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# INFLUENCE OF A NEIGHBORHOOD SHAPE ON THE EFFICIENCY OF CONTINUOUS VARIABLE NEIGHBORHOOD SEARCH

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**Abstract:** The efficiency of a Variable neighborhood search metaheuristic for continuous global optimization problems greatly depends on geometric shape of neighborhood structures used by the algorithm. Among the neighborhoods defined by balls in  $\ell_p$ ,  $1 \le p \le \infty$  metric, we tested the  $\ell_1$ ,  $\ell_2$ , and  $\ell_\infty$  ball shape neighborhoods, for which there exist efficient algorithms for obtaining uniformly distributed points. On many challenging high-dimensional problems, our exhaustive testings showed that, popular and the easiest for implementation,  $\ell_\infty$  ball shape of neighborhoods performed the worst, and much better efficiency was obtained with  $\ell_1$  and  $\ell_2$ .

**Keywords:** Global Optimization, Continuous Optimization, Metaheuristic Algorithms, Variable Neighbourhood Search.

MSC: 90C59, 90C06, 90C30.

#### 1. VNS FOR CONTINUOUS OPTIMIZATION

The goal of this paper is to explore the influence of neighborhood structure shapes on the efficiency of a Variable Neighborhood Search metaheuristic (VNS). The continuous unconstrained global optimization problem, with technically introduced box constraints, has the form

global min 
$$f(x)$$
,  $S = \{x \in \mathbb{R}^n \mid a_i \le x_i \le b_i, i = 1, 2, ..., n\}$ 

where  $f: \mathbb{R}^n \to \mathbb{R}$  is a continuous function. In many cases when local minima are present, such problem can be very difficult. For large dimensions of the problem, the number of local minima grows exponentially with the dimension, making

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the problem NP-hard. Exact methods can be applied only to the lower problem dimensions, so heuristic approaches are the only way to obtain good approximate solutions.

The VNS metaheuristic was first introduced by Mladenović and Hansen in [1, 2] for combinatorial optimization problems, and the applications to continuous optimization problems were given in [2, 3, 4]. The VNS approach has been implemented within the software package GLOB for unconstrained and constrained continuous optimization problems [5, 6, 7, 8] with several neighborhood structures and random point distributions.

The basic steps of the VNS metaheuristic are given as follows:

|    | Algorithm VNS   |
|----|---|
|    | /* Initialization */  |
| 01 | Select the set of neighborhood structures $\mathcal{N}_k$ , $k = 1, \ldots, k_{\text{max}}$ , |
|    | with corresponding random point distributions   |
| 02 | Choose an arbitrary initial point $x \in S$   |
| 03 | Set $x^* \leftarrow x$ , $f^* \leftarrow f(x)$  |
|    | /* Main loop */   |
| 04 | repeat the following steps <u>until</u> the stopping condition is met                         |
| 05 | Set $k \leftarrow 1$  |
| 06 | <b>repeat</b> the following steps <u>until</u> $k > k_{\text{max}}$                           |
| 07 | <b>Shake:</b> Generate at random a point $y \in \mathcal{N}_k(x^*)$                           |
| 08 | Apply some local search method from $y$ to obtain a local                                     |
|    | $\operatorname{minimum}\ y'$  |
| 09 | $\underline{\mathbf{if}} \ f(y') < f^* \ \underline{\mathbf{then}}$                           |
| 10 | Set $x^* \leftarrow y'$ , $f^* \leftarrow f(y')$ and <b>goto</b> line 05                      |
| 11 | $\underline{	ext{endif}}$   |
| 12 | Set $k \leftarrow k + 1$  |
| 13 | $\underline{\mathrm{end}}$  |
| 14 | $\underline{\mathrm{end}}$  |
| 15 | <b>Stop.</b> Point $x^*$ is an approximate solution of the problem.                           |

A good local optimizer is desirable to locate a local minimum efficiently, but for avoiding the local optima trap, the shaking step is crucial. Efficiency in finding better local minima depends on the geometry of neighborhoods and the random point distribution used in shaking step.

### 2. NEIGHBORHOODS INDUCED BY $\ell_p$ METRIC

In order to induce a set of neighborhood structures  $\mathcal{N}_k$  on the solution space S, the usual approach is to use some distance function  $\rho(x,y)$  that specifies the distance between points  $x, y \in S$ . For the continuous optimization problems, where  $S \subseteq \mathbb{R}^n$ ,  $\rho(x,y)$  is most often defined by Euclidean, rectangular, or other  $\ell_p$  metric:

$$\rho(x,y) = ||x - y||_p = \left(\sum_{i=1}^n |x_i - y_i|^p\right)^{1/p}, \ (1 \le p < \infty),$$

or

$$\rho(x,y) = ||x - y||_{\infty} = \max_{1 \le i \le n} |x_i - y_i|, \quad (p = \infty).$$

These metrics lead to different geometric shapes of neighborhoods that are to be explored. The neighborhood  $\mathcal{N}_k(x)$  denotes a set of points in the k-th neighborhood of x and, using the metric  $\rho$ , it is defined as a ball

$$\mathcal{N}_k(x) = \{ y \in S \mid \rho(x, y) \le \rho_k \},\$$

or spherical shell

$$\mathcal{N}_k(x) = \{ y \in S \mid \rho_{k-1} \le \rho(x, y) \le \rho_k \},$$

where  $\rho_k$  is the radius (size) of  $\mathcal{N}_k(x)$  monotonically increasing with k.

The simplest for implementation is to generate a uniformly distributed random point in  $\ell_{\infty}$  ball. If  $z_i$  are uniformly distributed points from the interval [0, 1], then

$$y_i = x_i + 2\rho_k(z_i - 0.5), \quad i = 1, \dots, n.$$

This simplicity is the main reason why  $\ell_{\infty}$  neighborhoods are so popular in implementations.

| n  | $\ell_1$   | $\ell_2$ | $\ell_{\infty}$ | n   | $\ell_1$    | $\ell_2$   | $\ell_{\infty}$ |
|----|------------|----------|-----------------|-----|-------------|------------|-----------------|
| 2  | 2          | 3.1416   | 4               | 20  | 4.3100e-13  | 2.5807e-02 | 1.0486e + 06    |
| 3  | 1.3333     | 4.1888   | 8               | 30  | 4.0480e-24  | 2.1915e-05 | 1.0737e + 09    |
| 4  | 0.66667    | 4.9348   | 16              | 40  | 1.3476e-36  | 3.6047e-09 | 1.0995e + 12    |
| 5  | 0.26667    | 5.2638   | 32              | 50  | 3.7019e-50  | 1.7302e-13 | $1.1259e{+15}$  |
| 6  | 0.088889   | 5.1677   | 64              | 60  | 1.3856e-64  | 3.0963e-18 | $1.1529e{+}18$  |
| 7  | 0.025397   | 4.7248   | 128             | 70  | 9.8559e-80  | 2.4323e-23 | 1.1806e + 21    |
| 8  | 0.0063492  | 4.0587   | 256             | 80  | 1.6892e-95  | 9.4265e-29 | 1.2089e + 24    |
| 9  | 0.0014109  | 3.2985   | 512             | 90  | 8.3323e-112 | 1.9676e-34 | 1.2379e + 27    |
| 10 | 0.00028219 | 2.5502   | 1024            | 100 | 1.3583e-128 | 2.3682e-40 | 1.2677e + 30    |

Table 1: Unit ball volumes in three different metrics

Uniformly distributed point in  $\ell_p$  ball for  $1 \leq p < \infty$  can be obtained with the acceptance-rejection method by repeatedly generating uniformly generated point in  $\ell_\infty$  ball until it is also within the  $\ell_p$  ball. For a large space dimension n this method is very inefficient due to huge volume differences between  $\ell_\infty$  and  $\ell_p$  balls, see Table 1 and Figure 1. Fortunately, there are efficient algorithms for generating uniformly distributed points inside  $\ell_2$  and  $\ell_1$  balls. Also, it is not hard to obtain uniformly distributed points in spherical shells for  $\ell_\infty$ ,  $\ell_2$  and  $\ell_1$  metrics.

Along with the uniformly distributed points in  $\ell_1$  ball (or spherical shell), a special random point distribution in  $\ell_1$  was proven to be very efficient for some problems. The random point y is obtained in two steps: first a random point  $z = (z_1, z_2, \ldots, z_n)$  on the  $\ell_1$  unit sphere is generated using the special distribution: (i)  $z_1$  is taken uniformly on [-1, 1],  $z_k$  is taken uniformly from  $[-A_k, A_k]$ , where

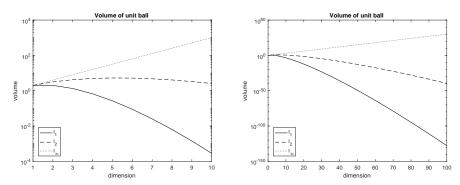


Figure 1: Volumes of  $\ell_1$ ,  $\ell_2$  and  $\ell_\infty$  unit balls

 $A_k = 1 - |z_1| - \ldots - |z_{k-1}|, k = 2, \ldots, n-1$ , and the last  $z_n$  takes  $A_n$  with random sign; (ii) coordinates of z are permuted randomly. After that, a random radius uniformly distributed in  $[0, \rho_k]$  (or  $[\rho_{k-1}, \rho_k]$ ) is determined in order to get a point y in  $\mathcal{N}_k(x)$ .

In the further analysis, we denote the shapes of neighborhoods as follows: S1, S2, and S3 for  $\ell_1$ ,  $\ell_2$ , and  $\ell_\infty$  balls and spherical shells with uniformly distributed random points, and S1s for  $\ell_1$  ball and the spherical shell with the special distribution, described above.

The main goal of this paper is to examine the effectiveness of neighborhood shapes in the shaking step of the VNS algorithm. This step represents the diversification part of the VNS metaheuristic, which is crucial for escaping from a local minimum to better solutions in the solution space. Local search represent the intensification part of the algorithm, responsible for efficiency of finding a local minimum reachable from the generated random point. In order to discover the influence of neighborhood shapes on the VNS algorithm efficiency, we test S1, S1s, S2 and S3 neighborhood shapes both in ball and spherical shell variants, while all other algorithm parameters are fixed. The results should be valuable to software developers implementing the VNS metaheuristic for continuous optimization problems.

#### 3. COMPUTATIONAL EXPERIMENTS

For all the tests, we used the software package GLOB, a test platform for numerical experiments with various variants of the VNS ([5]). GLOB is coded in ANSI C programming language as a single core console application. It supports neighborhood structures S1, S1s, S2, and S3, described in the previous section, and has a choice of several local minimizers. All the experimental results were obtained using a PC equipped with an Intel Core i7-6700 3.4 GHz processor with 16 GB RAM running 64bit Windows 7.

In all the tests, we used  $k_{\text{max}} = 10$  neighborhoods with radii  $r_i$  calculated automatically as a geometrical sequence of numbers. The tolerance for detecting that

the optimal solution was found was set to 1e-6 for smooth problems, and 1e-4 for non-smooth problems. Steepest descend local minimizer was used for smooth problems, and Nelder–Mead with restarts for non-smooth problems. Although some other local minimizers could be more effective, we did not use them because their role is not significant for testing effectiveness of different neighborhood shapes. In each test, the maximum run time limit was set to 30 sec. Execution time and the number of function and gradient evaluations were recorded until the global minimum was reached within the given tolerance, or the time limit was reached. A test run was considered successful if the global minimum was reached before the time limit. Each test was repeated 20 times with a different initial random point, and the average results are reported. The computer effort was calculated as  $N_f + nN_g$  for the steepest descend method, and  $N_f$  for Nelder–Mead method, where  $N_f$  and  $N_g$  are the number of function and gradient calls, and n is the dimension of the problem.

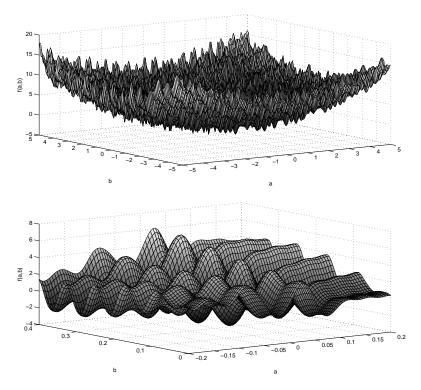


Figure 2: Trefethen 4 function with bounds  $[-5,5] \times [-5,5]$ , and  $[-0.2,0.2] \times [0.0,0.4]$ .

A set of test functions was chosen to represent challenging problems in high dimension solution spaces, or with many local minima, which makes them hard or impossible to solve by direct methods.

**Trefethen 4 function.** We start with a two dimensional problem with many local minima proposed in [9] (problem 4), see also [10]. This test instance has 2 variables  $a, b \in [-5, 5]$ :

$$f(a,b) = e^{\sin(50a)} + \sin(60e^b) + \sin(70\sin a) + \sin(\sin(80b)) - - \sin(10(a+b)) + (a^2 + b^2)/4.$$

The global optimum of f(a, b) is  $f_{\min} = -3.306868647$ . The graph of this function on two different scales is presented in Figure 2.

| _ |       | ball      |       | shell     |       |  |
|---|-------|-----------|-------|-----------|-------|--|
| n | shape | comp.eff. | time  | comp.eff. | time  |  |
| 2 | S1    | 101,549   | 0.021 | 134,690   | 0.028 |  |
|   | S1s   | 84,980    | 0.018 | 169,424   | 0.035 |  |
|   | S2    | 111,385   | 0.023 | 410,290   | 0.083 |  |
|   | S3    | 109,617   | 0.022 | 285,342   | 0.058 |  |

Table 2: Results for Trefethen 4 function

The computational results are presented in Table 2. The first column contains the dimension of the problem, and used neighborhood shape in the second, as denoted in the previous section. The average computer efforts and execution times in seconds from 20 runs are presented in the third and fourth columns for ball shape neighborhoods, and in the fifth and sixth column for spherical shell shapes. In every run, the global minimum was reached within the 30 sec time limit. It is evident from the results that ball neighborhood shapes are more efficient than shell shapes for the same metric. Comparing different metrics, shape S1s showed to be the most successful, although the other shapes did not perform significantly worse.

#### Rosenbrock function.

$$f(x) = \sum_{i=1}^{n-1} \left( 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2 \right)$$

for  $-10 \le x_i \le 10$ , i = 1, ..., n. The global minimum is  $f_{\min} = 0$ . This function is a standard problem for optimization algorithms performance testing. Local minimizers as steepest descend (used here within VNS) and Nelder-Mead exhibit poor performance if used alone, without VNS algorithm.

The results for Rosenbrock function for problem dimension up to 200 are presented in Table 3. In every run the global minimum was reached within the 30 sec time limit. The first observation is that there is no significant difference in performance between ball and spherical shell variant of neighborhoods. Neighborhood shape S3 performed the worst for both small and large space dimensions. Shape S1s was slightly better than S1 in all cases. Shape S2 was competitive with S1s and S1 for  $n \leq 150$ , but for n = 200, it was significantly less efficient.

|     |       | ball       |       | shell       |       |
|-----|-------|------------|-------|-------------|-------|
| n   | shape | comp.eff.  | time  | comp.eff.   | time  |
| 10  | S1    | 175,251    | 0.007 | 188,667     | 0.007 |
|     | S1s   | 125,028    | 0.005 | 106,047     | 0.004 |
|     | S2    | 134,256    | 0.006 | 135,278     | 0.006 |
|     | S3    | 379,827    | 0.014 | 336,029     | 0.013 |
| 20  | S1    | 272,472    | 0.012 | 249,717     | 0.011 |
|     | S1s   | 240,418    | 0.010 | 241,514     | 0.010 |
|     | S2    | 213,283    | 0.009 | 224,682     | 0.009 |
|     | S3    | 479,981    | 0.019 | 523,073     | 0.021 |
| 50  | S1    | 738,750    | 0.029 | 744,078     | 0.030 |
|     | S1s   | 670,541    | 0.026 | 697,932     | 0.027 |
|     | S2    | 1,001,924  | 0.044 | 827,911     | 0.036 |
|     | S3    | 10,132,164 | 0.440 | 8,279,130   | 0.361 |
| 100 | S1    | 2,342,324  | 0.090 | 2,352,889   | 0.091 |
|     | S1s   | 2,189,264  | 0.081 | 2,095,220   | 0.077 |
|     | S2    | 2,044,212  | 0.079 | 2,165,929   | 0.087 |
|     | S3    | 23,679,282 | 1.015 | 27,870,293  | 1.206 |
| 150 | S1    | 3,752,823  | 0.139 | 3,747,885   | 0.139 |
|     | S1s   | 3,375,741  | 0.120 | 3,315,324   | 0.119 |
|     | S2    | 3,957,138  | 0.152 | 3,679,985   | 0.140 |
|     | S3    | 40,560,739 | 1.695 | 30,906,761  | 1.290 |
| 200 | S1    | 6,678,584  | 0.249 | 6,318,854   | 0.236 |
|     | S1s   | 5,564,922  | 0.198 | 5,439,822   | 0.194 |
|     | S2    | 29,566,111 | 1.549 | 11,141,342  | 0.529 |
|     | S3    | 74,860,051 | 3.130 | 105,666,113 | 4.462 |

Table 3: Results for Rosenbrock function

Ackley function. Proposed in [11, 12]:

$$f(x) = 20 + e - 20 \exp\left(-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2}\right) - \exp\left(\frac{1}{n}\sum_{i=1}^{n} \cos(2\pi x_i)\right)$$

for  $-15 \le x_i \le 30$ , i = 1, ..., n, has a global minimum  $f_{\min} = 0$ , and  $45^n$  local minima. The graph of this function for n = 2 on two different scales is presented in Figure 3.

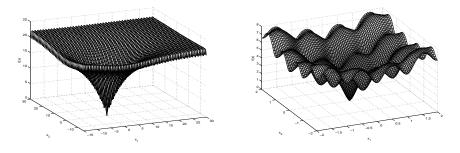


Figure 3: Ackley function for n=2 with bounds  $[-15,30] \times [-15,30]$ , and  $[-2,2] \times [-2,2]$ .

The results for Ackley function for problem dimension up to 50 are presented in Table 4. In every run, the global minimum was reached within the 30 sec time limit. As in the previous test problems, there is no significant difference in performance between ball and spherical shell variant of the neighborhoods. Contrary

|              |       | ball      |       | shel      | l     |
|--------------|-------|-----------|-------|-----------|-------|
| $\mathbf{n}$ | shape | comp.eff. | time  | comp.eff. | time  |
| 10           | S1    | 62,151    | 0.013 | 53,513    | 0.012 |
|              | S1s   | 63,889    | 0.014 | 65,680    | 0.014 |
|              | S2    | 49,823    | 0.011 | 50,588    | 0.011 |
|              | S3    | 43,811    | 0.009 | 42,456    | 0.009 |
| 20           | S1    | 194,772   | 0.054 | 200,953   | 0.055 |
|              | S1s   | 215,500   | 0.058 | 228,459   | 0.061 |
|              | S2    | 142,364   | 0.039 | 155,474   | 0.043 |
|              | S3    | 138,594   | 0.038 | 135,496   | 0.037 |
| 30           | S1    | 427,888   | 0.132 | 400,766   | 0.124 |
|              | S1s   | 486,548   | 0.145 | 528,480   | 0.158 |
|              | S2    | 263,078   | 0.082 | 281,063   | 0.087 |
|              | S3    | 255,680   | 0.078 | 261,403   | 0.081 |
| 40           | S1    | 824,502   | 0.273 | 817,231   | 0.269 |
|              | S1s   | 1,031,772 | 0.324 | 1,205,204 | 0.382 |
|              | S2    | 457,885   | 0.151 | 431,186   | 0.143 |
|              | S3    | 410,697   | 0.135 | 436,004   | 0.144 |
| 50           | S1    | 2,277,783 | 0.774 | 1,623,275 | 0.554 |
|              | S1s   | 2,247,472 | 0.732 | 2,195,793 | 0.720 |
|              | S2    | 632,166   | 0.218 | 616,375   | 0.215 |
|              | S3    | 756,055   | 0.259 | 762,336   | 0.262 |

Table 4: Experimental results for Ackley function

to Rosenbrock function, neighborhood shapes S2 and S3 performed significantly better than S1 and S1s, S1s beeing the worst overall. While S3 was better for smaller dimensions, S2 was the best for n=50. Good performance of S2 shape can be explained by spherical symmetry of the function on larger scale.

## Rastrigin function.

$$f(x) = 10n + \sum_{i=1}^{n} (x_i^2 - 10\cos(2\pi x_i))$$

for  $-5.12 \le x_i \le 5.12$ ,  $i=1,\ldots,n$ , has a global minimum  $f_{\min}=0$  and  $11^n$  local minima. The graph of this function for n=2 is presented in Figure 4.

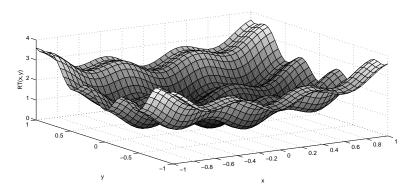


Figure 4: Rastrigin function for n = 2 for with bounds  $[-1,1] \times [-1,1]$ .

|     |       | I          | ball   |       |       |            | shell  |       |       |
|-----|-------|------------|--------|-------|-------|------------|--------|-------|-------|
| n   | shape | comp.eff.  | time   | succ. | error | comp.eff.  | time   | succ. | error |
| 10  | S1    | 49,021     | 0.009  | 20    |       | 60,399     | 0.012  | 20    |       |
|     | S1s   | 36,362     | 0.007  | 20    |       | 38,373     | 0.007  | 20    |       |
|     | S2    | 78,146     | 0.014  | 20    | İ     | 70,869     | 0.013  | 20    |       |
|     | S3    | 93,857     | 0.018  | 20    |       | 95,451     | 0.018  | 20    |       |
| 20  | S1    | 259,948    | 0.063  | 20    |       | 239,873    | 0.058  | 20    |       |
|     | S1s   | 126,846    | 0.030  | 20    | İ     | 121,491    | 0.029  | 20    |       |
|     | S2    | 407,110    | 0.095  | 20    |       | 462,573    | 0.108  | 20    |       |
|     | S3    | 585,289    | 0.136  | 20    |       | 544,657    | 0.129  | 20    |       |
| 30  | S1    | 540,162    | 0.147  | 20    |       | 599,701    | 0.165  | 20    |       |
|     | S1s   | 250,345    | 0.068  | 20    |       | 222,695    | 0.061  | 20    |       |
|     | S2    | 1,404,324  | 0.372  | 20    |       | 1,917,442  | 0.508  | 20    |       |
|     | S3    | 2,213,492  | 0.587  | 20    |       | 2,281,569  | 0.615  | 20    |       |
| 40  | S1    | 1,138,379  | 0.334  | 20    |       | 1,376,997  | 0.407  | 20    |       |
|     | S1s   | 435,630    | 0.125  | 20    |       | 451,957    | 0.132  | 20    |       |
|     | S2    | 2,651,781  | 0.763  | 20    |       | 2,980,924  | 0.862  | 20    |       |
|     | S3    | 8,193,466  | 2.351  | 20    |       | 8,323,397  | 2.413  | 20    |       |
| 50  | S1    | 1,950,614  | 0.598  | 20    |       | 1,953,808  | 0.608  | 20    |       |
|     | S1s   | 701,919    | 0.210  | 20    |       | 738,755    | 0.224  | 20    |       |
|     | S2    | 3,651,184  | 1.116  | 20    | i i   | 3,474,303  | 1.063  | 20    | İ     |
|     | S3    | 26,463,963 | 7.952  | 20    | i i   | 29,761,343 | 9.034  | 20    | İ     |
| 60  | S1    | 2,936,964  | 0.918  | 20    |       | 2,902,176  | 0.919  | 20    |       |
|     | S1s   | 1,011,087  | 0.311  | 20    |       | 972,489    | 0.303  | 20    |       |
|     | S2    | 3,605,867  | 1.140  | 20    |       | 3,100,591  | 0.984  | 20    |       |
|     | S3    | 62,799,699 | 19.333 | 10    | 0.60  | 54,233,167 | 16.777 | 12    | 0.50  |
| 70  | S1    | 4,199,080  | 1.336  | 20    |       | 4,166,472  | 1.339  | 20    |       |
|     | S1s   | 1,526,418  | 0.475  | 20    |       | 1,358,786  | 0.433  | 20    |       |
|     | S2    | 4,205,767  | 1.356  | 20    |       | 4,315,736  | 1.404  | 20    |       |
|     | S3    |            |        | 0     | 2.64  |            |        | 0     | 2.54  |
| 80  | S1    | 6,021,715  | 1.952  | 20    |       | 5,700,173  | 1.871  | 20    |       |
|     | S1s   | 1,680,877  | 0.535  | 20    |       | 1,846,936  | 0.595  | 20    |       |
|     | S2    | 5,729,992  | 1.899  | 20    |       | 5,669,393  | 1.879  | 20    |       |
|     | S3    |            |        | 0     | 5.32  |            |        | 0     | 5.42  |
| 90  | S1    | 7,157,711  | 2.367  | 20    |       | 7,237,914  | 2.429  | 20    |       |
|     | S1s   | 2,397,990  | 0.772  | 20    |       | 2,261,338  | 0.743  | 20    |       |
|     | S2    | 8,717,552  | 2.924  | 20    |       | 8,537,969  | 2.886  | 20    |       |
|     | S3    |            |        | 0     | 9.90  |            |        | 0     | 9.55  |
| 100 | S1    | 9,368,881  | 3.162  | 20    |       | 9,209,980  | 3.144  | 20    |       |
|     | S1s   | 2,971,556  | 0.971  | 20    |       | 2,845,786  | 0.945  | 20    |       |
|     | S2    | 14,066,449 | 4.844  | 20    |       | 12,093,366 | 4.207  | 20    |       |
|     | S3    |            |        | 0     | 14.32 |            |        | 0     | 14.78 |

Table 5: Results for Rastrigin function

The results for Rastrigin function for problem dimension up to 100 are presented in Table 5. Since not all runs were successful in finding the global minimum within the 30 sec time limit, two new columns are introduced. Columns marked "succ." contain the number of runs in which the global minimum was reached with proposed tolerance within the time limit. In cases when not all test runs were successful, columns marked "error" contain the average optimal function value error. Columns "comp.eff." and "time" contain average computer effort and execution time in seconds for the successful runs.

Results from Table 5 show that there is no significant difference between ball and spherical shell neighborhood variants, shell variant being slightly more efficient on average. Neighborhood shape S3 performed very inefficient, and for high problem dimensions it failed to provide the global minimum in every run. Shape S1s performed the best, while S1 and S2 were comparable, S1 being consistently

better than S2.

Molecular potential energy (MPE) function. Introduced in [13], see also [6], this function was proposed for testing methods for global minimization of potential energy of molecules:

$$f(x) = \sum_{i=1}^{n} \left( 1 + \cos 3x_i + \frac{(-1)^i}{\sqrt{10.60099896 - 4.141720682 \cos x_i}} \right)$$

for  $0 \le x_i \le 5$ ,  $i=1,\ldots,n$ , has a global minimum  $f_{\min}=-0.0411183034\cdot n$  and  $3^n$  local minima.

|     |             | 1          | ball   |          |         | shell      |             |          |         |
|-----|-------------|------------|--------|----------|---------|------------|-------------|----------|---------|
|     | ah a = a    |            |        |          | 07      |            |             |          | 07      |
| 10  | shape<br>S1 | comp.eff.  | time   |          | % error | comp.eff.  |             | succ.    | % error |
| 10  | S1s         | 30,015     | 0.010  | 20<br>20 |         | 34,439     | 0.011 0.004 | 20<br>20 |         |
|     |             | 13,809     |        |          |         | 13,359     |             | -        |         |
|     | S2<br>S3    | 34,772     | 0.011  | 20<br>20 |         | 34,596     | 0.011       | 20 20    |         |
| 20  | S1          | 118,409    | 0.038  |          |         | 80,510     | 0.026       | -        |         |
| 20  |             | 194,198    | 0.083  | 20       |         | 244,582    | 0.106       | 20       |         |
|     | S1s         | 46,391     | 0.021  | 20       |         | 51,333     | 0.023       | 20       |         |
|     | S2          | 166,932    | 0.072  | 20       |         | 178,088    | 0.076       | 20       |         |
|     | S3          | 10,794,746 | 4.489  | 20       |         | 7,722,668  | 3.228       | 20       |         |
| 30  | S1          | 552,584    | 0.267  | 20       |         | 739,538    | 0.362       | 20       |         |
|     | S1s         | 110,277    | 0.057  | 20       |         | 122,178    | 0.063       | 20       |         |
|     | S2          | 358,984    | 0.178  | 20       |         | 376,430    | 0.188       | 20       |         |
|     | S3          | 41,512,825 | 19.299 | 1        | 11.60   | 54,488,832 | 25.555      | 1        | 8.96    |
| 40  | S1          | 1,530,434  | 0.786  | 20       |         | 1,486,620  | 0.771       | 20       |         |
|     | S1s         | 185,029    | 0.104  | 20       |         | 198,909    | 0.113       | 20       |         |
|     | S2          | 583,497    | 0.317  | 20       |         | 594,570    | 0.324       | 20       |         |
|     | S3          |            |        | 0        | 27.13   |            |             | 0        | 30.86   |
| 50  | S1          | 3,315,594  | 1.763  | 20       |         | 2,696,179  | 1.442       | 20       |         |
|     | S1s         | 289,291    | 0.173  | 20       |         | 317,072    | 0.192       | 20       |         |
|     | S2          | 899,990    | 0.515  | 20       |         | 1,009,371  | 0.575       | 20       |         |
|     | S3          |            |        | 0        | 39.24   |            |             | 0        | 41.44   |
| 60  | S1          | 5,665,036  | 3.063  | 20       |         | 6,034,739  | 3.268       | 20       |         |
|     | S1s         | 455,756    | 0.282  | 20       |         | 514,346    | 0.323       | 20       |         |
|     | S2          | 1,941,462  | 1.143  | 20       |         | 1,555,161  | 0.914       | 20       |         |
|     | S3          |            |        | 0        | 50.98   |            |             | 0        | 55.29   |
| 70  | S1          | 7,844,683  | 4.273  | 20       |         | 8,460,620  | 4.628       | 20       |         |
|     | S1s         | 607,348    | 0.391  | 20       |         | 669,236    | 0.436       | 20       |         |
|     | S2          | 3,654,745  | 2.250  | 20       |         | 3,421,294  | 2.101       | 20       |         |
|     | S3          |            |        | 0        | 66.50   |            |             | 0        | 64.63   |
| 80  | S1          | 13,784,376 | 7.798  | 20       |         | 14,689,218 | 8.055       | 20       |         |
|     | S1s         | 788,130    | 0.520  | 20       |         | 836,788    | 0.555       | 20       |         |
|     | S2          | 6,237,038  | 4.039  | 20       |         | 6,767,309  | 4.363       | 20       |         |
|     | S3          |            |        | 0        | 76.38   |            |             | 0        | 73.89   |
| 90  | S1          | 18,575,697 | 10.219 | 20       |         | 18,658,937 | 10.264      | 20       |         |
|     | S1s         | 1,020,315  | 0.688  | 20       |         | 1,158,930  | 0.787       | 20       |         |
|     | S2          | 12,529,044 | 8.608  | 20       |         | 10,116,006 | 6.880       | 20       |         |
|     | S3          | ' '        |        | 0        | 78.86   | ' '        |             | 0        | 82.95   |
| 100 | S1          | 26,394,502 | 14.359 | 20       |         | 25,194,108 | 13.807      | 19       | 0.10    |
|     | S1s         | 1,357,828  | 0.925  | 20       |         | 1,530,488  | 1.061       | 20       |         |
|     | S2          | 17,011,040 | 11.940 | 20       |         | 17,261,623 | 12.228      | 20       |         |
|     | S3          |            |        | 0        | 86.93   | ' '        |             | 0        | 83.93   |

Table 6: Results for MPE function

The results for Molecular potential energy (MPE) function for problem dimensions up to 100 are presented in Table 6. Like in the case of Rastrigin function,

neighborhood shape S3 performed very inefficient, failing to provide global minima even for problem dimension n=30. Shape S1s performed the best, exceptionally better than others. Comparing shapes S1 and S2, shape S2 performed better than S1. Results also show that there is no significant difference between ball and spherical shell neighborhood variants, precedence varying from case to case. Nevertheless, for the most efficient S1s shape, ball variant performed slightly better than the spherical shell variant.

We also tested the efficiency of neighborhood shapes on four non-differentiable functions in high-dimensional space. From the set of 10 test problems proposed in [14], we chose 4 most challenging problems (see [15]). They are as follows:

#### Generalization of MXHILB function.

$$f(x) = \max_{1 \le i \le n} \left| \sum_{j=1}^{n} \frac{x_j}{i+j-1} \right|$$

for  $-10 \le x_i \le 10$ , i = 1, ..., n, has a global minimum  $f_{\min} = 0$ .

|    |       |           | bal    | l     |          | shell     |        |       |          |
|----|-------|-----------|--------|-------|----------|-----------|--------|-------|----------|
| n  | shape | comp.eff. | time   | succ. | error    | comp.eff. | time   | succ. | error    |
| 30 | S1    | 134,520   | 0.305  | 20    |          | 135,012   | 0.317  | 20    |          |
|    | S1s   | 123,354   | 0.281  | 20    |          | 123,354   | 0.283  | 20    |          |
|    | S2    | 138,366   | 0.314  | 20    |          | 138,366   | 0.321  | 20    |          |
|    | S3    | 142,601   | 0.324  | 20    |          | 142,601   | 0.328  | 20    |          |
| 40 | S1    | 1,831,959 | 6.834  | 20    |          | 1,880,604 | 6.999  | 20    |          |
|    | S1s   | 572,084   | 2.116  | 20    |          | 480,358   | 1.767  | 20    |          |
|    | S2    | 294,221   | 1.094  | 20    |          | 273,001   | 1.004  | 20    |          |
|    | S3    | 6,631,926 | 24.539 | 3     | 1.14E-04 | 5,080,383 | 19.171 | 6     | 1.08E-04 |
| 50 | S1    | 1,727,061 | 10.142 | 7     | 1.25E-04 | 3,386,658 | 19.828 | 6     | 1.21E-04 |
|    | S1s   | 1,056,715 | 6.152  | 19    | 9.96E-05 | 1,420,834 | 8.223  | 20    |          |
|    | S2    | 609,996   | 3.486  | 20    |          | 657,980   | 3.842  | 20    |          |
|    | S3    |           |        | 0     | 2.66E-04 |           |        | 0     | 2.63E-03 |

Table 7: Results for Generalization of MXHILB function

The results for Generalization of MXHILB function for problem dimensions n=30,40,50 are presented in Table 7. Ball and spherical shell neighborhood variants performed the same on average, with no significant difference. For n=30 all four neighborhood shapes were effective, S1s being slightly better. Neighborhood shape S3 led to optimal solutions only in several runs for n=40, and none for n=50. Shape S1 also couldn't reach optimal solutions in most runs for n=50, and for n=40 it was very inefficient. Although the shape S1s was the best for n=30, n=40 and n=50, the shape S2 performed the best with a significant margin.

#### Number of active faces function.

$$f(x) = \max_{1 \le i \le n} \left\{ g(-\sum_{j=1}^{n} x_j), \ g(x_i) \right\}, \quad g(y) = \ln(|y| + 1)$$

|    |       |           | bal    | 11    |          |           | she    | 11    |          |
|----|-------|-----------|--------|-------|----------|-----------|--------|-------|----------|
| n  | shape | comp.eff. | time   | succ. | error    | comp.eff. | time   | succ. | error    |
| 30 | S1    | 262,705   | 0.475  | 20    |          | 261,016   | 0.468  | 20    |          |
|    | S1s   | 187,764   | 0.336  | 20    |          | 187,764   | 0.336  | 20    |          |
|    | S2    | 188,018   | 0.338  | 20    |          | 188,018   | 0.337  | 20    |          |
|    | S3    | 302,300   | 0.542  | 20    |          | 259,477   | 0.466  | 20    |          |
| 40 | S1    | 4,420,157 | 11.805 | 10    | 1.22E-04 | 5,731,825 | 15.208 | 12    | 1.12E-04 |
|    | S1s   | 1,445,912 | 3.770  | 20    |          | 1,050,530 | 2.727  | 20    |          |
|    | S2    | 1,475,094 | 3.870  | 20    |          | 1,095,937 | 2.841  | 20    |          |
|    | S3    |           |        | 0     | 2.29E-04 | 5,393,734 | 14.292 | 1     | 2.63E-04 |
| 50 | S1    |           |        | 0     | 2.03E-04 | 5,601,173 | 22.458 | 1     | 2.31E-04 |
|    | S1s   | 2,503,346 | 9.856  | 13    | 1.07E-04 | 3,843,610 | 15.238 | 12    | 1.04E-04 |
|    | S2    | 3,965,567 | 15.544 | 6     | 1.10E-04 | 3,414,306 | 13.521 | 8     | 1.07E-04 |
|    | S3    |           |        | 0     | 6.91E-03 |           |        | 0     | 6.98E-04 |

Table 8: Results for Number of active faces function

The results for Number of active faces function for problem dimension up to n=50 are presented in Table 8. There was no significant difference between ball and spherical shell neighborhood variants, advantage varying from case to case. Neighborhood shape S3 performed the worst, particularly bad for n=40 and 50. Shape S1 follows, struggling to obtain optimal solutions for n=40. Neighborhood shapes S1s and S2 performed much better. Shape S1s was slightly more effective than S2 for n=30 and 40, and it reached optimal solutions in more cases than S2 for n=50.

#### Chained Mifflin 2 function.

$$f(x) = \sum_{i=1}^{n-1} (-x_i + 2(x_i^2 + x_{i+1}^2 - 1) + 1.75|x_i^2 + x_{i+1}^2 - 1|)$$

for  $-10 \le x_i \le 10$ , i = 1, ..., n, has a global minimum  $f_{\min} = -20.6535$  for n = 30,  $f_{\min} = -27.7243$  for n = 40 and  $f_{\min} = -34.7950$  for n = 50.

| -  |       |           | ball   | l     |         |           | shel   | l     |         |
|----|-------|-----------|--------|-------|---------|-----------|--------|-------|---------|
| n  | shape | comp.eff. | time   | succ. | % error | comp.eff. | time   | succ. | % error |
| 30 | S1    | 1,676,231 | 2.251  | 20    |         | 1,524,497 | 2.043  | 20    |         |
|    | S1s   | 948,998   | 1.241  | 20    |         | 832,751   | 1.091  | 20    |         |
|    | S2    | 1,202,220 | 1.587  | 20    |         | 1,228,610 | 1.618  | 20    |         |
|    | S3    | 3,156,177 | 4.299  | 20    |         | 4,078,934 | 5.561  | 20    |         |
| 40 | S1    | 3,723,598 | 7.522  | 19    | 0.02    | 4,160,843 | 8.467  | 20    |         |
|    | S1s   | 2,575,037 | 5.141  | 20    |         | 2,792,982 | 5.55   | 20    |         |
|    | S2    | 3,713,276 | 7.325  | 20    |         | 3,189,617 | 6.316  | 20    |         |
|    | S3    | 6,881,290 | 14.064 | 5     | 0.02    | 8,568,826 | 17.647 | 10    | 0.02    |
| 50 | S1    | 5,103,430 | 16.252 | 14    | 0.02    | 5,174,332 | 16.653 | 13    | 0.02    |
|    | S1s   | 4,133,162 | 12.829 | 18    | 0.02    | 4,214,633 | 13.095 | 19    | 0.02    |
|    | S2    | 4,464,450 | 13.864 | 19    | 0.02    | 3,748,401 | 11.663 | 20    |         |
|    | S3    |           |        | 0     | 0.05    |           |        | 0     | 0.04    |

Table 9: Results for Chained Mifflin 2 function

The results for Chained Mifflin 2 function for problem dimension up to n = 50 are presented in Table 9. Ball and spherical shell neighborhood variants performed

similarly, with no clear advantage between them. Neighborhood shape S3 again performed the worst, particularly for n=50. Among the other three shapes, S1 was the least competitive. Neighborhood shapes S1s and S2 performed the best, S1s being the most efficient in most cases, and S2 reaching the optimal solution in more cases than S1s for n=50.

#### Chained crescent II function.

$$f(x) = \sum_{i=1}^{n-1} \max\{x_i^2 + (x_{i+1} - 1)^2 + x_{i+1} - 1, -x_i^2 - (x_{i+1} - 1)^2 + x_{i+1} + 1\}$$

for  $-10 \le x_i \le 10$ , i = 1, ..., n, has a global minimum  $f_{\min} = 0$ .

|    |       |           | bal    | 11    |          |            | shel   | l     |          |
|----|-------|-----------|--------|-------|----------|------------|--------|-------|----------|
| n  | shape | comp.eff. | time   | succ. | error    | comp.eff.  | time   | succ. | error    |
| 30 | S1    | 1,113,540 | 1.615  | 20    |          | 1,015,723  | 1.470  | 20    |          |
|    | S1s   | 1,107,510 | 1.581  | 20    |          | 1,425,974  | 2.038  | 20    |          |
|    | S2    | 1,103,026 | 1.581  | 20    |          | 1,556,183  | 2.241  | 20    |          |
|    | S3    | 1,240,956 | 1.819  | 20    |          | 1,358,937  | 1.995  | 20    |          |
| 40 | S1    | 4,993,715 | 10.769 | 8     | 1.18E-04 | 5,277,355  | 11.286 | 10    | 1.23E-04 |
|    | S1s   | 4,854,389 | 10.093 | 17    | 1.08E-04 | 4,812,370  | 10.065 | 13    | 1.10E-04 |
|    | S2    | 4,903,779 | 10.184 | 17    | 1.01E-04 | 6,450,901  | 13.516 | 19    | 9.99E-05 |
|    | S3    | 8,035,215 | 17.272 | 7     | 1.22E-04 | 10,847,742 | 23.424 | 4     | 1.36E-04 |
| 50 | S1    | 3,063,428 | 10.147 | 20    |          | 2,810,161  | 9.259  | 16    | 1.04E-04 |
|    | S1s   | 2,628,553 | 8.488  | 20    |          | 1,359,642  | 7.521  | 18    | 1.02E-04 |
|    | S2    | 2,397,515 | 7.710  | 20    |          | 2,636,275  | 8.411  | 20    |          |
|    | S3    | 4,934,812 | 16.752 | 15    | 1.18E-04 | 3,904,913  | 13.144 | 13    | 1.11E-04 |

Table 10: Results for Chained Crescent II function

The results for Chained Crescent II function for problem dimension up to n=50 are presented in Table 10. Ball and spherical shell neighborhood variants performed similarly, without clear advantage between them. The VNS with restarted Nelder-Mead as a local minimizer performed noticeably more effective for n=50 than for n=40. The same effect was also noticed in [15] for some other modifications of Nelder-Mead minimizers. Neighborhood shape S3 was the least successful, followed by S1. Neighborhood shapes S1s and S2 were competitive in speed, S2 being better overall since it reached optimal solutions in more cases than S1s.

#### 4. CONCLUSIONS

In this study we examined the influence of a neighborhood shape to the efficiency of the VNS metaheuristic for continuous unconstrained global optimization problems. We considered neighborhoods defined as balls in  $\ell_p$  metrics for  $p=1,2,\infty$ , along with spherical shells, the spaces between two concentric spheres. The Most simple for software implementation, and thus most common, are  $\ell_{\infty}$  balls with uniform random point distribution (marked S3 in this study). Uniformly distributed points in  $\ell_2$  Euclidean ball (marked S2) and  $\ell_1$  ball (marked S1) can be

also used in the VNS by using efficient uniform random number generators for these balls. Finally, we define a special random number distribution in  $\ell_1$  ball (marked S1s), which proved to be very efficient for some problems.

Our exhaustive testing on a set of challenging smooth and non-differentiable functions led to the following conclusions:

First, there was no significant difference in efficiency of VNS between ball and spherical shell neighborhood shapes. They performed very similar, except for two-dimensional Trefethen 4 function, which is considered as an easier problem due to its low dimensionality. From the implementation point of view, introducing more complicated spherical shell neighborhoods is not justified regarding the algorithm efficiency.

Second, neighborhood shapes S1, S1s, S2, and S3 exhibited remarkably different performances, especially for high dimensional problems. S3 box-shaped neighborhood, the easiest to implement, was inefficient, and often unsuccessful in higher dimensions, for all test problems except for Ackley function, for which S2 performed slightly better than S3. So, using S3 alone, or together with the other neighborhood shapes, can degrade performance of the VNS. S1s shape performed the best overall, being the best in six test problems, and close to best S2 shape in two cases. Only in one case, for Ackley function, S1s performed badly. Neighborhood shape S2 performed badly only for low dimensional Trefethen 4 problem. It performed the best in three test problems and close to best in the fourth. Comparing shapes S1 and S1s with the same geometry but different random point distribution, S1 performed worse than S1s in all problems except the Ackley function, for which they both had poor performance. So, S1s and S2 are proved to be the most successful.

Neighborhood shape S1s performed the best overall. In a few problems, S2 performed the best, S1s being close. Only in one problem, S2 was the best, and S1s performed poorly. From implementation point of view, neighborhood shape S1s ( $\ell_1$  ball with special random distribution) is the best choice if used alone. If the implementation can combine more neighborhood shapes, neighborhood shape S1s in combination with S2 ( $\ell_2$  ball with uniform random distribution) would be overall more efficient than the other shape combinations for test problems from this study.

Future work will focus on experiments with more neighborhood shapes and more random distributions. Also, combinations of neighborhood shapes within the VNS will be tested.

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