Uncertainty and Operations Research

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Unconstrained Optimization and Quantum Calculus

Springer

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Decision analysis based on uncertain data is natural in many real-world applications, and sometimes such an analysis is inevitable. In the past years, researchers have proposed many efficient operations research models and methods, which have been widely applied to real-life problems, such as finance, management, manufacturing, supply chain, transportation, among others. This book series aims to provide a global forum for advancing the analysis, understanding, development, and practice of uncertainty theory and operations research for solving economic, engineering, management, and social problems.

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Foreword

This monograph primarily presents some important unconstrained optimization techniques in the setting of quantum calculus. This book begins with a historical note on the development of some gradient-based unconstrained optimization methods and presents the unconstrained optimization problems and a brief overview of quantum calculus. The seven chapters broadly cover q-gradient descent algorithm along with convergence proof, q-Fletcher-Reeves conjugate gradient method, q-Polak-Ribiére-Polyak conjugate gradient method, q-Dai-Yuan conjugate gradient algorithm based on q-gradient for solving unconstrained optimization problems, convergence results that take the Zoutendijk condition in the context of q-calculus for global convergence, unconstrained optimization problems using q-BFGS method using q-calculus and q-limited memory BFGS algorithm. The performance of the methods is illustrated with numerical examples. The monograph nicely builds the connection between theory, algorithms, convergence proofs, and implementation. Graduate or undergraduate students of mathematics and computer science and students from other engineering disciplines will find this book useful.

May 2024

Prof. Samir K. Neogy
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Preface

Optimization is a crucial tool used by decision-makers to solve any optimization problems. Making the best choice out of all the options available is the responsibility of decision-makers. An objective function defines the goodness of the options' performance in the field of optimization. The field of optimization has drawn numerous researchers from various fields to find highly effective solutions to their scientific issues. Optimization techniques are the most effective means of resolving real-world issues that are iterative in nature. Owing to the quick advancement of digital technology, a number of software programs are already in the market that function as "black boxes," providing input according to the optimization problem's nature and only producing the desired result. Serious researchers, on the other hand, are not constrained by logic, and they seek to understand every internal process involved in solving the issue. Thus, the goal of this monograph is to provide all techniques in an easy-to-understand format.

In the setting of quantum calculus, this monograph expands standard unconstrained optimization techniques. The unconstrained optimization involves minimizing a function with numerous dependent variables and no constraints on these variables. The complexity of the optimization issues increases with the number of variables. Algorithms are therefore more suited to address these kinds of issues. Every technique in this monograph uses algorithms for solving optimization issues that can be implemented in any computer language. This monograph can be used as a textbook by readers who wish to understand the traditional approaches to optimization in the context of quantum calculus. Therefore, there is a detailed discussion of several generalized gradient descent techniques for handling unconstrained optimization issues. These are iterative processes. They begin at any position and provide a series of better approximations until they reach a minimal point. The optimality conditions are examined in order to confirm that this point is, in fact, the solution to the problem. The present approximation of the solution may be enhanced if the optimality conditions are not met. The first- and second-order q-derivatives of the objective function, as well as the objective function value, are used in the described techniques.

This monograph is divided into seven chapters and is structured as follows:

In Chap. 1, we start with the introduction of unconstrained optimization (Sect. 1.1) and present the historical note on the development of some gradient-based unconstrained optimization methods in Sect. 1.2. We present a biography of Prof. Frank Hilton Jackson in Sect. 1.3 who is known as the founder of quantum calculus in the modern era. The history of q-calculus and the development of several unconstrained methods in the context of quantum calculus are discussed in Sect. 1.4. In Sect. 1.5, we present the unconstrained optimization problems and the necessary results associated with them to solve the optimization problems. In Sect. 1.6, we present the quantum calculus and performance profile.

In Chap. 2, we present the q-steepest descent method with the quasi-Fejér convergence. In Sect. 2.2, the q-gradient descent algorithm is given under some assumptions and its convergence proof is provided using q-Newton-Leibniz formula and quasi-Fejér convergence theorem in Sect. 2.3. The numerical experiments are performed in Sect. 2.4. First, we provide two examples to solve the problems by our method. Thereafter, 28 test problems are taken to compare our method with an existing method based on a number of iterations and function evaluations, respectively.

In Chap. 3, we propose a q-Fletcher-Reeves conjugate gradient method and start by presenting the development of the conjugate gradient method which is given in Sect. 3.1. In Sect. 3.2, we present the q-conjugate gradient algorithm for the modified Fletcher-Reeves method in the context of q-calculus. Section 3.3 proves the global convergence of the method with Armijo type line search with backtracking. In Sect. 3.4, 31 test problems with three separate examples are used to illustrate the performance of the proposed method based on a number of iterations and function evaluations.

In Chap. 4, a q-Polak-Ribiére-Polyak conjugate gradient method is presented by combining the classical method with q-calculus. Section 4.1 motivates to present this method and discusses some closely related works. The algorithm is given in Sect. 4.2 that proposes that the method has sufficient decent properties. Section 4.3 provides the global convergence results under some conventional conditions using standard and strong Wolfe conditions. In Sect. 4.4, we provide three numerical examples to illustrate the advantages of the present method, and with 51 different starting points, several test problems are solved to express the outstanding property of the method.

In Chap. 5, we propose a q-Dai-Yuan conjugate gradient algorithm based on q-gradient for solving unconstrained optimization problems. Section 5.1 turns our attention to the development of the q-Dai-Yuan conjugate gradient algorithm. In Sect. 5.2, we provide the global convergence of the algorithm under standard Wolfe conditions. Section 5.3 shows the convergence results that take the Zoutendijk condition in the context of q-calculus for global convergence. Section 5.4 reports numerical results to show the efficiency of the proposed method.

In Chap. 6, we solve unconstrained optimization problems using q-BFGS method. Section 6.1 gives a brief introduction about this method. Section 6.2 describes the BFGS update using q-calculus and presents an algorithm. In Sect. 6.3, we analyze the global convergence of the proposed algorithm. Section 6.4 reports numerical results and compares with the classical method. We offer some conclusions in the last section.

In Chap. 7, we propose a q-limited memory BFGS algorithm where the storage is critical. In Sect. 7.1, we briefly explore the several unconstrained optimization methods that motivate to present the limited memory BFGS method. In Sect. 7.2, an algorithm for this method is provided with an updated formula that generates matrices using information from the last m iterations, herein m is any number supplied by optimizers. In Sect. 7.3, the global convergence property is established under some suitable conditions like Armijo line search with backtracking and Wolfe conditions when the objective function is non-convex. In Sect. 7.4, we have taken 29 test problems. The resulting algorithm is tested numerically and compared with an existing method.

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Declarations

Competing Interests The authors have no conflicts of interest to declare that are relevant to the content of this chapter.

Ethics Approval No ethics approval was required.

Contents

Acronyms

Symbols

$\mathbb{N}$	Set of all natural numbers
$\mathbb{R}$	Set of all real numbers
$\mathbb{R}_+$	The set of all nonnegative real numbers
$\mathbb{R}_-$	The set of all nonpositive real numbers
$\mathbb{R}^n$	n-dimensional real vector space
$\mathcal{I}$	Identity matrix
∇_q	q-gradient operator
p_q	q-descent direction
$\Vert . \Vert$	Euclidean norm
D_q	q-derivative operator
$\pitchfork$	Pitchfork function

Abbreviations

USOP	Unconstrained Single Objective Optimization Problem
q-BFGS-QN	Quantum Broyden-Fletcher-Goldfarb-Shanno Quasi-Newton
q-DY	Quantum Day Yuan
q-FR	Quantum Fletcher-Reeves
q-LM-BFGS-QN	Quantum Limited Memory Broyden-Fletcher-Goldfarb-Shanno Quasi-Newton
q-PRP	Quantum Polak-Ribière-Polyak
q-SDQF	Quantum Steepest Descent Quasi-Fejér

Chapter 1
Introduction to Unconstrained Optimization and Quantum Calculus

1.1 Introduction

In this monograph, we explore certain mathematical programming techniques that are widely used to optimize nonlinear functions of single variables and multiple variables subject to no constraints. However, the structure of several problems involves the constraints that bound the design space. Instead, the methods of unconstrained optimization are important to study for several reasons. If no constraints are active for any problems, then the process of attaining a search direction and travel distance for minimizing the objective function involves an unconstrained minimization algorithm. However, there is a violation of constraints during the movement of search direction in search space. Second, a constrained optimization problem can be treated as an unconstrained optimization problem even if the constraints are active. In this case, the penalty and multiplier methods directly convert the constrained optimization problems into unconstrained optimization problems. Thus, unconstrained optimization methods are necessary to explore their different dimensions. Unconstrained optimization is the process of minimizing a function that depends on a number of real variables without putting any limits on how these variables should be set. When the number of variables is large, this problem becomes quite challenging. The most important gradient methods for solving unconstrained optimization problems are described in this monograph. These methods are iterative. They start with an initial guess of the variables and generate a sequence of improved estimates until they terminate with a set of values for the variables. We take the optimality conditions to check that this set of values for variables is indeed the solution to the problem. If the optimality conditions are not satisfied, then they may be used to improve the current estimate of the solution. The algorithms described in this book make use of the values of the function that minimizes the first and the second derivatives of the function. Most of what is said about unconstrained optimization methods are about steepest descent, conjugate gradient quasi-Newton, and limited-memory quasi-Newton.

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1.2 History of Unconstrained Optimization Methods

We are showcasing the historical remark on unconstrained optimization techniques in this part. Many scholars credit Prof. Augustin-Louis Cauchy, who first devised the gradient descent method in 1847 to solve a system of linear equations (Cauchy 1847). A comparable technique was separately developed by Prof. J. Hadamard (Fig. 1.1) for solving systems of linear equations (Hadamard 1908). Further, Curry (1944) provided the convergence properties of gradient descent method for solving non-linear optimization problems. Many scholars studied this strategy in-depth after that. A probabilistic method was proposed by Akaike (1959) to demonstrate the convergence of the gradient descent method. Zangwill (1969) demonstrated the deterministic approach to prove the global convergence which was linearly converged. Other scholars were motivated to create certain sophisticated kinds of optimization algorithms by this technique. Probably the most used optimization approach is called Newton's method. Nonetheless, Prof. Francois Vieta (1540–1603) developed a perturbation technique for solving scalar polynomial equations, which served as the inspiration for this method. Prof. Issac Newton improved on this process in 1669 by linearizing the polynomials that arose one after the other. In 1690, Prof. Joseph Raphson (1648–1715) reintroduced the same procedure, but he employed distinct derivations in order to avoid the tedious computation of successive polynomials.

Ultimately, in 1740, Prof. Thomas Simpson provided a summary of all of Newton's earlier accomplishments when he explained that Newton's method was an iterative way to solving generic nonlinear equations with general calculus. Additionally, Simpson expanded on the systems of two equations and pointed out that optimization issues can be resolved using Newton's approach by setting the function's gradient to

Fig. 1.1 Prof. A. L. Cauchy