the optimization environment TOMLAB. The tool includes both a broad range of optimization solvers, but also special tools e.g. for separable nonlinear least squares and parameter estimation in exponential models.

New algorithms and software in the area of global optimization makes it possible to optimize parameters for costly functions e.g. appearing in simulations. The TOMLAB nonlinear least squares solvers are robust and performs well on ill-conditioned problems. On-going research in our group in global optimization and nonlinear least squares will lead to more tools in these areas.

Table 2: Numerical test on the nonlinear least squares solution of 335 problems from radiotherapy planning supplied by Helax AB, Uppsala, Sweden.

Depth d	clsSolve GN	clsSolve FX†	lsqnonlin LM	lsqnonlin LS	NLSSOL	NPOPT
001	9 12 12	6 7 7	17 18 18	22 22 22	14 19 19	57 80 80
002	8 11 11	6 7 7	16 17 17	12 12 12	9 13 13	53 77 77
004	8 10 10	9 10 10	14 15 15	9 9 9	11 15 15	38 57 57
005	8 10 10	10 11 11	13 14 14	10 10 10	11 15 15	37 56 56
007	9 11 11	10 11 11	13 14 14	13 13 13	13 16 16	30 49 49
008	9 11 11	12 14 14	13 14 14	12 12 12	13 16 16	28 44 44
010	10 12 12	10 11 11	13 14 14	12 12 12	13 16 16	31 47 47
011	10 12 12	11 12 12	11 12 12	12 12 12	13 20 20	20 25 25
013	10 11 11	11 12 12	14 15 15	11 11 11	13 20 20	13 22 22
014	15 21 21	21 33 33	18 19 19	—	17 26 26	33 50 50
016	17 24 24	16 34 34	21 22 22	—	17 29 29	37 61 61
017	19 25 25	21 25 25	24 25 25	—	25 36 36	33 70 70
019	21 30 30	20 35 35	27 28 28	—	25 36 36	39 61 61
020	23 31 31	20 35 35	32 33 33	—	27 37 37	42 62 62
022	27 39 39	19 35 35	41 42 42	—	29 44 44	43 63 63
023	32 45 45	26 37 37	65 66 66	—	33 49 49	46 67 67
025	46 48 48	10 11 11	46 47 47	—	29 37 37	34 42 42
026	38 39 39	11 12 12	31 32 32	—	21 28 28	32 40 40
028	31 32 32	13 14 14	27 28 28	—	21 27 27	28 35 35
029	28 29 29	13 14 14	25 26 26	—	21 27 27	29 35 35
031	26 27 27	13 14 14	23 24 24	—	21 27 27	26 45 45
032	25 26 26	13 14 14	22 23 23	—	21 27 27	27 47 47
034	24 25 25	13 14 14	22 23 23	—	21 27 27	29 38 38
035	23 24 24	13 14 14	21 22 22	—	21 27 27	31 42 42
037	23 24 24	12 13 13	21 22 22	—	21 27 27	23 37 37
038	23 24 24	12 13 13	21 22 22	—	19 25 25	29 35 35
040	24 25 25	12 13 13	21 22 22	—	19 25 25	29 37 37
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497	9 10 10	5 6 6	9 10 10	20 20 20	7 9 9	18 26 26
499	9 10 10	5 6 6	9 10 10	20 20 20	7 9 9	17 25 25
500	9 10 10	5 6 6	9 10 10	20 20 20	7 9 9	17 25 25
Average	16 18 18	8 10 10	19 20 20	25 25 25	13 18 18	21 31 31
Failures	0	0	0	68	0	0

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