On a Property Analysis of Representations for Spanning Tree Problems

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Abstract. This paper investigates on some properties of encodings of evolutionary algorithms for spanning tree based problems. Although debate continues on how and why evolutionary algorithms work, many researchers have observed that an EA is likely to perform well when its encoding and operators exhibit locality, heritability and diversity. To analyze these properties of various encodings, we use two kinds of analytical methods; static analysis and dynamic analysis and use the Optimum Communication Spanning Tree (OCST) problem as a test problem. We show it through these analysis that the encoding with extremely high locality and heritability may lose the diversity in population. And we show that EA using Edge Window Decoder (EWD) has high locality and high heritability but nevertheless it preserves high diversity for generations.

1 Introduction

For a long time, many researchers have proposed various analytical methods to reveal the basic principle of encodings in EAs. Manderick et al. [6] used correlation coefficients for the fitness values of solutions before and after operators are applied. Sendhoff et al. [17] proposed the concept of "causality" to analyze the locality of EAs. Gottlieb et al. [1],[4],[9] proposed "mutation innovation", "crossover innovation" and "crossover loss" to emphasize the importance of locality and heritability. Merz et.al [7], Reeves et.al [11] and Watson et.al [19] used the fitness landscape analysis. Besides those, many literatures have dealt with methods for analyzing the properties of encodings [5],[12],[15]. In this paper, we concentrate on the analysis of locality, heritability and diversity of encodings based on Gottlieb et al.'s study and the fitness landscape analysis.

A difficulty of the population-based optimization is that once the search has narrowed near the previous optimal solution, the diversity in the population may not be enough for the search to get out of there and proceed towards the new optimal solution. Especially, if an evolutionary algorithm has very high locality or very high heritability as well, it may suffer from much serious problem. (Often, in these cases, diversity preserving mechanisms were used for avoiding these problems [9],[10].)

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In this paper we show it through empirical tests that locality, heritability and diversity are in conflict with each other. In other word, if an encoding has extremely high locality and extremely high heritability, it may lose the diversity in population after offsprings are created and lead the search toward the narrow space (exploitation) because offsprings generated by operators will be very similar to their parents. Therefore, as generation goes, it will be deprived of the ability of exploration. But, note that high diversity does not imply the loss of locality and heritability. However, to obtain a good performance of evolutionary algorithms the harmony of these properties is needed.

For empirical tests, we compare five encodings, the Prüfer encoding [3], the network random key encoding (NetKey) [12], the link and node bias encoding (LNB) [8], the edge set encoding (Edge Set With Heuristic (ESWH) and Edge Set Without Heuristic (ESWOH) : ESs) [9] and the edge-window-decoder encoding (EWD) [18]. These encodings have been applied very successfully to spanning tree based problems like optimum communication spanning tree problem, degree constrained minimum spanning tree problem and quadratic spanning tree problem. For more details about each encoding, refer to the references.

This paper is organized as follows. The optimum communication spanning tree problem is described in Section 2. Section 3 presents the analysis of encodings. We make some concluding remarks in Section 4.

2 Optimum Communication Spanning Tree Problem: OCST

We perform an empirical analysis with OCST problem, which is one of the well-known NP-hard constrained spanning tree problems.

Consider an undirected complete graph $G = (V,\ E)$, where $V = \{1,\ 2, ..., N\}$ is the set of N nodes and $E = \{1, 2, ..., M\}$ is the set of M edges with given distance (or cost). Generally, the MST is to find the minimal cost spanning tree. In the case of the OCST, there are also "communication requirements" associated with each pair of nodes, specified by $R(i, j)$. E.g. these may represent the number of expected daily telephone calls between two cities. For any spanning tree T of G, the communication cost between two cities i and j is defined to be the communications requirement multiplied by the distance between the two cities on T, and the communication cost of T itself is the total communication cost summed over all pairs of nodes.

The goal is to construct a spanning tree with minimum communication cost. That is to find a spanning tree T such that formula (1) is minimized, where $d_T(i, j)$ is the sum of the distance of edges along the route between i and j on T.

$$Min\ [\sum_{i,j \in V} R(i, j) d_T(i, j)] \qquad (1)$$

3 Analysis of Encodings

The properties, locality, heritability and diversity, of an encoding in evolutionary algorithms are the core factors for the effective search toward an optimal or near optimal solution. Though debate still continues on, many researchers have observed that an EA is likely to perform well when its encoding and operators exhibit these properties [8],[10]. Therefore, we want to analyze the difference among various encodings. To analyze this, we use the locality [1],[4], the heritability [5] and the fitness landscape analysis [7],[11],[19].

3.1 Metrics

In order to analyze the properties of an encoding, suitable metrics have to be defined.

First of all, there are two search spaces in computational space of evolutionary algorithms; the genotypic search space and the phenotypic search space. Most of the genetic operators work on the genotypes and the movement of genotypes on the genotypic search space by the genetic operators results in the change of corresponding phenotypes on the phenotypic search space. Finally, it makes the fitness value of corresponding solutions be changed. Therefore, the genotypic distance have to be defined preferentially. But since the genotypic distance is dependent on the encoding used, it must have universality.

Since the majority of the research follow the concept of evolutionary biology [16] when defining the genotypic distance, the genotypic distance is generally defined as follow;

- *The genotypic distance* is the smallest number of individual mutations required for the inter-conversion of two genotypes.

On the other hand, “the phenotypic distance” and “the fitness distance” are independent on the encoding used, but they are dependent on the problem used. So, these two metrics should be defined as the problem.

Next, we define “phenotypic distance (d_p)” and “fitness distance (d_f)” based on the OCST problem which is used as the test problem in this paper.

- *The phenotypic distance* is the total number of different edges between two phenotypes (spanning trees). Therefore, the phenotypic distance is *the Hamming distance.*

$$d_p(T_i,\ T_j) = \frac{1}{2} \sum_{u,v \in V} |E^i_{uv} - E^j_{uv}| \tag{2}$$

  where E^i_{uv} is 1 if an edge (u, v) exists in a tree T_i, otherwise 0.

- *The fitness distance* is the difference between the fitness values of two phenotypes (spanning trees).

$$d_f(T_i,\ T_j) = |f(T_i) - f(T_j)| \tag{3}$$

3.2 Locality

The locality can be defined as how well neighboring genotypes correspond to neighboring phenotypes [1], [4], [15]. Therefore, the locality of representation is high if small changes in the genotype result in small changes in the corresponding phenotype. In this context, it is appropriate to measure the locality of encodings using the mutation operator instead of the crossover operator, because the mutation operator is usually responsible for small steps in the phenotypic space, hence for gradual changes which we want to analysis.

Gottlieb and Eckert [1], [4] introduced *the mutation innovation* to measuring the locality. Mutation operators work in the genotype, but their effect can only be analyzed in the corresponding phenotype, which involves structural information of candidate solutions. So, the effect of mutation can be measured by the distance between the involved phenotypes. Therefore, the mutation innovation (MI) is equal to the phenotypic distance (d_p) but, only difference is to be compared between parent and its mutant.

$$MI = d_p(x, x^m) \tag{4}$$

where x and x^m indicate parent and its mutant respectively.

To analyze the locality of each encoding, we generated 1,000 random initial solutions in compliance with the used encoding, applied only a mutation operator to each encoding and performed the experiment on the selected benchmark instances (Palmer24 and Berry35U) and random generated instances ($N = 10 \sim 100$).

In this experiment, the reciprocal exchange mutation is used for Prüfer, NetKey and EWD, the random perturbation mutation is used for LNB and the specialized mutation operator is used for ESs [10]. If two genes with the identical gene value are selected when the reciprocal exchange mutation is applied to an encoding, it never generates a different offspring from the parent. So, in this case two genes with different gene values are selected again.

Table 1 shows the locality comparison among encodings and here a mutation was applied once to each encoding. In case of ESWH and ESWOH, all solutions had $MI = 1$ at all instances. The reason is for their specialized mutation operator; each mutation process changes exactly one edge on the genotype, and for the genotype and the phenotype are the same; non-redundant encoding. On the other hand, the others are a kind of redundant encodings except the Prüfer encoding. So, although a mutation operator is applied to encodings, sometimes it does not cause the change at the phenotype (the redundancy) or the different genotypes can be mapped to the same phenotype (the heuristic bias).

$P(MI = 0)$ represents these things. NetKey and LNB show higher frequency than Prüfer and EWD. It relates to *the degree of redundancy* and *the heuristic bias of encodings*. In case of NetKey, exactly two genes are exchanged by the mutation (the reciprocal exchange mutation) and it results in the change of sorting order at exactly two genes. So, if the selected genes are the genes which are not selected for the previous phenotype, it never makes a difference between the phenotypes. Therefore, $P(MI = 0)$ will be increased as the size of network is increased because only $N-1$ edges among the total edges $N(N-1)/2$ are selected

Table 1. Comparison of locality on Palmer24, Berry35U and random generated Instances (Rand10 $\sim$ 100), based on randomly generating 1,000 genotypes and applying mutation once to each

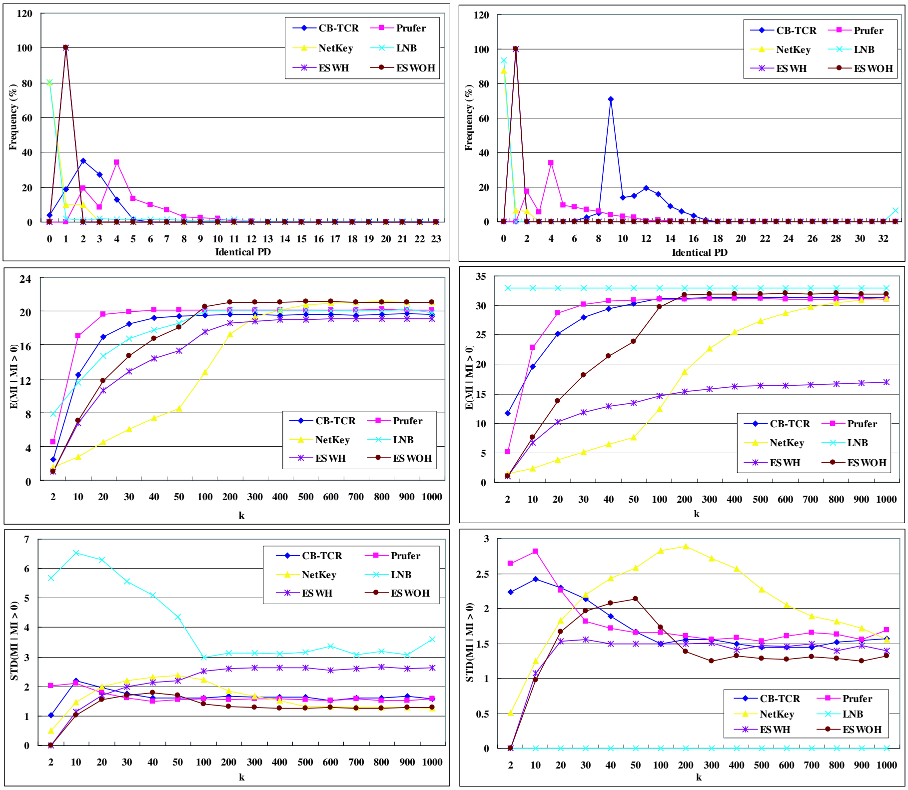
Palmer24	Prufer	LNB	NetKey	ESWH	ESWOH	EWD	Berry35U	Prufer	LNB	NetKey	ESWH	ESWOH	EWD
$P(MI = 0)(\%)$	0.00	80.5	80.3	0.00	0.00	4.10		0.00	93.5	87.3	0.00	0.00	0.00
$E(MI\|MI > 0)$	4.49	7.87	1.51	1.00	1.00	2.42		5.08	33.0	1.49	1.00	1.00	11.70
$Max(MI)$	12	22	2	1	1	7		17	33	3	1	1	18
$\sigma(MI\|MI > 0)$	2.01	5.67	0.50	0.00	0.00	1.02		2.64	0.00	0.51	0.00	0.00	2.24
Rand10							Rand20						
$P(MI = 0)(\%)$	0.00	55.7	61.9	0.00	0.00	70		0.00	56.3	77.7	0.00	0.00	4.7
$E(MI\|MI > 0)$	3.20	2.43	1.43	1.00	1.00	2.10		4.30	3.11	1.45	1.00	1.00	2.39
$Max(MI)$	6	8	2	1	1	5		10	11	2	1	1	6
$\sigma(MI\|MI > 0)$	1.12	1.71	0.49	0.00	0.00	0.89		1.65	2.05	0.49	0.00	0.00	0.96
Rand30							Rand40						
$P(MI = 0)(\%)$	0.00	61.1	84.0	0.00	0.00	3.90		0.00	64.8	87.2	0.00	0.00	2.60
$E(MI\|MI > 0)$	4.97	4.03	1.60	1.00	1.00	2.48		5.66	4.67	1.56	1.00	1.00	2.58
$Max(MI)$	14	22	2	1	1	9		19	18	2	1	1	7
$\sigma(MI\|MI > 0)$	2.39	3.46	0.49	0.00	0.00	1.01		3.19	3.47	0.49	0.00	0.00	1.00
Rand50							Rand60						
$P(MI = 0)(\%)$	0.10	64.5	89.7	0.00	0.00	3.80		0.00	66.7	91.6	0.00	0.00	2.80
$E(MI\|MI > 0)$	6.29	4.49	1.51	1.00	1.00	2.59		7.20	5.40	1.57	1.00	1.00	2.65
$Max(MI)$	21	23	2	1	1	6		27	25	3	1	1	8
$\sigma(MI\|MI > 0)$	3.87	3.91	0.50	0.00	0.00	0.98		4.86	4.44	0.54	0.00	0.00	1.00
Rand70							Rand80						
$P(MI = 0)(\%)$	0.00	68.1	91.0	0.00	0.00	2.40		0.00	70.1	90.1	0.00	0.00	2.80
$E(MI\|MI > 0)$	7.38	5.53	1.58	1.00	1.00	2.63		8.02	5.92	1.48	1.00	1.00	2.65
$Max(MI)$	31	22	2	1	1	7		29	23	3	1	1	9
$\sigma(MI\|MI > 0)$	5.56	4.22	0.49	0.00	0.00	1.01		5.94	4.52	0.54	0.00	0.00	1.01
Rand90							Rand100						
$P(MI = 0)(\%)$	0.00	71.1	92.2	0.00	0.00	1.70		0.00	69.4	90.5	0.00	0.00	1.50
$E(MI\|MI > 0)$	8.59	5.62	1.46	1.00	1.00	2.71		9.49	6.03	1.45	1.00	1.00	2.69
$Max(MI)$	36	23	3	1	1	6		38	23	3	1	1	5
$\sigma(MI\|MI > 0)$	6.88	4.41	0.55	0.00	0.00	1.01		7.99	4.84	0.57	0.00	0.00	0.98

to generate a spanning tree. The test results show that. And LNB has also the same redundancy as NetKey in terms of the length of the encoding, but in addition to that it has a strong heuristic bias in the context of having a preference toward a specific spanning tree [2]. Therefore, mutants over 80% at Palmer 24, over 93% at Berry35U and over avg. 70% at the random generated instances are the same as their parents. Especially, in Berry35U instance LNB shows much higher $P(MI = 0)$ value (93.5%) in comparison to those of the other encodings. That is for the strong heuristic bias of LNB using Prim's algorithm for sorting all edges with the modified cost matrix and for the instance's data set; all edge distances are the same (In this case LNB can only generate a star tree [2]). In all random instances, also LNB and NetKey show relatively higher values than the others. In case of EWD, even though it is a redundant representation, it has much lower redundancy comparing to NetKey and LNB. So, it exhibits relatively much lower probability at $P(MI = 0)$. The ESs and Prüfer show that all offsprings were different from their parents ($P(MI = 0) = 0$). As mentioned above, the reason is that the specialized mutation operator of ESs exactly changes one edge to a different edge which is not included in the tree and in case of the Prüfer encoding the mutation exchanges exactly two different genes. So, while $P(MI = 0)$ was 0%, $P(MI = 1)$ was 100%.

In addition, this table shows three other indicators of locality, $E(MI \mid MI > 0)$, $\sigma(MI \mid MI > 0)$ and $Max(MI)$. $E(MI \mid MI > 0)$ represents the expected mutation innovation in the case that some phenotypic property has actually been affected. So, high values represent low degree of locality. Especially, ESs can be seen as a very ideal case because single change in genotypes exactly causes 1 distance in phenotype. EWD shows low locality in comparison with NetKey and

ESs but high locality in comparison with Prüfer and LNB. But, when considering the redundancy of encodings, it is very difficult to distinguish which encoding has better locality between EWD and NetKey. In case of $\sigma(MI \mid MI > 0)$, also this table shows the similar results. NetKey, ESs and EWD are much stable than Prüfer and LNB. In Berry35U, LNB shows $E(MI \mid MI > 0) = 33$ and $\sigma(MI \mid MI > 0) = 0$. The reason is for LNB implies a strong heuristic bias. And the maximum number of edges modified ($Max(MI)$) does not exceed 38 at Prüfer, 33 at LNB, 3 at NetKey, 1 at ESs and 9 at ESW.

In figure. 1, the upper two figures indicate the frequency of solutions with the identical phenotypic distance (d_p) when a mutation is applied to each encoding once. EWD and Prüfer show that the solutions with various phenotypic distance are generated by a mutation. That means the exploration ability of EWD and Prüfer encoding. On the other hand, the other encodings exhibit their exploitation ability.



(a) Palmer24 (b) Berry35U

Fig. 1. The frequency of identical locality and the value of $E(MI \mid MI > 0)$ and $\sigma(MI \mid MI > 0)$ according to generation. In here, $E(MI \mid MI > 0)$ and $\sigma(MI \mid MI > 0)$ represent values obtained by the phenotypic distance between the original solution and its mutant generated after k generation (P_m=100).

The other figures show the value of $E(MI \mid MI > 0)$ and $\sigma(MI \mid MI > 0)$ according to generation. $E(MI \mid MI > 0)$ and $\sigma(MI \mid MI > 0)$ represent the values obtained by the phenotypic distance between the original solution and its mutant generated after k mutation. As k increases, it shows a significant difference within 200 generation. NetKey and ESWH exhibit lower mean values than the other encodings. That indicates high locality of the two encodings. But NetKey is very unpredictable at Berry35U and ESWH indicates slightly higher standard deviation values (STD) at Palmer24. On the other hand, even though LNB shows relatively high mean values and especially at Berry35U instance the mean values were all 33. As mentioned above, it is for strong bias toward a specific tree structure - a star tree. Moreover, at Palmer24 LNB is very unstable and unpredictable. Prüfer exhibits relatively high mean values -low locality- at both instances but $\sigma(MI \mid MI > 0)$ is very predictable at palmer24 instance.

Although ESWH and ESWOH start at the same $E(MI \mid MI > 0)$ value at the beginning of generation, the difference between ESWH and ESWOH becomes large because of the heuristic bias of ESWH. EWD starts slightly high mean value but finally the mean value becomes very similar to other encodings' mean value.

3.3 Heritability

The locality is a feature of the interaction between a coding and mutation operator. On the other hand, the heritability is a feature of the interaction between a coding and crossover operator. Julstrom [5] defined the heritability as the number of edges in the offspring's spanning tree that appeared in neither parent's tree. We define the heritability as a similar way.

- *The heritability* is the number of edges in the offspring's spanning tree that appeared in either parent's tree.

Table 2. Comparison of Average Heritability based on randomly generating 1,000 genotypes and applying crossover once to each

Heritability	Prufer	LNB	NetKey	ESWH	ESWOH	EWD
Palmer24	15.72	19.08	18.79	23.00	23.00	16.77
Berry35U	22.27	26.63	27.90	34.00	34.00	17.77
Rand10	6.92	7.80	7.67	9.00	9.00	7.46
Rand20	13.24	16.20	15.56	19.00	19.00	15.80
Rand30	19.39	24.11	23.57	29.00	29.00	24.34
Rand40	25.90	32.83	31.72	39.00	39.00	33.27
Rand50	31.60	40.05	39.96	49.00	49.00	41.67
Rand60	37.91	47.71	47.82	59.00	59.00	51.02
Rand70	43.94	57.01	56.17	69.00	69.00	60.04
Rand80	49.96	64.78	64.32	79.00	79.00	67.93
Rand90	55.57	73.46	72.73	89.00	89.00	77.51
Rand100	62.49	81.14	80.81	99.00	99.00	86.17

$$d_h(P_i, P_j, O) = |(P_i \cup P_j) \cap O| \quad (5)$$

where P and O represent parent and offspring.

Each encoding uses different crossover operators considering which crossover operator can give better performance for the considering encoding [18]. So, Prüfer uses two-point crossover, LNB one-point crossover, NetKey uniform crossover, ESs their specialized crossover and EWD adjacent node crossover.

Table. 2 exhibits the average heritability of each encoding and the high d_h values imply the high heritability.

ESs show very ideal case at all instances because of their specialized crossover operator. All of the generated offsprings are created by their parents' edges. However, they show the highest locality and heritability. In this empirical com-

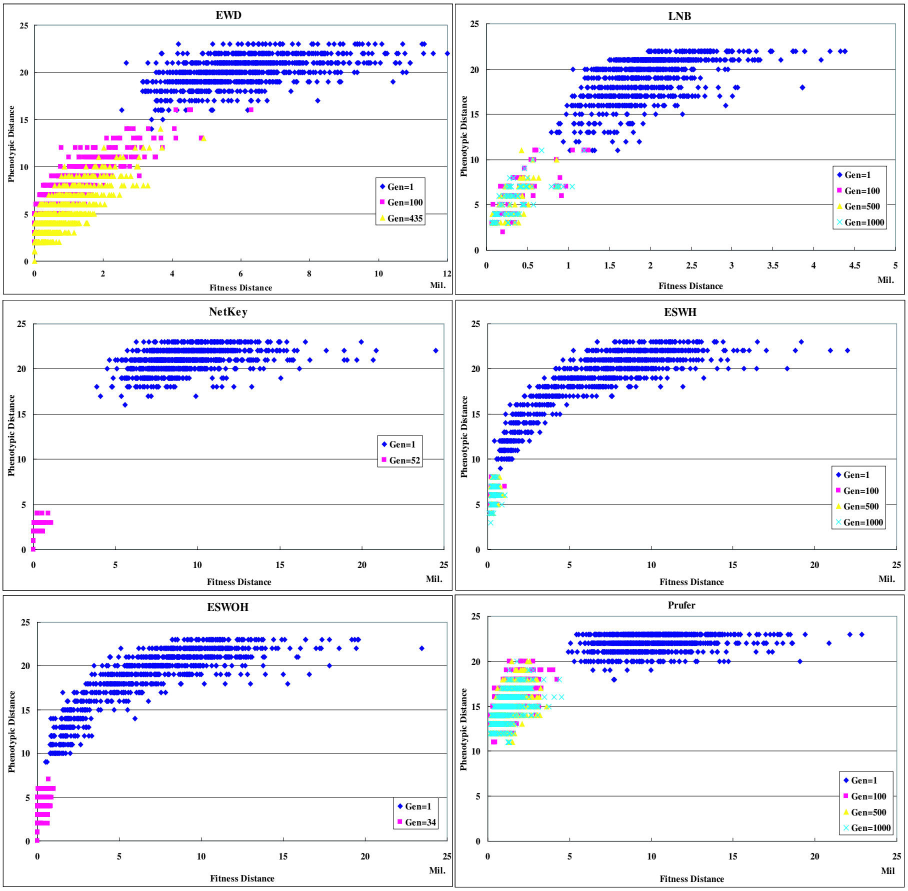


Fig. 2. The fitness landscape. 1,000 solutions are generated using each representation methods and genetic operators are applied to a representation (Palmer24).

parison, EWD exhibits higher heritability than the other encodings except ESs and Prüfer encoding exhibits the lowest heritability as the locality comparison.

3.4 Diversity

- If various different solutions coexist in population, the representation has high diversity. Otherwise, it has low diversity.

We analyzed the diversity of encodings at two instances (palmer24 and berry35U) and in this experiment all genetic operators were applied to encodings as following [18].

Figure. 2 and figure. 3 show the relation between phenotypic distance and fitness distance to optimum solution (palmer24) or the best known solution

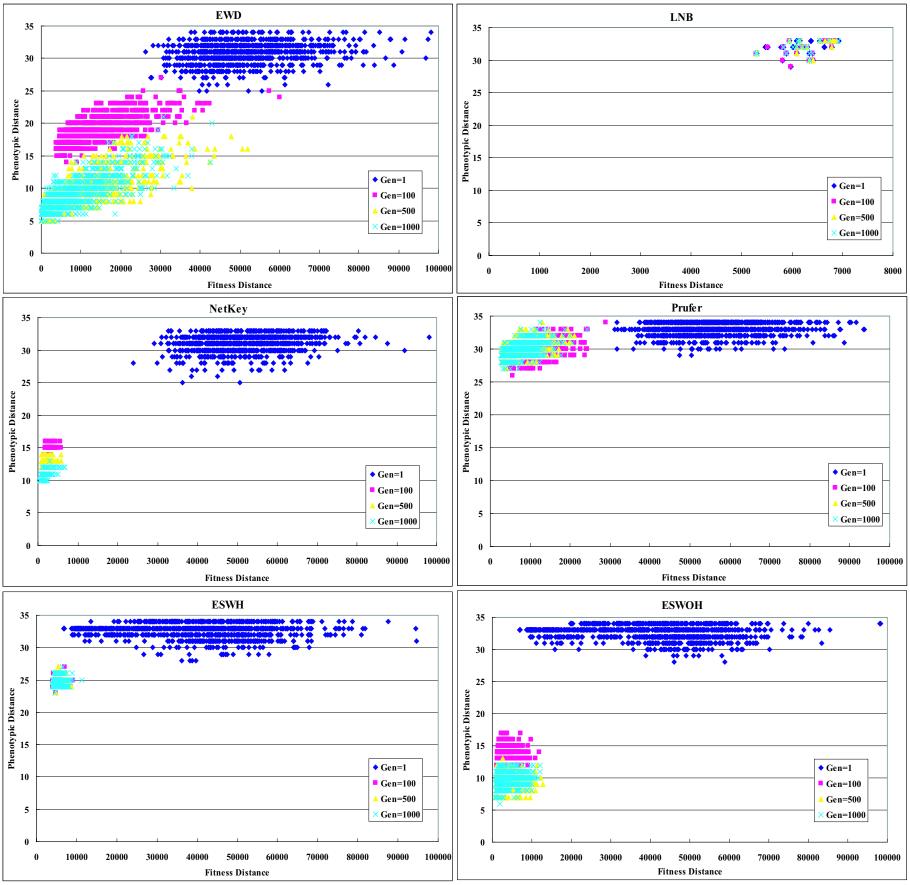


Fig. 3. The fitness landscape. 1,000 solutions are generated using each representation methods and genetic operators are applied to a representation (Berry35U).

(berry35U) according to generation. Here, different shape points represent the distribution of solutions scattered at each generation. Note that EWD keeps preserving the diversity of solution over generations at both instances and has high diversity in population. On the other hand, the other encodings dramatically lose the diversity of solution.

We conclude that the reason why the other encodings lose the diversity of population is for the strong heuristic bias or extremely high locality. If an encoding has extremely high locality, after operators are applied it keeps generating very similar offsprings or nearly the same offsprings, and finally the population will be filled by similar offsprings very fast as generation goes. As a result, the search space which the encoding explores will narrow and then it will become to lose the balance between “exploration” and “exploitation”. For example, at the locality comparison NetKey and ESs exhibited higher locality. But, if considering the diversity distribution, the solutions are distributed in a very limited space.

Observing the distribution of solutions, we can also estimate the difficulty of problems. In Palmer24 instance, the solution distribution of each encoding shows the positive correlation [15] between phenotypic distance and fitness distance. It means that an algorithm which guides toward solutions with small fitness value can easily find the optimum solution. On the other hand, in case of Berry35U, the solution distribution of each encoding shows no correlation between phenotypic distance and fitness distance. For example, ESWH and ESWOH use the specialized initialization operator, which is derived from Kruskal’s algorithm and the operator prefers to shorter edges. So, the initial solution distributions of ESs are scattered along x-axis and even though they find solutions with less fitness distance, the phenotypic distance is still large. As a result, the figure shows that if an algorithm guides toward a better fitness solution, it may fall into a local optima, and preserving the diversity of solution can give a help to escape the local optima.

4 Conclusions

We investigated the locality, heritability and diversity of encodings of evolutionary algorithms for spanning tree based problems and performed empirical tests on the optimum communication spanning tree problem.

Generally, the Prüfer encoding has low locality so that it did not give good performance in several literatures. We could also confirm low locality and low heritability of the Prüfer encoding. And it is known that if an encoding has high locality and high heritability, the evolutionary algorithm will give good performance. But, in our experiment, we showed that if an encoding has extremely high locality and heritability like ESs, it can lose the diversity of population. So, some researchers used the diversity preservation strategy [9], [10] to avoid this problem. However, it can be a good strategy. LNB and Netkey showed high locality and high heritability because of the heuristic bias or the redundancy of the encoding. But, these encodings also showed a feature of the diversity loss.

On the other hand, EWD showed slightly low locality and high heritability and the highest diversity in all test instances. And EWD showed a feature which it is independent on the property of problem. That shows EWD can be applied various spanning tree based problems and may give good performance.

As a result, EWD and ESs seem to be good encodings for the OCST, and potentially other spanning tree based problems.

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