Arbitrary Elementary Landscapes & AR(1) Processes

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Abstract

Neighborhood specification is a dominant consideration in assuring the success of a direct search approach to a difficult combinatorial optimization problem. Previous research has shown the efficacy of imposing an elementary landscape upon the search topology. Barnes, et. al. [1] generalize the notion of elementary landscapes to embrace arbitrary neighborhood digraphs. Stadler [2] shows, for the special case of symmetric-regular neighborhood digraphs, that the autocorrelation function associated with a smooth elementary landscape is consistent with an AR(1) time series. In this paper, we extend this idea to arbitrary neighborhood digraphs.

Keywords - Elementary landscapes, autocorrelation function, autoregressive processes, neighborhood digraphs

1 Introduction

A landscape for a combinatorial optimization problem (COP) is defined by $\mathcal{L} = (X, f, \mathcal{N})$ [1] , where $X = [x_i]$ is the finite solution space, $f = [f(x_i)] = [f_i]$ is the real objective function vector over all X, and $\mathcal{N}$ is the search neighborhood (defined by an associated digraph where the nodes are the $x_i \in X$) that governs the possible solutions that may be reached in a single *move* applied to any $x_i \in X$.

Let $A = [a_{ij}]$ be the ($|X| \times |X|$) adjacency matrix of the directed multigraph associated with $\mathcal{N}$. The nonzero elements of the diagonal *degree matrix*, D, give the cardinality of the set of adjacent neighbors of each $x_i \in X$, *i.e.*, $d_{ii} \equiv \sum_j a_{ij}$ and $T = D^{-1}A$ is the *transition matrix* associated with $\mathcal{N}$. Kemeny and Snell [3] define $\pi = [\pi_i]$ to be the *steady state vector* associated with T and show that $\alpha = \pi' Tf = \pi' f$ is the expected value of f_i for the discrete Markov process defined by T. A *realization* of this discrete Markov process may be generated by performing a *random walk* on the landscape associated with T. (The concept of a "random walk on T" is discussed in detail in section II.) For the special case of doubly stochastic T (which embraces symmetric-regular neighborhood digraphs as a subset) [4], $\pi = \left[\frac{1}{|X|}\right]$, i.e., π is a *uniform* vector, implying $\alpha = \mu \equiv \sum_{\forall X} f_i \big/ |X|$, the *arithmetic average* of the f_i. We define $f_\alpha = [f(x_i) - \alpha] = [f_{\alpha i}]$ to be the α-*normalized* objective function vector.

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The class of *elementary* $\mathcal{L}$ satisfies Grover's difference equation [5] and possesses a specific set of properties favorable for heuristic search. For such $\mathcal{L}$, f_α is an eigenvector of the *Laplacian*,

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

This implies that $L f_\alpha = \lambda f_\alpha$, where λ is a real eigenvalue of L. In this paper, we will show that α is unique.

2 The Autocorrelation Function of an Elementary $\mathcal{L}$

A random walk on a neighborhood, $\mathcal{N}$, is constructed by randomly selecting an $x_0 \in X$ as a starting incumbent solution. The next solution, x_1, is determined by randomly selecting a neighbor of the incumbent solution (with probability t_{ij}) and moving to it. The new solution then becomes the incumbent solution and the process repeats for *n-1* steps. At each step, $i = 0, 1, \ldots, n-1$, the value of each incumbent's associated $f_{\alpha i}$ is recorded yielding a sampled time series of length n. Weinberger [6] defines the *sample lag-s autocorrelation function* of a time series, $f_{\alpha i}$, of length n generated by a random walk on $\mathcal{N}$(or T) as

$$r_\pi(s) = \frac{\sum_{i,j} \pi_i T_{ij}^{\,s} f_{\alpha i} f_{\alpha j}}{\sum_{i,j} \pi_i f_{\alpha i} f_{\alpha j}} \tag{1}$$

For the x_i visited in a random walk on T, $E(f_i|T) = \alpha$ which implies that $E(f_{\alpha i}) = 0$ [6]. However, for the remainder of his paper, Weinberger [6] considered only the special case of a regular and symmetric transition matrix T. This assumption implies that

$$\pi = \left[\frac{1}{|X|}\right] \tag{2}$$

which, in turn, implies $\alpha \equiv \mu = \sum_{\forall i \in X} f_i \big/ |X|$.

The *theoretical* lag-s autocorrelation function for *any* $\mathcal{L}$ is

$$\rho_\pi(s) = \frac{f_\alpha' \Pi T^s f_\alpha}{f_\alpha' \Pi f_\alpha} \tag{3}$$

where Π is a diagonal matrix with $\Pi_{ii} = \pi_i$. The doubly stochastic T include the symmetric-regular T as a special case. Since $\pi = [\frac{1}{|X|}]$ is true if and only if T is doubly stochastic [4], the theoretical lag-s autocorrelation function for an $\mathcal{L}$ with doubly stochastic T is

$$\rho_\pi(s) = \frac{f_\alpha' T^s f_\alpha}{f_\alpha' f_\alpha}$$

If T is symmetric-regular, then $\mathcal{L}$ is elementary if and *only* if a univariate time series generated from a random walk on T is consistent with an autoregressive process of order 1, i.e., an AR(1) process [2]. For a symmetric-regular T, the set of f_α associated with an elementary $\mathcal{L}$ is identical to the set of f_α from a random walk on T that are consistent with an AR(1) process [2,6,7,8].

Let us now consider similar properties for an $\mathcal{L}$ with *arbitrary T:*

THEOREM 1. For *any* elementary $\mathcal{L}$, $\rho_\pi(s) = (1-\lambda)^S$ where λ is an eigenvalue of the *Laplacian, L*, and $\rho_\pi(s) = \rho_\pi^s(1)$.

PROOF: Since $\mathcal{L}$ is elementary if and only if $Tf_\alpha = (1-\lambda) f_\alpha$ [1], the equality $\rho_\pi(s) = (1-\lambda)^S$ follows directly. This is easily verified by noting that $T^s f_\alpha = (1-\lambda)^s f_\alpha$, substituting this relation into Equation (3), and reducing. □

(Note that an exponentially declining autocorrelation function, i.e., $\rho_\pi(s) = \rho_\pi^s(1)$, is a *fundamental characteristic* of AR(1) processes [8].)

THEOREM 2: Suppose a random walk on *any* $\mathcal{L}$ (T) is used to generate a time series on the $f_{\alpha i}$. If that time series is consistent with an AR(1) process, $\mathcal{L}$ is elementary.

PROOF: For any x_i visited by the random walk on T: $E(f_i) = \alpha = \pi Tf = \pi f$. Now define $[z_t] = [f_{i,t} - \alpha]$ to be the α normalized objective function values comprising the time series yielded from the random walk, i.e., the t^th^ normalized solution visited in the generation of the time series has objective function, $f_{\alpha i}$. Classically, a theoretical AR(1) process is defined by the recurrence equation,

$$z_t = \phi_1 z_{t-1} + a_t \tag{4}$$

where a_t is a random deviate taken from $N(0, \sigma^2)$, a normal distribution with mean 0 and variance σ^2.

Consider the temporally adjacent pair, z_t and z_{t-1}. By definition, $z_{t-1} \equiv f_{\alpha i}$ for *some* fixed i. For a given z_{t-1} (corresponding to an x_i), there are d_i possible values of z_t associated with the neighbors of z_{t-1}: $z_{t,j}$, $j = 1,\ldots, d_i$. In our random walk over a given finite $\mathcal{L}$, the parameters a_t are not distributed as $N(0, \sigma^2)$; rather, they are random deviates drawn from a finite discrete probability distribution with an expected value of zero. This follows directly from the fact that $E(z_t) = 0$ for all t and $a_t = z_t - \phi_1 z_{t-1}$.

Summing (4) over all possible values of z_t (i.e., the neighboring solutions of z_{t-1})and averaging yields

$$\sum_{j=1}^{d_i} \frac{z_{t,j}}{d_i} = \phi_1 \sum_{j=1}^{d_i} \frac{z_{t-1}}{d_i} + \sum_{j=1}^{d_i} \frac{a_{t,j}}{d_i} \tag{5}$$

Notice that

$$\sum_{j=1}^{d_i} \frac{z_{t,j}}{d_i} = \underset{x_j \in \mathcal{N}_i}{Avg}\, f_{\alpha j} = T_i f_\alpha \tag{6}$$

and

$$\sum_{j=1}^{d_i} \frac{z_{t-1}}{d_i} = f_{\alpha i} \tag{7}$$

Substituting (6) and (7) into (5) we obtain

$$T_i f_\alpha = \phi_1 f_{\alpha i} + \sum_{j=1}^{d_i} \frac{a_{t,j}}{d_i}, \; i=1, \ldots, /X/ \tag{8}$$

(Note that, by the Central Limit Theorem, the last term in Equation 8 will be distributed as an approximately Normal random variable given a sufficiently large d_i.)

Taking the expectation of (8) yields

$$T_i f_\alpha = \phi_1 f_{\alpha i}, \; i=1, \ldots, /X/. \tag{9}$$

In vector-matrix form, (9) can be written as $Tf_\alpha = \phi_1 f_\alpha$ which implies that the landscape $\mathcal{L}$ associated with T is elementary with eigenvalue $\lambda = 1-\phi_1 = 1-\rho(1)$. □

Theorems 1 and 2 show that for any *arbitrary* T, a landscape $\mathcal{L}$ is elementary if and *only* if a univariate time series on f_α generated from a random walk on T is consistent with an autoregressive process of order 1, i.e., an AR(1) process.

Let us define a *flat landscape* to be a landscape where all $f_{\alpha i} = 0$. We now consider four properties associated with the stationary distribution of T, π, and α, the expected value of the f_i given T.

PROPOSITION 1. For all landscapes $\mathcal{L}$ that share a given arbitrary transition matrix T (excluding flat landscapes), all f_α yielding elementary $\mathcal{L}$ are orthogonal to π, i.e., $\pi \perp f_\alpha$.

PROOF: If $\mathcal{L}$ is elementary, then $Tf_\alpha = (1-\lambda)f_\alpha$ which implies $\pi' Tf_\alpha = (1-\lambda)\pi' f_\alpha$. Since $\pi' T = \pi$ [2], *then* $\pi' f_\alpha = (1-\lambda)\pi' f_\alpha$ or equivalently $\lambda\pi' f_\alpha = 0$. Excluding the case of a flat landscape , where $\lambda=0$, we obtain $\pi' f_\alpha = 0$, i.e., $\pi \perp f_\alpha$. Hence, the weighted sum of the normed $f_{\alpha i}$ is zero. □

PROPOSITION 2. For all landscapes $\mathcal{L}$ that share an arbitrary aperiodic transition matrix T, all f_α , for which the random walk on T yields an AR(1) process, are orthogonal to π.

PROOF: Let $\mathcal{L}$ be a landscape for which a random walk yields an AR(1) process. For any AR(1) process, $\rho_\pi^{s}(1) = \rho_\pi(s)$. Thus $f_\alpha' \Pi T^s f_\alpha = \rho_\pi^{s}(1) f_\alpha' \Pi f_\alpha$, i.e., $f_\alpha' \Pi T^s f_\alpha$ is linearly proportional to $\rho_\pi^{s}(1)$.

If $|\rho_\pi(1)| < 1$, $\lim_{s\to\infty} \rho_\pi^{s}(1) = 0$. Hence $\lim_{s\to\infty} f_\alpha' \Pi T^s f_\alpha = 0$. Defining G to be a square matrix where $G_{ij} = 1\ \forall$ i,j, then $\lim_{s\to\infty} T^s = G\Pi$. Therefore, $\lim_{s\to\infty} f_\alpha' \Pi T^s f_\alpha = (\pi' f_\alpha)^2 = 0$ which can be true only if $\pi' f_\alpha = 0$. Therefore, $\pi \perp f_\alpha$.□

PROPOSITION 3. For doubly stochastic T , then $\pi' f = \mu$.

PROOF: For doubly stochastic T, $\pi = [\frac{1}{|X|}]$. Hence $\pi' f = \frac{\sum f_i}{|X|} = \mu$. □

LEMMA 1: For any fixed $\mathcal{L}$ (excluding flat landscapes), if there exists a normalization constant α, such that $\mathcal{L}$ is elementary then α is unique.

PROOF: Define $e = (1, 1, ..., 1)'$ and $0 = (0, 0, ..., 0)'$ to be $|X|$ dimensional vectors of ones, and zeros, respectively. Let $\alpha \neq \beta$ be two different normalization constants yielding elementary landscapes, i.e.,

$$Lf_\alpha = \lambda_\alpha f_\alpha$$

and

$$Lf_\beta = \lambda_\beta f_\beta$$

Subtracting (3.4) from (3.3) we obtain

$$\lambda_\alpha f_\alpha - \lambda_\beta f_\beta = L(f_\alpha - f_\beta) = (\beta - \alpha)Le = 0$$

Therefore, $\lambda_\alpha f_\alpha = \lambda_\beta f_\beta$.

We must consider two possibilities: $\lambda_\alpha = \lambda_\beta$ and $\lambda_\alpha \neq \lambda_\beta$.

- Let $\lambda_\alpha = \lambda_\beta = \lambda$ where $\lambda \neq 0$ (disallowing flat landscapes). Hence $f_\alpha = f_\beta \Rightarrow \alpha e = \beta e \Rightarrow \alpha = \beta$.
- Let $\lambda_\alpha \neq \lambda_\beta$ ($\lambda_\alpha \neq 0, \lambda_\beta \neq 0$)

  Hence $f_\alpha = \dfrac{\lambda_\beta}{\lambda_\alpha} f_\beta \Rightarrow f - \alpha e = \dfrac{\lambda_\beta}{\lambda_\alpha}(f - \beta e)$

  $$\Rightarrow (1 - \frac{\lambda_\beta}{\lambda_\alpha}) f = (\alpha - \frac{\lambda_\beta}{\lambda_\alpha}\beta) e$$

  $$\Rightarrow f = [(\alpha - \frac{\lambda_\beta}{\lambda_\alpha}\beta)\frac{\lambda_\alpha}{\lambda_\alpha - \lambda_\beta}] e$$

  which implies a flat landscape which are excluded in this proposition.

Therefore, if there exists an α such that $\mathcal{L}$ is elementary then α is unique.□

3. Conclusions and Future Research Directions

The primary contributions of this paper are:

(1) proving that *any* elementary $\mathcal{L}$ (arbitrary *T*) will possess an exponential decline in the autocorrelation spectrum consistent with an AR(1) process, i.e., $\rho_\pi(s) = \rho_\pi^{\,s}(1)$ and

(2) proving that a landscape $\mathcal{L}$ is elementary if and *only* if a univariate time series on f_α generated from a random walk on *T* is consistent with an AR(1) process.

These contributions are accompanied by the proof of four new properties associated with elementary $\mathcal{L}$.

Based on the insights provided by contribution (2), we are currently investigating the development of a methodology that will allow practitioners to generate random walks on landscapes associated with COPs and use the information gained to conclude whether their selected neighborhood yields an elementary landscape. In this effort, we are attempting to derive general guidelines on sufficient lengths of time series required to detect meaningful *departures* from AR(1) behavior.

An additional promising direction for future efforts would be to investigate structures of other possible neighborhoods that could possess properties favorable for heuristic search. Initial explorations of this type would be based upon other simple Box-Jenkins ARIMA models.

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