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Evolutionary Global Optimization, Manifolds and Applications

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Preface

Methods for solving global optimization problems with or without constraints find application in several disciplines like Game theory, Biology, Statistics, Engineering, Mathematics, Management Science, Economics, Physics, and in virtually every task that can be modeled by parametric systems. Many excellent methods have been developed so far, but several of them assume certain conditions about functions to be processed, as convexity or differentiability. However, when tackling real-world problems, we often get into situations in which objective functions to be optimized are not differentiable, convex, or even continuous. In such settings, many traditional methods are not so helpful, being necessary to find more general ways to get adequate results. In the past decades a large number of new global optimization methods were idealized aiming at reaching that more general objective, and a substantial part of them belong to the category of metaheuristic methods, being also known generically as metaheuristics. Many are based on probabilistic foundations, that is to say, use probability theory results to get to their objectives. Knowledge of the capabilities and limitations of these algorithms leads to a better understanding of their reach over various applications and indicates the way to future research on improving and extending algorithms' theoretical foundations and respective implementations. In another direction, almost all of them were developed to solve problems in linear spaces, not being able to deal with more general domains, like manifolds, for example. The main goal of this book is to present certain techniques for solving global optimization problems on manifolds by means of evolutionary algorithms, introducing certain applications chosen to complement the central presentation. In addition, the results will serve as a basis for constrained optimization in Euclidean spaces as well. By presenting detailed examples of applications we will try to stimulate the reader's intuition and make use of the proposed ideas easier to all wishing to solve constrained optimization problems on linear spaces or more general manifolds. In addition, applications tend to be concentrated on Game Theory, in particular Nash equilibrium problems related to several interesting real-world situations—they are reformulated as constrained global optimization problems and are solved with the help of Fuzzy ASA.

More abstract examples include minimization of well-known functions, in order to illustrate in detail the utilization of the proposed ideas. In order to offer usable material, the presented methods and examples use the Fuzzy ASA method, although many other paradigms could be adequate as well.

The insertion of an introductory chapter about metaheuristics is pertinent and justifiable because the algorithms presented in the book propose the use of existing evolutionary techniques when optimizing on manifolds. In this fashion, although Fuzzy ASA is used as the model optimizing paradigm, the suggested methods may be coupled to other metaheuristics. One big advantage of this viewpoint is that a great deal of tested knowledge may be applied in the new, expanded scope with almost null adaptation effort. The chapter also works as an indication and suggestion for future works, based on some of the fundamental ideas contained in the book.

Algorithms able to optimize functions defined on manifolds are important in that they may present lower computational complexity and frequently exhibit better numerical properties, as not getting caught in local minima attraction basins, for example. This becomes very clear when dealing with constrained optimization subject to equality constraints, given the inherent difficulty associated with such a type of restriction, due to its characteristic "bouncing" effect. This is so because it is not simple to keep evolving points exactly inside feasible regions using the conventional methods, giving rise to undesired oscillations along the optimization process. So, despite being important in more general contexts, even in traditional optimization tasks they may be quite effective. In this book it is presented a method for global optimization of functions defined on finite dimensional manifolds, which may be loosely described as configuration spaces that locally "look like" Euclidean spaces and, in truth, include them as particular cases, that is to say, $\mathbb{R}^n$ is a manifold as well. Pertinent elements of General and Differential Topology needed to develop the proposed algorithms are presented and it is possible to see that many already developed evolutionary paradigms can be applied almost directly, when faced and used in the adequate way. As many real-life problems can be naturally regarded as models whose defining parameters evolve on manifolds, like constrained optimization ones with equality constraints, for instance, new results in that direction are always welcome.

Prerequisites for reading this book include some knowledge of Linear Algebra, introductory Numerical Analysis and basic Probability Theory. Many necessary definitions and fundamental results are provided and formal mathematical requirements are kept to a minimum. The focus will be kept on continuous problems. This book can be used in courses related to optimization as well as by researchers and practitioners, and is adequate for self-study too.

The work is divided into three parts:

- Part I presents basic information about optimization algorithms, describing some well-known metaheuristics, their main characteristics, and overall architecture;
- Part II exposes fundamental facts about Topology, the Fuzzy ASA global optimization method along with its overall structure, well-known results about manifold theory, and the proposed methods themselves;

- Part III contains some important applications of (constrained) global optimization, with special emphasis on solutions of Generalized Nash equilibrium problems (GNEPs).

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Contents

Part I
Introductory Information

Chapter 1
The Many Aspects of Global Optimization

Abstract This chapter contains several considerations about global optimization methods, exposing in a condensed way several of their main qualitative characteristics. Taking into account that the focus in this book will be on the combination of an evolutionary method along with results of Topology and corresponding applications, we'll start to pave the way that will take us to the practical utilization of that approach, and stochastic optimization methods, in general.

1.1 Introduction

Being global optimization a difficult area of study, the discovery of all global optima of multimodal functions (having more than one local extremum) is one major challenge in this field. The difficulty associated to this operation has led researchers to develop many techniques aimed at solving several difficult problems.

The efficacy of many of these algorithms is highly dependent on the set of starting points, not existing a definitive technique that may assure convergence to all global optimizers without being caught in suboptimal regions (containing local, nonglobal extremes).

For traditional, deterministic paradigms such as those known as gradient-based methods, which work using the calculation of the first or second derivatives of the cost function, it is not uncommon to be captured and converge prematurely. The convergence to global optimizers is often guaranteed only when members of the initial populations reside in the neighborhood of global solutions and objective functions obey certain (somewhat restrictive) conditions, such as convexity, for instance.

On the other hand, stochastic techniques such as some evolutionary algorithms are developed under diverse principles and motivations, and strive for overcoming the premature convergence problem, often by employing strategies of exploration and exploitation. Such procedures normally work by sweeping domains of cost functions, identifying probable regions containing global optimizers, and in the final phase, the search is concentrated in precisely locating the possible global solutions. In this manner, it is theoretically possible for such a type of methods to "travel" along different attraction basins, not getting stagnated inside suboptimal locations.

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Optimization methods have been a necessity since time immemorial even though people may not be conscious of this. As humans have always tried to reach optimal results, be them maximum personal income or minimum costs in industries, it is somewhat evident that optimization problems have always been around. Even in Nature, the protein folding process is supposed to search for a minimum energy configuration state for instance, and molecules forming solid bodies during the process of freezing tend to assume energy-minimum crystal configurations. Another good example is the biological principle of survival of the fittest [17] which, conjugated to species evolution theory [9], tries to model adaptation of the species to their environment, and is definitely related to optimization principles. Hence, it is no exaggeration to say that optimization problems pervade the Universe itself, where (usually nonlinear) optimization processes happen all the time at the microscopic, mesoscopic or macroscopic levels—in General Relativity, for example, traveling along geodesics on smooth manifolds is a fundamental premise. As optimization problems may be global or local, there are techniques aimed at finding local or global optima—a local minimization problem, for example, requires finding a minimizer within a proper, specific neighborhood. In this way, the problem is local, not encompassing the whole domain of the given objective function. On the other hand, global optimization methods handle the case in which the search is for optimum points over the whole domain of the objective function. Therefore, the goal of global optimization methods is to find the best elements from a set, possibly subject to a set of constraints—these conditions are expressed as mathematical functions or relationships. The objective function works as the index we want to optimize and the constraints are the relationships we want to satisfy [11, 13].

In general the objective functions are real valued, that is, their images are subsets of $\mathbb{R}$. Their domains may contain many kinds of elements, like numbers, vectors of real or integer numbers, for example. In another dimension, objective function values may be obtained not only by mathematical expressions, but as results of simulations that can, for example, involve long and computationally expensive operations, justifying to a certain extent why a large number of publications takes the number of cost function evaluations as a measure of efficiency.

1.2 Main Approaches to Optimization Problems

Classifying existing global optimization methods is not a simple task but, in general, they can be separated into two groups: deterministic and stochastic. The deterministic methods are most often used whenever objective functions present certain analytical characteristics that make it possible to employ known theoretical results so as to find optimal points [6, 16, 18]. When using gradient methods, for instance, there is frequently a simulation of a dynamical system that evolves towards local optima, according to decreasing directions of the function under processing. Therefore, the feasible space can be explored using another complementary technique, for instance, so as to accelerate the whole optimization task. On the other hand, whenever the relationship between a solution candidate and its corresponding cost are too complicated, it may be hard to solve the global optimization problem by means of deterministic methods, even when dealing with small dimension problems. In those cases, stochastic algorithms can be a good alternative, particularly a specific and well-known family of probabilistic algorithms: the so-called Monte Carlo-based approaches. Typically they are able to find solutions in reduced time but don't guarantee convergence to global solutions. Their results might be non-global optima—when dealing with multimodal objective functions even deterministic algorithms could not, in general, ensure that they have reached global optima. In this fashion, we have an example of a heuristic paradigm - in particular, the decision is taken with basis in previous information and experimental data. Heuristics used in global optimization are useful when choosing which one of a set of possible solutions is to be examined in the sequence.

Heuristic approaches may be regarded (loosely speaking) as components of an optimization algorithm that use information currently gathered by a given algorithm to help in the decision of which candidate solution should be tested next or how the next individual can be produced, for example. On the other hand, metaheuristics are usually viewed as methods for solving general classes of problems, combining objective function values and reasoning rules in a somewhat abstract and reasonably effective way, often without exploring the structure of the particular problem at hand [12, 14, 20]. This association is often performed stochastically by using samples from the search space. Typical simulated annealing methods, for example, decide which candidate will be evaluated next according to the Boltzmann probability distribution. In another direction, biologically inspired algorithms try to follow the behavior of natural evolution and consider solution candidates as individuals that compete in an abstract setting. Considering other classification dimensions, metaheuristic methods tend to be population-based, like genetic or particle swarm intelligence algorithms. In addition to these nature-inspired and evolutionary approaches, there exist also methods that try to behave similarly to physical processes: simulated annealing, parallel tempering, and grenade explosion method [2, 12, 20].

1.3 Characteristics of Generic Global Optimization Problems

So far some global optimization algorithms were mentioned and we will have more to say about them in the chapters ahead. However, the methods introduced in this book will deal with only a small part of the actual number of available methods and we intend to focus even more later. Nevertheless, it is a natural question to ask why there are so many different algorithms and whether is this variety needed. One explanation could be that there are so many different kinds of global optimization tasks, creating different obstacles to optimizers and representing specific difficulties. Hence, in what follows we discuss concisely the most common problems usually encountered by existing paradigms during global optimization, namely, multimodality, stagnation, premature convergence, poor exploratory ability and related phenomena.

In practice, whenever a given implementation experiences even a single negative feature, as cited above, it can get "frozen" in a sub-optimal point and simply not be able to reach the global optimum. This is possible even if highly efficient optimization techniques are applied.

Figures 1.1, 1.2, 1.3, 1.4 and 1.5 show different types of configurations. As remarked before, all problems will be of the minimization type, and the graphs aim to illustrate the difficulties experienced when trying to obtain global minima starting from arbitrary points in the function's domain. Obviously the illustrations feature low dimensional cases, but when working in domains with higher dimensions there are similar scenarios.

To understand why these landscapes are hard to deal with, we should understand the situation in the optimization setting. One approach to obtain near-optimal solutions for complex problems in reasonable time is to apply metaheuristic optimization procedures—the fundamental fact is that optimization algorithms are guided primarily by values of objective functions. On the other hand, functions are considered hard from a numerical perspective if they are not continuous, not differentiable or

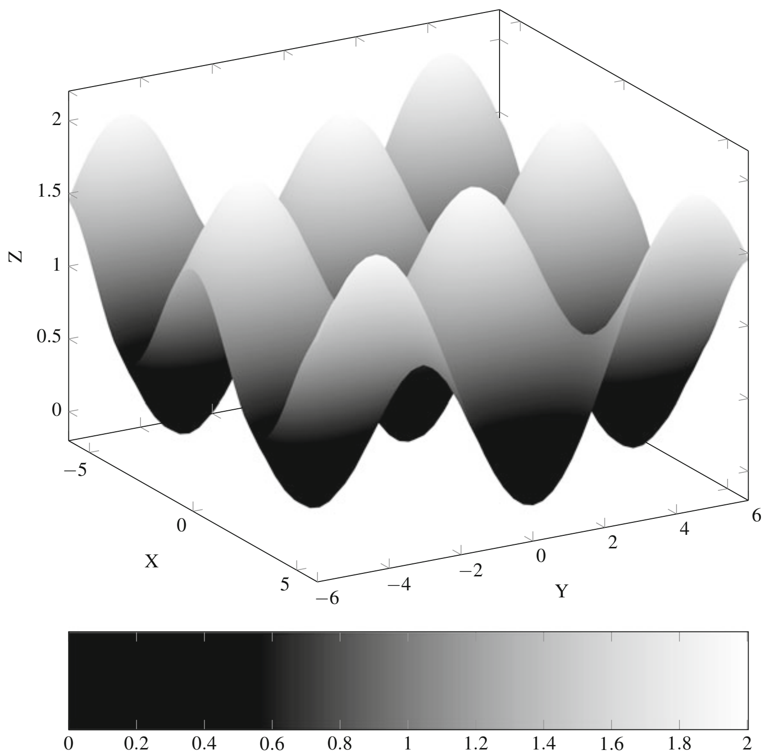

Fig. 1.1 Multimodal function

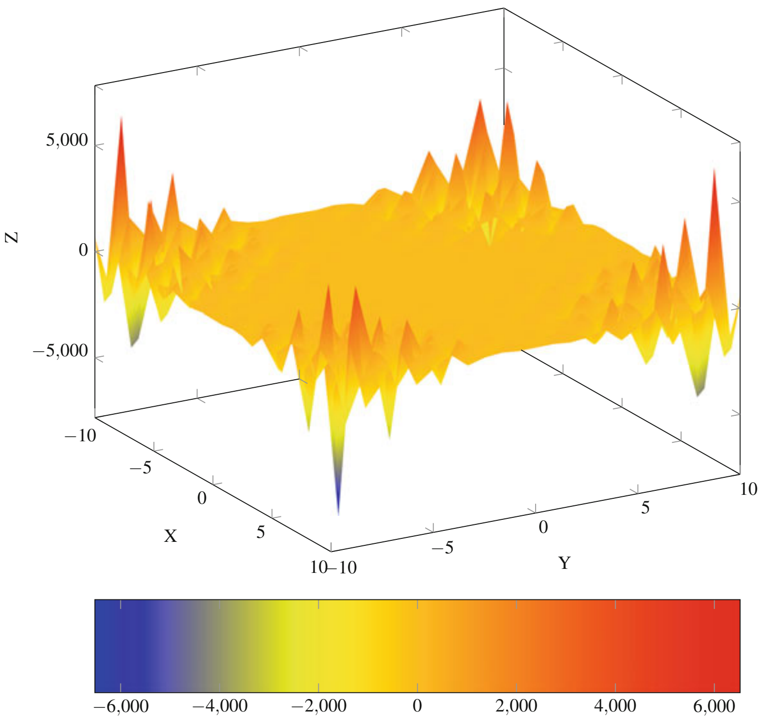

Fig. 1.2 Orientation is very difficult

multimodal. This conception of difficulty can be portrayed through the graphs shown in the figures mentioned above. In certain industrial applications of optimization techniques the analytical characteristics of the functions to be processed are not known in advance, and their values at different points are obtained from physical simulations or sampling operations. Hence it is seldom possible to predict the performance of optimizers when applied to these hard problems, in terms of having or not reached global optima, for instance. A reasonable and helpful strategy is to use models based on experimental data to improve the precision of final results.

As a generic rule, it is assumed that an optimization algorithm has converged if it cannot produce new candidates or continues producing solution candidates located inside a very limited region of the problem domain. Another typical issue associated to global optimization is that it is often not possible to decide whether the best solution currently known is a local or global optimum and thus if a true solution has been found. Therefore, it is usually unclear when the optimization process should be interrupted, concentrate on refining the current optimum, or explore different parts of the search space. This is specially significant when dealing with multimodal and/or nondifferentiable objective functions.

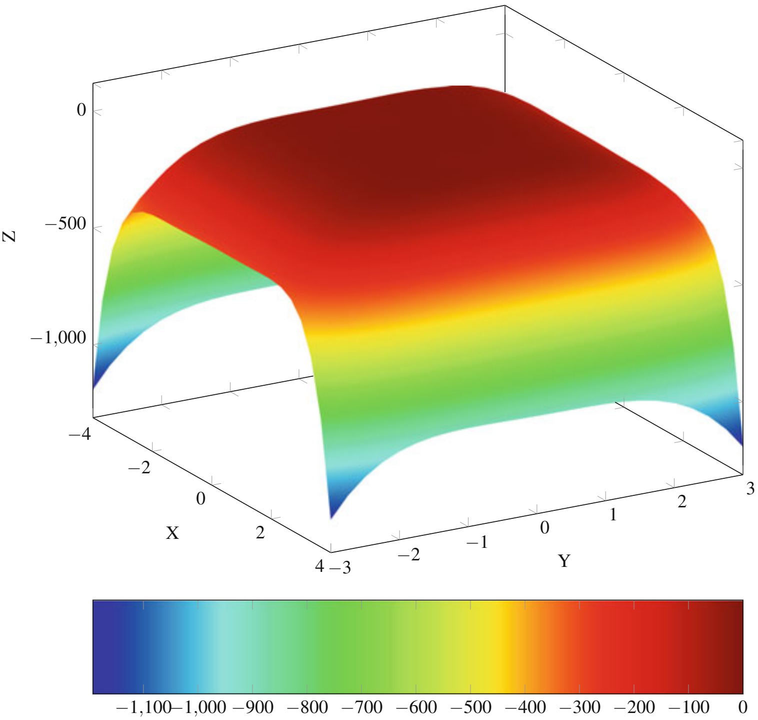

Fig. 1.3 Potential stagnation configuration

Premature convergence (to a local optimum) occurs if a given optimization process is no longer able to explore other parts of the search space except the area being currently visited (existing another region that contains a better solution) and stagnates at a sub-optimal point. Although the occurrence of multiple global optima is not very problematic, the existence of numerous local (and nonglobal) optima may originate problems, considering the possibility of premature convergence.

Yet another decision to be made is relative to the (exploration, exploitation) binomial. By exploration we mean visiting new sub-domains of the search space which have not been investigated earlier, and exploration processes try to find better solution states. Following this line, some operators are designed to create inferior solutions by destroying good individuals, but also have a small chance of finding more adequate candidates. On the other hand, exploitation processes incorporate small changes into existing individuals, leading to nearby solution candidates. Naturally, it is necessary to devise mechanisms that allow us to balance exploitation and exploration levels. It is worth to note that methods favoring exploitation over exploration have faster convergence but offer the risk of not finding the optimal solution, not forgetting the possibility of being caught at a local optimum. As expected, algorithms performing excessive exploration may never find the global optimum or spend too much

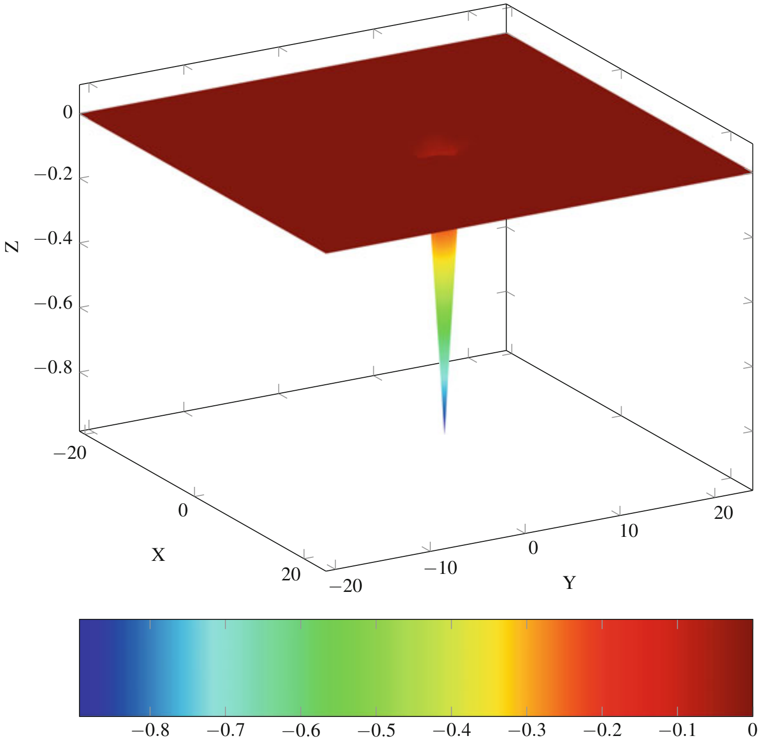

Fig. 1.4 Deep minimum

time trying to discover it. A good example might be the standard adaptive simulated annealing paradigm, that is able to do quenching, prioritizing exploitation over exploration and losing the guaranteed (theoretical) convergence in distribution to the global minimum.

Although there is no general method capable of avoiding premature convergence in all cases, the probability that an optimization process gets caught in a local optimum depends on several factors, including the properties of the function to be processed, for example. Typically, evolutionary global optimization methods adopt certain heuristics that tend to attenuate the risk of being caught in sub-optimal regions. As an example, increasing the degree of exploration may decrease the probability of premature convergence, taking into account that by doing so it is possible to improve the mapping of the objective function under study. As a matter of fact, some methods have been created to drive the search away from areas which have already been sampled. As an example, low selective pressure in a genetic algorithm decreases the chance of premature convergence but also delays the exploitation of good candidates. A possible alternative to avoid premature convergence is the use of self-adaptation, allowing the optimization algorithm to change strategies and its parameters, depending on the current state and performance figures. Such measures