Sampled Walk and Binary Fitness Landscapes Exploration

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Abstract. In this paper we present and investigate partial neighborhood local searches, which only explore a sample of the neighborhood at each step of the search. We particularly focus on establishing links between the structure of optimization problems and the efficiency of such local search algorithms. In our experiments we compare partial neighborhood local searches to state-of-the-art tabu search and iterated local search and perform a parameter sensitivity analysis by observing the efficiency of partial neighborhood local searches with different size of neighborhood sample. In order to facilitate the extraction of links between instances structure and search algorithm behavior we restrain the scope to binary fitness landscapes, such as NK landscapes and landscapes derived from UBQP.

1 Introduction

Fitness landscapes are nowadays used in various fields to better apprehend the behavior of complex systems. In particular, in evolutionary computation, the study of combinatorial and continuous search spaces through fitness landscapes analysis helps to understand and predict the behavior of evolutionary algorithms. The concept of fitness landscape was first introduced by Wright [15] in the field of theoretical biology. Originally, landscapes represent an abstract space of genotypes where each individual is surrounded by all individuals differing by a mutation on a single gene. Once an adaptation value (fitness) is assigned to each genotype, such a model illustrates the repartition of peaks, valleys, and plateaus which are helpful to highlight the effect of mutations on genotypes. In evolutionary computation, such a model can help to observe difficulties induced by a given problem when tackled with an optimization method. Some studies using the concept of fitness landscapes focus on basic methods in order to better isolate and study some mechanisms used among search algorithms. In particular many studies have investigated hill-climbing algorithms [12] [14] [2] which are basic methods often incorporated within more sophisticated metaheuristics.

The aim of this work is to obtain insights to conceive local search algorithms. We focus on establishing links between optimization problem structure and efficiency of local searches; the purpose here is not to tackle and optimize specifically a particular problem. More precisely, we present and focus on *partial neighborhood local search* algorithms, simple solution-based local searches which explore a sample of the neighborhood at each step of the search. In our experiments we perform a parameter sensivity analysis on partial neighborhood local searches and compare them to state-of-the-art local searches (iterated local search and tabu search) on two binary fitness landscapes: NK landscapes and the Unconstrained Binary Quadratic Programming problem (UBQP). Focusing on such landscapes facilitates the extraction of links between landscapes properties and search algorithms behavior. Here our experimental analysis highlights some links between ruggedness and both overall efficiency of considered methods as well as parameter sensivity of partial neighborhood local searches.

The paper is organized as follows. Section 2 introduces the concept of fitness landscapes and related features. In section 3 we introduce the *sampled walk* local search algorithm as well as a similar partial neighborhood search algorithm called ID walk, previously introduced by Neveu *et. al* [10]. In section 4, experiments are presented and analyzed. In the concluding section, we provide possible ways forward.

2 Fitness landscapes

A fitness landscape is a triplet $(\mathcal{X}, \mathcal{N}, f)$ where $\mathcal{X}$ denotes the search space, $\mathcal{N}$ the neighborhood relation which assigns a set of neighbors to each solution, and f the fitness value which assigns a score to each solution. The search space and fitness function are directly derived from the instance of the considered problem whereas the method used to tackle the instance often induces a particular neighborhood function. One of the main interests of fitness landscapes in evolutionary computation is to study the behavior of neighborhood-based optimization methods in function of landscapes properties (typically their size, neutrality and ruggedness). These properties and associated indicators are discussed in [9]. Yet, main landscape characterization features cannot be calculated exactly since it induces an exhaustive enumeration of the search space on landscapes that are usually derived from large-scale NP-hard problems. They are generally estimated through indicators which sample the search spaces.

The neutrality rate of a fitness landscape corresponds to the proportion of neighboring solutions which have the same fitness value. While some landscapes contain no neutrality, the presence of such a feature can have a non-negligible effect on the number and distribution of local optima. In fact, landscapes with high neutrality are in general harder to solve and induce questions about the acceptance of neutral moves within local searches.

The ruggedness of a landscape is a major property that determines the difficulty to optimize the underlying problem using the considered neighborhood relation. It mainly refers to the number of local optima, their distribution through the search space, and the size of their basins of attraction [11].

The autocorrelation function [13] is generally used to estimate the ruggedness of a fitness landscape. Such a measure requires the execution of several random walks through the considered landscape. It calculates the correlation between fitness and distances of solutions encountered during the random walk. The result is a plot of autocorrelation where correlations usually decrease from 1 to 0 with respect to increasing distances between solutions.

The definition of ruggedness is not clearly established and ruggedness can also refer to the epistasis phenomenon, related to the degree of variable interdependency between genes [4]. When the interdependence between genes is high, knowing if the presence of a given gene positively affects the individual is difficult, if not impossible. Such landscapes have high epistasis since the effect of a mutation depends on the presence of other mutations. The sign-epistasis phenomenon between two genes A and B is depicted in fig. 1 (in lower case when the gene is not present). Considering two solutions and a given mutation (or neighborhood operator application), there exists a sign epistasis when the sign of the fitness variation resulting from the application of the mutation on both solutions differs. The 1-ruggedness of a landscape corresponds to the rate of sign epistasis between neighboring solutions, whereas the k-ruggedness of a landscape corresponds to the rate of sign epistasis between k-distant solutions [2].

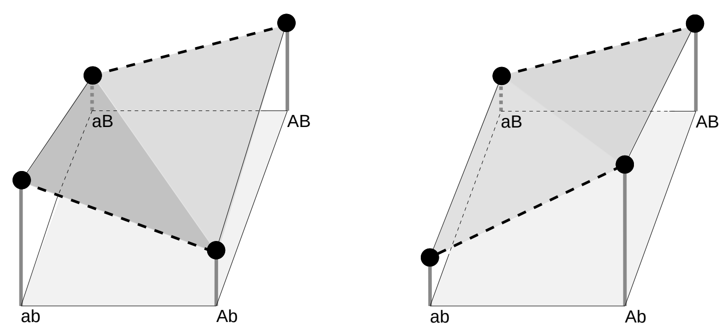

Fig. 1. Epistasis occurs when the presence of a mutation $a \to A$ affects the effect of another mutation ($ab \to aB$, $Ab \to AB$). We observe sign epistasis once a deteriorating mutation becomes beneficial when occuring after another mutation (left-hand side). Ride-hand side: no sign epistasis.

In the following, we mainly focus on the relation between ruggedness and behavior of partial neighborhood local searches.

3 Partial neighborhood local searches

This work follows previous studies related to the links between neutrality and ruggedness of combinatorial landscapes and the efficiency of hill-climbing algorithms. In particular, we investigated the ability of different neutral move policies within climbers to find good local optima.

First, it is obvious that accepting neutral solutions can potentially drive toward better local optima since it often helps not to be stuck in low-quality local optima. During the climbing process, most intensification mechanisms focus as a priority on improving the current solution rather than on considering neutral moves. In such cases, the selection of a neutral solution is only considered once a strict local optimum is reached. Yet a stochastic hill-climbing which indifferently selects the first improving or neutral neighbor encoutered clearly outperforms climbers which select improving neighbors as a priority [1].

Since accepting both improving and neutral neighbors during the search process helps to reach higher pikes, the effect of adding artificial neutrality in landscapes (by discretizing the fitness function) in order to reduce the ruggedness was studied in [3]. With an appropriate neutrality rate, stochastic climbers can efficiently tackle harder landscapes. Artificial neutrality-based climbers tend to favor better solutions without exclusively focusing on the improvement or deterioration of the real fitness values.

Here, we aim to simplify as far as possible the idea of favoring better neighbors. The key concept is to ignore if a move improves or not the current fitness value while maintaining a selection pressure. We then propose the *sampled walk* algorithm (SW), a local search which is based on randomly sampled neighborhoods (see alg. 1). At each step of the search, SW evaluates λ_{SW} random neighbors of the current solution and selects the one with the highest fitness value. Except λ_{SW}, the only choice to make concerns the stopping criterion. Yet, the stopping criterion is not necessarily fully considered as a parameter since in practice to be compared runs have to stop for any algorithm. Moreover such a parameter is irrelevant in an any-time optimization context.

λ_{SW} corresponds to a random walk whereas $\lambda_{SW} = N$ (with N is the neighborhood size) corresponds to a tabu search mechanism with an empty tabu list.

Due to the extreme simplicity of SW, its implementation is easy and does not require heavy design choices which depend upon the considered neighborhood function. Moreover, the SW simplicity greatly facilitates its analysis and allows many specific advanced variants. Note that SW, which is defined in a local search context, can also be viewed as an (1,λ) evolution strategy (with $\lambda = \lambda_{SW}$).

ID Walk (Intensification/Diversification Walk) [10] is based upon a similar concept. Like SW, ID Walk can be considered as a *partial neighborhood search* since it consists of evaluating (at most) λ_{ID} solutions at each step of the search. However, ID Walk selects the first encountered improving neighbor and therefore considers the fitness of the current solution to select the move to apply. When no improving solution is found among the λ_{ID} neighbors, the selected one depends upon the considered variant. ID_{best} selects the best one among the λ_{ID} deteriorating neighbors, whereas ID_{any} randomly selects one of them.

It is obvious that these partial neighborhood local seaches (SW, ID_{best}, ID_{any}), which use randomly generated subneigborhoods, leads to similar behaviors. As stated by Neveu *et al.* [10], ID walk was proposed with the aim to combine intensification and diversification during the search process. Although SW follows the same principle, it emphasizes that the diversification aspect (brought by the partial neighborhood) is not explicitly determined by the sign of the fitness variation. The next section experiments show that such approach is efficient even if its selection strategy does not consider the fitness of the current solution.

Algorithm 1 Sampled Walk algorithm

Choose $x_0 \in \mathcal{X}$ (initialization)
$x \leftarrow x_0$
$x^* \leftarrow x$
while stop criterion not reached **do**
    P $\leftarrow \lambda_{SW}$ random neighbors in $\mathcal{N}(x)$
    $x \leftarrow \text{argmax}_{x' \in P}(f(x'))$
    if $f(x) > f(x^*)$ **then**
        $x^* \leftarrow x$
    end if
end while
return x^*

4 Analysis on binary fitness landscapes

4.1 Experimental protocol

In order to properly assess the capacity of partial neighborhood local searches to lead toward good quality solutions, we compared the three variants SW, ID$_{best}$ and ID$_{any}$ to two widely-used local searches: tabu search (TS) [6] and iterated local search (ILS) [8]. Like SW, the classic tabu search does not use the current fitness for the selection process, but the whole neighborhood is considered. The tabu list prevents cycles which naturally occur by selecting iteratively the best neighbor among the complete neighborhood. ILS separates intensification and diversification phases. We choose here to use a first-improvement strategy during hill-climbing (intensification) phases, as first-improvement regularly reaches better local optima than best-improvement on landscapes difficult to climb [1]. Moreover, this leads to use for comparison two metaheuristics (ILS and TS) sufficiently different.

ILS and TS can be implemented with some variants which affect their behavior. Here we designed them as classical as possible. ILS performs λ_{ILS} random moves when a local optimum is reached. At each step of the algorithm, TS selects the best move using a tabu list of forbidden bit-flips of size λ_{TS}, that ensures a minimal distance between following solutions.

ILS, TS, ID$_{best}$, ID$_{any}$ and SW require to set two parameters: a stopping criterion and the aforementioned structuring parameter. In this study, the stopping criterion is a maximum number of evaluations to permit a fair comparison between methods. The maximum number of evaluations is fixed to 10^8 for all runs regardless to the landscape size. Such a value allows a sufficient convergence which ensures methods to almost never improve the best encountered solution after a significant number of evaluations. For each method we perform runs using several parameter values in order to establish appropriate settings.

For each triplet (landscape, method, parameter value) 100 runs are performed from the same initial set of 100 randomly generated solutions in order to reduce the stochastic bias. For each triplet, we retain the average of the 100 best encountered solutions (one per run). Since several values are tested, for each couple (landscape, method) only the best average is reported, i.e. the average obtained with the best considered parameter value. We also indicate if the method having the best average statistically dominates the other ones with respect to a binomial test (with a confidence level of 99%) for each considered couple.

In our experiments, we consider two types of fitness landscapes: NK landscapes and UBQP landscapes (ie. landscapes derivated from UBQP instances), the neighborhood operator under consideration being the one-flip operator.

NK landscapes are a model of binary fitness landscapes introduced by Kauffmann [7]. They are widely used when it comes to study the link between ruggedness and methods since their specificity is to have a tunable ruggedness. Such landscapes are defined by means of two parameters N and K. N specifies the number of variables and then the search space size (2^N). K determines the degree of variable interdependency (the fitness contribution of each variable being affected by K other variables) and greatly influences the ruggedness rate. Setting K to zero leads to a completely smooth landscape with no variable interdependency whereas setting K to $N-1$ leads to an extremely rugged (random) landscape. We used landscapes of various sizes $N \in \{128, 256, 512, 1024\}$ and ruggedness parameter $K \in \{1, 2, 4, 6, 8, 10, 12\}$.

The Unconstrained Binary Quadratic Programming problem (UBQP) is a NP-hard problem [5] which can reformulate a large scope of real-life problems in various fields. An instance of UBQP is composed of a matrix Q of size $n \times n$ of constants q_{ij} which can be positive or negative. A solution is a binary vector x of size n where $x_i \in \{0, 1\}$ corresponds to the i-th element of x. The UBQP objective function $f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij} x_i x_j$ has to be maximized.

We used an instance generator (proposed and provided by Gintaras Palubeckis on www.personalas.ktu.lt/∼ginpalu/ubqop_its.html) to generate some instances of different sizes and density. The density d affects the rate of values equal to zero in the matrix Q, $d = 0$ leads to a matrix full of zero except on the diagonal whereas a $d = 100$ leads to matrix with no zero.

4.2 Results

Results (see table 1) show in most cases that on the considered NK landscapes the sampled walk SW leads toward best solutions in average. SW efficiency does not seem to be affected by the ruggedness, which is mostly tuned by means of the parameter K. On smooth and small landscapes ($K \leq 4$ and $N = 128$) almost all methods lead toward the same solution which seems to be the global optimum. The explanation behind these results is that regardless the size and ruggedness

Land.	Average fitness					Best parameter value				
N K	SW	ID_{best}	ID_{any}	ILS	TS	λ_{SW}	λ_{IDb}	λ_{IDa}	λ_{ILS}	λ_{TS}
128 1	**.7245**	.7245	.7245	.7245	.7165	8, 12	8, 12	16 → 128	5 → 20	20
128 2	**.7424**	.7424	.7420	.7423	.7369	12, 16, 20	16	40	10	20
128 4	**.7959**	.7959	.7959	.7958	.7952	16, 20	16, 20	40 → 128	5	20
128 6	**.8004**	.8003	.8000	.7994	.7976	16	16	56	5	15
128 8	**.8021**	.8015	.7980	.7949	.7923	20	20	72	5	15
128 10	**.7937**	.7930	.7893	.7847	.7828	24	32	120	5	10
128 12	**.7819**	.7817	.7785	.7724	.7729	28	36	96	5	10
256 1	**.7220**	.7220	.7199	.7200	.7118	16	16	96	15	20
256 2	**.7444**	.7444	.7426	.7424	.7249	24	24	96	5, 10, 20	20
256 4	**.7934**	.7933	.7921	.7916	.7823	20	20	192	5	20
256 6	**.8048**	.8045	.8017	.8007	.8020	24	24	184	5	20
256 8	**.7964**	.7960	.7915	.7892	.7894	32	32	112	5	15
256 10	**.7869**	.7860	.7822	.7782	.7779	36	40	184	5	15
256 12	.7756	**.7756**	.7718	.7663	.7657	44	52	184	5	15
512 1	**.7079**	.7077	.7038	.7040	.7007	16	16	256	20	50
512 2	.7509	**.7509**	.7451	.7453	.7316	16	24	128	5	50
512 4	**.7860**	.7857	.7802	.7806	.7845	24	24	128, 256, 512	5	50
512 6	**.7989**	.7984	.7944	.7940	.7965	24	32	256	5	30
512 8	**.7939**	.7935	.7894	.7886	.7849	40	40	256	5	30
512 10	**.7829**	.7825	.7790	.7781	.7760	56	48	256	5	20
512 12	**.7720**	.7719	.7682	.7671	.7618	64	64	256	5	15
1024 1	**.7163**	.7160	.7083	.7087	.7051	16	16, 24	256	15	50
1024 2	**.7522**	.7521	.7427	.7428	.7274	24	24	256	5, 10, 20	50
1024 4	**.7878**	.7872	.7800	.7797	.7654	24	24	256	5	50
1024 6	**.7949**	.7943	.7893	.7890	.7899	32	32	256	5	50
1024 8	**.7901**	.7888	.7859	.7850	.7850	40	48	256	5	40
1024 10	**.7793**	.7786	.7758	.7753	.7740	56	64	256	10	30
1024 12	**.7694**	.7689	.7664	.7656	.7653	72	80	256	5	20

Table 1. Results on NK landscapes. Left-hand side: average fitness obtained with the best parameter value for each couple (landscape, method). For each landscape, the best average fitness obtained appears in bold, whereas non statistically dominated methods appear in shaded. Right-hand side: the best parameter value(s).

UBQP	SW	ID$_{best}$	ID$_{any}$	ILS	TS
2048 10	$_{100}4035.71$	$_{100}4052.02$	$_{100}3773.58$	$_{\mathbf{100}}\mathbf{4293.54}$	$_{100}4254.14$
2048 25	$_{164}0792.90$	$_{164}0823.45$	$_{164}0432.32$	$_{164}1183.63$	$_{\mathbf{164}}\mathbf{1192.63}$
2048 50	$_{239}7652.20$	$_{239}7695.08$	$_{239}7215.93$	$_{239}8106.97$	$_{\mathbf{239}}\mathbf{8443.35}$
2048 100	$_{309}7976.50$	$_{309}8266.91$	$_{309}7122.46$	$_{309}8566.65$	$_{\mathbf{309}}\mathbf{9318.75}$
4096 10	$_{280}7921.35$	$_{280}7955.71$	$_{280}6968.13$	$_{280}7632.68$	$_{\mathbf{280}}\mathbf{8263.77}$
4096 25	$_{459}4746.56$	$_{459}5136.29$	$_{459}3264.07$	$_{459}3665.15$	$_{\mathbf{459}}\mathbf{5741.73}$
4096 50	$_{652}6291.28$	$_{652}6692.46$	$_{652}4326.94$	$_{652}5133.66$	$_{\mathbf{652}}\mathbf{7995.10}$
4096 100	$_{90}90355.70$	$_{90}90761.04$	$_{90}86936.83$	$_{90}87492.74$	$_{\mathbf{90}}\mathbf{93039.30}$

Table 2. Results on UBQP landscapes. Average fitness obtained with the best parameter value for each couple (landscape, method). For each landscape, the best average fitness obtained appears in bold, whereas non statistically dominated methods appears in shaded.

of landscapes, runs are always performed with a credit of 100 million of evaluations. Since smaller and smoother landscapes tend to be easier to tackle, they require less computational effort to attain good solutions. On every considered landscapes, results obtained by ID walk are very close to those obtained by SW, but SW often statistically dominates on large landscapes.

Ruggedness does not seem to affect the overall comparative efficiency of the considered methods. Yet, best parameter values (among the considered ones) for each method evolve in function of the value of K. SW and ID$_{best}$ require very similar parameter values in order to reach good solutions. One can observe that the most appropriate parameter values increase when K increases. ID$_{any}$ parameters requirement does not evolve the same way as ID$_{best}$ and SW. For ILS and TS, the number of perturbations and the size of the tabu list also evolve in function of K. On very smooth landscapes, ILS requires more perturbations and TS a longer tabu list than on more rugged landscapes.

Such results, in addition to those observed on SW, seem indicate that the search process needs more diversification on smooth landscapes than on rugged ones. Actually smooth landscapes contain few local optima and then have large basins of attraction. On such a configuration, a more important diversification helps to get out of some basins and to attain different local optima.

All methods were also tested on several landscapes derived from UBQP instances and results differ from those obtained on NK landscapes. In table 2, we only report large landscapes results ($N = 2048$ and $N = 4096$) since on smaller ones the considered methods with various parameters value almost always lead toward the same solution (which is expected to be the global optimum). Such a fact indicates that for a given N, N-dimensional UBQP landscapes are *easier* to tackle than N-dimensional NK landscapes.

On large landscapes, the tabu search almost always leads toward the best average. ILS is rarely dominated when $N = 2048$, but always outperformed by TS when $N = 4096$.

4.3 Landscapes ruggedness and partial neighborhood LS efficiency

Experiments show that the sampled walk is particularly efficient on NK landscapes, regardless of the ruggedness level. Yet SW and other partial neighborhood local searches (ID walk) is less efficient on UBQP landscapes, which seem to be easier to tackle than NK landscapes. In order to determine if there is a link between those results and the structure of landscapes, we analyzed the ruggedness of landscapes by means of two indicators: autocorrelation and the k-ruggedness.

The plot of autocorrelation (fig. 2) on NK landscapes shows that its evolution is affected by K. Indeed, the more rugged a landscape is, the faster the correlation fitness-distance decreases. The plot of autocorrelation (fig. 3) on UBQP landscapes shows that its evolution is globally identical on all considered landscapes and evolves similarly as very smooth NK landscapes ($K = 1$).

The evolution of k-ruggedness (fig. 4) on NK landscapes follows the same scheme as the evolution of autocorrelation. Yet, the k-ruggedness indicator evolves quite differently on UBQP landscapes (fig. 5) than on smooth NK landscapes, especially on the first steps with a faster evolution. Such observation evokes locally-rugged landscapes.

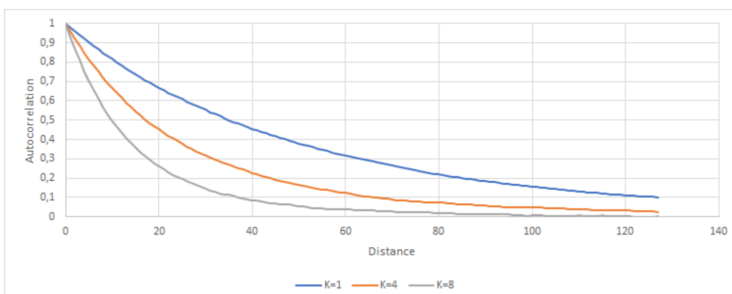

Fig. 2. Autocorrelation evolution on NK landscapes of size 128 (similar outputs can be observed for higher size of landscapes).

Considering NK landscapes, analogies between the evolution of autocorrelation and k-ruggedness seem to indicate that such landscapes have a uniform ruggedness repartition. On the contrary, it appears that UBQP landscapes have a less uniform ruggedness repartition, which we can describe as a local ruggedness and a global smoothness. This could also explain why smaller UBQP instances are easy to solve by local search as long as some diversification is applied. An hypothesis which could possibly explain the lower efficiency of partial neighborhood local searches on such landscapes is that such methods tends to explore solutions scattered through the entire landscape, whereas tabu search naturally intensifies around promising areas. In this type of landscapes, the correlation between

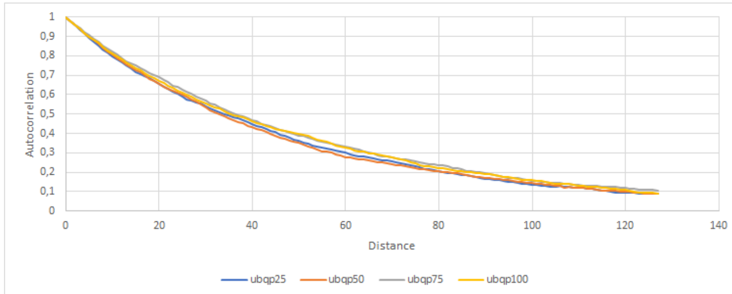

Fig. 3. Autocorrelation evolution on landscapes derived from UBQP of size 128 (similar outputs can be observed for higher size of landscapes).

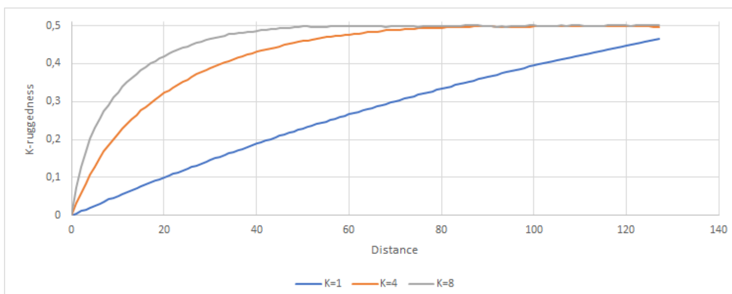

Fig. 4. K-ruggedness evolution on NK landscapes UBQP of size 128 (similar outputs can be observed for higher size of landscapes).

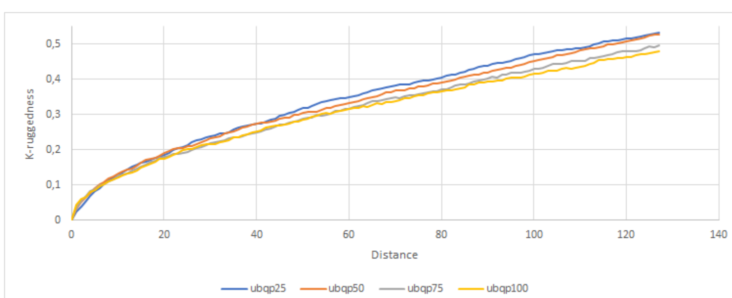

Fig. 5. K-ruggedness evolution on landscapes derived from UBQP of size 128 (similar outputs can be observed for higher size of landscapes).

fitness and distance of solutions decreases progressively. When the decorrelation fitness-distance is fast, the use of a sampled walk seems more appropriate to efficiently explore the search space.

5 Conclusion

In this paper we investigate partial neighborhood local searches and, more particularly, the sampled walk algorithm which can be viewed as a local search transposition of an (1,λ)-ES. We show that the sampled walk is efficient to tackle common binary landscapes. Conducted experiments on NK landscapes highlighted the fact that the sampled walk behavioral parameter can be principally set according to the landscape ruggedness. Experiments also show that such a method is globally competitive in comparison to metaheuristic searches like tabu search and iterated local search. Even if the sampled walk is outperformed by a tabu search on UBQP, we are able to establish links between respective efficiency of methods and ruggedness repartition thanks to the k-ruggedness indicator.

Future works include the consideration of permutation-based landscapes. The use of other solution representation brings some difficulties such as the criterion on which the tabu list is based, as well as the way to evaluate the k-ruggedness since this indicator is related to the concept of sign epistasis. It would provide useful information to analyze the behavior of the considered methods all along the search process (any-time optimization). Finally, this family of local searches like ID walk, based on a random sampling of the neighborhood, constitutes very simple search algorithms and have not been deeply investigated in the metaheuristics literature. There are thus many ways to differently use the sampled walk principle and to improve its efficiency, for instance by adapting its parameter during the search according to landscapes features.

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