Variable Interactions in Multi-Objective Optimization Problems*

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Abstract: Variable interaction is an important aspect of a problem, which reflects its structure, and has implications on the design of efficient optimization algorithms. Although variable interaction has been widely studied in the global optimization community, it has rarely been explored in the multi-objective optimization literature. In this paper, we empirically and analytically study the variable interaction structures of some popular multi-objective benchmark problems. Our study uncovers nontrivial variable interaction structures for the ZDT and DTLZ benchmark problems which were thought to be either separable or non-separable.

Keywords: Variable interaction analysis, differential grouping, large-scale optimization, evolutionary multi-objective optimization.

1 Introduction

Variable interaction is a major source of difficulty in numerical optimization, which hinders the performance of optimizers, especially on functions with complex variable interaction structures [1]. Variable interaction can be loosely defined as the extend to which the optimization of a variable is affected by the values taken by other variables. Complete lack of interaction between the decision variables is the simplest form of interaction structure in which case the variables can be optimized independently irrespective of the values take by other variables. The other extreme is when each variable interacts with every other variable. However, most real-world problems fall in between these two extremes [2]. Such problems, which are often called partially separable, have a modular structure and contain several clusters of interacting variables. It is clear that if the variable interaction structure is known, the problem can be decomposed into a set of simpler problems which are easier to optimize. Decomposition-based optimization algorithms have been widely studied in the field of large-scale global optimization to alleviate the adverse effects of high-dimensionality. Although there are numerous studies on both detecting and exploiting partial separability in global optimization [3, 4], very limited studies have been dedicated to the analysis of variable interaction in the context of multi-objective optimization. For example, [5] introduced variable interaction into some mulit-objective test problems; however, their proposed method did not account for a modular design with respect to variable interaction. In this paper, by using the recently developed differential grouping method [4] and mathematical analysis, we empirically and theoretically analyze the variable interaction structures of two popular benchmark suites, ZDT [6] and DTLZ [7], from the evolutionary multi-objective optimization (EMO) literature. Contrary to the conventional wisdom [8, 9], our analysis shows that most of the ZDT and DTLZ test problems exhibit nontrivial interaction structures which change with the number of objectives. A thorough understanding of variable interaction in the existing benchmarks can have implications on analyzing the behavior of existing algorithms, the design of new algorithms, and the design of future benchmark suites. The aim of this paper is to take a small step towards bridging this gap.

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2 Preliminaries

The multi-objective optimization problem (MOP) considered in this paper is as:

$$\begin{aligned} &\text{minimize} \quad \mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), \cdots, f_m(\mathbf{x}))^T \\ &\text{subject to} \quad \mathbf{x} \in \Omega \end{aligned} \tag{1}$$

where $\Omega = \prod_{i=1}^{n}[a_i, b_i] \subseteq \mathbb{R}^n$ is the feasible region of the decision (variable) space, and $\mathbf{x} = (x_1, \ldots, x_n)^T \in \Omega$ is a candidate solution. $\mathbf{F} : \Omega \to \mathbb{R}^m$ constitutes m objective functions, and $\mathbb{R}^m$ is the objective space.

Definition 1. *A function is partially additively separable if it takes the following general form [1]:*

$$f(\mathbf{x}) = \sum_{i=1}^{k} f_i(\mathbf{x}_i) \tag{2}$$

where $\mathbf{x}_i$ are mutually exclusive decision variables of f_i, and k is the number of independent subcomponents.

This property makes it easy to optimize $f(\mathbf{x})$, because each subcomponent $\mathbf{x}_i$ can be optimized independently.

$$\underset{(\mathbf{x}_1, \cdots, \mathbf{x}_k)}{\operatorname{argmin}} f(\mathbf{x}) = \left[\underset{\mathbf{x_1}}{\operatorname{argmin}} f(\mathbf{x}), \cdots, \underset{\mathbf{x_k}}{\operatorname{argmin}} f(\mathbf{x})\right] \tag{3}$$

Definition 2. *Given a continuously differentiable function $f(\mathbf{x})$, for any pair of variables x_i and x_j, if $\frac{\partial^2 f}{\partial x_i \partial x_j} \neq 0$, then x_i and x_j are said to interact with each other; otherwise, they are said to be independent from each other.*

The differential grouping method for detecting the variable interaction structure is derived from the following theorem [4].

Theorem 1. *For an additively separable function $f(\mathbf{x})$, $\forall a, b_1 \neq b_2, \delta \in \mathbb{R}, \delta \neq 0$, if the following condition holds:*

$$\Delta_{\delta, x_p}[f](\mathbf{x})|_{x_p=a, x_q=b_1} \neq \Delta_{\delta, x_p}[f](\mathbf{x})|_{x_p=a, x_q=b_2} \tag{4}$$

then x_p and x_q are non-separable where

$$\Delta_{\delta, x_p}[f](\mathbf{x}) = f(\cdots, x_p + \delta, \cdots) - f(\cdots, x_p, \cdots) \tag{5}$$

refers to the forward difference of f with respect to variable x_p with interval δ.

Before the analysis, we describe the test problems used in this paper. ZDT benchmark suite [6] has been extensively used to benchmark numerous EMO algorithms for more than a decade and has the following general structure [10]:

$$\begin{aligned} &\text{minimize} \quad \mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}_I), f_2(\mathbf{x}_{II})) \\ &\text{subject to} \quad f_2(\mathbf{x}_{II}) = g(\mathbf{x}_{II}) \cdot h(f_1(\mathbf{x}_I), g(\mathbf{x}_{II})), \end{aligned} \tag{6}$$

where $\mathbf{x} = (\mathbf{x}_I, \mathbf{x}_{II})$ is partitioned into two non-overlapping sets. In particular, $\mathbf{x}_I = x_1$ and $\mathbf{x}_{II} = (x_2, \cdots, x_n)^T$ for all ZDT test problems. DTLZ [7] is another popular benchmark suite in the EMO literature. In essence, the DTLZ is developed based on the same principle as that of the ZDT. However, unlike ZDT, DTLZ test problems are scalable to any number of objectives. To help with the clarity of the analysis in the following section, the mathematical definitions of ZDT and DTLZ test problems are summarized in Table 1.

Table 1: Mathematical Definitions of ZDT and DTLZ Benchmark Suites

Name	Definition	Domain
ZDT1	$f_1 = x_1$ $g = 1 + 9 \cdot \sum_{i=2}^{n} x_i/(n-1)$ $h = 1 - \sqrt{f_1/g}$	$[0,1]$
ZDT2	as ZDT1, except $h = 1 - (f_1/g)^2$	$[0,1]$
ZDT3	as ZDT1, except $h = 1 - \sqrt{f_1/g} - (f_1/g)\sin(10\pi f_1)$	$[0,1]$
ZDT4	as ZDT1, except $g = 1 + 10 \cdot (n-1) + \sum_{i=2}^{n}(x_i^2 - 10\cos(4\pi x_i))$	$x_1 \in [0,1]$ $x_i \in [-5,5]$
ZDT6	$f_1 = 1 - \exp(-4x_1)\sin^6(6\pi y_1)$ $g = 1 + 9 \cdot (\sum_{i=2}^{n} x_i/(n-1))^{0.25}$ $h = 1 - (f_1/g)^2$	$[0,1]$
DTLZ1	$f_1 = (1+g)0.5\prod_{i=1}^{m-1} x_i$ $f_{j=2:m-1} = (1+g)0.5(\prod_{i=1}^{m-j} x_i)(1 - x_{m-j+1})$ $f_m = (1+g)0.5(1-x_1)$ $g = 100[n - m + 1 + \sum_{i=m}^{n}((x_i - 0.5)^2 - \cos(20\pi(x_i - 0.5)))]$	$[0,1]$
DTLZ2	$f_1 = (1+g)0.5\prod_{i=1}^{m-1}\cos(x_i\pi/2)$ $f_{j=2:m-1} = (1+g)0.5(\prod_{i=1}^{m-j}\cos(x_i\pi/2))(\sin(x_{m-j+1}\pi/2))$ $f_m = (1+g)\sin(x_1\pi/2)$ $g = \sum_{i=m}^{n}(x_i - 0.5)^2$	$[0,1]$
DTLZ3	as DTLZ2, except g is replaced by the one from DTLZ1	$[0,1]$
DTLZ4	as DTLZ2, except x_i is replaced by x_i^α, where $i \in \{1, \cdots, m-1\}, \alpha > 0$	$[0,1]$
DTLZ5	as DTLZ2, except x_i is replaced by $\frac{1+2gx_i}{4(1+g)}$, where $i \in \{2, \cdots, m-1\}$	$[0,1]$
DTLZ6	as DTLZ5, except the equation for g is replaced by $g = \sum_{i=m}^{n} x_i^{0.1}$	$[0,1]$
DTLZ7	$f_{j=1:m-1} = x_m$ $f_m = (1+g)(m - \sum_{i=1}^{m-1}[\frac{f_i}{1+g}(1 + \sin(3\pi f_i))])$ $g = 1 + 9\sum_{i=m}^{n} x_i/(n-m+1)$	$[0,1]$

3 Variable Interaction Analysis via Differential Grouping

Differential grouping [4] is a popular technique that can identify the underlying variable interaction structure of black-box continuous functions with a high accuracy. In this study, we employ its modified version (as shown in Algorithm 1) to analyze the ZDT and DTLZ benchmark suites. Due to the existence of multiple objective functions[1], Algorithm 1 applies differential grouping to each objective function independently, which results in m interaction structure matrices.

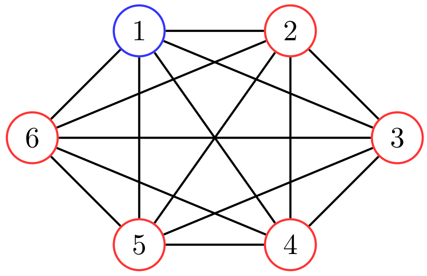
3.1 Variable Interaction Analysis on ZDT Benchmark Suite

Table 1 clearly shows that f_1 of all ZDT test problems is a fully separable function because it is only a function of x_1. Thus, we only need to analyze the variable interaction for the second objective function f_2. To keep the interaction matrices and the graphs within a manageable size, we set the number of variables to $n = 6$ which is large enough to reveal the patterns and regularities of the benchmark functions. The experimental results show that, by running Algorithm 1, f_2 of all ZDT test problems share the same variable interaction matrix, as shown in Fig. 1(a). The graphical representation of this interaction matrix is a fully connected graph which is shown in Fig. 1(b). This clearly shows that all

[1]The objective functions of ZDT and DTLZ test suites are genuinely independent.

$$
\begin{array}{c|c}
\begin{matrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{matrix} &
\begin{pmatrix}
0 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 1 & 1 \\
1 & 1 & 1 & 0 & 1 & 1 \\
1 & 1 & 1 & 1 & 0 & 1 \\
1 & 1 & 1 & 1 & 1 & 0
\end{pmatrix} \\
 & \begin{matrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \end{matrix}
\end{array}
$$

(a) variable interaction matrix



(b) variable interaction graph

Figure 1: Variable interaction structures of the f_2 function of ZDT test suite.

Algorithm 1: Interaction Analysis via Differential Grouping

Output: Interaction Structure Matrices $\mathrm{I}^{(1)}_{n\times n}, \cdots, \mathrm{I}^{(m)}_{n\times n}$

```
for i ← 1 to m do
    Initialize all entries of I^(i)_{n×n} to be 0;
    for j ← 1 to n do
        for k ← 1 to n ∧ k ≠ j do
            p^1 ← rand(1, n), p^2 ← p^1 /* rand: random number generator */
            repeat
                ξ_1 ← rand, ξ_2 ← rand;
            until |ξ_1 − p^1_j| > ε_1 ∧ |ξ_2 − p^1_k| > ε_1;
            p^2_j ← ξ_1;
            Δ_1 ← f_i(p^1) − f_i(p^2);
            p^1_k ← ξ_2, p^2_k ← ξ_2;
            Δ_2 ← f_i(p^1) − f_i(p^2);
            if |Δ_1 − Δ_2| > ε_2 then
                I^(i)_{jk} ← 1;
return I^(1)_{n×n}, ··· , I^(m)_{n×n}
```

the decision variables of f_2 interact with each other, making f_2 a fully non-separable function. In order to validate the correctness of this non-separability property, we use Definition 2 to prove Proposition 1.

Proposition 1. *f_2 of the ZDT benchmark suite is fully non-separable.*

Proof. Let us start from ZDT1. By taking the derivative of f_2 with respect to x_1, we have:

$$\frac{\partial f_2}{\partial x_1} = \frac{\partial(g - (1 - \sqrt{x_1/g}))}{\partial x_1} = \frac{\partial(g - \sqrt{x_1 g})}{\partial x_1}. \tag{7}$$

Since g is a function of x_2 to x_n, we can treat it as a constant in equation (7):

$$\frac{\partial f_2}{\partial x_1} = -0.5\sqrt{g/x_1}, \tag{8}$$

where $x_1 \neq 0$. According to Table 1, g is a summation of terms involving x_2 to x_n. Therefore:

$$\frac{\partial g}{\partial x_i} = 9/(n-1), \tag{9}$$

where $i \in \{2, \cdots, n\}$. Based on equation (8) and equation (9), we have:

$$\frac{\partial^2 f_2}{\partial x_1 \partial x_i} = -\frac{1}{4\sqrt{x_1 g}} \cdot \frac{\partial g}{\partial x_i} = -\frac{9}{4(n-1)\sqrt{x_1 g}}, \tag{10}$$

$$
\begin{array}{cc}
\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{array} &
\begin{pmatrix}
0 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 1 & 1 \\
1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 & 0
\end{pmatrix} \\
& \begin{array}{cccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \end{array}
\end{array}
$$

(a) f_1 and f_2

$$
\begin{array}{cc}
\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{array} &
\begin{pmatrix}
0 & 1 & 0 & 1 & 1 & 1 \\
1 & 0 & 0 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0
\end{pmatrix} \\
& \begin{array}{cccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \end{array}
\end{array}
$$

(b) f_3

$$
\begin{array}{cc}
\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{array} &
\begin{pmatrix}
0 & 0 & 0 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \\
& \begin{array}{cccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \end{array}
\end{array}
$$

(c) f_4

Figure 2: Variable interaction matrices of DTLZ1 to DTLZ4 .

where $i \in \{2, \cdots, n\}$. Since $g > 0$, we have $\frac{\partial^2 f_2}{\partial x_1 \partial x_i} \neq 0$. Based on Definition 2, we can see that x_1 interacts with all other variables, i.e., x_2 to x_n.

By taking the derivative of f_2 with respect to x_i for $i \in \{2, \cdots, n\}$, we have:

$$\frac{\partial f_2}{\partial x_i} = \frac{\partial g}{\partial x_i} - \frac{\partial \sqrt{x_1/g}}{\partial x_i} = \frac{9}{n-1}(1 - \frac{\sqrt{x_1}}{2\sqrt[4]{g}}). \tag{11}$$

By taking the derivative of equation (11) with respect to x_1, we have:

$$\frac{\partial^2 f_2}{\partial x_i \partial x_1} = -\frac{9}{4(n-1)\sqrt[4]{g}\sqrt{x_1}}, \tag{12}$$

where $x_1 \neq 0$. Since $g > 0$, we have $\frac{\partial^2 f_2}{\partial x_i \partial x_1} \neq 0$. Furthermore, by taking the derivative of equation (11) with respect to x_j, $j \in \{2, \cdots, n\}$ and $i \neq j$, we have:

$$\frac{\partial^2 f_2}{\partial x_i \partial x_j} = \frac{81\sqrt{x_1}}{8(n-1)^2 g^{-5/4}}, \tag{13}$$

where $x_1 \neq 0$. Since $g > 0$, we have $\frac{\partial^2 f_2}{\partial x_i \partial x_j} \neq 0$. In summary, we can see that all variables interact with each other, which means that the f_2 function of ZDT1 is fully non-separable. This agrees with the output of differential grouping. Since the other ZDT test problems share a similar form of h and g functions as that of ZDT1, we can use the above procedure to prove their non-separability. ■

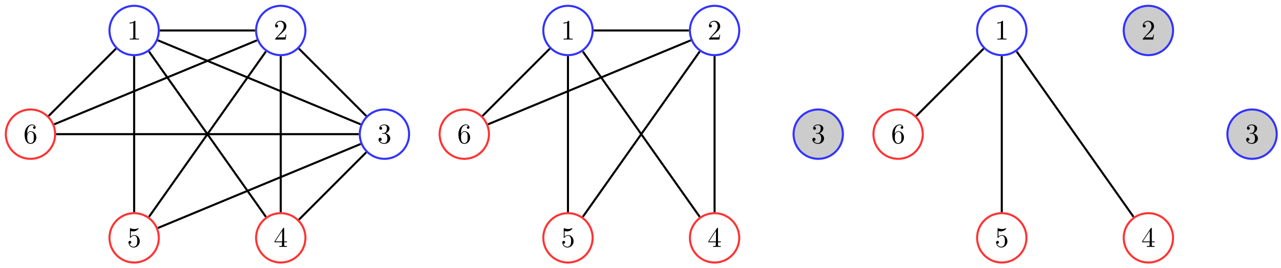
3.2 Variable Interaction Analysis on DTLZ Benchmark Suite

According to Table 1, the mathematical forms of DTLZ functions can be classified into three groups: DTLZ1 to DTLZ4, DTLZ5 to DTLZ6, and DTLZ7. Thus, we investigate the variable interaction structure of each group separately. Without loss of generality, we set $m = 4$ and $n = 6$ in the experiments. By running Algorithm 1 on DTLZ1 to DTLZ4, we can empirically verify that they share the same variable interaction matrices as shown in Fig. 2. Moreover, Fig. 3 is the graphical representation of the matrices in Fig. 2. To validate the correctness of this result, we again use Definition 2 to prove Proposition 2.

Proposition 2. *For DTLZ1 to DTLZ4, $\forall f_i, i \in \{1, \cdots, m\}$, we divide the corresponding decision variables into two non-overlapping sets: $\mathbf{x}_I = (x_1, \cdots, x_\ell)^T$, $\ell = m-1$ for $i \in \{1, 2\}$ while $\ell = m-i+1$ for $i \in \{3, \cdots, m\}$; and $\mathbf{x}_{II} = (x_m, \cdots, x_n)^T$. All members of $\mathbf{x}_I$ not only interact with each other, but also interact with those of $\mathbf{x}_{II}$; all members of $\mathbf{x}_{II}$ are independent from each other.*

Proof. From Table 1 and equation (6), we re-write the objective functions of DTLZ1 to DTLZ4 in the following abstract form:

$$f_i(\mathbf{x}) = h(\mathbf{x}_I) \cdot g(\mathbf{x}_{II}), \tag{14}$$



(a) f_1 and f_2 (b) f_3 (c) f_4

Figure 3: Variable interaction graphs of DTLZ1 to DTLZ4 .

where $i \in \{1, \cdots, m\}$. $\mathbf{x}_I = (x_1, \cdots, x_\ell)^T$, $\ell = m-1$ for $i \in \{1, 2\}$ while $\ell = m-i+1$ for $i \in \{3, \cdots, m\}$; and $\mathbf{x}_{II} = (x_m, \cdots, x_n)^T$. Notice that h function is a multiplication term of all individual variables of $\mathbf{x}_I$, while g function is some independent summations of terms involving all individual variables of $\mathbf{x}_{II}$.

Let us start from DTLZ1. By taking the derivative of f_i, where $i \in \{1, \cdots, m\}$, with respect to each member of $\mathbf{x}_I$, i.e., x_j, where $j \in \{1, \cdots, \ell\}$, we have:

$$\frac{\partial f_i}{\partial x_j} = 0.5(1+g) \cdot \prod_{p=1, p\neq j}^{\ell} x_p. \tag{15}$$

Now by differentiating equation (15) with respect to x_k, where $k \in \{1, \cdots, n\}$ and $k \neq j$, we have:

$$\frac{\partial^2 f_i}{\partial x_j \partial x_k} = \begin{cases} 0.5(1+g) \cdot \prod_{p=1,p\neq i,j}^{m-1} x_p, & k \in \{1, \cdots, m-1\} \\ 0.5\frac{\partial g}{\partial x_k} \cdot \prod_{p=1,p\neq i}^{m-1} x_p, & k \in \{m, \cdots, n\}. \end{cases} \tag{16}$$

In particular, when $k \in \{m, \cdots, n\}$, we have:

$$\frac{\partial g}{\partial x_k} = 200(x_k - 0.5) + 2000\pi \sin(20\pi(x_k - 0.5)). \tag{17}$$

Note that both g and $\frac{\partial g}{\partial x_k}$ are not 0, when $x_k \neq 0.5, k \in \{m, \cdots, n\}$. In this case, we have $\frac{\partial^2 f_i}{\partial x_j \partial x_k} \neq 0$, where $i \in \{1, \cdots, m\}$, $j \in \{1, \cdots, \ell\}$, $k \in \{1, \cdots, n\}$ and $k \neq j$. According to Definition 2, we can see that all members of $\mathbf{x}_I$ not only interact with each other, but also interact with those of $\mathbf{x}_{II}$. Note that since f_i, where $i \in \{3, \cdots, m\}$, is without of x_p, where $p \in \{m-i+2, \cdots, m-1\}$, we can treat x_p be independent/non-separable from the other variables for f_i.

In addition, by taking the derivative of f_i, where $i \in \{1, \cdots, m\}$, with respect to each member of $\mathbf{x}_{II}$, i.e., x_j, where $j \in \{m, \cdots, n\}$, we have:

$$\frac{\partial f_i}{\partial x_j} = 0.5 \prod_{p=1}^{\ell} x_p \cdot \frac{\partial g}{\partial x_j}. \tag{18}$$

According to equation (17), we can see that $\frac{\partial g}{\partial x_j}$ is a function of x_j. Thus, $\frac{\partial^2 f_1}{\partial x_j \partial x_k} = 0$, where $k \in \{m, \cdots, n\}$ and $k \neq j$. According to Definition 2, we can see that all members of $\mathbf{x}_{II}$ are independent/non-separable from each other.

Since DTLZ2 to DTLZ4 have a similar form as DTLZ1, but are with some different exponentials, we can use the above proof procedure to derive the same variable interaction structure as DTLZ1. ■

Then, by running Algorithm 1 on DTLZ5 and DTLZ6, we obtain the variable interaction matrices and graphs, as shown in Fig. 4 and Fig. 5, respectively. The correctness of this result is validated by the proof of Proposition 3.

$$\begin{array}{cc} \begin{array}{c} x_1\\ x_2\\ x_3\\ x_4\\ x_5\\ x_6 \end{array} & \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1\\ 1 & 0 & 1 & 1 & 1 & 1\\ 1 & 1 & 0 & 1 & 1 & 1\\ 1 & 1 & 1 & 0 & 1 & 1\\ 1 & 1 & 1 & 1 & 0 & 1\\ 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix} \\ & \begin{array}{cccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \end{array} \end{array}$$

(a) f_1 and f_2

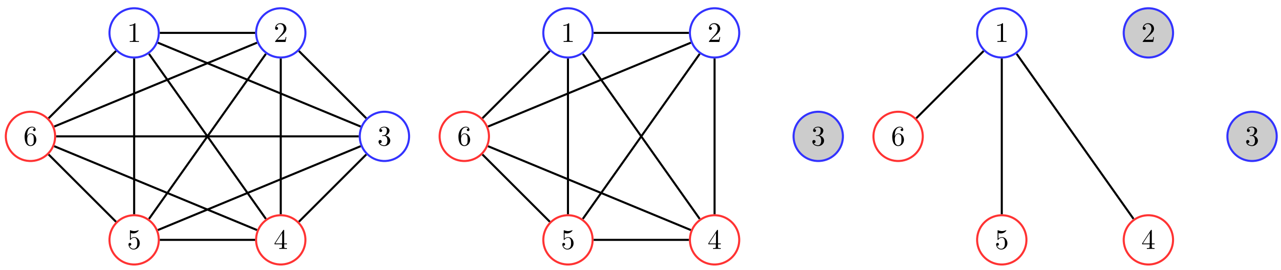
$$\begin{array}{cc} \begin{array}{c} x_1\\ x_2\\ x_3\\ x_4\\ x_5\\ x_6 \end{array} & \begin{pmatrix} 0 & 1 & 0 & 1 & 1 & 1\\ 1 & 0 & 0 & 1 & 1 & 1\\ 0 & 0 & 0 & 0 & 0 & 0\\ 1 & 1 & 0 & 0 & 1 & 1\\ 1 & 1 & 0 & 1 & 0 & 1\\ 1 & 1 & 0 & 1 & 1 & 0 \end{pmatrix} \\ & \begin{array}{cccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \end{array} \end{array}$$

(b) f_3

$$\begin{array}{cc} \begin{array}{c} x_1\\ x_2\\ x_3\\ x_4\\ x_5\\ x_6 \end{array} & \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \\ & \begin{array}{cccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \end{array} \end{array}$$

(c) f_4

Figure 4: Variable interaction matrices of DTLZ5 and DTLZ6.



(a) f_1 and f_2 (b) f_3 (c) f_4

Figure 5: Variable interaction graphs of DTLZ5 and DTLZ6.

Proposition 3. *For DTLZ5 and DTLZ6, $\forall f_i, i \in \{1, \cdots, m\}$, we divide the corresponding decision variables into two non-overlapping sets: $\mathbf{x}_I = (x_1, \cdots, x_\ell)^T$, $\ell = m-1$ for $i \in \{1, 2\}$ while $\ell = m-i+1$ for $i \in \{3, \cdots, m\}$; and $\mathbf{x}_{II} = (x_m, \cdots, x_n)^T$. For f_i, where $i \in \{1, \cdots, m-1\}$, all members of $\mathbf{x}_I$ and $\mathbf{x}_{II}$ interact with each other; for f_m, we have the same interaction structure as Proposition 2.*

Proof. From Table 1 and equation (6), we re-write the objective functions of DTLZ5 and DTLZ6 in the following abstract form:

$$f_i(\mathbf{x}) = h(\mathbf{x}_I, g(\mathbf{x}_{II})) \cdot g(\mathbf{x}_{II}), \tag{19}$$

where $i \in \{1, \cdots, m-1\}$. $\mathbf{x}_I = (x_1, \cdots, x_\ell)^T$, $\ell = m-1$ for $i \in \{1, 2\}$ while $\ell = m-i+1$ for $i \in \{3, \cdots, m\}$; and $\mathbf{x}_{II} = (x_m, \cdots, x_n)^T$. Comparing equation (19) with equation (14), the only difference lies on the h function which consists of both $\mathbf{x}_I$ and $\mathbf{x}_{II}$. Note that the objective functions of DTLZ5 and DTLZ6 have a similar form as that of DTLZ2, we can use the proof procedure of Proposition 2 to prove that all members of $\mathbf{x}_I$ not only interact with each other, but also interact with those of $\mathbf{x}_{II}$.

In addition, due to the additional term of $\mathbf{x}_I$ within the h function, we can derive that $\frac{\partial f_i}{\partial x_j}$, where $j \in \{m, \cdots, n\}$, should be a function of both x_j and members of $\mathbf{x}_I$. Thus, $\frac{\partial^2 f_i}{\partial x_j \partial x_k} \neq 0$, where $k \in \{m, \cdots, n\}$ and $k \neq j$. This means that all members of $\mathbf{x}_{II}$ also interact with each other.

As for f_m, it still obeys the form of equation (14). According to the proof of Proposition 2, we can easily derive the same interaction structure as described in Proposition 2. ■

At last, we run Algorithm 1 on DTLZ7 and find that all its objective functions are fully separable. This means that all entries of its interaction matrices should be 0, and the corresponding interaction graphs consist of n independent nodes. The proof of Proposition 4 validates the correctness of this result.

Proposition 4. *All objective functions of DTLZ7 are fully separable.*

Proof. From Table 1, we can see that f_i of DTLZ7 is a function of x_i for $i \in \{1, \cdots, m-1\}$. Thus, it is obvious that these objective functions are fully separable. As for f_m, we can re-write it as follows:

$$f_m = (1+g)m - \sum_{i=1}^{m-1} (f_i + f_i \sin(3\pi f_i)) \tag{20}$$

In this case, f_m is the function of some independent summation terms involving x_1 to x_n. Therefore, it is also a separable function. ■

4 Conclusions and Future Directions

We have seen that some of the ZDT and DTLZ test problems have complex variable interaction structures that change with the number of objectives. More specifically, some objective functions are fully separable (e.g., f_1 of ZDT problems and all objectives of DTLZ7), some are fully non-separable (e.g., f_2 of ZDT problems and f_1 to f_{m-1} of DTLZ5 and DTLZ6), while the others are in between these two extreme cases, i.e., partially non-separable. This result is in contrast with the existing literature that coarsely classified the functions as separable or non-separable [8, 9].

An interesting observation about the DTLZ functions is the existence of overlapping components within the objective functions. For example, in Fig. 3, at a first glance, the first two objective functions of DTLZ1 to DTLZ4 may be seen as a single non-separable component. However, upon a closer inspection, we can see that the variables form three components containing a set of shared decision variables. Concretely, $\{x_1, x_2, x_3, x_4\}$, $\{x_1, x_2, x_3, x_5\}$ and $\{x_1, x_2, x_3, x_6\}$ can be seen as three components with $\{x_1, x_2, x_3\}$ being the shared variables. This is analogous to functions with overlapping components in the large-scale global optimization literature [11]. Although differential grouping can discover the full variable interaction structure matrix, the optimal decomposition of functions with overlapping components is still an open question [11]. Based on the analysis in Section 3, it appears that objective functions with overlapping components are commonplace in multi-objective optimization. The analysis that we presented in this paper facilitates the study of this phenomenon with respect to both algorithm and benchmark designs.

Overall, variable interaction can affect various aspects of the EMO community, ranging from operator design to the choice of aggregation functions within decomposition-based EMO algorithms [12–16]. We believe that variable interaction is an under-explored area in this literature, which might be due to extreme focus of the current research on small to medium sized problems. It is clear that when the dimensionality of a problem grows beyond a certain level, using a divide-and-conquer strategy becomes inevitable in which case considering variable interaction becomes a necessity. In the future, we plan to analyze a wider range of common benchmark suites within the EMO community. Additionally, similar to the large-scale global optimization [11], we plan to develop benchmark problems with challenging yet controllable variable interaction structures, which can better resemble the modular nature of real-world optimization scenarios.

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