



International Conference on Computational Science, ICCS 2010

Computational optimization, modelling and simulation – a paradigm shift

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Abstract

Computational optimization forms an integrated part of modern computational science. Any good design should intend to achieve certain optimality, though optimal solutions are often difficult to find in practice since uncertainty and nonlinearity always present in almost all real-world problems. As resources, time and money are always limited, optimization becomes even more important in practice. This workshop on Computational Optimization, Modelling and Simulation (COMS 2010) at ICCS 2010 will summarize the latest developments of optimization and modelling and their applications in science, engineering and industry.

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Keywords: algorithm; black-box modelling; computational optimization; derivative-free method; optimization algorithm; modelling; nonlinear optimization; surrogate-based optimization; simulation;

1. Introduction

Computational modelling is becoming the third paradigm of modern sciences, as predicted by the Nobel Prize winner Ken Wilson in 1980s at Cornell University. This so-called third paradigm complements theory and experiment to problem solving. In fact, a substantial amount of research activities in engineering, science and industry today involves mathematical modelling, data analysis, computer simulations, and optimization. The main variations of such activities among different disciplines are the type of problem of interest and the degree and extent of the modelling activities. This is especially true in the subjects ranging from engineering design to oil industry and from climate changes to economics.

Computational optimization is an important paradigm itself with a wide range of applications. In almost all applications in engineering and industry, we are always trying to optimize something – whether to minimize the cost and energy consumption, or to maximize the profit, output, performance and efficiency. In reality, resources, time and money are always limited; consequently, optimization is far more important [1,2]. The optimal use of available resources of any sort requires a paradigm shift in scientific thinking, this is because most real-world applications

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have far more complicated factors and parameters to affect how the system behave; and subsequently, it is not always possible to find the optimal solutions. We have to settle for suboptimal solutions or even feasible solutions which are good enough and practically achievable in a reasonable time scale.

This search for optimality is complicated further by the fact that uncertainty almost always presents in the real-world systems. For example, materials properties such as Young's modulus and strength always have a certain degree of inhomogeneous variations. The available materials which are not up to the standards of the design will affect the chosen design significantly. Therefore, we seek not only the optimal design but also robust design in engineering and industry [2,3]. Optimal solutions, which are not robust enough, are not practical in reality. Suboptimal solutions or good robust solutions are often the choice.

Another complication to optimization is that most problems are nonlinear and often NP-hard. That is, the solution time for finding optimal solutions is exponential in terms of problem size. For such problems, there is no efficient algorithm of polynomial time exists in general. For example, the travelling salesman problem (TSP) intends to visit each city exactly once, for a given set of n cities, so as to minimize the overall travelled distance. This is an NP-hard problem and the number of combinations of possible solutions is the order of $n!$. In fact, many engineering applications are usually NP-hard indeed.

Contemporary engineering design is heavily based on computer simulations. This introduces additional difficulties to optimization. Growing demand for accuracy and ever-increasing complexity of structures and systems results in the simulation process being more and more time consuming. In many engineering fields, the evaluation of a single design can take as long as several days or even weeks. On the other hand, simulation-based objective functions are inherently noisy, which makes the optimization process even more difficult. Still, simulation-driven design becomes a must for a growing number of areas, which creates a need for robust and efficient optimization methodologies that can yield satisfactory designs even at the presence of analytically intractable objectives and limited computational resources.

This workshop on Computational Optimization, Modelling and Simulations (COMS 2010) at the ICCS 2010 intends to provide an opportunity to review and discuss the latest developments concerning optimization and modelling with a focus on applications in science, engineering and industry. In the rest of this brief summary paper, we will briefly consider the type of optimization, algorithms and approximation techniques for objective functions. We will then introduce the topics and papers in this workshop.

2. Optimization and Modelling

2.1. Optimization and Algorithms

There are many ways to formulate optimization problems. However, it is possible to write a nonlinear optimization problem in the following generic form

$$\begin{array}{ll} \text{Minimize} & f_i(\mathbf{x}), \quad (i=1,2, \dots, p), \\ \text{Subject to} & h_j(\mathbf{x})=0, \quad (j=1,2,\dots, M), \\ & g_k(\mathbf{x}) \leq 0, \quad (k=1,2,\dots, N), \end{array}$$

where $\mathbf{x} = (x_1, x_2, \dots, x_n)$ is the vector of the design or independent variables. Here the objective functions $f_i(\mathbf{x})$, equality constraints $h_j(\mathbf{x})$, inequality constraints $g_k(\mathbf{x})$ are typically nonlinear. If $p=1$, there is only a single objective, and this is the case discussed in most literature. In reality, most optimization problems are multiobjective ($p>1$), and different concepts such as the Pareto front come into play. Even for single objective optimization, the algorithms are as diverse as the optimization itself.

If the objective is linear, and all constraints are linear as well, the optimization becomes a linear programming problem. Dantzig's simplex method is an efficient algorithm for solving such problems. For nonlinear optimization, efficient algorithms only exist for certain special cases such as convex optimization [4]. Under the right conditions, interior-point or barrier methods are very efficient.

However, in general, we do not have efficient algorithms for solving all nonlinear optimization problems. There are various algorithms which have certain advantages and disadvantages. Gradient-based algorithms such as

hill-climbing require the problem functions (constraints and objective) are relatively smooth. If there is some discontinuity, we have to use gradient-free or derivative-free methods such as Nelder-Mead downhill simplex method and Hooke-Jeeves style pattern search. However, all these methods are local search methods. As most optimization problems are nonlinear and multimodal, global search methods should be used. Global search algorithms are mostly heuristic and metaheuristic with stochastic components. Genetic algorithms and particle swarm optimization are two excellent examples [5,7].

For a given problem, the chosen algorithm may depend on the type of problem, solution quality and available resources. As the No-Free-Lunch theorems [6] dictate, there is no universally efficient algorithm for all optimization problems. Therefore, a substantial amount of effort in optimization research is to identify the appropriate algorithm for a given type of problem.

2.2 Objectives and Simulators

Even with an efficient optimization algorithm, the evaluations of the objective functions are often time-consuming. In most engineering design and industrial applications, the objective cannot be expressed in terms of explicit functions, as the dependence of the objective on design variables is complex and implicit. This black-box type of optimization often requires a numerical simulator such as computational fluid dynamics and finite element analysis. Such simulators are very computationally expensive. Furthermore, almost all optimization algorithms are iterative, and require quite many times of function evaluations. Therefore, any technique in improving the efficiency of simulators or function evaluations is crucially important [7,8].

Surrogate-based and knowledge-based optimization uses certain approximations to the objective so as to reduce the cost of objective evaluations [8]. The approximations are often local, while the quality of approximations is evolving as the iterations proceed.

Applications of optimization in engineering and industry are diverse. This is reflected in the papers submitted to this workshop. The responses and interests to our call for papers are overwhelming; however, due to limited space and time slots for presentations, many high-quality papers cannot be included in the workshop. The accepted papers are quite representative and cover almost all important topics of computational optimization and modelling [9].

3. New Developments

The accepted papers of this workshop COMS2010 at ICCS 2010 have spanned a wide range of applications and reflect the state-of-the-art developments in computational optimization, modeling and simulations. New algorithms and improved performance are often formulated by hybridization. N. Saadouli presented a computationally efficient solution algorithm for a large scale stochastic dynamic program, while D. Clever et al. present a combination of an adaptive multilevel SQP method and a space-time adaptive PDAE solver for optimal control problems. At the same time, G. A. Gray et al. discuss hybrid optimization schemes for simulation-based problems.

Algorithm development and analysis include a wide range of techniques. From the integer simulation-based optimization by local search by J. Sklenar and P. Popela, stochastic programming with binary second-stage variables by T. Shiina, to the election campaign optimization algorithm by W. Lv et al. In addition to these exciting development, O. Kolb et al. present a modified QR decomposition technique to avoid non-uniqueness in water supply networks with extension to adjoint calculus, while M. Thaher and T. Takaoka discuss an efficient algorithm for the k-maximum convex sums, and H. I. Sayed et al. present SWOOP -- an adjustable global optimization technique. On the other hand, M. Simsek et al. outline the recent developments in knowledge-based neural modeling with extensive discussion in applications. S. Benhammada and S. Chikhi discuss a semi-formal specification for a generic model of artificial stock markets.

Applications range from the application of derivative-free methodologies to generally constrained oil production optimization problems by D. Echeverría Ciaurri et al., to the multi-fidelity design optimization of transonic airfoils using shape-preserving response prediction by L. Leifsson and S. Koziel, followed by the optimization and data mining for fracture prediction in geosciences by G. Shi and X. S. Yang. In addition, P. Domschke et al. present an adaptive model switching and discretization algorithm for gas flow on networks, while G. Gharooni-fard et al. discuss the scheduling of scientific workflows using a chaos-genetic algorithm.

Meanwhile, F. Li et al. present a rule-based optimization approach for airline load planning system. Furthermore, D. Lozovanu and S. Pickl study the optimal stationary control of discrete processes and a polynomial time algorithm for stochastic control problems on networks; K. Wendt et al. present a knowledge-guided genetic algorithm for input parameter optimization in environmental modeling.

As we have seen, the algorithms and applications of computational optimization and modeling are diverse and wide-ranging. There is no doubt that new efficient algorithms will emerge, and more and more applications will appear in the near future. This workshop may well pave the way for further discussions and development in optimization and modelling.

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