CONSTRAINED NONLINEAR OPTIMIZATION WITHOUT DERIVATIVES

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Abstract.

In real optimization problems, usually the analytical expression of the objective function is not known, nor its derivatives, or they are complex. In those cases it becomes essential to use optimization methods where the calculation of the derivatives, or the verification of their existence, is not necessary: the Direct Search Methods.

When the problem has constraints (Constrained Nonlinear Programming Problems), the Direct Search Methods are not enough, because they only solve Unconstrained Nonlinear Problems.

Traditionally, this kind of problems is solved using Penalty or Merit functions, that are a linear combination of the objective function and a measure of the constrained violation.

Unfortunately the choice of suitable penalty parameters is, frequently, very difficult, so as an alternative appeared the Filter Methods which were introduced by Fletcher and Leyffer.

In this work we present a synopsis of the existing techniques to solve optimization problems with constraints, without using derivatives or approximations of them.

1 Introduction

Mathematical programming has been to the study and real understanding of many problems and phenomenas, in engineering, economy, medicine, etc. Optimization problems are abundant, where it is necessity to determine the best suitable solutions for a given reality. The techniques or strategies used in each method depends on the amount of usable information, the efficiency and robustness of the algorithm , the easiness of implementation, and, obviously, the properties of the problem to solve.

In real optimization problems, usually the analytical expression of the objective function is not known, nor its derivatives, or they are complex. In these cases it becomes essential to use optimization methods where the calculation of the derivatives, or even the verification of their existence, is not necessary: the Direct Search Methods.

Direct Search Methods are suitable when some of the functions that define the problem are given as black boxes, not assuring enough precision to approximate derivatives.

Black box problems occur frequently in science and engineering, where the evaluation of the objective function usually requires complex deterministic simulations. Those simulations are required to properly describe the underlying physical phenomena. Also the computational noise, associated with the simulations, indicates that obtaining derivatives is difficult and unreliable.

Direct Search Methods are nonlinear optimization methods that neither require explicitly nor approximate derivatives to solve the problem. Instead, at each one iteration it is generated a set of trial points and their function values are compared with the best previously obtained solution. This information is then used to determine the next set of trial points.

2 Unconstrained Nonlinear Programming Problems

2.1 Direct Search Methods for Unconstrained Minimization

Consider the following general Unconstrained Nonlinear Programming Problem, $P1$:

$$\text{minimize } f(x), \tag{1}$$

where $x \in R^n$ and f is the objective function.

In accordance with Lewis et al. [20], the most popular Direct Search Methods (or Derivative-free Methods) for Unconstrained Minimization (for $P1$ - (1)), can be organized into three basic categories:

- Pattern Search Methods;
- Simplex Methods;
- Methods With Adaptive Sets of Search Directions.

Pattern Search Methods include methods like the Hooke and Jeeves Method, [17], Nelder and Mead, [22], is a good example of a Simplex Method and the Powell Method, [24], is a Method With Adaptive Set of Search Directions. A review of Direct Search Methods is presented in the paper of Lewis et al. [20].

3 Constrained Nonlinear Programming Problems

3.1 Penalty Methods

Whenever a problem has constraints (Constrained Nonlinear Programming Problems), the Direct Search Methods (or Derivative-free Methods) for Unconstrained Minimization are not enough, because they only solve Unconstrained Nonlinear Problems.

Consider the fallowing general Constrained Nonlinear Programming Problem (NLP), P:

$$\begin{array}{ll} \text{minimize} & f(x) \\ x \in R^n & \\ \text{subject to} & c_i(x) \leq 0, \end{array} \tag{2}$$

where $f : R^n \to R \cup \{\infty\}$ is the objective function and $c_i : R^n \to R^m$ are the constraint functions with $C = (c_1, ..., c_m)^T$. The feasible region is the region defined by the constraint functions and it is usually denoted by X.

Traditionally, this kind of problems are solved using Penalty or Merit functions, that are a linear combination of the objective function and a measure of the constrained violation. It is thus possible to solve constrained Nonlinear Problems using methods that are usually used for unconstrained problems.

In a Penalty Method, the feasible region X is expand to R^n, but a larger cost or penalty is added to the objective function for points that lie outside of the original feasible region, X. The Penalty Methods construct a new objective function, Φ, which contains information about the initial objective function, f, and the problem constraints. A sequence of Unconstrained Problems is constructed, dependent of the positive parameter r witch solutions, $x^*(r)$, converge to the solution of the initial problem, x^*.

The new objective function Φ, will be:

$$\Phi(x,r) = f(x) + r\, p(x), \tag{3}$$

where r is a positive parameter, named **Penalty Parameter** and $p(x)$, is the **Penalty Function**.

Definition. The function $p : R^n \to R$ is the **Penalty Function** for P, if:

- $p(x) = 0$ if $c_i(x) \leq 0$
- $p(x) > 0$ if $c_i(x) > 0$

Then we must solve a sequence of unconstrained problems P_m (4), that substituted the P problem (2), with a new objective function:

$$P_m : \text{minimize } f(x) + r_m p(x) \tag{4}$$

where $x \in R^n$ and being r_m a sequence of constants that verify $r_m \to +\infty$.

In recent years, there has been a resurgence of interest in Penalty Methods, mainly for Exact Penalty Methods, [3], Byrd et al., [9], Chen et al., [11], Fletcher et al., [15], Gould et al., [19], Leyffer et al., [21], Mongeau et al., and [27], Zaslavski, because their ability to handle degenerate problems and inconsistent constrained linearizations.

The Penalty Methods are designed to solve this problem by solving a sequence of constructed Unconstrained Problems. Then they are seen as vehicle to solve Constrained Optimization Problems using Unconstrained Optimization techniques. A review of Penalty Methods is presented in the paper of Correia et al. [7], and in Byrd et al., [3].

3.2 Filter Methods

The difficulties of choosing appropriate values for penalty parameters, in Penalty Methods, caused nonsmooth Penalty Methods to fall out of favor during the early 1990's. It led to the development of Filter Methods which do not require a penalty parameter.

So as an alternative to penalty function appeared the Filter Methods, which were introduced by Fletcher and Leyffer. A filter algorithm introduces a function that aggregates the constrained violations and constructs a bi-objective problem. In this problem, a step is accepted if it either reduces the objective function or the constrained violation. This implies that the Filter Methods are less parameter dependent than a penalty function.

The SQP-filter approach was also applied to interior point algorithms by Ulbrich et al., [26]. Audet and Dennis [1] presented a Pattern Search Filter Method for Derivative-free Nonlinear Programming. Gould et al., [14], introduced a multidimensional filter algorithm to solve nonlinear feasibility problems. Gould et al., [16], extended the multidimensional filter techniques to general Unconstrained Optimization Problems. Filter Methods were also used in the context of nonsmooth optimization by Fletcher and Leyffer, [11] and by Karas et al. [18].

A review of Filter Methods is presented by Fletcher et al. in [12]. Global convergence for Filter Methods in SLP problems was obtained by Fletcher et al.[10] and a proof of its convergence for SQP was given by Fletcher et al. in [13]. In both cases, this convergence is only to a point that satisfies the Fritz John optimally conditions. Thus, previous filter algorithms require explicit use of the derivatives of both the objective and the objective constrains.

3.3 Dynamic Penalty Methods

Afterwards, a new approach for updating the penalty parameter, the Dynamic Penalty Methods, promised to solve those difficulties. They automatically increase the penalty parameter and overcome this undesirable behavior. These methods adjust the penalty parameter at every iteration, to achieve a prescribed level of linear feasibility. Consequently the choice of the penalty parameter becomes an integral part of the step computation.

An earlier form of the penalty update strategy is presented for Byrd et al., [3], in the context of a successive linear quadratic programming algorithm (SLQP).

Other penalty strategies have been proposed recently: Chen et al., [9], proposed rules that update the penalty parameter as optimality of the penalty problem is approached; they are based in part on feasibility and the size of the Lagrange multipliers; Leyffer et al., [19], considered Penalty Methods for MPCCs and described dynamic criteria for updating the penalty parameter based on the average decrease in the penalized constraints.

The method of Byrd et al., [3], differ from those strategies because they test the effect of the penalty parameter on the step to be taken, based on the current problem model.

4 Web Application

Our goal is to create a Web Application able of solving any Constrained or Unconstrained Nonlinear Problem. It will have a computation engine, to solve the problems and Web Interface, available to clients using a Web Browser. Clients will interact with the computation engine using and Web page. The methods are being implemented using Java Technology. It is an multi-platform technology, that has a rich variety of classes that abstracts the Internet protocols like HTTP, FTP, IP, TCP-IP, SMTP, DNS, making it suitable for networked applications. In fact it was the Internet that made it so popular, embeded in applets, running in web pages.

An Java application is compiled once and then it can run anywhere, as long as the target platform supports Java. This is one of Java key features, compile once and run anywhere.It has also a good performance, despite the fact it is an interpreted language. It was compared with other programming languages to test its performance. It was compared with C, in finite element analysis [23] and against C and FORTRAN in scientific applications [4]. In both cases it was concluded that Java had a good relative performance.

To solve a Constrained Nonlinear Programming Problem (NLP), (2), without the use of derivatives or approximations of them, we can apply Penalty Methods or Filter Methods. Penalty Methods construct a new objective function, that contains information about the initial objective function and the problem constraints. It generates a sequence of Unconstrained Problems witch solutions converge to the initial problem solution. Filter Methods introduces a function that aggregates the constrained violations and constructs a bi-objective Unconstrained problem. Then we can solve Unconstrained Nonlinear Problems by means of Direct Search Methods.

Thus, our application will give to the user the option to indicate the type of problem he wants to solve: Constrained or Unconstrained Nonlinear Problem. If he wants to solve an Unconstrained Nonlinear Problem he can use immediately the Direct Search Methods. If he wants to solve an Constrained Nonlinear Problem he must first choose between Penalty Methods or Filter Methods and them to apply one of the Direct Search Methods. **Figure 1.**, **Figure 2.** and **Figure 3.** illustrates the options that the application will have available.

$\boxed{\text{Unconstrained Nonlinear Problem}} \quad \longleftrightarrow \quad \boxed{\text{Constrained Nonlinear Problem}}$

Figure 1: First, our application will give to the user the option to indicate the type of problem he wants to solve: Constrained or Unconstrained Nonlinear Problem.

Our first step, to build the application, was the implementation, in Java language, of the Direct Search Methods. This implementation was described in [5], Correia et al. In this work we present a brief description of Pattern Search Methods and Simplex Methods and have presented some numerical results. The test problems used had been selected by Bagirov in [2] , Schittkowski in [25] and Maratos test problems. We concluded that Pattern Search

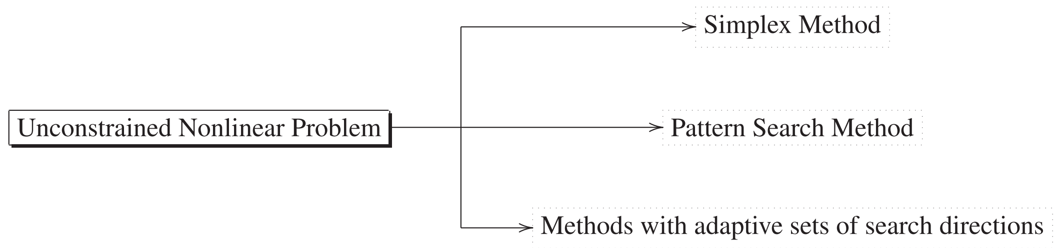

Figure 2: If the user wants to solve a Unconstrained Nonlinear Problem he can use immediately the Direct Search Methods.

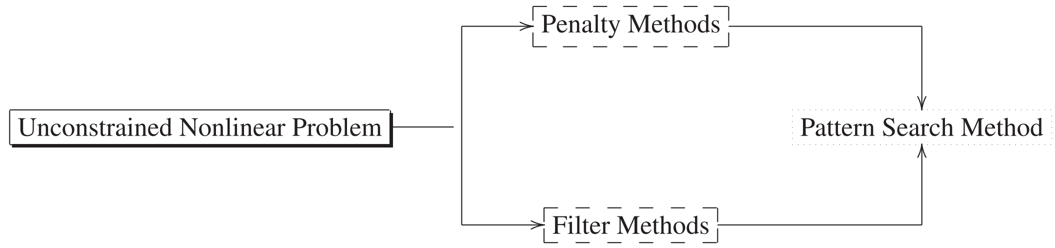

Figure 3: If the user wants to solve a Constrained Nonlinear Problem he must first choose between Penalty Methods or Filter Methods and them to apply one of the Direct Search Methods.

Method is faster than Simplex Method, when applied in the Schittkowski problems presented, but it is unsuccessful for the Bagirov and Maratos problems.

Then, in [6], Correia et al., we presented an alternative to Penalty Methods and another way to solve Constrained Nonlinear Problems. In this paper it is present a new Direct Search Method, based on Simplex Methods, for general Constrained Optimization, that combines the features of the Simplex Method and Filter Methods. This method does not compute or approximate any derivatives. The proposed methods were implemented in Java and we illustrate the behavior of our algorithm through some examples by [8].

Next we have as objective the implementation of the Exact Penalty Methods and the Dynamic Penalty Methods.

5 Final Considerations

In this work we present a synopsis of the most popular methods to solve Constrained and Unconstrained Nonlinear Problems, without using derivatives or approximations of them.

We briefly present the general structure of our future Web Application, that will be able of solving those problems.

Then we describe summary some results that were achieved through the implementation that has been made in Java Technology.

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