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ICRS-Filter: A randomized direct search algorithm for constrained nonconvex optimization problems

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ABSTRACT

This work presents a novel algorithm and its implementation for the stochastic optimization of generally constrained Nonlinear Programming Problems (NLP). The basic algorithm adopted is the Iterated Control Random Search (ICRS) method of Casares and Banga (1987) with modifications such that random points are generated strictly within a bounding box defined by bounds on all variables. The ICRS algorithm serves as an initial point determination method for launching gradient-based methods that converge to the nearest local minimum. The issue of constraint handling is addressed in our work via the use of a filter based methodology, thus obviating the need for use of the penalty functions as in the basic ICRS method presented in Banga and Seider (1996), which handles only bound constrained problems. The proposed algorithm, termed ICRS-Filter, is shown to be very robust and reliable in producing very good or global solutions for most of the several case studies examined in this contribution.

1. Introduction

Optimization of nonconvex programming problems has an important role in Applied Mathematics, Computer Science as well as scientific and engineering practices. The significance of the global solution in some cases is ‘non-negotiable’, as it could signify “profit or loss” for chemical manufacturers, or “make-or-break” functional properties of proteins in drugs research by predicting their conformational structure.

There are two main approaches to addressing global optimization problems: deterministic and stochastic methods. Reviews of the deterministic global optimization methods are given in Floudas (1999) and Floudas and Misener (2009). For a given problem, deterministic methods are able to provide a certificate of global optimality of the final solution. Deterministic methods generally tend to be computationally expensive with computational times growing very quickly with problem sizes.

The other approach, which is based on stochastic algorithms, improves an initial point using stochastic perturbations. In the stochastic approach, the objective function is evaluated at randomly generated points and the process terminates when there is no further improvement in the objective function value as well as satisfaction of convergence criteria. Stochastic methods can only guarantee solutions which are local optima, without being able to certify global optimality. However, the methods’ ability in efficiently and reliably locating local optima has been proven in various practical applications, especially for very large problems when “good enough” solutions are acceptable. Stochastic methods frequently employ multiple starting points to increase the chance of finding the global optimum (Hickernell and Yuan, 1997; Torn, 1978; Fouskakis and Draper, 2002).

Our work falls into the latter category of optimization methods and a new method, termed ICRS-Filter Method, will be presented which is the combination between the Integrated Controlled Random Search (ICRS) algorithm originally developed by Casares and Banga (1987) and the Filter approach (Fletcher and Leyffer, 2000) to deal with generally constrained NLP problems.

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2. The generic ICRS method

The ICRS method was first developed by Casares and Banga (1987). Banga proposed the ICRS method as a stochastic search method for global optimization of problems with bounds on variables. The method operates by generating random points obeying a normal distribution within the bounds. As the iterations progress, and as acceptances of improving points become fewer, the standard deviation of the normal distribution is suitably reduced thus inducing a more localized search around a current point desired to be improved.

The original ICRS algorithm applies to an unconstrained problem, which is assumed to have the following formulation (**P1**):

Problem P1

$$\min_{x} \ f(x) \tag{2.1a}$$

subject to

$$x^L \le x \le x^U \tag{2.1b}$$

where $x \in \mathbb{R}^n$.

The Algorithm is presented as Algorithm 1. The ICRS algorithm is a search method, which instead of employing a set of search directions, it uses randomly generated points. As the Algorithm generates points closer to a local minimum, the standard deviation σ is reduced, hence the "contracting spheres" picture as shown in Fig. 2.1.

Algorithm 1. ICRS algorithm.

Initial Guess $\leftarrow x_0$
Initial Deviation Factor $\leftarrow k_1$
Reduction Deviation Factor $\leftarrow k_2$
Expansion Deviation Factor $\leftarrow k_3$
Maximum Number of Samples $\leftarrow N_{Sample}$
Maximum Number of Failures $\leftarrow N_{Failure}$
Variable Convergence Tolerance $\leftarrow \varepsilon$
Evaluate Best Objective Function Value $f_{Best} \leftarrow f(x_0)$
Compute Initial Deviation Factor $\sigma \leftarrow k_1 \cdot (x^U - x^L)$
Set Current Solution Vector $x_{Best} \leftarrow x_0$
Set *ifailure* $\leftarrow 0$
for $i \leftarrow 1$ to N_{Sample} **do**
  Generate a new point x_{New} which is Normally distributed between x^U and x^L, given the Mean x_{Best} and Standard Deviation σ
  $f_{New} \leftarrow f(x_{New})$
  if $f_{New} < f_{Best}$ **then**
    Variable Tolerance $\leftarrow \phi(x_{New}, x_{Best})$
    Update Objective Value $f_{Best} \leftarrow f_{New}$
    Update Current Solution $x_{Best} \leftarrow x_{New}$
    Expand Deviation Factor $\sigma \leftarrow k_3 \cdot \sigma$
    if Variable Tolerance $< \varepsilon$ **then**
      Exit Sampling Loop
    end if
  else
    if $f_{New} \ge f_{Best}$ **then**
      $ifailure \leftarrow ifailure + 1$
      if $ifailure > N_{Failure}$ **then**
        Reduce Deviation Factor $\sigma \leftarrow k_2 \cdot \sigma$
        Reset Counter $ifailure \leftarrow 0$
      end if
    end if
  end if
end for
return Best Solution x_{Best} and Best Objective Value f_{Best}

It is important to note that the ICRS algorithm is a *randomized* direct search method and this is to be contrasted with other well-known methods in which the search directions are generated deterministically, such as the Nelder-Mead Simplex Algorithm (Correia et al., 2010; Nelder and Mead, 1965). Their algorithm is evidently unable to handle any other constraints on the variables' domain, which can be easily induced by adding equalities or inequalities to the original (**P1**) problem. Consequently, the ICRS approach is only effective at solving unconstrained optimization problems.

The most important step in the ICRS algorithm is the generation of normally distributed points within given bounds. The following methods have been attempted in this work:

1. Projection to bounds method

The principle behind the method is very simple: given x_0 and σ, generate a random point x which is normally distributed with mean x_0 and with a standard deviation σ. The method used to generate the points x is adapted from Box and Muller (1958). Furthermore, if *any* elements in x are falling below the lower bound or exceeding the upper bound, they will be replaced by the corresponding lower or upper bound values, i.e. "clipped to the bounds".

The "*Projection to bounds method*" often causes the sampling points to "stick" onto the bounds too often and leads to an uneven distribution in the interior of the sampling region. Furthermore, in problems containing functions, which are undefined at the bounds, the method could lead to numerical instabilities. Therefore, the method is not strongly recommended, but it is still included in the discussion as a legacy of the original implementation.

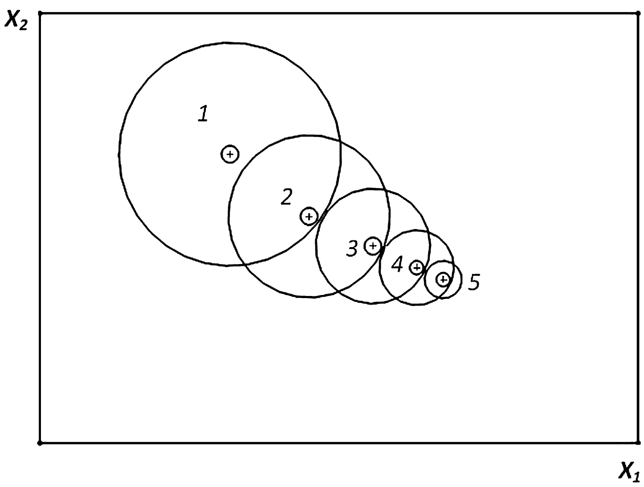

Fig. 2.1 – Illustration of the ICRS algorithm.