New knowledge about the Elementary Landscape Decomposition for solving the Quadratic Assignment Problem

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ABSTRACT

Previous works have shown that studying the characteristics of the Quadratic Assignment Problem (QAP) is a crucial step in gaining knowledge that can be used to design tailored meta-heuristic algorithms. One way to analyze the characteristics of the QAP is to decompose its objective function into a linear combination of orthogonal sub-functions that can be independently studied. In particular, this work focuses on a decomposition approach that has attracted considerable attention: the Elementary Landscape Decomposition (ELD).

The main drawback of the ELD is that it does not allow an understandable characterization of what is being measured by each component of the decomposition. Thus, it turns out difficult to design new efficient meta-heuristic algorithms for the QAP based on the ELD. To address this issue, in this work, we delve deeper into the ELD by means of an additional decomposition of its elementary components. Conducted experiments show that the performed analysis may be used to explain the behaviour of ELD-based methods, providing critical information about their potential applications.

CCS CONCEPTS

• **Mathematics of computing → Combinatorial optimization**; • **Theory of computation → Random search heuristics**.

KEYWORDS

Quadratic Assignment Problem, Elementary Landscapes

ACM Reference Format:
Xabier Benavides, Josu Ceberio, Leticia Hernando, and Jose A. Lozano. 2023. New knowledge about the Elementary Landscape Decomposition for solving the Quadratic Assignment Problem. In *Genetic and Evolutionary Computation Conference (GECCO '23), July 15–19, 2023, Lisbon, Portugal.* ACM, New York, NY, USA, 9 pages. https://doi.org/10.1145/3583131.3590369

GECCO '23, July 15–19, 2023, Lisbon, Portugal

ACM ISBN 979-8-4007-0119-1/23/07…$15.00
https://doi.org/10.1145/3583131.3590369

1 INTRODUCTION

The "no free-lunch" theorem [31] states that there is no single meta-heuristic algorithm that performs the best for all Combinatorial Optimization Problems (COPs). Therefore, considering the specific characteristics of the problem to be solved is crucial when designing the best possible algorithm for a particular context. However, due to the NP-hard nature of many COPs [1, 27], studying their characteristics may be a task as complex as optimizing them. A possible solution for this issue is to decompose the problem into a set of orthogonal sub-problems that are easier to work with, using techniques such as Elementary Landscape Decomposition (ELD).

The ELD [12] is a decomposition method that allows us to split a COP into a linear combination of independent elementary components. The ELD has already been used to analyze and improve the performance of meta-heuristic algorithms. For example, Ceberio et al. [8] used the ELD as a multi-objectivization method that allowed them to obtain a diverse set of promising solutions for a series of COPs. Moreover, Benavides et al. [2] proposed a new algorithm called the Variable Function Search (VFS) that uses the components of the ELD to guide a local search. Although these works illustrated the benefits of ELD-based meta-heuristics, it is still not clear why considering information about the decomposition during the optimization process seems to be a good policy in some cases.

Among all the COPs with a known ELD, we are interested in the Quadratic Assignment Problem (QAP) [10]. The QAP was originally introduced as a mathematical model for the location of a set of indivisible economic activities [22], and has since been extended to many areas such as facility layout design [17], parallel production scheduling [18] or backboard wiring [4]. Moreover, some other relevant COPs can be seen as particular cases of the QAP, as for example the Linear Ordering Problem (LOP) [9], the Traveling Salesman Problem (TSP) [21], or the DNA Fragment Assembly Problem (DNA-FA) [24]. For these reasons, the QAP has been extensively studied in the literature about the ELD [2, 7, 10, 11], and thus, will be the subject of this work.

The ELD of the QAP lacks a straightforward interpretation that would allow us to design ELD-based meta-heuristics in an informed manner. In this paper, we try to further understand the ELD of the QAP by performing an additional decomposition of its elementary components (for simplicity, we focus on symmetric instances with null main diagonals). This decomposition will allow us to characterize each component of the ELD as a linear combination of three common sub-functions, which in turn will help us to analyze the effects of including the ELD in the optimization process. Then, we will use the acquired knowledge to decide how to use this approach for solving different QAP instances.

This paper is organized as follows. Sections 2 and 3 introduce the concepts that are needed to understand this work. Section 4 explains the proposed decomposition of the components of the ELD, which is analytically studied in Sections 5 and 6 from both theoretical and experimental perspectives. The results of these analyses are further discussed in Section 7. Finally, the general conclusions and future research lines are highlighted in Section 8.

2 QUADRATIC ASSIGNMENT PROBLEM

Given a set of n facilities and n possible locations, the goal of the Quadratic Assignment Problem (QAP) [22, 23] is to find the facility-location assignment that minimizes the costs derived from the communications between facilities. In order to do that, we need to consider the distances between locations (stored in a distance matrix $D_{n\times n} = [d_{i,j}]$) and the work flows between facilities (stored in a flow matrix $H_{n\times n} = [h_{p,q}]$). The objective function uses this information to measure the quality of any given solution σ:

$$f(\sigma) = \sum_{i=1}^{n}\sum_{j=1}^{n} d_{i,j} h_{\sigma(i),\sigma(j)} \tag{1}$$

where σ is a permutation of size n that represents the facility-location assignment and $\sigma(i)$ is the facility assigned to the location i. Thus, the search space of the problem is the set of all the permutations of size n, denoted as S_n. The goal in the QAP is to find the assignment $\sigma^* \in S_n$ that minimizes Equation 1.

3 ELEMENTARY LANDSCAPE DECOMPOSITION

Given a COP defined by the search space Ω and the objective function f, a neighborhood function is defined as $N : \Omega \mapsto \mathcal{P}(\Omega)$, where $\mathcal{P}(\Omega)$ is the power set of Ω. In other words, the neighborhood function assigns to each solution $x \in \Omega$ a set of solutions $N(x) \subset \Omega$, known as the neighborhood of x. This creates a neighborhood structure that interconnects the solutions in the search space. From now on, we will only consider symmetric ($y \in N(x) \Leftrightarrow x \in N(y)$) and regular ($|N(x)| = d$ for all $x \in \Omega$) neighborhood functions.

A landscape of a combinatorial optimization problem [26, 28] is represented as a triplet (Ω,f,N), where Ω is the search space of the problem, f is the objective function and N is a neighborhood function. Among all possible landscapes, it has been shown that those that satisfy the Grover's wave equation [19], known as elementary landscapes, have some properties that make them promising candidates for being solved using local search-based algorithms [28, 30]. The Grover's wave equation is expressed as

$$\underset{y\in N(x)}{avg}\{f(y)\} = f(x) + \frac{k}{|N(x)|}\left(\bar{f} - f(x)\right) \tag{2}$$

where k is a characteristic constant and $\bar{f}$ is the average objective value of all the solutions in the search space. The objective function of any landscape that satisfies Equation 2 is denoted as elementary function [19, 28].

One of the advantages of elementary landscapes is that the Grover's wave equation allows computing the average objective value of the neighborhood of any solution $x \in \Omega$ based on the objective value of that particular solution x. Moreover, the Grover's wave equation can also be used to compute the average objective value of a partial neighborhood $M \subset N(x)$ [30]. From a practical perspective, this can be helpful if we have an algorithm that considers the neighborhood of multiple solutions at the same time, since we can use it to decide which neighborhood should be explored at each step of the search. As the solution evaluation may be costly, this feature may be used to create efficient local search-based methods.

In addition to the potential efficiency improvements, elementary landscapes are also interesting due to their common properties. In particular, this type of landscapes always satisfy the following [13]:

(1) $f(x) < \bar{f} \Longrightarrow f(x) < \underset{y\in N(x)}{avg}\{f(y)\} < \bar{f}$
(2) $f(x) = \bar{f} \Longrightarrow f(x) = \underset{y\in N(x)}{avg}\{f(y)\} = \bar{f}$
(3) $f(x) > \bar{f} \Longrightarrow f(x) > \underset{y\in N(x)}{avg}\{f(y)\} > \bar{f}$

This implies that in an elementary landscape the objective value of any local minimum is always equal to or lower than the average objective function value $\bar{f}$ (first condition), while the opposite happens in the case of the local maxima (third condition). Furthermore, the properties above also prove that certain types of plateaus cannot exist in elementary landscapes [30].

All these characteristics are common to every landscape that follows the Grover's wave equation. Therefore, we can observe that elementary landscapes always have a well-known structure, which is particularly useful for dealing with COPs. However, many of the most relevant COPs cannot be expressed as a single elementary landscape based on any known neighborhood. Nevertheless, given a symmetric neighborhood function, any landscape that is not elementary can be expressed as a linear combination of a set of elementary landscapes. This decomposition process is known as Elementary Landscape Decomposition (ELD) [12].

3.1 Elementary Landscape Decomposition of the QAP

The ELD for the Quadratic Assignment Problem that was proposed in [10] is based on the *swap* neighborhood operator, which has been widely used in the literature for solving the QAP [25]. Given a permutation $\sigma = (\sigma(1)...\sigma(i)...\sigma(j)...\sigma(n))$, this neighborhood operator consists of exchanging two items $\sigma(i)$ and $\sigma(j)$ in order to obtain a new neighbor solution $\sigma' = (\sigma(1)...\sigma(j)...\sigma(i)...\sigma(n))$. Hence, the original landscape used in the decomposition is (S_n, f, N_s), where S_n is the set of all permutations of size n, f is the objective function of the QAP, and N_s is the neighborhood function based on the swap operator. In what follows, we denote this landscape as L.

The ELD of L consists of finding a set of m elementary functions $\{f^1, f^2, ..., f^m\}$ that form m elementary landscapes along with the original search space and neighborhood function. These elementary

Table 1: $\alpha^m, \beta^m, \gamma^m, \epsilon^m, \zeta^m$ parameter values ($m = 1, 2, 3$).

	α	β	γ	ϵ	ζ
ϕ^1	$n-3$	$1-n$	-2	0	-1
ϕ^2	$n-3$	$n-3$	0	0	1
ϕ^3	$2n-3$	1	$n-2$	0	-1

functions must satisfy that $f(\sigma) = f^1(\sigma) + f^2(\sigma) + ... + f^m(\sigma)$ for every $\sigma \in S_n$, so we can see that the goal of the ELD is to decompose the objective function of the QAP into a sum of sub-functions. In order to do that, we first rewrite Equation 1 as follows:

$$f(\sigma) = \sum_{i,j=1}^{n} \sum_{p,q=1}^{n} d_{i,j} h_{p,q} \delta^{p}_{\sigma(i)} \delta^{q}_{\sigma(j)} \tag{3}$$

where δ^b_a represents the Kronocker delta function that returns 1 if $a = b$, and 0 otherwise. Equation 3 can be easily separated into two different parts: the instance related part that depends on the distance and flow matrices ($\psi_{i,j,p,q} = d_{i,j} h_{p,q}$) and the problem related part that depends on σ ($\varphi_{(i,j)(p,q)}(\sigma) = \delta^{p}_{\sigma(i)} \delta^{q}_{\sigma(j)}$). Hence,

$$f(\sigma) = \sum_{i,j=1}^{n} \sum_{p,q=1}^{n} \psi_{i,j,p,q} \varphi_{(i,j)(p,q)}(\sigma) \tag{4}$$

It is important to remark that the value of $\psi_{i,j,p,q}$ does not vary depending on the input solution, so f is just a linear combination of $\varphi_{(i,j)(p,q)}(\sigma)$. Since any linear combination of elementary functions (with the same characteristic constant k) is also an elementary function, the work in [10] focuses on decomposing $\varphi_{(i,j)(p,q)}(\sigma)$, that is, the problem related part. Thus, f can be decomposed into three orthogonal functions [10]:

$$f^1(\sigma) = \sum_{\substack{i,j,p,q=1 \\ i \neq j, p \neq q}}^{n} \psi_{i,j,p,q} \frac{\phi^1_{(i,j)(p,q)}(\sigma)}{2n} \tag{5}$$

$$f^2(\sigma) = \sum_{\substack{i,j,p,q=1 \\ i \neq j, p \neq q}}^{n} \psi_{i,j,p,q} \frac{\phi^2_{(i,j)(p,q)}(\sigma)}{2(n-2)} \tag{6}$$

$$f^3(\sigma) = \sum_{i,p=1}^{n} \psi_{i,i,p,p} \varphi_{(i,i)(p,p)}(\sigma) + \sum_{\substack{i,j,p,q=1 \\ i \neq j, p \neq q}}^{n} \psi_{i,j,p,q} \frac{\phi^3_{(i,j)(p,q)}(\sigma)}{n(n-2)} \tag{7}$$

where $f(\sigma) = f^1(\sigma) + f^2(\sigma) + f^3(\sigma)$ for every $\sigma \in S_n$. The $\phi^m_{(i,j)(p,q)}$ auxiliary functions are defined as:

$$\phi^m_{(i,j)(p,q)}(\sigma) = \begin{cases} \alpha^m & \text{if } \sigma(i) = p \wedge \sigma(j) = q \\ \beta^m & \text{if } \sigma(i) = q \wedge \sigma(j) = p \\ \gamma^m & \text{if } \sigma(i) = p \oplus \sigma(j) = q \\ \epsilon^m & \text{if } \sigma(i) = q \oplus \sigma(j) = p \\ \zeta^m & \text{if } \sigma(i) \neq p, q \wedge \sigma(j) \neq p, q \end{cases} \tag{8}$$

where $1 \leq i, j, p, q \leq n$ and $\alpha^m, \beta^m, \gamma^m, \epsilon^m, \zeta^m \in \mathbb{R}$. The parameter values for each of the functions $m = 1, 2, 3$ are shown in Table 1. The operator $\oplus$ stands for the exclusive OR operator.

Considering the search space and the neighborhood function of L, the functions f^1, f^2 and f^3 are elementary with characteristic constants $k^1 = 2n$, $k^2 = 2(n-1)$ and $k^3 = n$, respectively (obtained from Equation 2). Thus, they form three independent elementary landscapes $L^1 = (S_n, f^1, N_s)$, $L^2 = (S_n, f^2, N_s)$ and $L^3 = (S_n, f^3, N_s)$. These elementary landscapes are, precisely, the components of the ELD of the QAP.

Although the ELD of the problem consists of three components, this does not mean that all the instances of the QAP are composed of three non-constant elementary landscapes. For example, [2] proved that the objective function of L_1 is constant when at least one of the matrices that form the QAP is symmetric with respect to the main diagonal. Something similar happens in the case of the Traveling Salesman Problem (TSP), which is a special case of the QAP. In TSP-like instances, the objective function of L_3 becomes constant for all the solutions in the search space [10]. As a result, if a QAP instance meets certain characteristics, some of the elementary landscapes may be irrelevant for optimization purposes.

4 DECOMPOSITION OF THE ELEMENTARY FUNCTIONS

One of the main drawbacks of the ELD is that it is not easy to interpret the aspects of the solutions that are being evaluated by each of the individual components. Thus, it is difficult to design new meta-heuristic algorithms that exploit the advantages of working with elementary landscapes. In order to address this issue, in this section we propose an additional decomposition of the components of the ELD of the QAP that tries to provide an understandable characterization of each of them.

Before explaining the proposed decomposition, it is important to remark that this approach focuses on decomposing the objective functions of the elementary landscapes, that is, the elementary functions. Thus, for the sake of clarity, in what follows we mainly talk about the f^1, f^2 and f^3 functions, and not about the landscapes as a whole (which also include the search space and the neighborhood function). However, the reader should keep in mind that the landscape concept is always implicitly present.

Let us consider a symmetric QAP instance ($d_{i,j} = d_{j,i} \wedge h_{i,j} = h_{j,i}$ for every $i, j = 1, ..., n$) with null main diagonals ($d_{i,i} = 0 \wedge h_{i,i} = 0$ for every $i = 1, ..., n$). The vast majority of the benchmark instances in the literature satisfy these two conditions [5, 16], so from now on, we will focus on this particular case to simplify the decomposition process. However, it is important to notice that similar analyses can be conducted for other types of instances. Taking this into account, let us rewrite the elementary functions of the ELD (Equations 5, 6, 7) as follows.

$$f^1(\sigma) = \sum_{a=1}^{n-1} \sum_{b=a+1}^{n} \sum_{c=1}^{n-1} \sum_{d=c+1}^{n} \frac{g^1_{(a,b),(c,d)}(\sigma)}{2n} \tag{9}$$

$$f^2(\sigma) = \sum_{a=1}^{n-1} \sum_{b=a+1}^{n} \sum_{c=1}^{n-1} \sum_{d=c+1}^{n} \frac{g^2_{(a,b),(c,d)}(\sigma)}{2(n-2)} \tag{10}$$

$$f^3(\sigma) = \sum_{a=1}^{n-1} \sum_{b=a+1}^{n} \sum_{c=1}^{n-1} \sum_{d=c+1}^{n} \frac{g^3_{(a,b),(c,d)}(\sigma)}{n(n-2)} \tag{11}$$

where f^m is the elementary function that corresponds to the L^m elementary landscape, and $g^m_{(a,b)(c,d)}(\sigma) = \psi_{a,b,c,d}\phi^m_{(a,b)(c,d)}(\sigma) + \psi_{b,a,c,d}\phi^m_{(b,a)(c,d)}(\sigma) + \psi_{a,b,d,c}\phi^m_{(a,b)(d,c)}(\sigma) + \psi_{b,a,d,c}\phi^m_{(b,a)(d,c)}(\sigma)$. As can be seen, the $\sum_{i,p=1}^{n} \psi_{i,i,p,p}\varphi_{(i,i)(p,p)}(\sigma)$ term has been removed from the f^3 function since its value is 0 when all the elements in the main diagonal of the distance and flow matrices are zero. As the instance is symmetric, $\psi_{a,b,c,d} = \psi_{b,a,c,d} = \psi_{a,b,d,c} = \psi_{b,a,d,c}$, so we can simplify the previous auxiliary function as $g^m_{(a,b)(c,d)}(\sigma) = \psi_{a,b,c,d}\big(\phi^m_{(a,b)(c,d)}(\sigma)+\phi^m_{(b,a)(c,d)}(\sigma)+\phi^m_{(a,b)(d,c)}(\sigma)+\phi^m_{(b,a)(d,c)}(\sigma)\big)$. Based on Equation 8, $g^m_{(a,b)(c,d)}$ has three possible outcomes:

- If $\sigma(a) = c \wedge \sigma(b) = d$ or $\sigma(a) = d \wedge \sigma(b) = c$, then $g^m_{(a,b)(c,d)} = (2\alpha^m + 2\beta^m)\psi_{a,b,c,d}$.
- If $\sigma(a) = c \oplus \sigma(b) = d$ or $\sigma(a) = d \oplus \sigma(b) = c$, then $g^m_{(a,b)(c,d)} = (2\gamma^m + 2\epsilon^m)\psi_{a,b,c,d}$.
- If $\sigma(a) \neq c, d \wedge \sigma(b) \neq c, d$, then $g^m_{(a,b)(c,d)} = 4\zeta^m\psi_{a,b,c,d}$.

where the parameters α^m, β^m, γ^m, ϵ^m and ζ^m depend on the value of m (Table 1). Considering the three cases separately, we can decompose $g^m_{(a,b)(c,d)}$ as

$$\chi^m_{(a,b)(c,d)}(\sigma) = \begin{cases} (2\alpha^m + 2\beta^m)\psi_{a,b,c,d} & \text{if } \sigma(a) = c \wedge \sigma(b) = d \text{ or} \\ & \sigma(a) = d \wedge \sigma(b) = c \\ 0 & \text{otherwise} \end{cases} \tag{12}$$

$$\omega^m_{(a,b)(c,d)}(\sigma) = \begin{cases} (2\gamma^m + 2\epsilon^m)\psi_{a,b,c,d} & \text{if } \sigma(a) = c \oplus \sigma(b) = d \text{ or} \\ & \sigma(a) = d \oplus \sigma(b) = c \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

$$\tau^m_{(a,b)(c,d)}(\sigma) = \begin{cases} 4\zeta^m\psi_{a,b,c,d} & \text{if } \sigma(a) \neq c, d \wedge \sigma(b) \neq c, d \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

where $g^m_{(a,b)(c,d)}(\sigma) = \chi^m_{(a,b)(c,d)}(\sigma)+\omega^m_{(a,b)(c,d)}(\sigma)+\tau^m_{(a,b)(c,d)}(\sigma)$. For the sake of simplicity, we define the following three auxiliary functions that are just Boolean versions of χ^m, ω^m and τ^m:

$$\chi'_{(a,b)(c,d)}(\sigma) = \begin{cases} 1 & \text{if } \sigma(a) = c \wedge \sigma(b) = d \text{ or} \\ & \sigma(a) = d \wedge \sigma(b) = c \\ 0 & \text{otherwise} \end{cases} \tag{15}$$

$$\omega'_{(a,b)(c,d)}(\sigma) = \begin{cases} 1 & \text{if } \sigma(a) = c \oplus \sigma(b) = d \text{ or} \\ & \sigma(a) = d \oplus \sigma(b) = c \\ 0 & \text{otherwise} \end{cases} \tag{16}$$

$$\tau'_{(a,b)(c,d)}(\sigma) = \begin{cases} 1 & \text{if } \sigma(a) \neq c, d \wedge \sigma(b) \neq c, d \\ 0 & \text{otherwise} \end{cases} \tag{17}$$

where we have that

- $\chi^m_{(a,b)(c,d)}(\sigma) = (2\alpha^m + 2\beta^m)\psi_{a,b,c,d}\chi'_{(a,b)(c,d)}(\sigma)$
- $\omega^m_{(a,b)(c,d)}(\sigma) = (2\gamma^m + 2\epsilon^m)\psi_{a,b,c,d}\omega'_{(a,b)(c,d)}(\sigma)$
- $\tau^m_{(a,b)(c,d)}(\sigma) = 4\zeta^m\psi_{a,b,c,d}\tau'_{(a,b)(c,d)}(\sigma)$

Finally, these auxiliary functions χ', ω' and τ' can be used to decompose each elementary function f^m such that $m = 1, 2, 3$ into three (non-elementary) sub-functions:

$$f^m_\chi(\sigma) = \frac{2\alpha^m + 2\beta^m}{r^m}\sum_{a=1}^{n-1}\sum_{b=a+1}^{n}\sum_{c=1}^{n-1}\sum_{d=c+1}^{n}\psi_{a,b,c,d}\chi'_{(a,b)(c,d)}(\sigma) \tag{18}$$

$$f^m_\omega(\sigma) = \frac{2\gamma^m + 2\epsilon^m}{r^m}\sum_{a=1}^{n-1}\sum_{b=a+1}^{n}\sum_{c=1}^{n-1}\sum_{d=c+1}^{n}\psi_{a,b,c,d}\omega'_{(a,b)(c,d)}(\sigma) \tag{19}$$

$$f^m_\tau(\sigma) = \frac{4\zeta^m}{r^m}\sum_{a=1}^{n-1}\sum_{b=a+1}^{n}\sum_{c=1}^{n-1}\sum_{d=c+1}^{n}\psi_{a,b,c,d}\tau'_{(a,b)(c,d)}(\sigma) \tag{20}$$

where $r^1 = 2n$, $r^2 = 2(n-2)$, $r^3 = n(n-2)$ and $f^m(\sigma) = f^m_\chi(\sigma) + f^m_\omega(\sigma) + f^m_\tau(\sigma)$ for every $\sigma \in S_n$.

The main advantage of the proposed decomposition is that each of the sub-functions (f^m_χ, f^m_ω, f^m_τ) evaluates different aspects of a given solution. For every combination of values a, b, c and d such that $1 \leq a < b \leq n$ and $1 \leq c < d \leq n$, we have that:

- The only non-null terms in f^m_χ are the ones that satisfy that $\sigma(a) = c \wedge \sigma(b) = d$ or $\sigma(a) = d \wedge \sigma(b) = c$. That is, this function only evaluates the combinations of locations-facilities in which both current facilities (c and d) are in the current locations (a and b) in the solution σ.
- The only non-null terms in f^m_ω are the ones that satisfy that $\sigma(a) = c \oplus \sigma(b) = d$ or $\sigma(a) = d \oplus \sigma(b) = c$. That is, this function only evaluates the combinations of locations-facilities in which just one of the current facilities (c or d) is in one of the current locations (a or b) in the solution σ.
- The only non-null terms in f^m_τ are the ones that satisfy that $\sigma(a) \neq c, d \wedge \sigma(b) \neq c, d$. That is, this function only evaluates the combinations of locations-facilities in which neither of the current facilities (c and d) is in the current locations (a and b) in the solution σ.

Thus, not only do the elementary functions of the ELD consider the quality of the current facility-location assignment (f^m_χ), but also the quality of the solutions that could be reached by modifying one (f^m_ω) or both (f^m_τ) of the facilities assigned to each pair of locations. Since the cases β, γ, ϵ and ζ of Equation 8 cancel each other out when the elementary landscapes are combined [10], this additional information is not explicitly present in the original landscape of the QAP, and only arises when the ELD is computed.

5 THEORETICAL ANALYSIS

Once we have defined the decomposition of the elementary functions, we can now use this new framework to analyze the ELD of the QAP. First, let us replace the parameters in the proposed sub-functions (Equations 18, 19, 20) with their actual values according to Table 1. To avoid unnecessary repetition, we only show the value of the common coefficients that depend on α^m, β^m, γ^m, ϵ^m, ζ^m and r^m, which is the only part of the equations that varies according to the elementary function (Table 2).

Based on these coefficient values, we can now study the characteristics of the proposed sub-functions in order to gain knowledge about the characterization of each component in the ELD. With this purpose, we first compute the expected values of the sub-functions[1]

[1]See supplementary material for further details.

Table 2: Common coefficients in f_χ^m, f_ω^m and f_τ^m for $m = 1, 2, 3$.

	χ	ω	τ
f^1	$\frac{-2}{n}$	$\frac{-2}{n}$	$\frac{-2}{n}$
f^2	$\frac{2(n-3)}{n-2}$	0	$\frac{2}{n-2}$
f^3	$\frac{4(n-1)}{n(n-2)}$	$\frac{2}{n}$	$\frac{-4}{n(n-2)}$

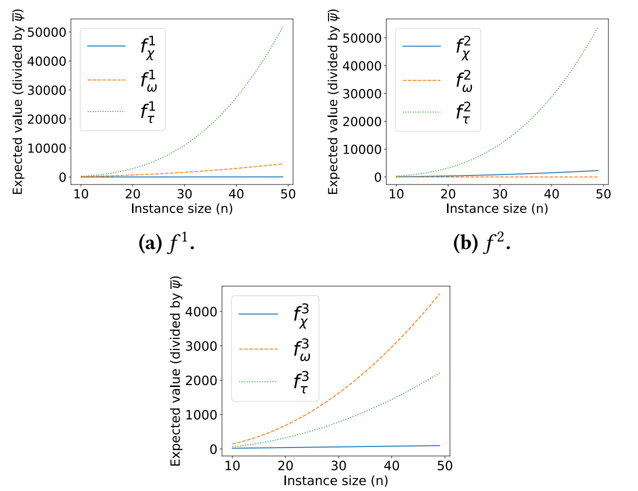
Table 3: Expected value and variance of the sub-functions. $\bar{\psi}$ represents the average value of $\psi_{a,b,c,d}$ such that $1 \leq a < b \leq n$ and $1 \leq c < d \leq n$. Moreover, s_χ^2, s_ω^2 and s_τ^2 represent the variances of the summations in f_χ^m, f_ω^m and f_τ^m, respectively.

		Expected value	Variance
f^1	f_χ^1	$-(n-1)\bar{\psi}$	$\frac{4}{n^2}s_\chi^2$
	f_ω^1	$-2(n-1)(n-2)\bar{\psi}$	$\frac{4}{n^2}s_\omega^2$
	f_τ^1	$-\frac{(n-1)(n-2)(n-3)}{2}\bar{\psi}$	$\frac{4}{n^2}s_\tau^2$
f^2	f_χ^2	$\frac{n(n-1)(n-3)}{n-2}\bar{\psi}$	$\frac{4(n-3)^2}{(n-2)^2}s_\chi^2$
	f_ω^2	0	0
	f_τ^2	$\frac{n(n-1)(n-3)}{2}\bar{\psi}$	$\frac{4}{(n-2)^2}s_\tau^2$
f^3	f_χ^3	$\frac{2(n-1)^2}{n-2}\bar{\psi}$	$\frac{16(n-1)^2}{n^2(n-2)^2}s_\chi^2$
	f_ω^3	$2(n-1)(n-2)\bar{\psi}$	$\frac{4}{n^2}s_\omega^2$
	f_τ^3	$-(n-1)(n-3)\bar{\psi}$	$\frac{16}{n^2(n-2)^2}s_\tau^2$

as a measure of the average contribution of the α, β, γ, ϵ and ζ cases to the value of the f^1, f^2 and f^3 elementary functions (Table 3).

As can be seen, the expected values of the f_χ^m, f_ω^m and f_τ^m sub-functions vary greatly from one elementary function to another. In order to visualize these differences, Figure 1 shows the magnitude of the expected values of the sub-functions for different n sizes (the $\bar{\psi}$ factor has been removed since it is common to all sub-functions).

The plots show that, for large enough instances, the f_τ^m sub-function (which measures the ζ case) is the one with the highest average contribution to the value of f^1 and f^2. In the case of f^3, however, the f_ω^m sub-function (which measures the γ and ϵ cases) has a slightly higher contribution than f_τ^m. Moreover, it is also worth mentioning that f_χ^m has a generally small contribution to the value of all the elementary functions. This may be non-intuitive since this sub-function includes the α and β cases, that is, the information that is taken into account by the original objective function of the QAP. Nevertheless, it is important to recall that the γ, ϵ and ζ cases cancel out when the landscapes are combined, which means that the sum of the f_ω^m and f_τ^m sub-functions is always 0. Thus, we have that $E[f_\omega^1]+E[f_\omega^2]+E[f_\omega^3]+E[f_\tau^1]+E[f_\tau^2]+E[f_\tau^3] = 0$, and hence, $E[f_\chi^1] + E[f_\chi^2] + E[f_\chi^3] = E[f]$. This is caused by the values of the common coefficients in the sub-functions (Table 2), which have different signs depending on the elementary function.



(a) f^1.

(b) f^2.

(c) f^3.

Figure 1: Expected value magnitude ($|E[X]|$) of the sub-functions for each elementary function (Table 3). We observe constant (f_ω^2), linear (f_χ^1, f_χ^3), quadratic (f_ω^1, f_χ^2, f_ω^3, f_τ^3) and cubic (f_τ^1, f_τ^2) behaviours.

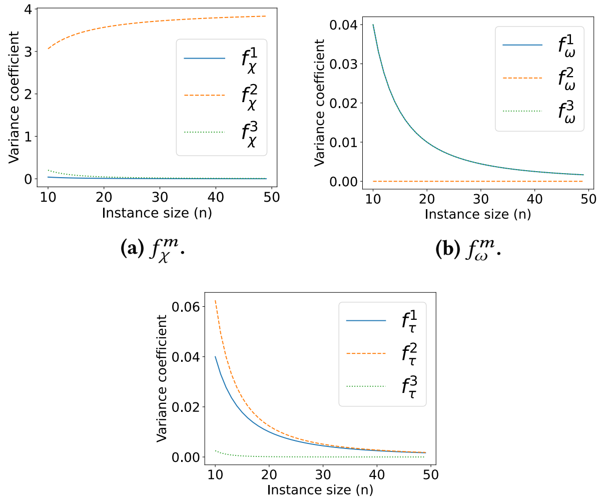
Therefore, it is not possible to minimize (or maximize) all the f_χ^m, f_ω^m or f_τ^m sub-functions at the same time.

Another characteristic that is worth studying is the variance of the sub-functions. This feature is especially relevant when we work with meta-heuristic algorithms, since the sub-functions that have higher variance are those that most influence the search process. The variances of the sub-functions are shown in Table 3.

If we look at f_χ^1, f_χ^2 and f_χ^3 in the variance column, we notice that the only variable part in the variance equations is the coefficient by which the variance of the summation (s_χ^2) is multiplied. The same happens in the case of f_ω^m and f_τ^m (considering that the coefficient in f_ω^2 is 0), and thus, we can compare the variance of a specific sub-function for different elementary functions by comparing the corresponding coefficients. Figure 2 shows the evolution of the coefficients in the variance equations of the sub-functions according to the instance size. In general, we have that:

- The variance of the f_χ^m sub-function is higher in f^2 than in the rest of the elementary functions.
- The variance of f_ω^2 is 0. Therefore, the f_ω^m sub-function has no influence in the optimization of f^2. Regarding the remaining elementary functions, the variance of f_ω^m is exactly the same in both cases.
- The variance of the f_τ^m sub-function is similar in the f^1 and f^2 elementary functions, while it is lower in f^3.

It seems that the variance contribution of the f_χ^m sub-function is particularly relevant in the case of f^2. That is, from an optimization point of view, the α and β cases (the ones already present in f) may play an important role in f^2. This is consistent with the experimental analysis made in [2], where they found that the f^2 elementary function under the swap neighborhood shares a significant number of local optima with the original landscape of the QAP.



(a) f_χ^m. (b) f_ω^m. (c) f_τ^m.

Figure 2: Evolution of the coefficients in the variance equations of f_χ^m, f_ω^m and f_τ^m (Table 3). We observe quadratic (f_χ^1, f_ω^1, f_τ^1, f_τ^2 f_χ^3, f_ω^3) and quartic (f_τ^3) decrements. The remaining cases have a (nearly) constant behaviour (f_χ^2, f_ω^2).

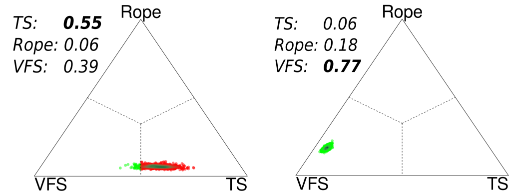
On the other hand, the variance contribution of f_ω^m also seems to be remarkable in the case of f^3. Thus, not only does f^3 take into account the information already present in f, but also the extra information given mainly by the γ and ϵ cases. In conclusion, as f^2 and f provide similar information and f^1 is constant in symmetric instances, optimizing f^3 may be a good diversification policy that exploits the benefits given by the ELD.

6 EXPERIMENTAL ANALYSIS

With all this information given by the proposed decomposition, we now use the acquired knowledge to study the impact of the ELD during the optimization process of the QAP. For this purpose, we perform an experimental study on some of the most challenging QAP instances in the literature: the *Drezner* and *Taixxeyy* instances [16]. These benchmarks are composed of 112 instances ranging from size 15 to 175 that are specifically designed to be difficult for meta-heuristic algorithms. Moreover, all the instances in the benchmarks are symmetric and have null main diagonals, so the proposed additional decomposition can be applied to them.

The experimental analysis consists of applying two different local search-based algorithms under the swap neighborhood for solving the previously mentioned QAP instances[2]: a short-term memory Tabu Search (TS) [15] and the Variable Function Search (VFS) algorithm proposed in [2]. The VFS is a modified version of the TS that takes into account the ELD during the search process. That is, when the VFS reaches a local optimum of the original objective function f, it only allows non-improving movements that lead to solutions that have a better objective value in at least one of the elementary functions of the decomposition. In doing so, it ensures that the search always moves to solutions that are better than the current one in at least one of the sub-problems, which may help us to avoid exploring poor-quality regions of the search space.

[2]Source code available in https://github.com/Av-Repos/GECCO_2023.



(a) *Drezner.* (b) *Taixxeyy.*

Figure 3: Results of the statistical analyses. The obtained expected probabilities are shown in the upper left corner.

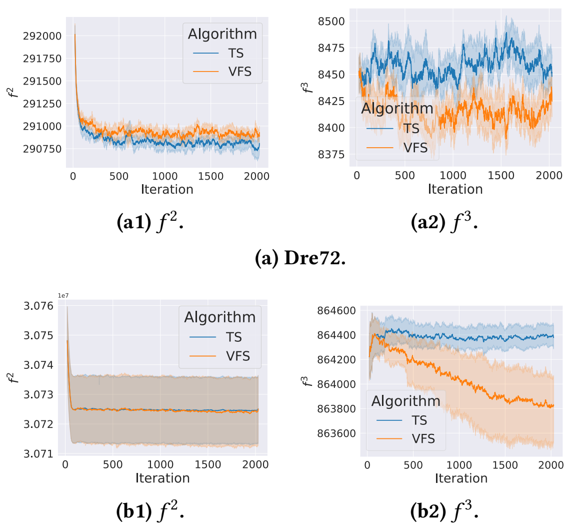
Thus, our goal in this section is to better understand the behaviour of the TS and the VFS with the help of the information gathered in the previous theoretical analysis. With this aim, we first run each of the algorithms 10 times for each of the *Drezner* and *Taixxeyy* instances. The size of the tabu list in all cases is equal to the instance size (n). Regarding the stopping criterion, a maximum number of solution evaluations has been set: $1{,}000n^2$.

Based on the obtained results, we conduct an analysis to statistically assess the difference between the performance of both algorithms. In particular, we conduct a Bayesian signed rank-test [3, 6] for each of the considered benchmarks. Given a set of performance measures obtained by two meta-heuristic algorithms, this method estimates the expected probability of each algorithm being the best for solving the test instances. The data used to compute the statistical analyses consists of the relative errors with respect to the best known solutions obtained in the experimentation.

The Bayesian signed-rank test requires defining the interval of performance difference under which both algorithms are considered to be equivalent (*rope*). Due to the differences in the scale of the relative errors, in this work the *rope* interval has been set independently for each benchmark of instances. In particular, the limits of the *rope* interval are calculated as ±1% of the average relative error obtained by both the TS and the VFS in the corresponding benchmark. Taking this into account, the results of the statistical analyses are shown as simplex plots in Figure 3.

Each point in the simplex plots represents a sample of the posterior distribution of the probability of win-lose-tie. The closer a point is to a vertex, the higher the probability of the corresponding option. If the points are closer to the TS vertex, for example, it means that the TS algorithm has a higher probability of being the best, and the same happens in the case of the VFS and *rope* vertices. Moreover, the dispersion of the point clouds gives us information about the uncertainty of the statistical analysis. If the points are close together, it means that the results of the analysis have a low uncertainty. In contrast, if the points are far apart, then the uncertainty of the analysis is higher. Thus, the Bayesian signed-rank test allows us to distinguish between the uncertainty of the behaviour of the algorithms and the uncertainty of the statistical analysis (which is caused by the lack of data).

As can be seen in Figure 3, the performance of the algorithms differs greatly depending on the benchmark. On the one hand, the TS



(a1) f^2. (a2) f^3.

(a) Dre72.

(b1) f^2. (b2) f^3.

(b) Tai75e01.

Figure 4: Evolution of the average f^2 and f^3 values during the 10 runs of the TS and VFS. The shaded areas represent the corresponding 95% confidence intervals.

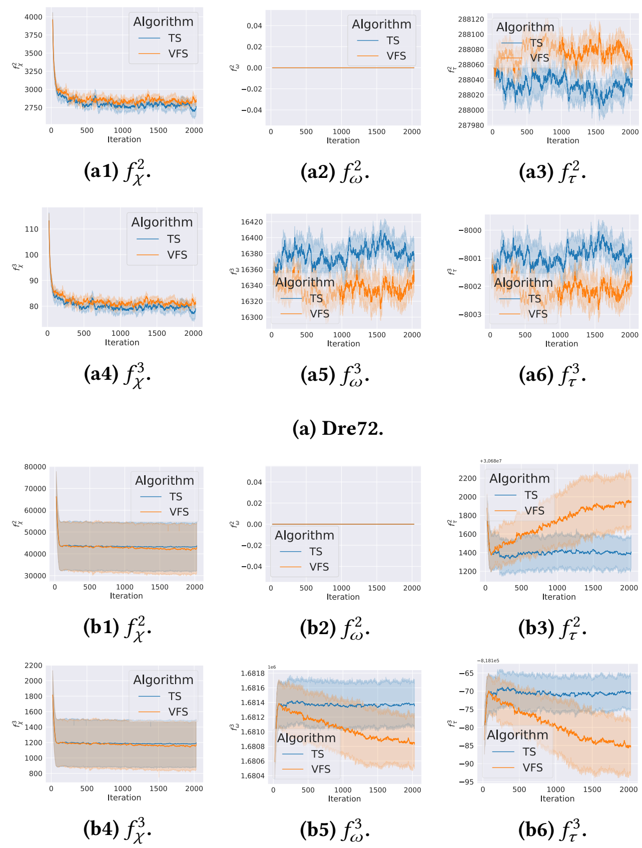
seems to be the most promising algorithm for the *Drezner* instances, although the dispersion of the point cloud shows that there is some uncertainty in the obtained results. The opposite happens in the case of the *Taixxeyy* instances, where the VFS algorithm seems to be the best with a 0.77 probability and a very low uncertainty.

Once we have seen that the performance of both algorithms (the classical approach and the one that considers the ELD) is different, the next step is to try to understand what is happening during the optimization process. Just as an example, we focus on studying one representative instance from each of the benchmarks: the *Dre72* (*Drezner*) and *Tai75e01* (*Taixxeyy*) instances.

First, let us plot the evolution of the elementary function values during the executions of the TS and VFS algorithms for the *Dre72* and *Tai75e01* instances (Figure 4). We also plot the evolution of the corresponding sub-function values to gain a deeper insight into what is being optimized at each step of the search (Figure 5). The f^1 elementary function has been left out since its value is constant in all the considered benchmark instances.

As shown in Figure 4, the behaviour of the algorithms is pretty different. First, it seems like both methods implicitly optimize the f^2 component of the problem. As explained in Section 5, this means that they first focus on the elementary function in which the variance of the α and β cases is higher, hence focusing on the information already available in the original objective function of the QAP. This can be noted in Figure 5, where the shapes of the optimization curves of the f^2_χ sub-function are nearly identical to those of the f^2 elementary function (Figure 4). This suggests that the α and β cases are the most relevant cases during the optimization of f^2, while γ, ϵ and ζ just add noise that has a low influence on the search process.

When a local optimum of f^2 is reached, the VFS algorithm tries to escape from it by optimizing the f^3 component. Thus, at this



(a1) f^2_χ. (a2) f^2_ω. (a3) f^2_τ.

(a4) f^3_χ. (a5) f^3_ω. (a6) f^3_τ.

(a) Dre72.

(b1) f^2_χ. (b2) f^2_ω. (b3) f^2_τ.

(b4) f^3_χ. (b5) f^3_ω. (b6) f^3_τ.

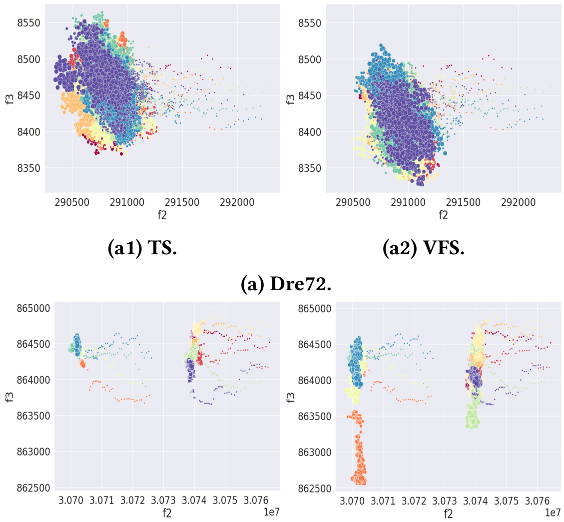
(b) Tai75e01.

Figure 5: Evolution of the average sub-function values during the 10 runs of the TS and VFS. The shaded areas represent the corresponding 95% confidence intervals.

point, the VFS uses the extra information given by the ELD to try to explore new promising regions of the search space. Once again, this can be observed in Figure 5, since the shapes of the optimization curves of f^3_ω and f^3_τ are very similar to those of f^3 (Figure 4). Therefore, as concluded in Section 5, it seems that the γ, ϵ and (to a lesser extent) ζ cases are the ones that control the optimization process of f^3. Since the TS does not incorporate the additional knowledge given by the ELD, it cannot continue improving the solution once the optimization of f^2 converges.

Although the behaviour of each algorithm remains similar across benchmarks, their performance differs depending on the target instance. In particular, the optimization of the f^3 elementary function is much more effective in *Tai75e01*, while it seems to be unnecessary in *Dre72*. To better visualize the dissimilarities between benchmarks, Figure 6 shows the comparison between the f^2 and f^3 values of the solutions visited by the TS and the VFS in both cases.

As shown in the plots, the objective value space of both instances is different. For example, in the case of *Dre72*, improving f^3 seems to worsen the f^2 value. Thus, as the variance of f^2 is generally higher than the variance of f^3 in symmetric instances [2], focusing



(a1) TS. (a2) VFS.

(a) Dre72.

(b1) TS. (b2) VFS.

(b) Tai75e01.

Figure 6: Comparison between the f^2 (x axis) and f^3 (y axis) values obtained during the 10 runs of the TS and VFS. Different colors represent different runs, and the size of the points is directly proportional to the iteration number.

on optimizing f^2 (TS) seems to be a better idea than looking for a trade-off between elementary functions (VFS) in *Drezner* instances.

On the other hand, if we look at *Tai75e01*, we do not find any negative correlation between f^2 and f^3. What is more, the solutions explored by the algorithms seem to be grouped in certain regions of the objective value space, creating *clusters* of solutions with similar f^2 and f^3 values. This grouping is particularly evident in the f^2 function (x axis), in which two different clusters can be easily distinguished. Therefore, it appears that the f^2 value of the starting solution determines, to a great extent, the solutions that are visited during the search. This suggests that there are sub-optimal regions of the search space that are difficult to escape using local search processes, similar to the *funnels* or *sinks* that arise when studying Local Optima Networks (LON) [14, 20, 29]. Consequently, considering just the α and β cases causes a premature convergence of the algorithm that may lead to sub-optimal results. This is why the VFS performs better than the TS in the *Taixxeyy* benchmark, since, in this case, the VFS can further improve the solution by focusing on f^3 once the optimization of f^2 stagnates.

7 DISCUSSION

In previous sections, we have used the proposed decomposition to characterize the components of the ELD of the QAP from both theoretical and practical points of view. During the analysis, we have found that the f^2_χ sub-function (which measures the α and β cases) is the one that has the most significant influence in the optimization process of f^2. In contrast, the f^3_ω sub-function (which measures the γ and ϵ cases) is the most relevant sub-function for the optimization of f^3.

These findings are particularly important for integrating the ELD into meta-heuristic algorithms that solve the QAP. They allow us to make more informed decisions about which elementary landscapes should be taken into account at each step of the search process, instead of just trying to jointly optimize all the elementary components as done in previous works [2, 8]. For example, a possible good policy is to first focus on the information already present in the original objective function of the QAP (f^2), and then use the f^3 elementary function to try to further improve the solution when the search converges. Although this strategy may not be suitable for all possible instances, it may provide good results if f^2 and f^3 are not negatively correlated and the search space structure of f^2 under the swap neighborhood contains sub-optimal funnels.

Finally, the proposed decomposition can also be used to deal with one of the problems of the ELD of the QAP: the computational complexity of the elementary functions. As can be observed in Equations 5, 6 and 7, the complexity of the elementary functions is $O(n^4)$, which makes it impractical to use ELD-based methods for solving large instances. However, as some sub-functions have a weak impact on the optimization process, we can just ignore the calculations that correspond to those sub-functions in order to save time. For example, f^3_ω can be efficiently calculated in $O(n^3)$. Thus, computing f^3_ω instead of f^3 would reduce the complexity of the objective function while maintaining the general behaviour of meta-heuristic algorithms. Obviously, this approach would not benefit from the advantages of an elementary landscape, but it may be an interesting strategy if we have strict computational limitations.

8 CONCLUSIONS AND FUTURE WORK

This work has shown that all the elementary landscapes that form the decomposition of the QAP under the swap neighborhood are just linear combinations of a set of smaller non-elementary components. By studying these components separately, we have been able to find interesting patterns that can be used to find general optimization policies. As some of the most studied COPs in the literature are just particular cases of the QAP (for example, TSP and LOP), the results of this work can be extended to other relevant problems with minor modifications.

It is important to remark that this work has focused on symmetric instances with null main diagonals. For the sake of completeness, similar studies should be conducted for other types of instances. However, our goal in this work was not to characterize all possible QAPs, but to provide useful tools for better understanding the ELD of the problem and its effects on meta-heuristic methods. Thus, future research lines could be aimed at designing specific optimization algorithms that take advantage of the ELD approach using the knowledge provided by our analysis.

ACKNOWLEDGMENTS

This work has been funded by the Basque Government (IT1504-22, BERC 2022-2025 program, projects KK-2021/00065 and KK-2022/00106 through Elkartek Program), the Spanish Ministry of Science and Innovation (projects PID2019-106453GA-I00 and PID2019-104966GB-I00, BCAM Severo Ochoa accreditation CEX2021-001142-S) and the Spanish Ministry of Universities (FPU21/00607 grant).

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