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A Crystal Growth Approach for Topographical Global Optimization

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Abstract. A new approach for topographical global minimization of a function $f(x)$, $x \in A \subset R^n$ by using sampled points in A is presented. The globally sampled points are firstly obtained by uniform random sampling or uniform sampling with threshold distances. The point with the lowest function value is used as the nucleus atom to start a crystal growth process. A first triangular nucleus includes the nucleus atom and two nearest points. Sequential crystal growth is continued for which a point next closest to the nucleus atom is bonded to the crystal by attaching to two nearest solidified points. A solidified point will be marked during the crystal growth process if any of two connected points has a lower function value. Upon completion of entire crystal growth process, all unmarked points are then used as starting points for subsequent local minimizations. Extension of the topographical algorithms to constrained problems is exercised by using penalty functions. Formulas for estimation on the number of sampled points for problems with an assumed number of local minima are provided. Results on three global minimization problems by two topographical algorithms are discussed.

Key words: Global optimization, Topography graph, Crystal growth

1. Introduction

The objective of this work is to develop a new approach in topographical global optimization algorithms for solving the global minimum of an unconstrained function $f(x)$ in $A \subset R^n$. The global optimization methods comprise two major branches: the deterministic methods (Horst and Tuy, 1992) and probabilistic methods. The probabilistic methods primarily comprise random search methods, clustering methods (Törn and Zilinskas, 1989) and emergent nature-simulated methods such as genetic algorithms (Goldberg, 1989) and simulated annealing (Kirkpatrick et al., 1983). The topographical global optimization algorithms (Törn and Viitanen, 1992, 1994) that we tried to improve belong to a general category of clustering methods. Topographical information about the objective functions of sampled points located in the search space is used to construct a directed topograph. In the topograph, any point with all k nearest neighbors having higher objective function values becomes a near-minimum point in a simulated basin consisting of at least the k compared points. The crystal growth approach proposed in this paper belongs to topograph-

ical global optimization methods. It serves to provide an algorithm in which no performance-depending parameters are required so that the search efficiency and reliability will be increased.

The paper has the following structure. Section 2 contains a more detailed description of the topographical global optimization method proposed in (Törn and Viitanen, 1992, 1993). The major drawback of the topographical algorithm is also explained. In Section 3, the crystal growth approach in the topographical algorithm will be described in detail. An estimation formula on the size of sampled points needed to obtain a good covering based on an assumed number of basins in the search domain is also proposed. Section 4 comprises results of experiments applying both topographical algorithms in three illustrative problems consisting of one constrained minimization problem and two unconstrained minimization problems.

2. The topographical algorithm

The topographical algorithm proposed by Törn and Viitanen (1994) consists of two parts. The undirected topograph is first constructed in the 'sampler' process by accepting N randomly generated points in which any two points are separated at least with a prespecified threshold distance. The sampled points accordingly created will form a uniform distribution to cover the region better than a uniform random sampling. The coordinates of accepted points are stored in a C-matrix. The sampler process is terminated after the construction of a knn-matrix containing the identifications of k nearest neighbors to every point, sorted by distance.

The second part of the topographical algorithm mainly consists of the construction of the directed topograph and subsequent local minimizations. The construction of the directed topograph starts from evaluating the function value for each point in the C-matrix. Function values are compared between each element in one of all rows in the knn-matrix and the point from which the k elements are nearest. The element in the row will be marked if it has a higher function value, otherwise it will be unmarked. Finally the knn-matrix will be scanned for all rows that contain only marked elements. These rows represent points for which all k nearest neighboring points have higher function values and they can be used as initial points for subsequent local minimizations. These points should also be checked so as to make sure that they are not marked anywhere in the knn-matrix. The number of local minima in a directed topograph is heavily dependent on the value of k selected. If k is chosen too small, the number of possible minima will be large that consequently demands extra computational cost to obtain the global minimum. For k equal to N the number of potential minima will be 1 since only the point with the smallest function value will be qualified.

Although the topographical optimization algorithm is simple and robust, two drawbacks remain. Two most important parameters needed to be defined by the user in the topographical optimization algorithm are k and N. There exist no guidelines to select appropriate values for them. The method may fail to locate the global

optimum or waist unnecessary computational resources for a poor selection of k value even if N is properly defined. These is a need to create a modification on this part of topographical optimization algorithm in which the modified version will search the potential minima without any parameter other than N. It will be all agreed that N is difficult to properly define without a thorough understanding on the space A. However, it would be useful to have estimation formulas for proper N values to use based on an assumption of the number of local minima in the space A. The crystal growth approach was proposed to provide a more stable algorithm in which no parameters other than N have to be defined. The guideline to select proper values of N based on an assumption of the number of basins is described in the following section.

3. Topographical optimization with crystal growth approach

The algorithm consists of three parts: the sampled point placement process, the potential local minima determination process and the local minimizations to find the global optimum. The sampling process using a prespecified threshold value to obtain uniform distribution of sampled points in the space is also suggested in the crystal growth approach. Sampled points obtained by other sampling procedures can also be used for the crystal growth approach with varied effects depending on the distribution of points and local basins.

3.1. CRYSTAL GROWTH PROCESS

The crystal growth approach for topographical optimization is basically responsible for the discovery of points serving as initial points for potential local minima. The crystal growth approach consists of the following steps:

1. Rank all sampled points according to their objective function values.
2. The point with the lowest function value is defined as the core of the nucleus.
3. The core and two nearest points form a triangular nucleus from which a crystal growth process starts.
4. The third (next) nearest point to the core will be bonded to the two nearest points among all points in the polycrystal and form a new triangular single crystal. If the new point has a higher objective function value than any of two connected points in the polycrystal the new point is marked.
5. Process (4) is continued until all points are bonded to the polycrystal.
6. Sequentially repeat steps from (3) to (5) by using the unmarked point with the next lowest function value as the new nucleus core until all unmarked points have been used as cores.
7. All final unmarked points are promising initial points for local minima.

The procedure of the crystal growth approach may be illustrated by following examples. Assume that total of six sampled points are created in the space ($n = 2$) as shown in Figure 1. The function value for each point is evaluated and used as

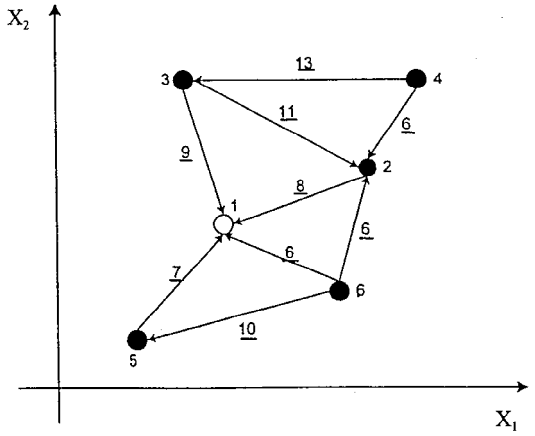

Figure 1. The directed topograph for six sampled points.

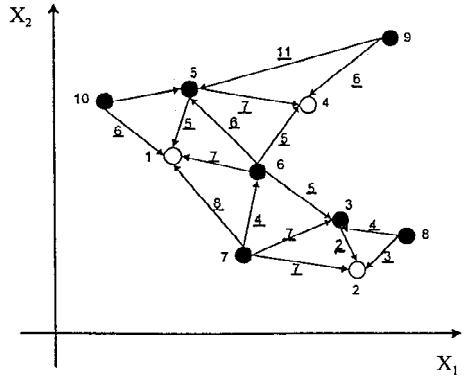

Figure 2. The directed topograph comprising three local minima.

the index number for each point for convenience. The point 1 is used as the core of the nucleus to form the triangular nucleus that consists of the core and two nearest points 6 and 5 with a distance 6 and 7 from the core, respectively. Since both points have higher function values than the core, points 6 and 5 are marked and shown in black circles in the figures. Once a new single crystal is formed, an arrowed arc will be drawn from a point of a higher function value to a point of a lower value. The third (next) nearest point from the nucleus core is now point 2 which is thus bonded to two nearest points 6 and 1 from all solidified points 1, 6 and 5 and forms a second single crystal. The point 2 is marked because it has a higher function value than one of two points to which it is connected. The next nearest point from the core is point 3 and a new crystal is formed by attaching point 3 to points 1 and 2. For the same reason as for point 2, point 3 is marked. The next nearest point from the core and also the last point in the space is point 4. A last single crystal is formed by attaching point 4 to points 2 and 3 which are two nearest points among all solidified points to point 4. Point 4 is marked since point 2 has a lower function value. After

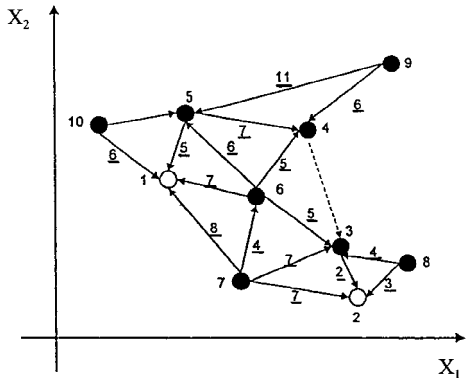

Figure 3. The directed topograph comprising two local minima.

all sampled points have been solidified, only point 1 leaves unmarked. Therefore, point 1 will be used as the sole promising initial point for a local minimization.

Another example involves 10 sampled points in a 2-dimensional space. Identical usage of indices as used in the first example is used in this example. A first run of crystal growth will result in a directed topograph as shown in Figure 2. There are three unmarked points 1, 2 and 4 at the end of the first crystal growth process. Since point 2 is still unmarked and has the second lowest function value of all, it will be used as a new core to start a second crystal growth process. After three crystals are formed points 2, 3, 8, 7 and 6 are sequentially solidified. When the next nearest neighbor, point 4, is connected to points 6 and 3 and forms a new crystal, point 4 is then marked due to its higher function value than point 3 as shown in Figure 3. At the end of the second crystal growth process, points 1 and 2 remain unmarked. A third crystal growth process using point 2 as the core fails to create new results. Finally, points 1 and 2 are considered as near local minimum candidates. It is noted that there is no parameter needed to be defined by the user in order to apply the crystal growth approach. Chances of failure to discover the global minimum and unnecessary computational cost resulted from an improper k value can be reduced by using the parameter-light crystal growth techniques.

3.2. ESTIMATION OF N

A larger value of N will demand a larger number of function analyses before and during the local minimizations. A small value of N will result in incorrect judgment in the topograph construction process for which a large number of unnecessary points for an identical minimum may be selected. In order to find the global optimum using the topographical approach effectively, the value of N needs to be large enough to place a couple of sampled points around each basin containing a local minimum. An estimation formula for a "proper" value of N based on a predicted number of basins is provided and explained as follows:

Assume that m basins exist in a space of n variables and the valid range between the lower bound and the upper bound is represented as l_i for the i-th variable. The effective number of m basins in the i-th dimension can be expressed as

$$m_i = int\left[m \frac{l_i}{\sum_{k=1}^{n} l_k} \right] \tag{1}$$

where int represents an integer function.

The effective number of basins for each dimension can be then used to compute the necessary sampling points for the topographical algorithms to have good results. At least one point needs to be located in each of effective basins in the i-th dimension and at least one point will need to be located in each side of a basin, the minimum number of sampled points N_i required by the distributed basins in the i-th dimension will be as follows:

$$N_i = 2m_i + 1 \tag{2}$$

The total number N of required sampled points for m basins is therefore as follows:

$$N = N_1 \times N_2 \times N_3 \cdots \times N_n \tag{3}$$

It is noted that although the equation (3) provides a proper number of sampled points for a design space with an assumed number of local minima based on an assumption that all sampled points are ideally distributed. The actual number of sampled points required will be larger according to different sampling techniques. For a same number of sampled points in a design space, the probability for two points to become too close by using the uniform distribution with a threshold distance will be significantly lower than other random sampling techniques. The equation which suggests the enlarged number of sampled points N^* required according to different sampling techniques is defined as follows:

$$N^* = \frac{N}{|\log_{10}(1-p)|} \quad (0.1 \leqslant p \leqslant 0.9) \tag{4}$$

where p represents the clustering parameter for different sampling techniques.

For a random uniform sampling, an appropriate value of p is between 0.4 and 0.5. The uniform sampling with a maximum threshold distance will have a highest value of p, 0.9, therefore less sampled points defined by (3) are needed to cover the space with equal effectiveness. Although the number and sizes of basins in a given space are generally unknown, the estimation formulas offer a unique advantage. If the number of basins is known or can be estimated using any algorithm, formulas defined in (1–4) will provide an economic size of sampled points which can cover the nonconvex space with reasonable effectiveness.

4. Experimental results

The crystal growth approach was tested and compared with the topographical algorithm by Törn and Viitanen in three global minimization problems. The first problem is the Himmeblau's function containing four minima of equal function values. The second problem is a constrained global optimization problem containing six design variables and six linear constraints. The last problem involves a modified exponential bump function with ten design variables and at least twenty local minima.

4.1. HIMMEBLAU'S FUNCTION

The Himmeblau's function and its bounds are defined as follows:

$$F(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2 \qquad -5 \leqslant x \leqslant 5; \quad -5 \leqslant y \leqslant 5 \tag{5}$$

Two sampling methods consisting of the uniform threshold sampling and the uniform random sampling are used. The value of p in (4) is set as 0.9 and 0.5 for the uniform threshold sampling and the uniform random sampling, respectively and accordingly 25 (5×5) and 83 ($5 \times 5/0.301$) points are created in two cases for the topographical minimization. The distribution of the 25 sample points (threshold distance 1.61) represented by solid circles in the space is shown in Figure 4, in which four potential minima or unmarked points obtained by the crystal growth approach are identified by single circles. The four unmarked points can lead to all four existing minima after local minimizations are executed. The performance of Törn and Viitanen's algorithm based on identical 25 sampled points with varied k values ranging from 2 to 15 is shown in Figure 5. It is noted that as k equals 2, the number of potential minima is 7 of which 3 are redundant. When k is greater than 5, the number of potential minima is less than 4 so that some relative minima fail to be identified.

A topograph comprising 83 randomly generated sampled points and the four potential local minima formed after the crystal growth process was completed is shown in Figure 6. The four following local minimizations discovered also all four local minima in the space. The performance of Törn and Viitanen's algorithm based on identical 83 sampled points is shown in Figure 7. With sufficient sampled points, all four relative minima are eventually located in all k values. Compared with four in crystal growth approach, sixteen local minimizations were required in the $k = 2$ case. Results of two sampling cases showed that the crystal growth approach performed more accurate and efficient than the counterpart algorithm with varied k values.

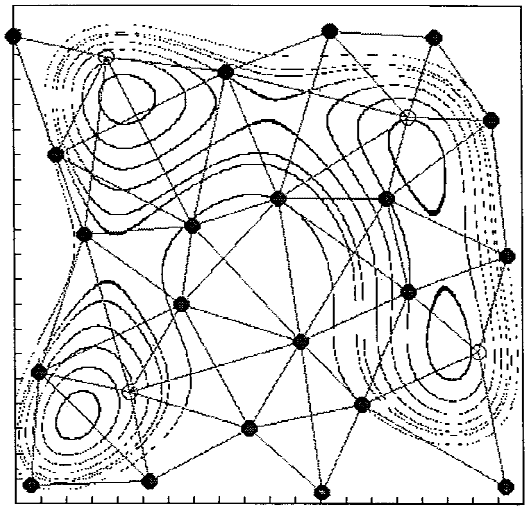

Figure 4. The topograph and local minima of 25 sampled points generated with a threshold distance for Himmeblau's function.

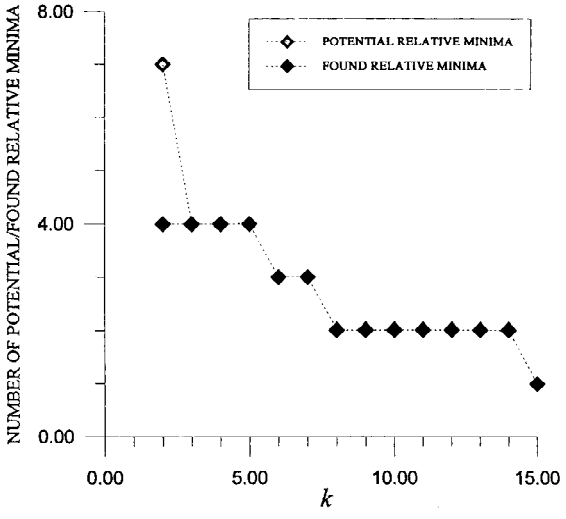

Figure 5. Numbers of potential and located minima from 25 sampled points with varied k values.

4.2. CONSTRAINED GLOBAL MINIMIZATION

To test both topographical algorithms in problems of higher complexity and dimensionality, this constrained problem consisting of six variables and six linear constraints was used. This problem is included in a collection book of constrained global optimization problems (Floudas and Pardalos, 1990). The problem state-

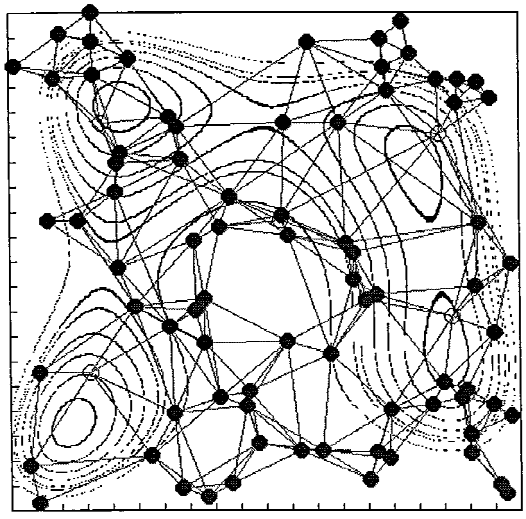

Figure 6. The topograph and local minima of 83 randomly generated sampled points for Himmeblau's function.

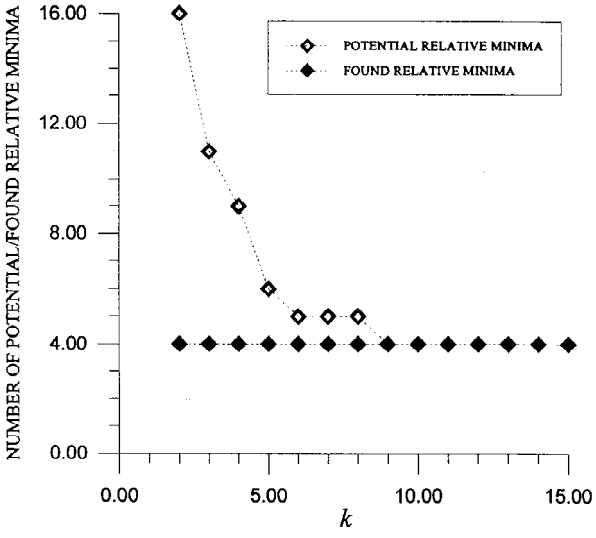

Figure 7. Numbers of potential and located minima from 83 sampled points with varied k values.

ment is as follows:

$$\begin{aligned} \text{MIN}\ \ & F(\mathbf{X},\mathbf{U}) = x_1^{0.6} + x_2^{0.6} + x_2^{0.4} + 2u_1 + 5u_2 - 4x_3 - u_3 \\ \text{s.t.}\ \ & x_2 - 3x_1 - 3u_1 = 0 \\ & x_3 - 2x_2 - 2u_2 = 0 \\ & 4u_1 - u_3 = 0 \\ & x_1 + 2u_1 \leqslant 4 \end{aligned} \tag{6}$$

$$
\begin{aligned}
x_2 + u_2 &\leqslant 4 \\
x_3 + u_3 &\leqslant 6 \\
x_1 &\leqslant 3 \\
u_2 &\leqslant 2 \\
x_3 &\leqslant 4 \\
x_1, x_2, x_3, u_1, u_2, u_3 &\geqslant 0
\end{aligned}
$$

In order to extend the topographical algorithms to constrained minimization problems, a pseudo-objective function often encountered in the sequential unconstrained minimization techniques (Fiacco and McCormick, 1968) is defined as follows:

$$\Phi(\mathbf{X}, \mathbf{U}) = F(\mathbf{X}, \mathbf{U}) + P(\mathbf{X}, \mathbf{U}) \tag{7}$$

where $P(\mathbf{X}, \mathbf{U})$ is the penalty function which transfers the constraint violations into the penalty on the objective function. The parameter r_p represents the multiplier which controls the magnitude of the penalty. The penalty function is defined as follows:

$$P(\mathbf{X}, \mathbf{U}) = r_p \left\{ \sum |h(\mathbf{X}, \mathbf{U})| + \sum [g^+(\mathbf{X}, \mathbf{U})] \right\} \tag{8}$$

where $h(\mathbf{X}, \mathbf{U})$ represents the equality constraint functions, and $g(\mathbf{X}, \mathbf{U})$ represents the inequality constraint functions.

In this problem, r_p was selected as the absolute value of the mean of the objective functions of the 350 sampled points obtained by a threshold distance. The directed topographies of the 350 sampled points by both algorithms are exclusively

Table 1. Comparison of two algorithms in the constrained problem

	k	Number of potential minima	Number of relative minima	Number of function evaluation used
	2	64	11	4802
	3	35	8	3036
Törn and	4	25	6	2087
Viitanen's	5	17	5	1659
algorithm	6	13	4	1320
	7	11	3	1162
	8	10	3	1092
Crystal growth approach	–	11	7	1106

based on the pseudo-objective function values. The crystal growth approach and the topographical algorithm with k varied from 2 to 8 were executed on 350 threshold sampled points. The results are listed in Table 1. All approaches led to the global minimum despite of varied number of relative minima obtained. It is clearly shown that the crystal growth approach provided a relatively stable and efficient algorithm than the counterpart algorithm in which lower k values demanded a great amount of computation while higher k values located less relative minima.

4.3. TEN-VARIABLE EXPONENTIAL BUMP FUNCTION

The third problem involves a modified exponential bump function defined as follows:

$$F(\mathbf{X}) = 100 - \sum_{i=1}^{20} [\mathbf{W}_i \times \mathrm{EXP}(-\mathbf{Y}_i)] \tag{9}$$

where

$$\mathbf{Y}_i = \mathbf{PP}_i \left[\sum_{j=1}^{10} (\mathbf{X}_j - \mathbf{P}_{i,j})^2 \right]; \quad i = 1 \sim 20 \tag{10}$$

$$\mathbf{P} = \begin{bmatrix}
2 & -4 & 2 & -4 & 2 & -4 & 2 & -4 & 2 & -4 \\
-2 & 4 & -2 & 4 & -2 & 4 & -2 & 4 & -2 & 4 \\
-3 & -3 & -3 & -3 & -3 & -3 & -3 & -3 & -3 & -3 \\
3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\
-4 & 3 & 4 & 3 & 4 & -3 & 4 & 3 & 4 & 3 \\
4 & -3 & 4 & 3 & 4 & 3 & -4 & 3 & 4 & 3 \\
4 & 3 & -4 & 3 & 4 & 3 & 4 & -3 & 4 & 3 \\
4 & 3 & 4 & -3 & 4 & 3 & 4 & 3 & -4 & 3 \\
-3 & 2 & 3 & 2 & -3 & -2 & 3 & 2 & 3 & -2 \\
3 & -2 & 3 & 2 & -3 & 2 & -3 & 2 & 3 & -2 \\
3 & 2 & -3 & 2 & -3 & 2 & 3 & -2 & 3 & -2 \\
3 & 2 & 3 & -2 & -3 & 2 & 3 & 2 & -3 & -2 \\
-4 & -3 & -2 & 3 & 4 & 4 & -3 & -2 & -3 & 4 \\
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-3 & -3 & -3 & 4 & -2 & 2 & -4 & -3 & -3 & -3 \\
-3 & -3 & 3 & -4 & -2 & -2 & 4 & -3 & -3 & -3 \\
-3 & 3 & -3 & -4 & -2 & -2 & -4 & 3 & -3 & -3 \\
3 & -3 & -3 & -4 & -2 & -2 & -4 & -3 & 3 & -3
\end{bmatrix}$$

Table 2. Comparison of two algorithms in exponential function

	k	Number of potential minima (relative minima) for 1000 sampled points	Number of potential minima (relative minima) for 2000 sampled points
Törn and	2	226 (18)	405 (18)
Viitanen's	3	119 (14)	223 (15)
algorithm	4	82 (11)	144 (13)
	5	61 (11)	95 (13)
	6	41 (9)	72 (11)
	7	33 (8)	55 (11)
	8	29 (6)	46 (10)
	9	25 (5)	37 (9)
	10	22 (5)	29 (9)
	11	21 (5)	23 (8)
	12	18 (5)	20 (7)
	13	16 (5)	18 (7)
	14	13 (5)	17 (7)
	15	13 (5)	15 (7)
Crystal growth approach	–	16 (13)	23 (17)

$$\mathbf{PP} = [0.04, 2 * 0.05, 2 * 0.04, 0.05, 4 * 0.04, 0.05, 0.03, 0.05, 0.04, 3 * 0.05, 0.04, 0.05, 0.04]^T$$

$$\mathbf{W} = [2 * 100, 2 * 90, 8 * 80, 8 * 70]^T$$

The design space of this problem consists of 20 customized valleys of varied depths and widths, therefore, generally comprises at least 20 relative minima. The best solution obtained from thousands of local minimizations is $\mathbf{X} = \{1.825, -3.876, 1.908, -3.953, 1.724, -3.835, 1.901, -3.881, 1.790, -3.869\}$ with an objective function of -7.536. For this problem of 10 variables, the number of sampled points suggested by (3) is prohibitively large so that two cases, 1000 (threshold distance 6.15) and 2000 (threshold distance 5.80) sampled points, were studied for both topographical algorithms. The results are shown in Table 2. All algorithms reported in Table 2 located the best solution despite of varied number of relative minima finally obtained. A consistent trend was also found in this problem that the crystal growth approach performed the best in the ratio of the potential minima over the relative minima. With an improved covering, from 1000 to 2000 sampled points, the crystal growth approach obtained 17 relative minima by execution of only 23 local minimizations. The Törn and Viitanen's algorithm

($k = 2$) obtained the most 18 relative minima after 405 local minimizations which are almost as much as 18 times required in the crystal growth case. With enlarged values of k, the Törn and Viitanen's algorithm obtained less relative minima.

5. Concluding remarks

The crystal growth approach for the topographical algorithm overcomes the major drawback of the algorithm by Törn and Viitanen. No sensitive and critical parameters such as k need to be defined by the user for the use of the crystal growth algorithm. The crystal growth algorithm equipped with an interconnecting checking system performs more efficient and reliable in locating minima with moderate computation investment. The topographical algorithm by Törn and Viitanen is still superior than the crystal growth approach in two items. The simpler algorithm for programming, and the possibilities to discover more minima in very low k values, especially $k = 2$, with a great amount of computational effort. The large number of local minimization prevents Törn and Viitanen's algorithm from being practical in global optimization problems in which the evaluation of the objective function is time consuming. The extension of the topographical algorithms to constrained problems was successfully exercised by using a penalty function approach. Formulas for the estimation of N needed to provide an effective covering was derived based on the assumed number of basins in the search domain. These estimation formulas provide the user a good estimation on N values in problems of low dimensionality if the information on the number or sizes of basins in the space is partly revealed.

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