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The Theory of Elementary Landscapes

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Abstract—When joined to a stipulated neighborhood digraph, an objective function defined on the solution space of a real combinatorial optimization problem forms a landscape. Grover shows that landscapes satisfying a certain difference equation have properties favorable to local search.

Studying only symmetric and regular neighborhood digraphs, Stadler defines *elementary* landscapes as those which can be realized as an eigenvector of the Laplacian of the neighborhood digraph, and shows that such landscapes satisfy Grover's difference equation.

Recent developments in algebraic graph theory support a new definition of the graph Laplacian which we use to extend the notion of elementary landscapes to neighborhood digraphs which may be neither regular nor symmetric. This paper uses the new definition to extend the notion of elementary landscapes so that they characterize landscapes satisfying Grover's wave equation.

We extend some known results to these more general elementary landscapes and analyse the types which may occur. © 2003 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

In the context of a local search procedure applied to a *real* combinatorial optimization problem (COP), a *move* is an operation on an incumbent solution $x \in X$ (the solution space) that transforms x into a *neighboring* solution, y. A stipulated set of such moves for each and every $x \in X$ defines the *neighborhood* $\mathfrak{N}$. Each $\mathfrak{N}(x)$ may contain duplicates since distinct moves may produce the same neighboring solution. Given an objective function $f : X \to \mathbb{R}$, the triple $\mathfrak{L} = (X, f, \mathfrak{N})$ is a *landscape*. While combinatorial optimization is a focus of this paper, the definition of a landscape presented here is completely abstract and the results in this paper apply to the many situations [1] in which landscapes occur.

Grover [2] and Codenotti and Margara [3] showed that landscapes arising from certain classes of COPs satisfy Grover's difference equation. Grover stated that if a landscape satisfies this equation then local optima are superior to the average value μ of the objective function over the solution

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space, and, the number of steps to reach a solution at least as good as μ from any starting point is linear in the problem size. Codenotti and Margara stated that the average value of a solution's neighbors is between the solution's value and μ. Barnes and Colletti [4] investigate a large number of neighborhoods that satisfy Grover's difference equation for all symmetric traveling salesman problems (STSPs). Solomon *et al.* [5] extend this previous work on STSPs to a much larger class of TSPs with weakly symmetric distance matrices.

Like Grover [2] and Codenotti and Margara [3], Stadler [1] studied only symmetric and regular neighborhood digraphs and showed that landscapes satisfying Grover's difference equation, elementary landscapes, embodied a normalized objective function as an eigenvector of a graph Laplacian. He argued that any COP with an elementary landscape is a favorable candidate for solution by local search methods.

In Section 2, using a graph Laplacian *similar* (as a linear operator) to Chung's [6] we extend Stadler's definition of elementary landscapes to arbitrary neighborhood digraphs, enabling us to characterize landscapes satisfying Grover's wave equation. In Section 3, existing results on elementary landscapes are extended to this larger class, and two general types of elementary landscapes are identified and are related using the two-step neighborhood. In the final section, we summarize the contributions of this paper and suggest areas for future research.

2. ELEMENTARY LANDSCAPES

We begin by reviewing Grover's equation and explaining its relation to the graph Laplacian.

2.1. Mathematical Preliminaries

For an objective function f, let $[f(x) : \forall x \in X]$ be the associated vector in $\mathbb{R}^{|X|}$. It will cause no confusion to identify f with its vector of values. For any $\alpha \in \mathbb{R}$, f_α defined by $f_\alpha(x) = f(x) - \alpha$ is the objective function *normalized* at α. Denote by μ the average value of f over X.

A neighborhood $\mathfrak{N}$ on the solution space defines a directed multigraph with adjacency matrix $A \in \mathbb{N}^{|X| \times |X|}$ where $A(x, y)$ is the number of times y occurs in $\mathfrak{N}(x)$. The degree matrix D is the diagonal matrix whose $D(x, x)$ entry is $|\mathfrak{N}(x)|$. If every diagonal entry of D is the same number, d, then the digraph associated with A is *regular*.

2.2. Grover's Equation

Grover defines the difference operator ∇^2 by

$$\nabla^2 f(x) = \frac{\sum\limits_{y \in \mathfrak{N}(x)} [f(y) - f(x)]}{|\mathfrak{N}(x)|},$$

and identifies the class of landscapes for which, after an appropriate normalization, there is some constant $\lambda > 0$ such that the following 'wave' equation is satisfied:

$$\nabla^2 f + \lambda f = 0. \tag{1}$$

While Grover's definition allows landscapes whose neighborhood graph is of any type, all his results assume landscapes whose neighborhood graph is regular and symmetric. Grover shows this class to have a number of properties favorable to local search. We extend these results to general neighborhood graphs below. He also shows that landscapes arising from certain well known COPs satisfy equation (1).

2.3. Stadler's Definition of Elementary Landscapes

Considering only regular and symmetric $\mathfrak{N}$, Stadler [1] defines the Laplacian matrix to be $L_S = dI - A$ where I is an $|X| \times |X|$ identity matrix, and d is the degree of every vertex. For regular, symmetric neighborhoods, it can be shown that $L_S = -d\nabla^2$. As a consequence, we have *sufficient* conditions for a landscape to satisfy equation (1): in a regular, symmetric landscape for which f_μ is an eigenvector of L_S, f_μ satisfies equation (1). Stadler calls such landscapes *elementary*.

As shown in the Appendix, because Grover and Stadler limited their studies to regular and symmetric $\mathfrak{N}$, they needed only to investigate f_μ. Other classes of $\mathfrak{N}$ require consideration of general normalized objective function vectors, f_α.

2.4. Extending the Definition of Elementary Landscapes

For any digraph associated with an adjacency matrix A we define the *Laplacian* by

$$L = I - D^{-1}A.$$

L has a number of important properties. $D^{-1}A$ is a stochastic matrix (i.e., its row sums are all 1), and so its (possibly complex) eigenvalues have modulus in the interval $[0,1]$ [7]. Consequently, the eigenvalues of L have modulus in the interval $[0,2]$.

Lemma 1. *For any $f : X \to \mathbb{R}$, $D^{-1}Af(x)$ is the average value, $\mathrm{Avg}_{y\in\mathfrak{N}(x)} f(y)$, of f on $\mathfrak{N}(x)$. That is,*

$$D^{-1}Af(x) = \frac{\sum\limits_{y\in\mathfrak{N}(x)} f(y)}{|\mathfrak{N}(x)|}.$$

Proof. Routine. ∎

Definition 2. *An elementary landscape is one in which f_α is an eigenvector of L for some real number α, i.e.,*

$$L f_\alpha = \lambda f_\alpha. \tag{2}$$

A simple consequence of Lemma 1 is the following.

Theorem 3. *As linear operators on the space of functions $f : X \to \mathbb{R}$, $L = -\nabla^2$.*

The following corollary provides the promised characterization.

Corollary 4. *A landscape $(X, f, \mathfrak{N})$ is elementary if and only if $(X, f_\alpha, \mathfrak{N})$ satisfies Grover's wave equation for some α.*

With this characterization, the classical mathematical tool of spectral analysis can now be applied in studying different types of landscapes for a given neighborhood [1].

3. TYPES OF ELEMENTARY LANDSCAPES

This section explains the properties of elementary landscapes which make them amenable to local search and we distinguish two classes of elementary landscapes which result from varying the parameter λ.

While it is possible to define COPs where the objective function f can achieve complex values, for the purposes of this paper we limit ourselves to COPs (and therefore, landscapes) where f can achieve only *real* values. This limits us to elementary landscapes where both the eigenvector (f), and therefore, the eigenvalue (λ) are real, since the Laplacian of a neighbourhood is real by definition.

As noted previously (and by [6]), the eigenvalues of L lie in the interval $[0,2]$, so that an elementary landscape can only exist with λ in this range. The feasible range of the normalizing parameter α may be deduced from Theorem 5 below.

We now relate elementary landscapes to local optima of COPs. A solution x is said to be a *local minimum* if $f(x) \le f(y)$ for every $y \in \mathfrak{N}(x)$. The notion of *local maximum* is defined similarly.

THEOREM 5. *In an elementary landscape with $\lambda > 0$, local minima have values at most α, and local maxima have values at least α.*

PROOF. Equation (2) with Lemma 1 yields, for each $x \in X$,

$$\mathrm{Avg}_{y \in \mathfrak{N}(x)} f_\alpha(y) = (1 - \lambda) f_\alpha(x). \tag{3}$$

If x^* is a local minimum, then it is no greater than the least of its neighbors, and therefore,

$$f_\alpha(x^*) \leq \mathrm{Avg}_{y \in \mathfrak{N}(x^*)} f_\alpha(y) = (1 - \lambda) f_\alpha(x^*).$$

From this we immediately have $\lambda f_\alpha(x^*) \leq 0$, and since $\lambda > 0$, $f(x^*) \leq \alpha$ as required.

The corresponding proof for local maxima is symmetrical. ∎

In the next section, we describe how the value of λ determines the properties of an elementary landscape.

3.1. Smooth and Rugged Landscapes

In general, a neighborhood $\mathfrak{N}$ defines a directed multigraph, with an edge from x to y for each occurrence of y in $\mathfrak{N}(x)$. If, for each $x, y \in X$ there is a directed path from x to y, the neighborhood digraph is *connected*.

The following proposition explains why elementary landscapes with eigenvalue 0 or 2 are often degenerate and permits us to restrict further investigations to elementary landscapes with $\lambda \in (0, 2)$.

PROPOSITION 6. *If $\mathfrak{N}$ defines a connected digraph, then*

- *an elementary landscape with $\lambda = 0$ has constant objective function, i.e., a flat landscape where $f(x)$ has the same value $\forall\, x \in X$;*

and if in addition $x \in \mathfrak{N}(x)$ for at least one $x \in X$, then

- *there is no elementary landscape with $\lambda = 2$.*

PROOF. First, notice that corresponding to an eigenvalue λ of L is an eigenvalue $1 - \lambda$ of $D^{-1}A$. If the neighborhood digraph is connected, then $D^{-1}A$ is a nonnegative irreducible matrix.

Suppose f_α is an eigenvector for the eigenvalue $\lambda = 0$ of L. Then the corresponding eigenvalue of $D^{-1}A$ is 1, which is the eigenvalue of maximum modulus, and so, by the Perron-Frobenius Theorem, 1 is a simple root of the characteristic equation of $D^{-1}A$ which implies that it corresponds with a single eigenvector. Since the vector $\mathbf{1}$ whose entries are all 1 is an eigenvector of L with eigenvalue $\lambda = 0$, we conclude that this is the only eigenvector corresponding to that eigenvalue. Hence, the objective function $f = \mathbf{1} + \alpha$ is a constant vector.

If in addition $x \in \mathfrak{N}(x)$ for some $x \in X$, then the irreducible $D^{-1}A$ has positive trace, which implies that $D^{-1}A$ is a primitive matrix. Once again, by Perron-Frobenius [8, Theorem 0.3], such a matrix has unique eigenvalue of maximum modulus, therefore $1 - \lambda \neq -1$, i.e., $\lambda \neq 2$. ∎

We identify two types of elementary landscapes depending on the value of $\lambda \in (0, 2)$.

TYPE 1. If $0 < \lambda \leq 1$, then equation (3) implies that

$$f_\alpha(x) \leq \mathrm{Avg}_{y \in \mathfrak{N}(x)} f_\alpha(y) \leq 0 \quad (\text{i.e., } f(x) \leq \mathrm{Avg}_{y \in \mathfrak{N}(x)} f(y) \leq \alpha), \qquad \text{for } f_\alpha(x) \leq 0$$

and

$$f_\alpha(x) \geq \mathrm{Avg}_{y \in \mathfrak{N}(x)} f_\alpha(y) \geq 0 \quad (\text{i.e., } f(x) \geq \mathrm{Avg}_{y \in \mathfrak{N}(x)} f(y) \geq \alpha), \qquad \text{for } f_\alpha(x) \geq 0.$$

This implies that "on average" all $x \in X$ have neighbors whose $f(y)$ are similar to $f(x)$ (on the same side of α), i.e., the landscape is characterized by smooth "rolling hills and valleys" [1]. This relation was also observed by Codenotti and Margara [3]. However, in the general case where α need not equal μ, stronger information may be inferred. For example, if $\alpha < \mu$, then local minima have lesser values than when $\alpha = \mu$.

TYPE 2. If $1 \leq \lambda < 2$, then (3) implies that

$$f_\alpha(x) \leq 0 \leq \mathrm{Avg}_{y \in \mathfrak{N}(x)} f_\alpha(y), \qquad \text{for } f_\alpha(x) \leq 0$$

and

$$f_\alpha(x) \geq 0 \geq \mathrm{Avg}_{y \in \mathfrak{N}(x)} f_\alpha(y) \geq 0, \qquad \text{for } f_\alpha(x) \geq 0.$$

This relation implies that all solutions are neighbored, on average, by solutions with values on the opposite side of α.

At the intersection of these two cases (when $\lambda = 1$) we clearly have

$$\mathrm{Avg}_{y \in \mathfrak{N}(x)} f_\alpha(y) = 0.$$

Henceforth, we shall refer to landscapes of Type 1 as *smooth-elementary* and landscapes of Type 2 as *rugged-elementary*.

While rugged-elementary landscapes would present a more difficult challenge for a simple greedy local search, knowledge that such a landscape is present would enhance the strategic search possibilities of more sophisticated reactive and adaptive metaheuristic approaches like tabu search. The identification of rugged-elementary landscapes extends the incomplete results of Codenotti and Margara [3] and Stadler [1] who apparently were only aware of smooth-elementary landscapes.

3.2. Smoothing Rugged Landscapes

Let adjacency matrix A define a regular neighborhood $\mathfrak{N}_A$ which yields an elementary landscape. We now consider cases where the associated *two-step* neighborhood $\mathfrak{N}_{A^2}$ must yield a smooth ($\lambda < 1$) landscape.

THEOREM 7. *Every regular neighborhood $\mathfrak{N}_A$ defines a two-step regular neighborhood $\mathfrak{N}_{A^2}$ such that if $(X, f, \mathfrak{N}_A)$ is an elementary landscape with a real eigenvalue, then $(X, f, \mathfrak{N}_{A^2})$ is a smooth elementary landscape.*

PROOF. Let d be the degree of regularity of the neighborhood $\mathfrak{N}_A$. It is easy to see that $\mathfrak{N}_{A^2}$ is regular with degree d^2. The Laplacian L_A of $\mathfrak{N}_A$ is $I - (1/d)\,A$ while the Laplacian of $\mathfrak{N}_{A^2}$ is $L_{A^2} = I - (1/d^2)\,A^2$.

Suppose $(X, f, \mathfrak{N}_A)$ is elementary. Then

$$\lambda f_\alpha = L_A f_\alpha = \left(I - \frac{1}{d} A\right) f_\alpha$$

so that

$$A f_\alpha = d(1-\lambda) f_\alpha.$$

Therefore,

$$\begin{aligned} L_{A^2} f_\alpha &= \left(I - \frac{1}{d^2} A^2\right) f_\alpha \\ &= f_\alpha - \frac{d^2}{d^2}(1-\lambda)^2 f_\alpha \\ &= \left(1 - (1-\lambda)^2\right) f_\alpha \\ &= \left(2\lambda - \lambda^2\right) f_\alpha \end{aligned}$$

so that $(X, f, \mathfrak{N}_{A^2})$ is elementary with eigenvalue $(2\lambda - \lambda^2)$. Since $2\lambda - \lambda^2$ has maximum value 1, $(X, f, \mathfrak{N}_{A^2})$ is smooth. ∎

Recalling that every real symmetric matrix has real eigenvalues we have the following.

COROLLARY 8. *If A defines a regular, symmetric neighborhood, then for every elementary landscape $(X, f, \mathfrak{N}_A)$, the two-step landscape $(X, f, \mathfrak{N}_{A^2})$ is smooth.*

If the one-step adjacency matrix, A, is irregular *and* symmetric, then a smooth two-step landscape exists. To see this, note that A^2 is positive semidefinite. Hence, $D_2^{-1}A^2$ is also positive semidefinite (e.g., [9, p. 218]), where D_2 is the two-step diagonal degree matrix. Therefore, the eigenvalues, λ_2, of the two-step Laplacian $L_{A^2} = I - D_2^{-1}A^2$ correspond to the $(1-\lambda_2)$ eigenvalues of $D_2^{-1}A^2$ which are nonnegative, i.e., $\lambda_2 \leq 1$. Unfortunately, unlike the case where A is regular, f_α is not necessarily invariant when one moves from the one-step to the two-step neighborhood.

Studying irregular and asymmetric one- and two-step neighborhoods and answering the question when the latter yields smooth landscapes is an interesting area for future research.

4. CONCLUSIONS

This paper extends the definition of elementary landscapes to arbitrary neighborhood digraphs. This facilitates the understanding of elementary landscapes for COPs where irregular and/or asymmetric neighborhoods may be considered. Asymmetric neighborhood digraphs may yield complex eigenvalues and eigenvectors. Their use and meaning is an intriguing area for further investigation.

Two general classes of elementary landscapes, smooth and rugged, are characterized. For a regular adjacency matrix, rugged elementary landscapes can be smoothed by using the corresponding two-step neighborhood. Empirical evidence indicates that Glover and Laguna's ejection chain method [10] of generating compound neighborhoods enhances a metaheuristic search method. The findings in this paper may provide theoretical insight into the success of such techniques. The development of neighborhoods always yielding smooth landscapes is an important area for research. The existing neighborhoods possess $\alpha \equiv \mu$, so the development of neighborhoods yielding elementary landscapes where $\alpha \neq \mu$, and studying the properties of such landscapes is another area for future research.

Using the single agent traveling salesman problem as an analysis base, we are currently applying eigenvector analysis for investigating the form and character of elementary neighborhoods for arbitrary adjacency matrices. A directly related, and more complex, area of study would be to develop methods to determine what neighborhood or neighborhoods would yield an elementary landscape for a stipulated distance matrix or class of distance matrices.

APPENDIX

The Appendix briefly explains why previous researchers were not aware that α could differ in values from μ.

PROPOSITION 9. *If the adjacency matrix is regular and symmetric then the eigenvalues and eigenvectors of the Laplacian must be real.*

PROOF. As noted earlier, the Laplacian is clearly symmetric if the adjacency matrix is. The result now follows immediately from the well-known fact that the eigenvalues and eigenvectors of a symmetric matrix are real. ∎

All the COP landscapes explicitly considered by earlier researchers such as Grover and Stadler have regular and symmetric neighbourhood graphs, therefore only regular and symmetric neighborhood graphs were considered in the theoretical formulations. As a consequence of symmetry (see [2, Lemma 6.1]) the normalization parameter α is forced to be the global average μ. In fact, it can easily be shown that $\alpha = \mu$ for a larger class of landscapes which includes those with symmetric neighborhood graphs as a subclass. That larger class is the set of those whose normalized adjacency matrices, $D^{-1}A$, are *doubly stochastic*, i.e., the row and column sums are all unity.

THEOREM 10. *If* $(X, f, \mathfrak{N}_A)$ *is* (α, λ)*-elementary with* $D^{-1}A$ *doubly stochastic, then* $\alpha = \mu$, *the global average of* f.

PROOF. Recall, a matrix is doubly stochastic if its rows and columns all sum to 1. Therefore, if $D^{-1}A$ is doubly stochastic then the columns of $L = I - D^{-1}A$ sum to zero, that is,

$$\mathbf{1}^\top L = \mathbf{0}^\top, \tag{4}$$

where $\mathbf{1} = (1, 1, \dots, 1)^\top$ is an $|X|$-dimensional vector of ones, and $\mathbf{0} = (0, 0, \dots, 0)^\top$ is an $|X|$-dimensional vector of zeros. Starting with the fact that $\lambda f_\alpha = L f_\alpha$ and premultiplying both sides by $\mathbf{1}^\top$ yields

$$\begin{aligned} \lambda \left(\sum_{x \in X} f_\alpha(x) \right) &= \lambda \left(\mathbf{1}^\top f_\alpha \right) \\ &= \left(\mathbf{1}^\top L f_\alpha \right) \\ &= \mathbf{0}^\top f_\alpha \text{ from (4)} \\ &= 0. \end{aligned}$$

Therefore, if $\lambda \neq 0$ then we must have that

$$\sum_{x \in X} f_\alpha(x) = 0,$$

which is to say, $\alpha = \mu$ as required. ∎

It is an interesting problem to find elementary COP landscapes which do not have $D^{-1}A$ doubly stochastic.

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