Nonlinear Systems Modeling and Optimization Using AIMMS /LGO

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Summary

This brief article reviews the quantitative decision-making paradigm, with an emphasis on nonlinear models that frequently have multiple (global and local) optima. We introduce the AIMMS /LGO software implementation to analyze and solve such models. A list of illustrative applications of global optimization (including LGO applications) is provided, with further topical references.

Decision-Making and Optimization

In today's competitive global economy, government organizations and private businesses all aim for 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 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, and many other areas.

Operations Research (O.R.) provides a comprehensive, scientifically established methodology to assist analysts and decision-makers. The key objective of O.R. is *optimization*: that is, "to do things best under the given circumstances". Closely related disciplines (with significant overlaps) include decision analysis, systems analysis, management science, control theory, game theory, optimization theory, constraint logic programming, artificial intelligence, fuzzy decision-making, multi-criteria analysis, and so on: these are all aimed at finding better decisions. The same comment applies, *mutatis mutandis*, to O.R. related 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.

Global Optimization

According to the general optimization paradigm, the decision-maker selects the key *variables* that influence the quality of decisions. This quality 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, and so on). In addition to the objective function, typically a set of (physical, technical, economic, environmental, legal, societal) *constraints* is also considered. Then, by (algorithmically) adjusting the value of the decision variables, we wish to select a "good" (*feasible*) solution or – ideally – the "best possible" (*optimal*) solution, in the context of the given model formulation.

Here we will consider the general class of *nonlinear* models, in which some of the model objective or constraint functions are nonlinear. Within this context, the objective of *global optimization* is to find the *globally best* solution, in the (possible or known) presence of multiple local optima. Formally, we want to find the global solution(s) of the constrained optimization model

$$\min f(x)$$
$$x \in D := \{x_l \le x \le x_u,\ g(x) \le 0\} \subset R^n \quad (1)$$

In the model formulation (1), x is an n-dimensional real vector; the corresponding n-vector bounds x_l and x_u are interpreted component-wise. We assume that x_l and x_u are finite, the objective f and the constraints $g(x)=(g_1(x), \ldots, g_m(x))$ are all continuous functions, and the feasible set D is non-empty. These assumptions guarantee that the model is well-posed, and hence it has a global solution (set).

As an example, the figure below shows the error function related to solving a pair of equations: here we wish to find the smallest possible error, by changing the parameters x and y. (In the notation of model (1), these two parameters are the components of the decision vector.)

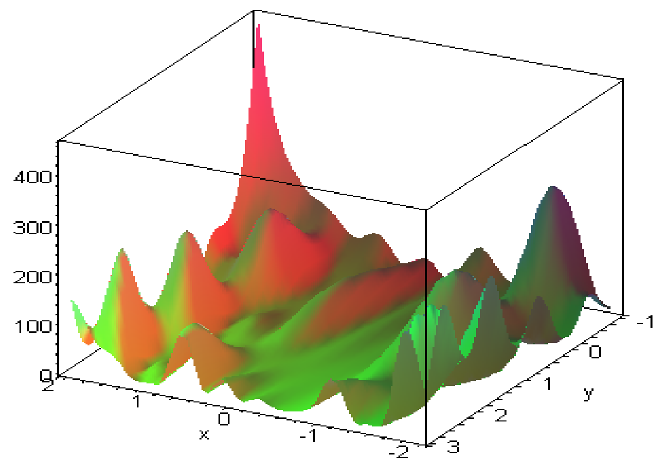

Figure 1 *A box-constrained global optimization model: objective function.*

Let us point out that if we use traditional local scope search methods to solve this problem, then – depending on the starting point of the search – we will often find only *locally optimal* solutions of varying quality. (Notice the many “valleys” in Figure 1 that could easily trap local search methods.) In order to find the *globally optimal* solution, a genuine global scope search effort is needed. Nonlinear models are ubiquitous in many applications, including advanced engineering design, biotechnology, data analysis, environmental management, financial planning, process control, risk management, scientific modeling, and other areas. The solution of such models often requires a global scope search approach.

LGO Solver Suite for Nonlinear Optimization

Since 1986, we have been developing nonlinear optimization software, with both global and local search capabilities. For the underlying theory and some key implementation details, consult (Pintér, 1996, 2001, 2002, 2006b). Here we review the core LGO (Lipschitz-Continuous Global Optimizer) software implementation and its AIMMS platform-specific version.

The LGO software is based on the research summarized in (Pintér, 1996); however, numerous features have been added to enhance its current implementation. LGO offers an integrated suite of global and local search algorithms, to handle optimization models with efficiency and speed. In contrast to several widely used nonlinear local optimization solver engines (such as CONOPT or MINOS), LGO's main scope of application is global optimization. However, LGO also has its own built-in local nonlinear optimization capability.

A practically important point to emphasize here is that a specialized model structure is not assumed or exploited by LGO. Therefore nonlinear models handled by LGO can be defined by arbitrary computable functions that – for reasons of theoretical validation of the numerical results obtained – should be continuous or Lipschitz-continuous over a given finite "box" range of the (continuous) decision variables, recall the model form (1). These very basic analytical requirements are met by great many practical models. Without going into details, note that e.g. all models defined by smooth (continuously differentiable) functions on the variable range $[x_l, x_u]$ have a suitable Lipschitz-continuous structure.

AIMMS /LGO Implementation

AIMMS – abbreviating Advanced Integrated Multidimensional Modeling Software – (Paragon Decision Technology, 2006) offers a sophisticated, fully integrated model development and solution environment, for the creation of high-performance decision support applications. AIMMS helps organizations to rapidly improve the quality, service, profitability, and responsiveness of their operations.

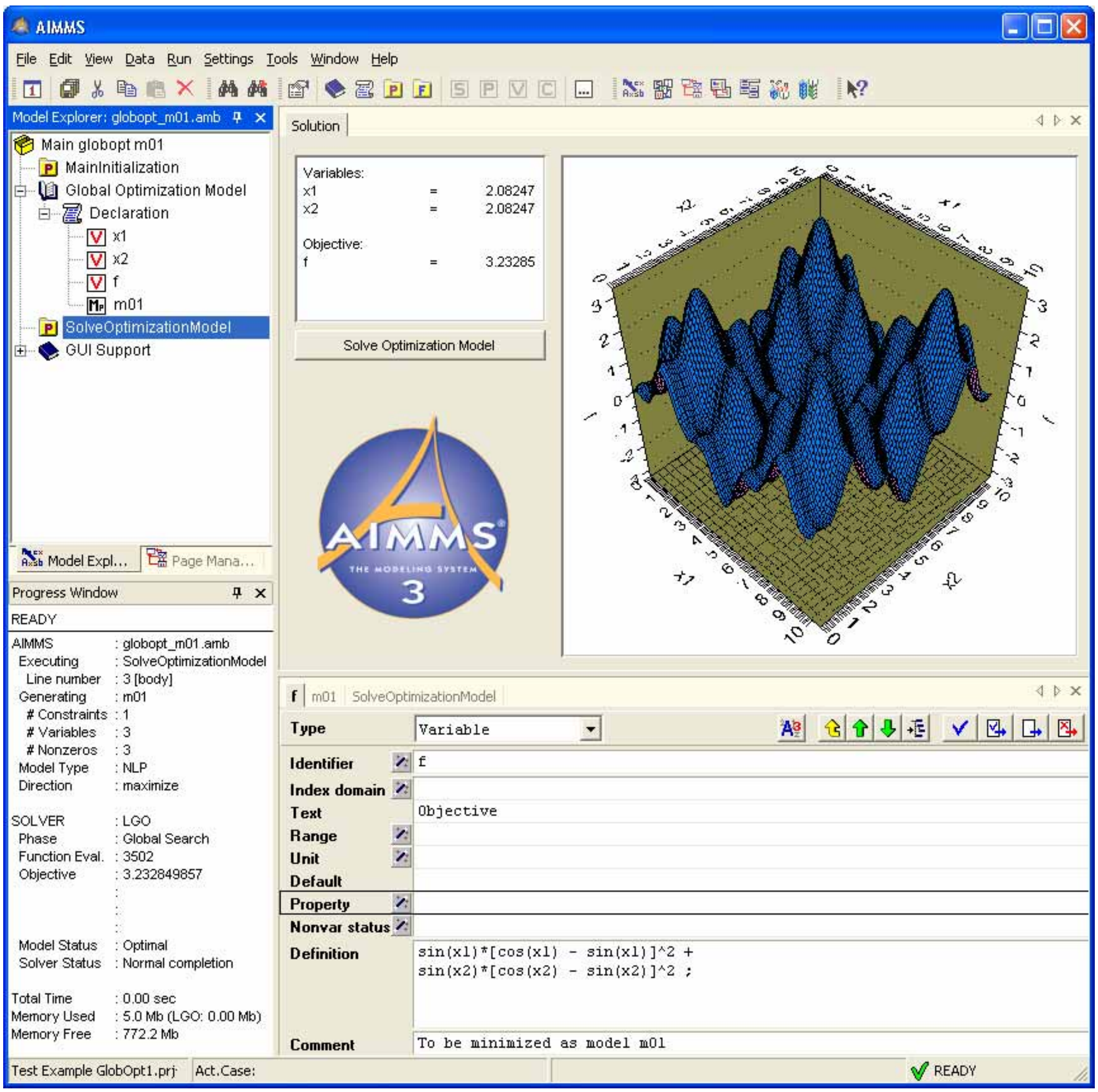

Figure 2 *AIMMS with the LGO solver: formulating, solving, and visualizing model (2).*

The AIMMS development environment offers a unique combination of advanced features and design tools, such as the graphical model explorer, which allow users to build and maintain complex decision support applications and advanced planning systems, in a fraction of the time required by conventional programming tools. It also offers a range of solvers to handle specific model types.

Recently, Paragon Decision Technology and PCS have made available the AIMMS /LGO solver option based on the core LGO technology. Figure 2 shows an example of using AIMMS /LGO to solve a merely two-dimensional, but visibly rather difficult test model.

The test model in question is

$$\min \sin(x_1)(\cos(x_1)-\sin(x_1))^2+\sin(x_2)(\cos(x_2)-\sin(x_2))^2 \quad (2)$$

$$0\leq x_1\leq 10,\ 0\leq x_2\leq 10.$$

The numerical solution of model (2), obtained in a fraction of a second on today's desktop machine, is $x_1=x_2=5.22406$; the numerical optimum estimate is -3.23285, see Figure 2.

In the AIMMS /LGO implementation, the LGO solver suite is seamlessly integrated with AIMMS. This implementation has been thoroughly tested using standard nonlinear and global optimization model libraries, as well the developers' (Paragon and PCS) test model libraries.

For further information regarding AIMMS /LGO, please visit Paragon Decision Technology's web site http://www.aimms.com. In addition to general information about AIMMS, see specifically http://www.aimms.com/aimms/product/solvers/lgo.html: the website also includes the downloadable user guide (Pintér, 2005) and a free trial license of AIMMS with LGO.

Global Optimization Applications and Perspectives

We see particularly strong application potentials for AIMMS /LGO in cases when the decision model to solve cannot be brought to one of the simple "standard" model forms – notably, continuous linear programming and its immediate extensions. Broad classes of such applications originate from the following areas: optimization of complex models, including confidential (or other) "black box" systems; optimal control of dynamic systems; and decision-making under uncertainty. Model-instances that belong to these broad categories are ubiquitous in research and commercial applications of mathematics, physics, chemistry, biochemistry, environmental science, pharmaceuticals, medicine, engineering, economics, finance, and other related industries and services.

A few specific (past and present LGO) application examples are: acoustics equipment design, cancer therapy planning, chemical process modeling, data classification and visualization, economic and financial forecasting, environmental risk assessment and management, industrial product design, laser equipment design, model fitting to data (calibration), optimization in numerical mathematics, 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, waste water treatment systems management, and numerous others. For a range of engineering and scientific applications of global optimization, consult e.g. (Pintér, 2006a, b).

In conclusion, global optimization methods and software can be put to good use in a rapidly growing range of professional applications, as well as in research and education.

Acknowledgements

I wish to thank Johannes Bisschop, Gertjan de Lange, and Marcel Hunting for useful discussions and valuable contributions to the AIMMS /LGO solver link development project.

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