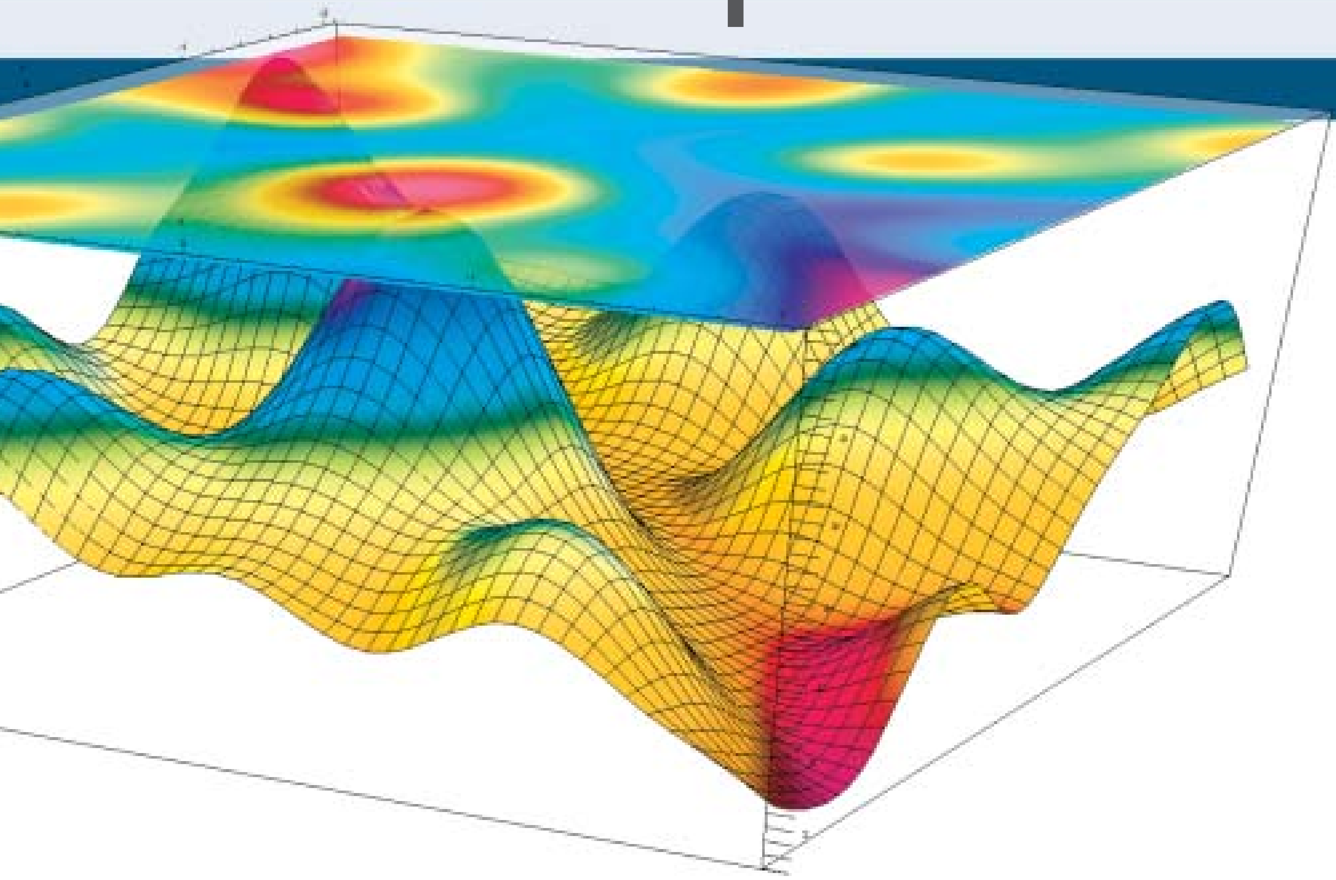
maple

Professional Toolbox SERIES™

Global Optimization



This document presents a concise review of the quantitative decision-making, modeling and optimization paradigm, with an emphasis on nonlinear models. We introduce the Global Optimization Toolbox to solve such models and illustrate its use.

Maplesoft

command the brilliance

The Maple Global Optimization Toolbox

by János D. Pintér

Pintér Consulting Services, Inc.

Summary

This document presents a concise review of the quantitative decision-making, modeling and optimization paradigm, with an emphasis on nonlinear models. We introduce the Global Optimization Toolbox to solve such models and illustrate its use.

Decision-Making and Optimization

In today's competitive global economy, government organizations and private businesses all aim for resource-efficient operations that deliver high quality products and services. This demands prudent, effective and timely decisions in an increasingly complex and dynamically changing environment.

To illustrate this point, one can think of decisions related to strategic, tactical, and real-time decision-making in areas such as:

- agricultural planning
- biotechnology
- data analysis
- distribution of goods and resources
- emergency and rescue operations
- engineering systems design
- environmental management
- financial planning
- food processing
- health care management
- inventory control
- manpower and resource allocation
- manufacturing of goods
- military operations
- production process control
- risk management
- sequencing and scheduling of operations
- telecommunications
- traffic control

Operations Research (O.R.) is a comprehensive, scientifically established approach: its practical purpose is to assist analysts and decision-makers in making well-established quantitative decisions. The central objective of O.R. is *optimization*: that is, "to do things best under the given circumstances".

With varying emphasis on certain parts of this "definition" of O.R., many closely related disciplines have emerged (with significant overlaps among them): decision analysis, systems analysis, management science, control theory, game theory, optimization, constraint logic programming, artificial intelligence, fuzzy decision-making, multi-criteria analysis, and so on are all aimed at finding better decisions. Also included are business applications such as supply-chain management, enterprise resource planning, total quality management, just-in-time production and inventory management, materials requirements planning, and others. All of these are ultimately related to making efficient quantitative decisions.

Following the optimization paradigm, the decision-maker selects the key variables that will influence the quality of decisions. The latter is expressed by the objective function that is maximized (profit, quality, speed of service or job completion, and so on), or minimized (cost, loss, risk of some undesirable event, etc.). In addition, a set of (physical, technical, economic, environmental, legal, societal) constraints is also considered, when selecting a "good" (feasible) solution or the "very best" (optimal) solution, in the context of the problem formulation.

This document reviews the main steps of quantitative decision modeling and problem solution, with a particular emphasis on using Maple™ and the Global Optimization Toolbox in this process. A list of illustrative references is also provided.

Modeling and Solution Procedure

A formal procedure aimed at making optimal decisions includes the following main stages:

1. Conceptual description of the decision problem at a suitable level of abstraction, retaining only the essential attributes, while omitting secondary details and circumstances.
2. Development of a quantitative model that captures the key elements of the decision problem, in terms of decision variables and the relevant functional relationships among these (as expressed by constraints and objectives).
3. Development and/or adaptation of a systematic (algorithmic) solution procedure, in order to explore the set of feasible solutions, and to select the best decision, or a list of good alternative decisions.
4. Numerical solution and its verification; interpretation and summary of results.
5. Posterior analysis and implementation of the decision(s) found.

The problems tackled by O.R. and related disciplines are often so complex that the correct model and solution procedure may not be clear at the beginning. For example, drawbacks to a model or solution approach that looked promising in Steps 2 and 3 may only become apparent at Step 4, either because the solution failed to capture the key attributes of the decision problem identified in Step 1, or because the solution approach was not computationally tractable.

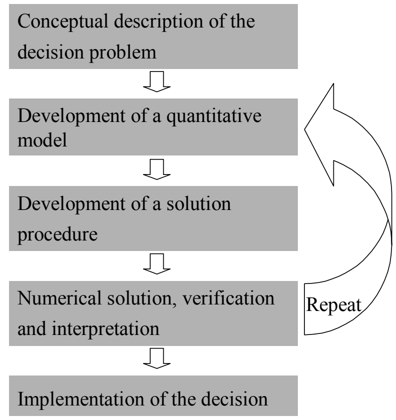


Figure 1 *Formal modeling and solution process for making optimal decisions*

Therefore, decision makers often must carry out the steps outlined above in an iterative fashion (see Figure 1). That is, they repeatedly refine the model formulation and solution procedure until the numerical solution captures the essence of the problem, is computationally tractable, and is deployable in a real setting. When the solution meets these three criteria (in the eyes of the decision makers), the decision can be implemented.

One can see that Steps 1 and 2 require an element of modeling "art" in addition to mathematical knowledge. Step 3 requires not only knowledge but also "taste" to find a suitable, computationally tractable approach to solving the problem. Steps 1, 4 and 5 greatly benefit from interaction with the actual decision-makers or users of the decision support system (DSS) developed. The importance of these points to obtaining meaningful, deployable solutions to real-life decision problems (and thereby also to increasing the visibility that the field of O.R. rightly deserves) can not be overemphasized.

Optimization Models and Solution Strategies

To formalize the constrained optimization paradigm, we shall use the following notation:

- x decision vector, an element of the real Euclidean n-space $\boldsymbol{R}^n$
- $f(x)$ objective function, f: $\boldsymbol{R}^n \rightarrow \boldsymbol{R}$
- D non-empty set of admissible decisions, defined by
- xl, xu explicit, finite bounds of x (an embedding "box" in $\boldsymbol{R}^n$)
- $g(x)$ m-vector of continuous constraint functions, g: $\boldsymbol{R}^n \rightarrow \boldsymbol{R}^m$.

In this notation, the optimization model can be concisely stated as

(1) $\quad min\ f(x) \quad x \in \mathrm{D} = \{x:\ xl \leq x \leq xu,\ g(x) \leq 0\}$

Under fairly general analytical conditions, the model (1) has one or more optimal solutions. (For example, if D is non-empty, and f is continuous, then the model has a global solution set.) At the same time, finding globally best solutions may be numerically difficult.

To illustrate this point, consider the following simple one-dimensional instance of (1).

(2) $min\ x^2 - 10\sin(x^2 - 3x + 2),\ -5 \le x \le 5$

A plot of this function is shown in Figure 2.

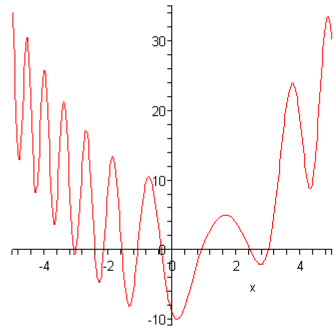


Figure 2 *A multi-extremal function*

Now, if we use “traditional” local scope search methods, then – depending on the starting point of the search – we will arrive at *locally optimal* solutions of varying quality. (See the “valleys” in this figure that could trap local search methods.) In order to find the globally optimal solution, a genuine global scope search effort is needed. In higher dimensions, the complexity can increase rapidly, as shown by the direct two-dimensional analogue of the model. Note that we have changed the box region bounds in order to make the generated example a bit more realistic (by removing some artificial symmetry). See Figure 3.

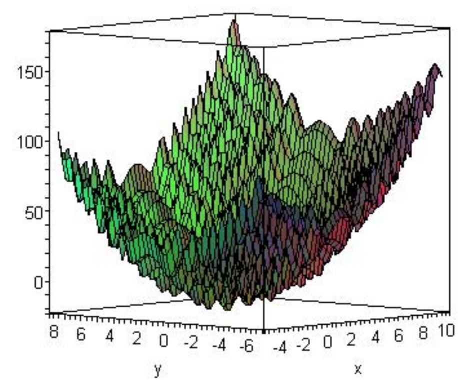


Figure 3 *A two-dimensional extension of the model in Figure 2*

Nonlinear models are ubiquitous in many applications in advanced engineering design, biotechnology, data analysis, environmental management, financial planning, process control, risk management, scientific modeling, and others. In many of these models, a global search approach is effective in finding the globally optimal solution.

Maple for O.R. Modeling and Optimization

Maple is a fully integrated scientific and technical modeling and computing environment. It enables the development of sophisticated documents that combine description, calculations and visualization, with numerous supporting features, such as on-line documentation, debugging, code generation, and so on. All of these capabilities accelerate and expand the scope of optimization model development and solution.

Features of Maple that pertain especially to the modeling and solving of optimization problems include the following:

- performance scales well to modeling large, complex problems
- supports rapid prototyping and model development
- has an extensive set of built-in mathematical and computational functions
- has comprehensive symbolic calculation capabilities
- supports advanced computations with arbitrary numeric precision
- is fully programmable (thus extendable by adding new functionality)
- has sophisticated visualization tools
- supports advanced technical documentation, desktop publishing, and presentation
- provides links to external software products
- is portable across a broad range of hardware platforms and operating systems
- can export its results into source code for other programming languages, such as C and MATLAB

The Global Optimization Toolbox

The core of the Toolbox is the LGO (Lipschitz Global Optimizer) solver suite. LGO is based on award-winning research published e.g. in professional books and articles (see the related references). LGO has been used in both commercial and academic applications for more than a decade.

LGO offers a combined implementation of global and local scope nonlinear solvers. The current LGO implementation includes the following solver algorithms:

- branch-and-bound based global search
- adaptive global random search (single-start)
- random multi-start based global search
- reduced gradient approach based local search.

The Maple Global Optimization Toolbox implementation of LGO provides a powerful combination of Maple's model development, numerics, and visualization capabilities with the robustness and solver speed of LGO.

Illustrative Applications

Example 1

Let us first show how to solve the model stated in formula (2) using the Global Optimization Toolbox. To load the Toolbox into a Maple session, we simply use the statement

```
> with(GlobalOptimization):
```

The model (2) is then solved by the one-line command below; Maple's result is in blue.

```
> GlobalSolve(x^2-10*sin(x^2-3*x+2), x=-5..5);
```

$$[-9.9779, [x = 0.14662]]$$

By contrast, the local solver (that comes with standard Maple releases, invoked using the Minimize function) gives one of the sub-optimal solutions:

```
> Minimize(x^2-10*sin(x^2-3*x+2), x=-5..5);
```

$$[-2.1125, [x = 2.7651]]$$

Needless to say, this is not a criticism of the local solver: however, it shows the limitations of a local scope approach – unless one knows a priori where to initiate the search. Clearly, this would not always be a very simple task: recall the (merely two-dimensional) function in Figure 3.

Example 2

Let us consider next a somewhat more complicated optimization model as shown below:

$$min\ \sin^2(2x^2 + xy^2) + \sin^2(4y + x^2 - 12xy)$$

$$\log(1 + x^4) + 8\sin(x^2 - y) \leq 0.01,$$

$$x + y^2 - x^2 + \sin(x) - 5y \leq -1.2\},$$

$$-2 \leq x \leq 3$$

$$-4 \leq y \leq 2$$

The next two Maple statements and corresponding answers show the difference between local and global searches in a somewhat more complicated model. Notice the constraint definitions, which for added emphasis we place here on the second line, and the variable bounds (third line):

```
> Minimize(sin(2*x^2+x*y^2)^2+sin(4*y+x^2-12*x*y)^2,
     {log(1+x^4)+8*sin(x^2-y)<=0.01, x+y^2-x^2+sin(x)-5*y<=-1.2},
     x=-2..3, y=-4..2);
```

$$[0.49683, [x = 0.47921, y = 2.0000]]$$

```
> GlobalSolve(sin(2*x^2+x*y^2)^2+sin(4*y+x^2-12*x*y)^2,
     {log(1+x^4)+8*sin(x^2-y)<=0.01, x+y^2-x^2+sin(x)-5*y<=-1.2},
     x=-2..3, y=-4..2);
```

$$[1.491\ 10^{-19}, [x = 1.016\ 10^{-10}, y = 1.5708]]$$

Maple for O.R. Modeling and Optimization

Maple is a fully integrated scientific and technical modeling and computing environment. It enables the development of sophisticated documents that combine description, calculations and visualization, with numerous supporting features, such as on-line documentation, debugging, code generation, and so on. All of these capabilities accelerate and expand the scope of optimization model development and solution.

Features of Maple that pertain especially to the modeling and solving of optimization problems include the following:

- performance scales well to modeling large, complex problems
- supports rapid prototyping and model development
- has an extensive set of built-in mathematical and computational functions
- has comprehensive symbolic calculation capabilities
- supports advanced computations with arbitrary numeric precision
- is fully programmable (thus extendable by adding new functionality)
- has sophisticated visualization tools
- supports advanced technical documentation, desktop publishing, and presentation
- provides links to external software products
- is portable across a broad range of hardware platforms and operating systems
- can export its results into source code for other programming languages, such as C and MATLAB

The Global Optimization Toolbox

The core of the Toolbox is the LGO (Lipschitz Global Optimizer) solver suite. LGO is based on award-winning research published e.g. in professional books and articles (see the related references). LGO has been used in both commercial and academic applications for more than a decade.

LGO offers a combined implementation of global and local scope nonlinear solvers. The current LGO implementation includes the following solver algorithms:

- branch-and-bound based global search
- adaptive global random search (single-start)
- random multi-start based global search
- reduced gradient approach based local search.

The Maple Global Optimization Toolbox implementation of LGO provides a powerful combination of Maple's model development, numerics, and visualization capabilities with the robustness and solver speed of LGO.

Application Perspectives

We see particularly strong application potentials for the Global Optimization Toolbox in advanced nonlinear optimization, when the decision model cannot be brought to one of the simple "standard"' forms – notably, continuous linear programming and its immediate extensions. Three broad classes of such prospective applications come from the following areas:

- optimization of complex "black box" systems
- optimal control of dynamic systems
- decision-making under uncertainty

Such models are ubiquitous in both academic research and in commercial applications of mathematics, physics, chemistry, biochemistry, environmental science, pharmaceuticals, medicine, finance, industrial engineering, and other related industries and services.

A few more concrete examples (case studies from the author's practice) are listed below:

- acoustics equipment design
- cancer therapy planning
- chemical process modeling
- data analysis, classification and visualization
- economic and financial forecasting
- environmental risk assessment and management
- industrial design
- laser equipment design
- model fitting to data (calibration)
- optimization in numerical mathematics (parametric integrals and differential equations)
- optimal operation of "closed" (confidential) engineering or other systems
- potential energy models in computational physics and chemistry
- packing and other object arrangement design problems
- robot design and manipulations
- systems of nonlinear equations and inequalities
- wastewater treatment systems management.

Further prospective and actual application areas and examples are welcome: please feel free to contact Maplesoft™ or the author of this document, to discuss the applicability of the Toolbox regarding specific areas.

In conclusion, we believe the Maple Global Optimization Toolbox can be put to good use in a rapidly growing range of professional applications, as well as in research and education.

References

Literally, thousands of books have been written on Operations Research, nonlinear systems modeling, and nonlinear/global optimization. The following list provides a sample of such works.

Aris, R. (1999) *Mathematical Modeling: A Chemical Engineer's Perspective*. Academic Press, San Diego, CA.

Bazaraa, M.S., Sherali, H.D. and Shetty, C.M. (1993) *Nonlinear Programming: Theory and Algorithms*. Wiley, New York.

Bell, P.C. (1999) *Management Science / Operations Research: A Strategic Perspective*. South-Western College Publishing, Cinicinnati, OH.

Beltrami, E., (1993) *Mathematical Models in the Social and Biological Sciences*. Jones and Bartlett, Boston.

Bertsekas, D.P. (1999) *Nonlinear Programming. (2nd Edition.)* Athena Scientific, Cambridge, MA.

Bertsimas, D. and Freund, R.M. (2000) *Data, Models, and Decisions: The Fundamentals of Management Science*. South-Western College Publishing, Cincinnati, OH.

Birge, J.R. and Louveaux, F. (1997) *Introduction to Stochastic Programming. (2nd Edition.)* Springer-Verlag, Berlin.

Carter, M.W. and Price, C.C. (2001) *Operations Research: A Practical Introduction*. CRC Press, Boca Raton, FL.

Casti, J.L. (1990) *Searching for Certainty*. Morrow & Co., New York.

Chong, E.K.P. and Zak, S.H. (2001) *An Introduction to Optimization. (2nd Edition.)* Wiley, New York.

Courant, R. and Hilbert, D, (1989) *Methods of Mathematical Physics, Vol. 1*. Wiley, New York.

Edgar, T.F., Himmelblau, D.M. and Lasdon, L.S. (2001) *Optimization of Chemical Processes. (2nd Edition.)* McGraw-Hill, New York.

Eigen, M. and Winkler, R. (1975) *Das Spiel*, Piper & Co., München.

Gershenfeld, N.A. (1999) *The Nature of Mathematical Modeling.* Cambridge University Press, Cambridge, UK.

Horst, R. and Pardalos, P.M., Eds. (1995) *Handbook of Global Optimization, Vol. 1*. Kluwer Academic Publishers, Dordrecht.

Hillier and Lieberman, G.J. (1986) *Introduction to Operations Research. (4th Edition.)* Holden Day, Oakland, CA.

Liebling, T.M. and de Werra, D., Eds. (1997) *Lectures on Mathematical Programming* (ISMP97). Elsevier Science, Amsterdam.

Liberatore, M.J. and Nydick, R.L. (2003) *Decision Technology: Modeling, Software, and Applications*. Wiley, Hoboken, NJ.

Murray, J.D. (1983) *Mathematical Biology*. Springer-Verlag, Berlin.

Nocedal, J. and Wright, S.J. (1999) *Numerical Optimization*. Springer-Verlag, New York 1999.

Operations Research (2002) *50th Anniversary Issue* INFORMS, Linthicum, MD.

Papalambros, P.Y. and Wilde, D.J. (2000*) Principles of Optimal Design.* Cambridge University Press, Cambridge, UK.

Pardalos, P.M. and Resende, M.G.C., Eds. (2002) *Handbook of Applied Optimization*. Oxford University Press, Oxford.

Pardalos, P.M. and Romeijn, H.E., Eds. (2002) *Handbook of Global Optimization, Vol. 2*. Kluwer Academic Publishers, Dordrecht.

Parlar, M. (2000) *Interactive Operations Research with Maple: Models and Methods*. Birkhäuser, Boston.

Pearson, C.E. (1986) *Numerical Methods in Engineering and Science.* Van Nostrand Reinhold, New York.

Pintér, J.D. (1996) *Global Optimization in Action*. Kluwer Academic Publishers, Dordrecht.

Pintér, J.D. (2001) *Computational Global Optimization in Nonlinear Systems: An Interactive Tutorial*. Lionheart Publishing, Inc. Atlanta, GA.

Pintér, J.D. (2004) *Applied Nonlinear Optimization in Modeling Environments*. CRC Press, Boca Raton, FL. (To appear.)

Schittkowski, K. (2002) *Numerical Data Fitting in Dynamical Systems*. Kluwer Academic Publishers, Dordrecht.

Sethi, S.P. and Thompson, G.L. (2000) *Optimal Control Theory: Applications to Management Science and Economics*. Kluwer Academic Publishers, Dordrecht.

Schroeder, M. (1991) *Fractals, Chaos, Power Laws*. Freeman & Co., New York.

Terlaky, T., Ed. (1996) *Interior Point Methods of Mathematical Programming*. Kluwer Academic Publishers, Dordrecht.

Waterloo Maple Inc. (2004) *Maple 9.5*. Maplesoft, a division of Waterloo Maple Inc. Waterloo, ON.

Waterloo Maple Inc. (2004) *Applications of the Global Optimization Toolbox*. Maplesoft, a division of Waterloo Maple Inc. Waterloo, ON.

Williams, H.P. (1999) *Model Building in Mathematical Programming. (4th Edition.)* Wiley, New York.

Winston, W.L. (1994) *Operations Research: Applications and Algorithms.* Duxbury Press, Belmont, CA.

Zwillinger, D. (1989) *Handbook of Differential Equations. (3rd Edn.)* Academic Press, New York.

About the Author

János D. Pintér, Ph.D., D.Sc., is a researcher and practitioner with three decades of experience. His main area of interest is advanced modeling and optimization, including algorithm and software development. He has written books, numerous articles and technical reports. His software products, marketed with partners and through his company, have been in use by academia, government and business organizations in over 20 countries.

Dr. Pintér is a member of INFORMS, the Mathematical Programming Society, the Canadian and Hungarian O.R. Societies, and SIAM. He serves on the Editorial Board of the *Journal of Global Optimization*, the *Journal of Applied Mathematics and Decision Sciences*, and two online forums maintained by the GAMS Corporation. He received the 2000 INFORMS Computing Society Prize for his book *Global Optimization in Action*, as well as other research awards and fellowships (e.g., in Australia, Austria, Canada, Germany, Hungary, Italy, Netherlands, and the United States). Dr. Pintér has presented lectures, tutorials, and workshops in over 25 countries.