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THE MULTI LEVEL SINGLE LINKAGE METHOD FOR UNCONSTRAINED AND CONSTRAINED GLOBAL OPTIMIZATION

by

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Abstract

The more successful methods for unconstrained global optimization of an arbitrary multimodal objective function are of a stochastic nature and involve a combination of sampling and local search techniques. In this class, the recently developed Multi Level Single Linkage method combines attractive theoretical properties with excellent computational properties. We describe this method below, and discuss its computational behaviour and its extension to constrained global optimization.

1. INTRODUCTION

The global optimization problem is to find the global optimum (say, the global minimum) x_* of a real valued twice continuously differentiable objective function $f: \mathbb{R}^n \to \mathbb{R}$. For computational reasons one usually assumes that a set $S \subset \mathbb{R}^n$ which is convex, compact and contains the global minimum as an interior point, is specified in advance. Nevertheless, the problem to find

$$y_* = \min_{x \in S}\{f(x)\} \tag{1.1}$$

remains essentially one of unconstrained optimization.

Only a few solution methods for this problem have been developed so far, certainly in comparison with the multitude of nonlinear programming methods that aim for an arbitrary local minimum. For a survey of global optimization methods we refer to Dixon and Szegö [10], Dixon and Szego [11], Rinnooy Kan and Timmer [23] and Timmer [27]. It appears not to be possible to design methods which offer an absolute guarantee of success for arbitrary f. Therefore, most methods are of a stochastic nature and provide an asymptotic guarantee in a stochastic sense. For instance, if the function is evaluated in points which are drawn from a uniform distribution over S, then it can be shown that the smallest function value found converges to the global minimum value y_* with probability 1 (i.e. almost surely) (cf. Rubenstein [26]).

In Section 2, we describe a folklore method in this category, known as Multistart, paying particular attention to an appropriate stopping rule for this method. The Multi Level Single Linkage method eliminates the inherent inefficiencies of Multistart while retaining its theoretical properties; it is briefly described in Section 3. In Section 4, we review its computational performance. Finally, in Section 5 we discuss at some length our initial attempts to extend Multi Level Single Linkage to constrained global optimization.

2. MULTISTART

Most successful methods for global optimization involve local searches from some or all of the sample points. This presupposes the availability of some local search procedure P which starting from an arbitrary point $x \in S$,

produces a local minimum x*. Depending on what may be assumed avout f, a large number of such procedures is available from the nonlinear programming literature. We assume that P is strictly descent (Timmer [27]), such that if P is started from any point $x \in S$ and converges to a local minimum x*, there exists a path from x to x* along which the function values are nonincreasing. We also assume that this path is completely contained in S. Finally we assume that the number of stationary points of f, i.e. points where the gradient of f is zero, is finite.

The simplest way to make use of the local search procedure P occurs in a folklore method known as Multistart. Here, P is applied to every point in a sample, drawn from a uniform distribution over S, and the local minimum with the lowest function value found in this way is the candidate value for y_*.

An interesting analysis of Multistart was initiated in Zielinski [31] and extended in Boender and Zielinski [2], Boender and Rinnooy Kan [3], and Boender [5]. It is based on a Bayesian estimate of the number of local minima W and of the relative size of each region of attraction $\theta_\ell = m(R(x^*))/m(S)$, $\ell = 1, \ldots, W$, where m(.) denotes Lebesque measure and a region of attraction R(x*) is defined to be the set of all points in S starting from which P will arrive at x*.

In [5] a so-called non-informative prior distribution is specified for the unknowns W, $\theta_1, \ldots, \theta_W$. Given the outcome of an application of Multistart, Bayes' rule is then used to compute the posterior distribution, which incorporates both the prior beliefs and the sample information.

After lengthly calculations, surprisingly simple expressions emerge for the posterior distribution and posterior expectation of several interesting parameters (Boender [5]). For instance, if w different local minima have been found as the result of M local searches started in uniformly distributed points, then the posterior expectation of the number of local minima is

$$\frac{w(M-1)}{M-w-2} \qquad (2.1)$$

This Bayesian analysis is quite an attractive one, the more so since it can be easily extended to yield optimal Bayesian stopping rules (Boender and Rinnooy Kan [4]).

3. MULTI LEVEL SINGLE LINKAGE

In spite of the scope that Multistart offers for analysis, the procedure is lacking in efficiency. The main reason is that it will inevitably cause each local minimum to be found several times. To avoid all these time consuming local searches, P should be applied no more than once, or better still exactly once, in every region of attraction. For this purpose, the Multi Level Single Linkage method has been developed. Unlike the Single Linkage method described in Boender et al. [1], Multi Level Single Linkage focuses on the function values of the sample points to obtain an extremely simple but powerful method.

In the Multi Level Single Linkage method the local search procedure P is applied to every sample point except if there is another sample point or a previously detected local minimum within some critical distance which has a smaller function value.

Actually, the method is implemented in an iterative fashion, where points are sampled in groups of fixed size, say N. In each iteration the above rule is applied to the points of the expanded sample to determine from which sample points P should be started.

In spite of its simplicity, the theoretical properties of Multi Level Single Linkage are quite strong (Timmer [27]). If, for some $\sigma > 0$, the critical distance in iteration k is chosen to be

$$r_k = \pi^{-\frac{1}{2}}\left[\left(\Gamma\left(1 + \frac{n}{2}\right)m(S)\ \sigma \frac{\log kN}{kN}\right]^{1/n}, \qquad (3.1)$$

then any local minimum x^* will be found by Multi Level Single Linkage within a finite number of iterations with probability 1. At the same time we can prove that, if $\sigma > 4$, the total number of local searches ever started by Multi Level Single Linkage is finite with probability 1 even if the sampling continues forever. In [27] it is indicated that these results are in some sense the strongest possible ones. (Actually, the above results were obtained for a slightly different version of Multi Level Single Linkage, modified to ensure that P is never applied in a point which is very close to the boundary of S or to a stationary point detected previously.)

Since Multi Level Single Linkage and Multistart result in the same set of minima with a probability that tends to 1 with increasing sample size, we can simply use the stopping rules which were designed for Multistart

(Boender and Rinnooy Kan [4]).

One might believe that it is unlikely that the global minimum will be found by applying P to a sample point with a relatively high function value. It is then possible to reduce the sample by removing a certain fraction, say $1-\gamma$, of the sample points with the highest function values and to apply Multi Level Single Linkage to the reduced sample points only. Such a reduction of the sample does not significantly affect the theoretical properties of Multi Level Single Linkage. In [27] it is observed that in case of a reduction of the sample to γkN sample points in iteration k, the critical distance should still equal (3.1), but that in (2.1) M should equal γkN and not kN.

Because of the extreme simplicity of the Multi Level Single Linkage method it can be implemented very efficiently. Of course, it is not advisable to start the calculations necessary for applying the method from scratch in every iteration. Since the sample of iteration k-1 is a subset of the sample of iteration k, and since it is known in what way the critical distance varies with k, it turns out to be possible to develop an efficient dynamic implementation of the method (Timmer [27]). In this dynamic implementation, the information which is necessary to determine the starting points of the local search procedure in iteration k is determined by updating the corresponding information from iteration k-1. It turns out to be possible to implement Multi Level Single Linkage in such a way that the running time needed up to iteration k is only O(k) in expectation. Hence, the calculations needed to update the information in iteration k do not vary with the size of the complete sample, but only with the number of newly sampled points.

A fuller description of the results described in this section, including proofs, can be found in [24, 25, 27].

4. COMPUTATIONAL RESULTS

To examine the computational behaviour of Multi Level Single Linkage it has been coded in Fortran IV and run on the DEC 2060 computer of the Computer Institute Woudestein.

We tested Multi Level Single Linkage on the standard set of test functions (Dixon and Szegö [12]), which is commonly used in global optimization. These test functions are listed in Table 1.

Table 1

TEST FUNCTIONS

GP	Goldstein and Price
BR	Branin (RCOS)
H3	Hartman 3
H6	Hartman 6
S5	Shekel 5
S7	Shekel 7
S10	Shekel 10

In this section Multi Level Single Linkage will be compared with a few leading contenders whose computational behaviour is described in Dixon an Szegö [11]. In this reference methods are compared on the basis of two criteria: the number of function evaluations and the running time required to solve each of the seven test problems. To eliminate the influence of the different computer systems used, the running time required is measured in units of standard time, where one unit corresponds to the running time needed for 1000 evaluations of the S5 test function in the point (4,4,4,4).

Since both the number of function evaluations and the units of standard time required are sensitive to the peculiarities of the sample at hand, the results reported for Multi Level Single Linkage represent the average outcome of four independent runs. We applied Multi Level Single Linkage to 20% of the sample points ($\gamma = 0.2$) and choose σ to be equal to 4. After an initial sample of size 100, we increased the sample and applied Multi Level Single Linkage iteratively until the expected number of minima (2.1) exceeded the number of different minima found by less than 0.5. We did not implement the method as efficiently as possible since this is not really necessary if the sample size is moderate. Since all test functions are twice differentiable, we could use the VA10AD variable metric routine from the Harwell Subroutine Library as a local search procedure.

In Table 2 and Table 3 we summarize the computational results of Multi Level Single Linkage and compare them to those obtained for a few leading contenders as reported in Dixon and Szegö [12].

Table 2

NUMBER OF FUNCTION EVALUATIONS

	FUNCTION						
METHOD	GP	BR	H3	H6	S5	S7	S10
Gomulka [12]	-	-	-	-	5500	5020	4860
Bremmerman [7,12]	300	160	420L	515	375L	405L	336L
Price [21]	2500	1800	2400	7600	3800	4900	4400
Törn [28,29]	2499	1558	2584	3447	3649	3606	3874
De Biase and Frontini [9]	378	597	732	807	620	788	1160
Multi Level Single Linkage	148	206	197	487	404	432*	564

L: the method did not find the global minimum.

*: the global minimum was not found in one of the four runs.

Table 3

NUMBER OF UNITS STANDARD TIME

	FUNCTION						
METHOD	GP	BR	H3	H6	S5	S7	S10
Gomulka [12]	-	-	-	-	9	8.5	9.5
Bremmerman [7,12]	0.7	0.5	2L	3	1.5L	1.5L	2L
Price [21]	3	4	8	46	14	20	20
Törn [28,29]	4	4	8	16	10	13	15
De Biase and Frontini [9]	15	14	16	21	23	20	30
Multi Level Single Linkage	0.15	0.25	0.5	2	1	1*	2

L: the method did not find the global minimum.

*: the global minimum was not found in one of the four runs.

5. CONSTRAINED GLOBAL OPTIMIZATION

In this section we shall consider the constrained global optimization problem which is to find the global minimum x_* of an objective function f given a set of equality and inequality constraints. We assume that a set S which contains all feasible solutions (including the global one) as interior points is specified in advance. Hence, we consider the problem to find

$$y_* = \min_{x \in S} f(x) \tag{5.1}$$

$$\text{s.t. } h_i(x) = 0 \qquad i \in M_1 = \{1,\ldots,m_1\}, \tag{5.2}$$

$$h_i(x) \leqq 0 \qquad i \in M_2 = \{m_1+1,\ldots,m_2\}. \tag{5.3}$$

where $h_i : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable ($i \in M_1 \cup M_2$).

Given a point $x \in S$ it is convenient to define the following index sets

$$I(x) = \{i \in M_1 \mid h_i(x) \neq 0\}, \quad J(x) = \{j \in M_2 \mid h_j(x) > 0\}, \tag{5.4}$$

$$\overline{I}(x) = \{i \in M_1 \mid h_i(x) = 0\}, \quad \overline{J}(x) = \{j \in M_2 \mid h_j(x) = 0\}. \tag{5.5}$$

We define a constraint to be <u>violated</u> in x if it is not satified in x, i.e. if its index is in the set I(x) or J(x). A constraint is said to be <u>active</u> in x if it is violated or if its index belongs to the set $\overline{I}(x)$ or $\overline{J}(x)$. The index set of the active constraints in x is denoted by M(x) and we have $M(x) = M_1 \cup J(x) \cup \overline{J}(x)$. The gradients of f(x) and $h_i(x)$ ($i \in M_1 \cup M_2$) in a point x will be denoted by $\nabla f(x)$ and $\nabla h_i(x)$ respectively. $\nabla^2 f(x)$ and $\nabla^2 h_i(x)$ ($i \in M_1 \cup M_2$) will indicate the matrix of second order derivatives of f respectively h_i in x. To be able to derive necessary and sufficient conditions for a point to be a local minimum of (5.1)-(5.3), we need a so-called <u>constraint qualification</u>: we assume that the gradients of the active constraints, i.e. the vectors $\nabla h_i(x)$ ($i \in M(x)$) are <u>linearly independent</u> for every $x \in S$. Under such a constraint qualification, the Kuhn-Tucker conditions are <u>necessary</u> for a point x* to be a local minimum of (5.1)-(5.3). The <u>second order sufficient conditions</u> for local optimality specify that, in addition to satisfying the Kuhn-Tucker conditions, the multiplier vector $\lambda_* \in \mathbb{R}^{m_2}$ (with components $\lambda_*^{(i)}$) has to satisfy

$$z^T\Big(\nabla^2 f(x^*) + \sum_{i \in M_1 \cup M_2} \lambda_*^{(i)} \nabla^2 h_i(x^*)\Big)\, z > 0 \tag{5.6}$$

for every nonzero vector $z \in \mathbb{R}^n$ satisfying $z^T \nabla h_i(x^*) = 0$ if $i \in M_1 \cup \{j \in \overline{J}(x^*) \mid \lambda_*^{(j)} > 0\}$ and $z^T \nabla h_i(x^*) \leq 0$ if $i \in \{j \in \overline{J}(x^*) \mid \lambda_*^{(j)} = 0\}$.

Only very few methods have been developed to solve the constrained global optimization problem. In [18] it is shown that the Tunneling Method can be generalized to solve problem (5.1)-(5.3). However, this approach has the same disadvantages as it has in the unconstrained case in that no guarantee of success can be provided. Some attention has been given to certain subclasses of problem (5.1)-(5.3). For instance, the case that f is concave and the constraints are convex has been described in [17, 22]. In [19] it is assumed that f is concave and that the constraints are linear. Of course, these kinds of assumptions change the structure of the problem considerably.

What happens if we try to generalize the successful method described in Section 3 to solve the constrained problem? If it would be possible to use feasible points only, i.e. points in S satisfying (5.2) and (5.3), then such a generalization would be straightforward. More precisely, if we draw the sample points from a uniform distribution over the feasible region and use an interior point minimization technique [13] as local search procedure, then we would not have to adapt our clustering procedures at all. However, it is not known how to draw points from a uniform distribution over the feasible region. Of course, one can draw the points from a uniform distribution over S and ignore the points that are not feasible. But if there are equality constraints we will never draw a feasible point, and even if M_1 is empty, such a procedure would be very inefficient for large n. Actually, even if M_1 is empty and all constraints are linear, then there is still no efficient way known to obtain points that are distributed according to a uniform distribution over the feasible region (cf. [5] for a method of generating points which are asymptotically uniform). Finally, an interior point minimization technique is not very efficient and cannot be used if there are equality constraints. We conclude that this approach does not seem very promising.

It follows that we cannot avoid infeasible points in our calculations. Recall that in the method described in Section 3, the function value of the sample points plays a crucial role: in Multi Level Single Linkage, we do not apply the local search procedure to a sample point x if another sample point is within the critical distance of x and has a smaller function value than f(x). Furthermore, one of the reasons that Multi Level Single Linkage has strong theoretical properties is that the local search procedure is descent with respect to f. If we are doomed to treat infeasible points, how

should we then compare the function values of a feasible and an infeasible point? If the infeasible point has a smaller f-value this does not mean that we should not start a local search from a feasible point close to it, since the constrained local search may very well generate a sequence with increasing f-values. We conclude that we must measure the relative attractiveness of the sample points in a different way.

For this purpose we will use a penalty function. Such a penalty function measures the f-value in a point together with the extent to which it is feasible, so as to give a single value for the attractiveness of the point. Of course, it would be very helpful if we could use a penalty function ψ which has the property that there is a 1-1 correspondence between the local minima of ψ and the local minima of (5.1)-(5.3). We will call a penalty function with the above 1-1 property a doubly exact penalty function. Note that a doubly exact penalty function has stronger properties than the well known exact penalty functions [15] which are used in local constrained optimization and only have the property that all constrained local minima are also minima of the penalty function.

A doubly exact penalty function can be derived from the familiar ℓ_1-penalty function (Zangwill [30], Pietrzykowski [20])

$$\psi(x,\alpha) = f(x) + \sum_{i\in M_1} \alpha^{(i)}|h_i(x)| + \sum_{i\in M_2} \alpha^{(i)}\max(0,h_i(x)). \qquad (5.7)$$

In [20] it has been proved that for every local minimum x^* of (5.1)-(5.3), there exists an $\alpha_o \in \mathbb{R}^{m_2}$ such that for all $\alpha \geq \alpha_o$, x^* is a local minimum of (5.7) as well. More precisely (Charalambous [8]), if x^* is a local minimum of (5.1)-(5.3) which satisfies the second order sufficient conditions with Lagrange multipliers $\lambda_*^{(i)}$ ($i \in M_1 \cup M_2$) and if $\alpha^{(i)} > |\lambda_*^{(i)}|$, for all $i \in M_1 \cup M_2$, then x^* is a local minimum of $\psi(x,\alpha)$.

It is also possible to choose α in such a way that each minimum of $\psi(x,\alpha)$ is a minimum of (5.1)-(5.3). For this purpose we introduce the following notation.

The matrix whose i-th row consists of the gradient $\nabla h_i(x)$ ($i=1,2,\ldots,m_2$) will be denoted by $A(x)$. $\bar{A}(x)$ is equal to $A(x)$ except for the fact that all rows that correspond to constraints which are inactive in x are deleted. Hence, the i-th row of $\bar{A}(x)$ corresponds to the gradient of the i-th active constraints in x. If all constraints are active in x, we define a vector $\lambda(x) \in \mathbb{R}^{m_2}$ by

$$\lambda(x) = - \left(A(x)A(x)^T\right)^{-1} A(x)\nabla f(x). \qquad (5.8)$$

Note that $\left(A(x)A(x)^T\right)^{-1}$ is well defined since we assumed the gradients of the active constraints in every x to be linearly independent. If certain constraints are not active in x, then let i(j) be the j-th active constraint in x. For every active constraint in x, we now take $\lambda^{(i(j))}(x)$ to be equal to the j-th element of $\left(\overline{A}(x)\overline{A}(x)^T\right)^{-1} \overline{A}(x)\nabla f(x)$. Elements of $\lambda(x)$ corresponding to constraints that are inactive in x are taken to be equal to 0.

The function $\lambda(x) : \mathbb{R}^n \to \mathbb{R}^{m_2}$ defined in this way is bounded. To see this, let M' be an arbitrary subset of $M_1 \cup M_2$ and let S' be the largest subset of S such that for all points x in S', M' is the index set of the active constraints in x. Furthermore, let $\overline{C}(x)$ be the matrix containing the gradients of the active constraints in S', i.e. $\overline{C}(x) = \overline{A}(x)$ for all $x \in S'$. Finally, let $\overline{S}'$ be the closure of S'. It is easy to check that the constraints that are active in S' are also active in $\overline{S}'$. Since the active constraints are assumed to be independent, it follows that $\left(\overline{C}(x)\overline{C}(x)^T\right)^{-1}$ exists for all $x \in \overline{S}'$. (Note that $\overline{C}(x)$ is not equal to $\overline{A}(x)$ if $x \in \overline{S}'$ S'.) Hence, $\left(\overline{C}(x)\overline{C}(x)^T\right)^{-1} \overline{C}(x)\nabla f(x)$ is a continuous function of x over the compact set $\overline{S}'$ and therefore it attains a maximum over this set. It follows that the supremum of $\left(\overline{C}(x)\overline{C}(x)^T\right)^{-1} \overline{C}(x)\nabla f(x)$ over S' is also bounded. Finally, since there are only a finite number of subsets M' of $M_1 \cup M_2$, and since $\overline{A}(x)$ equals $\overline{C}(x)$ in every corresponding set S', it follows that $\sup_{x \in S} \left(\overline{A}(x)\overline{A}(x)^T\right)^{-1} \overline{A}(x)\nabla f(x)$ is bounded so that a vector $\alpha \in \mathbb{R}^{m_2}$ exists which satisfies

$$\alpha^{(i)} > \sup_{x \in S} |\lambda^{(i)}(x)| \qquad (i \in M_1 \cup M_2). \qquad (5.9)$$

Given the above observation, we are now in a position to prove that, if α is chosen to satisfy (5.9) and if $x^* \in S$ is a local minimum of $\psi(x,\alpha)$, then x^* is a local minimum of (5.1)-(5.3). We can also prove that, if α satisfies (5.9) and if x^* is a local minimum of (5.1)-(5.3) which satisfies the second order sufficient conditions of (5.6), then x^* is a local minimum of $\psi(x,\alpha)$. The proofs for these results will appear elsewhere.

Thus, if α satisfies (5.9), then we almost know that ψ is a doubly exact penalty function. We only need the provision that a local minimum x^* of

(5.1)-(5.3) satisfies the second order sufficient conditions (5.6) to show that it is also a minimum of ψ. This provision is not unusual in the theory of exact penalty functions (Fletcher [14], Charalambous [8]), and actually we do not believe that it is strictly necessary.

One might argue that the requirement (5.9) prevents $\psi(x,\alpha)$ from being practically useful, since (5.9) itself defines a global optimization problem. However, this turns out to be not a serious drawback in our context; the latter global problem does not need to be solved explicitly. Moreover, we believe that a requirement like (5.9) is unavoidable in a doubly exact penalty function. We can view α as a parameter which contains global information about the problem, so that the value of ψ in a point x does not only depend on the specification of the constrained problem in x alone. Let us say that a penalty function is parameter-free if its value in any point x only depends on the properties of the constrained problem in x. We conjecture that for every continuous penalty function whose value in an arbitrary point x depends only on $f(x)$, $h_i(x)$ $(i \in M_1 \cup M_2)$ and the values of a finite number of derivatives of f and h_i in x, there exist smooth (e.g. continuous differentiable) functions f and h_i $(i \in M_1 \cup M_2)$ such that there is no 1-1 correspondence between the minima of the penalty function and the minima of (5.1)-(5.3). The truth of this conjecture would imply that there is no parameter free doubly exact penalty function.

Through the theoretical results described above, we have laid the foundation for a stochastic method for constrained global optimization that is similar in spirit to the Multi Level Single Linkage method. The (nontrivial) details of this method do appear in [27], but we do not discuss them here. For one thing, they are beyond the scope of this contribution; for another thing, it is conceivable that there are more appropriate theoretical frameworks in which such an extension could be carried out. Even more than unconstrained global optimization, constrained global optimization represents a virgin territory that is well worth exploring in more detail.

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