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Proceedings of MAGO 2014, pp. 141 – 143.

Networks of Optimization Methods and Problems

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Abstract Benchmarking optimization methods and meaningful characterization of optimization problems have been the focal points of many research projects done in the field of global optimization. Our approach aims at investigating this topic with the usage of the computational and mathematical tools of network science. For a particular test problem a network formed by all the minima found by an optimization method can be constructed. Given these networks the analysis of their particular properties (e.g. degree distribution, path lengths, centrality measures, etc.) can lead to novel characterization of optimization problems and methods.

Keywords: benchmarking, network science

1. Introduction

Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable. This work deals with optimization *problems* of the type

$$\min_{x \in D} f(x)$$

together with optimization *methods* belonging to the class of incomplete and asymptotically complete methods [1]. Several benchmarking techniques have been proposed already (see, e.g. [2, 3]) with the goal of giving hints on which optimization methods should be used in order to solve certain type of optimization problems in an efficient way. Our method complements these works with the help of the emerging field of network science.

2. Methodology

The proposed methodology takes inspirations from the early work of Stillinger and Weber [4], in which potential energy landscapes of some atomic clusters were formed into networks. The idea was that these landscapes can be divided into basins of attractions surrounding each locally minimal energy level. This approach was later successfully applied to the analysis of network topology of the potential function of small Lennard-Jones clusters [5]. In this case the so-called inherent structure network can be built in which nodes correspond to the minima and the edges link those minimum which are directly connected by a transition state. The same idea can be used for combinatorial optimization problems [6]. We give here a possible extension of these ideas to the space of continuous optimization problems and methods.

Given an optimization test problem, define a reasonable fine grid in its search space. Let x_S be a point on this grid. We take x_S as the starting point of the investigated optimization method. For each and every starting point the results of the optimization methods (i.e. the stationary points found from that starting point) is recorded. Now the stationary point network (SPN) can be constructed: the vertices of this graph are the stationary points found by the optimization method, and two vertices are connected if they were found from the same starting point. Note that in case of a deterministic solver this definition would never produce any edge, so in that case the definition needs to be modified. A simple example is given in

Section 3. Similar construction is used in [5] (and called inherent structure network) and in [6] (called local optima network).

Once these SPN graphs are constructed for each method and for each test functions, their properties could be used as comparison of the methods and problems in question.

Graph measures In the following we give an incomplete list of graph measures, taken from network science, together with their interpretations in the local optima networks context.

Size of the network is defined as the number of nodes. Clearly, this represents the number of local minima found by the optimizer.

Node degree is the number of edges a node has to other nodes. In our case this measures the number of adjacent stationary points. Related to this, it is worth considering the nodes degree distribution.

Average path length is defined as the average value of all shortest paths in the network. This measure indicates that how many non-local jumps should be taken, on average, from one basin to another to reach the one representing the global optimum value.

Diameter is the size of the longest of all shortest paths. This gives a worst-case scenario regarding the number of non-local jumps to reach the global minimum.

Betweenness centrality for a given node is calculated as the fraction of paths connecting all pairs of nodes and containing the node of interest. We hypothesize that the global optima have the highest betweenness centrality value.

3. Preliminary results

Currently we have a prototype framework in which two methods (a simple steepest decent (SD), and Differential Evolution (DE) [7]) are implemented along with some standard optimization tests from the classical Dixon-Szegő problem sets. We choose these two methods because their application in the proposed methodology must be clarified.

Firstly, SD is a simple example of the deterministic methods, i.e. it always produces the same result if it is started from a single point. Thus, the corresponding SPN does not contain any edge. In order to override this issue we propose here that upon starting from x_S it is checked if $\nabla f(x_S) = 0$, e.g. whether we start from a stationary point. (Practically, this is tested by checking if $\|\nabla f(x_S)\| < \epsilon$.) If x_S is a stationary point then the following 'multistart' type procedure is applied: give a small perturbation to x_S and start SD from there; repeat this for, say, 10 times. The resulting graph is shown on Figure 1. Note that for better visualization we do not show all the different points found by SD, only with those with positive degree.

Secondly, DE is a population based method, i.e. it uses more than one point during its run. Our proposed solution here is that the starting point x_S is always included in the first population (and obviously the other points in the population are selected randomly, as it is done in the standard DE). Regarding the result, the connected component of the graph produced by DE contains 665 nodes and 3848 edges. This case shows that the resulting graph contains much more vertices than the number of local/global minima of the function, which indicates the need for the introduction of further properties in the SPN, for example node weights.

Finally, we notice that the whole approach has particular relevance for problems with multiple local minima. In that case the resulting graph is expected to be large enough for the analysis by the network science tools. Detailed results will be given in the full version of the paper.

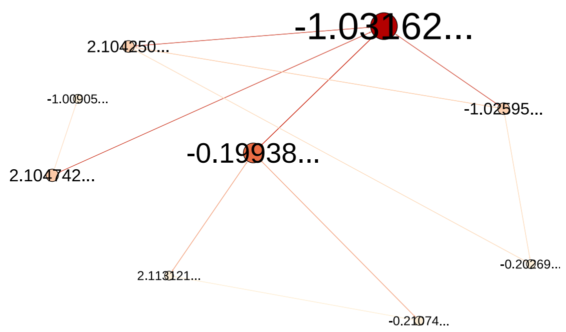

Figure 1: Stationary point network of SHCB using Steepest Decent method. Larger nodes represents higher betweenness centrality value.

Acknowledgments

This work was partially supported by the European Union and the European Social Fund through project FuturICT.hu (grant no.: TAMOP-4.2.2.C-11/1/KONV-2012-0013) and by the grant Aktion Österreich-Ungarn 87öu3. T. Vinkó was supported by the Bolyai Scholarship of the Hungarian Academy of Sciences.

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