Multi-Objectivizing Sum-of-the-Parts Combinatorial Optimization Problems by Random Objective Decomposition

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Abstract

Multi-objectivization is a term used to describe strategies developed for optimizing single-objective problems by multi-objective algorithms. This paper focuses on the multi-objectivization of the sum-of-the-parts Combinatorial Optimization Problems (COPs), which include the Traveling Salesman Problem (TSP), the Unconstrained Binary Quadratic Programming (UBQP) and other well-known COPs. For a sum-of-the-parts COP, we propose to decompose its original objective into two sub-objectives with controllable correlation. Based on the decomposition method, two new multi-objectivization techniques called Non-Dominance Search (NDS) and Non-Dominance Exploitation (NDE) are developed, respectively. NDS is combined with the Iterated Local Search (ILS) metaheuristic (with fixed neighborhood structure), while NDE is embedded within the Iterated Lin-Kernighan (ILK) metaheuristic (with varied neighborhood structure). The resultant metaheuristics are called ILS+NDS and ILK+NDE, respectively. Empirical studies on some TSP and UBQP instances show that with appropriate correlation between the sub-objectives, there are more chances to escape from local optima when new starting solution is selected from the non-dominated solutions defined by the decomposed sub-objectives. Experimental results also show that ILS+NDS and ILK+NDE both significantly outperform their counterparts on most of the test instances.

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1. Introduction

The so-called multi-objectivization approach deals with a single-objective problem by converting it into a multi-objective (in most cases, bi-objective) one and then optimizing it by a multi-objective algorithm. Its effectiveness has been confirmed in many studies [1, 2]. The core of multi-objectivization is on how to do the conversion. Existing multi-objectivization techniques acquire multiple objectives either through decomposing the original objective into sub-objectives or by combining it with helper objectives.

This paper focuses on multi-objectivizing a subclass of the Combinatorial Optimization Problems (COPs), the sum-of-the-parts COPs, through decomposition. In a sum-of-the-parts COP, its objective function can be represented as the summation of a finite number of sub-functions over unit costs. The well-known Traveling Salesman Problem (TSP), Unconstrained Binary Quadratic Programming (UBQP) problem, Quadratic Assignment Problem (QAP) and Vehicle Routing Problem (VRP) all belong to this type.

We propose to decompose a sum-of-the-parts COP’s objective function $f$ into two sub-objectives $f_1$ and $f_2$ by splitting each unit cost into two parts. The decomposed $f_1$ and $f_2$ are subject to $f(x) = f_1(x) + f_2(x)$ for any solution $x$ in the solution space. The cost splitting follows a probability distribution, while the sub-objectives’ correlation can be controlled by varying the probability distribution. Based on the proposed objective decomposition method, two new multi-objectivization techniques are developed.

The first one is called Non-Dominance Search (NDS) which is suitable to be combined within search based metaheuristics with fixed neighborhood structure\footnote{A search based metaheuristic is an iterative optimization algorithm for COPs. At each iteration, it searches for a better solution in the neighborhood of current solution. If a local optimum is found, it tries to escape from it by starting the search from a new point.}. The idea behind NDS is similar to that of Variable Neighborhood Search (VNS)\footnote{Variable Neighborhood Search (VNS) is a metaheuristic that alternates between local search and exploration of other neighborhoods.} who enlarges the neighborhood size when a local optimum is found. NDS also tries to find a better solution in the neighborhoods of the neighboring solutions of the local optimum. At a local optimum $x_*$, NDS first...
looks for neighboring solutions of \( x^* \) that are non-dominated to \( x^* \) in terms of \((f_1, f_2)\). If the set of solutions is denoted as \( \mathcal{N}(x^*|f_1, f_2) \), NDS explores the neighborhoods of all solutions in \( \mathcal{N}(x^*|f_1, f_2) \) for a better solution than \( x^* \). If there is no such solution, it returns \( x^* \), otherwise the better solution will be used as the new starting point for next round of local search.

NDS is motivated by the hypothesis that it is more likely to find a better solution in the neighborhood of a non-dominated neighboring solution of \( x^* \) than that of the dominated neighboring solution of \( x^* \). We call this hypothesis the “neighborhood non-dominance” hypothesis. Obviously, if such a hypothesis holds, NDS can help reduce the search complexity of local search based metaheuristics.

To investigate the hypothesis, we carry out empirically study on two sum-of-the-parts COPs, namely, the Traveling Salesman Problem (TSP) and the Unconstrained Binary Quadratic Programming (UBQP). Empirical results confirm that the hypothesis does hold for the considered TSP and UBQP instances. Further, it is found that the effectiveness of the decomposition depends highly on the correlation between the two sub-objectives.

A limitation of NDS is that it requires that the neighborhood structure is fixed, i.e., given a solution, one can list all the neighboring solutions. However, NDS cannot be combined within a local search with varied neighborhood structure, e.g., the Lin-Kernighan (LK) local search [4] for the TSP. To overcome this problem, we propose another multi-objectivization technique, called Non-Dominance Exploitation (NDE). NDE looks for local optima that are non-dominated to the current best solution. The search region close to these local optima will be further exploited.

In this paper, we combine NDS with the well-known Iterated Local Search (ILS) and NDE with the Iterated Lin-Kernighan algorithm (ILK) [5]. The resultant algorithms are called ILS+NDS and ILK+NDE, respectively.

In the experimental studies, we compare ILS+NDS against the basic ILS and a variant of ILS+NDS (in which the guidance of \((f_1, f_2)\) is eliminated) on some TSP instances and UBQP instances, and compare ILK+NDE against the basic ILK and a variant of ILK+NDE (in which the the guidance of \((f_1, f_2)\) is eliminated) on some middle- and large-size TSP instances. In addition, in the ILS+NDS implementation, different levels of sub-objectives’ correlation are tested. The experimental results show that ILS+NDS and ILK+NDE both significantly outperform their counterparts on most of the test instances in case that a relative high correlation between the sub-objectives \((f_1, f_2)\) is exerted.
Preliminary work of this paper has been published in a conference [6]. This paper differs significantly from the conference version in the following aspects. In this paper,

- the decomposition method is generalized to all the sum-of-the-parts COPs. Besides the TSP, the UBQP is also used as testbed.
- a method to control the correlation between the sub-objectives $f_1$ and $f_2$ is proposed.
- systematic experiments are carried out to analyze the neighborhood non-dominance hypothesis.
- a new multi-objectivization technique, NDE, is proposed for local search metaheuristics with varied neighborhood structure.

The rest of the paper is organized as follows. Section 2 presents the related work. Section 3 formalizes the sum-of-the-parts COP and introduces the proposed objective decomposition method. The TSP and the UBQP are used to show the procedure of the decomposition method. In Section 4, two new multi-objectivization techniques, NDS and NDE, based on the proposed objective decomposition method, are presented. Section 5 presents the empirical study on the neighborhood non-dominance hypothesis. Experimental results of the proposed methods for the TSP and the UBQP instances are also presented in Section 5. Section 6 concludes the paper and discusses future work.

2. Related Work

The study of multi-objectivization can be dated back to 2001 when Knowles et al. [1] first invented the term “multi-objectivization”. In their work, a continuous optimization problem and the TSP were used as the testbeds. The authors proposed to decompose the TSP by cutting a tour into two sub-tours. Their experimental results showed that the multi-objective algorithm can return better solutions compared to a broadly equivalent single-objective algorithm. The authors claimed that this is because the multi-objectivization technique reduced the number of local optima in the search space. Ishibuchi and Nojima [7] focused on single-objective problems which are in the form of a scalarizing function. They decomposed the original objective into sub-objectives that are similar to the scalarizing function and
found that Evolutionary Multi-Objective algorithm (EMO) helps a local solver escape from local optima.

The aforementioned work found that multi-objectivization is beneficial to single-objective optimization. However, Handl et al. [8] argued that multi-objectivization through decomposition can equally render a single-objective optimization problem easier or harder, since the incomparable nature of multiple objectives creates plateaus in the fitness landscape which may reduces the number of local optima, but may hinder the search. In literature, the decomposition multi-objectivization method has been successfully applied to logic circuit design [9], sorting and shortest paths problem [10], robotic control [11], protein structure prediction [12] and others.

Compared to the decomposition based multi-objectivization methods, much work have been carried out on using helper objectives to multi-objectivize a single-objective problem. For constrained optimization problems, it is a common practice to transform the constraints as a helper objective. There has an extensive study of constrained optimization using EMO, see e.g. [13, 14, 15, 16, 17, 18, 19].

For continuous problem, the helper objectives usually are related to the properties of the solution population or the properties of the problem. For example, Abbass and Deb [20] used the age of individual solution as an additional objective to maintain the population diversity and to slow down the selection pressure. Jiao et al. [21] converted a single-objective problem to a dynamic multi-objective problem by considering a niche-count objective to maintain the diversity. Deb and Saha [22] converted a multi-modal problem into a bi-objective problem by considering the gradient or neighborhood information as the second objective.

For COPs, some studies defined the helper objectives based on the segments of the original objective. Jahne et al. [23] proposed the so-called Multi-Objectivization via Segmentation (MOS) method for the TSP. In MOS, costs of the edges passing through certain cities were selected as the helper objectives. For the Job Shop Scheduling Problem (JSSP), Jensen [24, 25] used the flow-times of individual jobs as the helper objectives which are designed to dynamically change during the search in a random order. Experimental results showed that using NSGA-II [26] to optimize the generated multi-objective problem significantly outperforms using a traditional GA. Syberfeldt and Rogstrom [27] proposed a two-step multi-objectivization method. In the first step, the helper objective was set to conflict with the original objective and in the second step the helper objective
was in harmony with the original objective. Alsheddy proposed a helper objective by a penalty-based approach. Bleuler et al. tried to reduce the ‘bloat’ phenomenon in genetic programming by considering the program size as a second objective.

Lochtefeld and Ciarallo conducted a series of studies on helper-objective-based and decomposition-based methods. They found that problem specific knowledge should be incorporated for a good helper-objective sequence. In a recent study, they showed that the decomposition based method has a better on-average performance compared to the helper objective method on their tested JSSP instances. Brockhoff et al. showed that a multi-objectivized problem can become either harder or easier depending on the definitions of the helper objectives.

In addition to the previous studies, multi-objectivization has been proved to be helpful in timetabling problem, dynamic environment, minimum spanning tree, computational mechanics design, chemical phase-equilibrium detection, short-term unit commitment problem, compliant mechanism design and others.

From the above literature review we observe that first few studies have been tried to develop a universal multi-objectivization method for a wide range of problems. Second, existing EMO algorithms are applied in most studies. In this paper, we propose a universal objective decomposition method which is suitable for the sum-of-the-parts COPs. Further, based on the decomposition method, we propose two new techniques which can improve the global search ability of local search based metaheuristics.

3. Objective Decomposition

A Combinatorial Optimization Problem (COP) is defined as

\[
\text{minimize} / \text{maximize} \quad f(x) \\
\text{subject to} \quad x \in S,
\]

where \( f : S \to \mathbb{R} \) is the objective function and \( S \) is the solution space which is a finite discrete set, e.g., an \( n \)-dimensional binary vector space \( \{0, 1\}^n \) for the UBQP or an \( n \)-dimensional permutation space \( \mathcal{P}_n \) for the TSP. In this paper we focus on the sum-of-the-parts COPs. A sum-of-the-parts COP satisfies the following constraints:

(i) The problem is uniquely determined by a finite discrete set of units \( U = \{u_i|i = 1, 2, \ldots, |U|\} \) and each unit \( u_i \) has a fixed cost \( c_i \);
(ii) A feasible solution $x$ is a subset of $U$ and satisfies certain rules of composition;

(iii) The objective function $f(x)$ is the summation (or weighted summation) of the costs of units in $x$.

Formally, the sum-of-the-parts COP can be expressed as

$$\min / \max f(x) = \sum_{i=1}^{\left|U\right|} I_i(x) \cdot w_i \cdot c_i,$$

subject to $x \subset U,$

$x$ satisfies certain composition rules, \hspace{1cm} (2)

where $I_i(x)$ is an indicator function:

$\quad I_i(x) = \begin{cases} 
1 & \text{if } u_i \in x, \\
0 & \text{otherwise}, 
\end{cases}$ \hspace{1cm} (3)

and $c_i$ is the cost associated with $u_i$ and $w_i$ is the weight.

The well-known TSP belongs to the sum-of-the-parts COPs. In a TSP, the edges between any two cities forms a finite set and each edge has a fixed travel cost. A TSP solution is a subset of edges that forms a tour visiting every city exactly once then returning to the first city. The function value of a TSP solution is the total cost of the edges in the tour. Hence, in the TSP, the total edge set can be seen as the unit set $U$ and the edge costs can be seen as the unit costs. Besides the TSP, we can deduce that the Quadratic Assignment Problem (QAP), the Vehicle Routing Problem (VRP), the Knapsack Problem (KP) and the Unconstrained Binary Quadratic Programming (UBQP) all belong to the sum-of-the-parts COPs.

For the sum-of-the-parts COPs, we propose a new method to decompose the original objective function $f$ into two sub-objective functions $f_1$ and $f_2$ such that $f(x) = f_1(x) + f_2(x)$ for any solution $x$ in the solution space. The proposed decomposition method is quite simple. For each unit $u_i$ in the finite set, the method splits its cost into two new values $c_i^{(1)}$ and $c_i^{(2)}$ such that $c_i = c_i^{(1)} + c_i^{(2)}$ following a probability distribution $p$. The decomposition is independent of the unit set, i.e. the splitting of all the unit costs follows the same probability distribution. As a result, $f_1$ and $f_2$ are defined by the new unit costs $\{c_i^{(1)} | i = 1, 2, \ldots, |U|\}$ and $\{c_i^{(2)} | i = 1, 2, \ldots, |U|\}$, respectively:

$$f_1(x) = \sum_{i=1}^{\left|U\right|} I_i(x) \cdot w_i \cdot c_i^{(1)}, \quad \text{and} \quad f_2(x) = \sum_{i=1}^{\left|U\right|} I_i(x) \cdot w_i \cdot c_i^{(2)}.$$
\[ f_2(x) = \sum_{i=1}^{\lvert U \rvert} I_i(x) \cdot w_i \cdot c_i^{(2)}. \] (5)

It is obvious that \( f(x) = f_1(x) + f_2(x) \) for any \( x \in U \).

The relationship between the original objective function \( f \) and the two sub-objective functions \((f_1, f_2)\) can be illustrated in Figure 1. In Figure 1, we plot a new axis in the middle of the \( f_1 \) and \( f_2 \) axis. For any point \((f_1(x), f_2(x))\) in the bi-objective space, its projection on the middle axis is denoted as \((f_1(x'), f_2(x'))\). Then we can have \( f_1(x') = f_2(x') \) and \( f_1(x) + f_2(x) = f_1(x') + f_2(x') = 2f_1(x') \). The distance between \((f_1(x'), f_2(x'))\) and \((0, 0)\) is \( \sqrt{(f_1(x') - 0)^2 + (f_2(x') - 0)^2} = \sqrt{2(f_1(x'))^2} = \sqrt{2|f_1(x')|} = \frac{1}{\sqrt{2}} \cdot 2|f_1(x')| = \frac{1}{\sqrt{2}}|f_1(x') + f_2(x')| = \frac{1}{\sqrt{2}}|f_1(x) + f_2(x)| = \frac{1}{\sqrt{2}}|f(x)| \), which means the middle axis measures \( \frac{1}{\sqrt{2}} f(x) \).

From Eq. (4) and Eq. (5), it is seen that \( f_1(x) \) and \( f_2(x) \) are different only by \( \{c_i^{(1)}|i = 1, 2, \ldots, |U|\} \) and \( \{c_i^{(2)}|i = 1, 2, \ldots, |U|\} \). We thus use their Pearson correlation coefficient to measure the correlation between the sub-objectives \( f_1(x) \) and \( f_2(x) \). The correlation coefficient is defined as:

\[ \rho = \frac{\text{cov}(\{c_i^{(1)}\}, \{c_i^{(2)}\})}{\sigma(\{c_i^{(1)}\}) \cdot \sigma(\{c_i^{(2)}\})}, \] (6)

where \( \text{cov}(\cdot, \cdot) \) is the covariance operator and \( \sigma(\cdot) \) the standard deviation operator. If \( c_i^{(1)} = c_i^{(2)} = c_i/2 \) for all \( i \in \{1, 2, \ldots, |U|\} \), then we have \( f_1(x) = f_2(x) = f(x)/2 \) for any \( x \) in the solution space and \( \rho = 1 \). Conversely, if \( |c_i^{(1)} - c_i^{(2)}| >> 0 \) for all \( i \in \{1, 2, \ldots, |U|\} \), then we have \( |f_1(x) - f_2(x)| >> 0 \) for any \( x \) in the solution space and \( \rho \rightarrow -1 \). Hence, by controlling the ratio between \( c_i^{(1)} \) and \( c_i^{(2)} \), we can control the correlation between \( f_1 \) and \( f_2 \).
In the following, we show how to apply the proposed decomposition method to the TSP and the UBQP respectively.

3.1. Decomposition of the TSP

Given \( n \) cities and travel cost between every pair of cities, the TSP is to find the most cost-effective tour that visits every city exactly once and returns to the first city. Formally, let \( G = (\mathcal{V}, \mathcal{E}) \) be a fully connected graph with cities as vertexes, where \( \mathcal{V} \) is the vertex set and \( \mathcal{E} \) the edge set. Denote \( c_{i,j} > 0 \) the cost of the edge between vertex \( i \) and vertex \( j \), the objective function of a TSP is defined as

\[
\text{minimize } f(x) = c_{x(n), x(1)} + \sum_{i=1}^{n-1} c_{x(i), x(i+1)},
\]

subject to \( x = (x(1), x(2), \ldots, x(n)) \in \mathcal{P}_n \), where \( f : \mathcal{P}_n \rightarrow \mathbb{R} \) is the objective function and \( \mathcal{P}_n \) is the permutation space of \( \{1, 2, \ldots, n\} \). In this paper we focus on the symmetric TSPs, i.e., \( c_{i,j} = c_{j,i} \) for all \( i, j \in \{1, 2, \ldots, n\} \).

As mentioned above, the TSP belongs to the sum-of-the-parts COP. In the TSP, the edge set \( \mathcal{E} \) can be seen as the finite unit set \( U \) in Eq. (2) with the edge costs as the unit costs. A TSP solution \( x \) corresponds to a subset of \( \mathcal{E} \), i.e., \( \text{edge}(x(1), x(2)), \text{edge}(x(2), x(3)), \ldots, \text{edge}(x(n-1), x(n)), \text{edge}(x(n), x(1)) \) and the function value of \( x \) is the summation of the edge costs in \( x \). Hence the proposed objective decomposition method can be directly applied to the TSP.

To decompose a TSP, for each edge \((i, j)\), first \( c_{i,j}^{(1)} \) is randomly sampled from a pre-defined probability distribution \( p \) in \((0, c_{i,j})\), where \( c_{i,j} \) is the original edge cost, then \( c_{i,j}^{(2)} = c_{i,j} - c_{i,j}^{(1)} \). It is obvious that \( c_{i,j}^{(1)} > 0, c_{i,j}^{(2)} > 0 \) and \( c_{i,j}^{(1)} + c_{i,j}^{(2)} = c_{i,j} \) for any \( i, j \in \{1, 2, \ldots, n\} \), hence \( \{c_{i,j}^{(1)} | i, j \in \{1, 2, \ldots, n\}\} \) and \( \{c_{i,j}^{(2)} | i, j \in \{1, 2, \ldots, n\}\} \) define two legal TSPs \( f_1 \) and \( f_2 \) and \( f(x) = f_1(x) + f_2(x) \) for any \( x \) in the solution space. Note here that, the generated TSPs \( f_1 \) and \( f_2 \) are both non-Euclidean TSP.

We find that the correlation between \( f_1 \) and \( f_2 \) by such a decomposition can be controlled by the shape of \( p \). In Figure 2, we show three examples of \( p \) with different shapes, including “bell”, “valley” and “line”.

When \( p \) is of the shape of a “bell” (Figure 2(a)), the greatest probability is obtained in the middle of \((0, c_{i,j})\). Sampling \( c_{i,j}^{(1)} \) from the bell distribution
is therefore of high probability to be $c_{i,j}/2$. Since $c_{i,j}^{(2)} = c_{i,j} - c_{i,j}^{(1)} \approx c_{i,j}/2$, it means that the probability that $c_{i,j}^{(1)} \approx c_{i,j}^{(2)}$ is very high and the correlation coefficient $\rho$ will be roughly 1.

When $p$ is of the shape of a “valley” (Figure 2(b)), the probability that $c_{i,j}^{(1)} \approx 0$ or $c_{i,j}^{(1)} \approx c_{i,j}$ is very high. Hence it is very likely that the difference between $c_{i,j}^{(1)}$ and $c_{i,j}^{(2)}$ is relatively large, which means $\rho$ is close to $-1$.

When $p$ is of the shape of a “line”, it is actually the uniform distribution (Figure 2(c)). $c_{i,j}^{(1)}$ takes any value in $(0, c_{i,j})$ with equal probability, so does $c_{i,j}^{(2)}$. As a result, the correlation coefficient $\rho \approx 0$.

In summary, it is seen that with different $p$s, positively correlated, negatively correlated or nearly independent sub-TSPs can be obtained after decomposition. To illustrate how the two sub-objectives behave w.r.t. $\rho$, we carried out the following experiment taking the TSP instance eil51 as an example. First the objective of eil51 is decomposed according to different $p$s, and eight pairs of $(f_1, f_2)$ with different $\rho$ values ranging from $-0.5657$ to $0.9330$ are selected. Then 1000 solutions of eil51 are randomly generated. The $(f_1, f_2)$ values of the 1000 solutions for each pair are shown in each subplot of Figure 3.

The maximum and minimum objective value, denoted as $f(x_{\text{max}})$ and $f(x_{\text{min}})$, respectively, of the 1000 solutions are also shown in Figure 3 in red lines. From Figure 3, it is seen that along the increasing of $\rho$, the solutions become more and more concentrated along the middle axis.
3.2. Decomposition of the UBQP

The Unconstrained Binary Quadratic Programming problem (UBQP) is defined as follows:

\[
\text{maximize } f(x) = x^T Q x = \sum_{i=1}^{n} \sum_{j=1}^{n} q_{i,j} x_i x_j \\
\text{subject to } x \in \{0, 1\}^n,
\]

where \( Q = [q_{i,j}] \) is a \( n \times n \) matrix, and a feasible solution \( x \) is a vector of \( n \) binary variables. The UBQP is \( \mathcal{NP} \)-hard and has been widely studied [45].

The UBQP belongs to the sum-of-the-parts COP. In the UBQP, \( Q \) can be seen as the finite set \( U \) with \( q_{i,j} \) as the unit costs. A UBQP solution \( x \) defines a subset \( \{q_{i,j} | x_i = 1 \land x_j = 1\} \) and the function value of \( x \) is the summation of the members in the subset. Hence, the proposed objective decomposition method can be applied to the UBQP.

Different from the positiveness of the edge cost in the TSP, the element value of \( Q \) can be negative. The decomposition method proposed for the TSP is thus not entirely applicable for the UBQP, but similar idea can be used.
For each pair \((i, j)\), we propose to sample \(q_{i,j}^{(1)}\) from a pre-defined probability distribution \(p\) defined in the interval \((\frac{q_{i,j}}{2} - q', \frac{q_{i,j}}{2} + q')\) where \(q' > 0\) is a pre-defined positive constant. The rest procedure is the same to that of the TSP decomposition. Similarly, we can control the correlation coefficient \(\rho\) by choosing a bell-like, valley-like or uniform \(p\).

4. The Proposed Multi-Objectivization Techniques

Based on the proposed objective decomposition method, we propose two new multi-objectivization techniques, named as Non-Dominance Search (NDS) and Non-Dominance Exploitation (NDE), respectively. They can be used to improve the global search ability of local search based metaheuristics. Particularly, NDS is applicable for metaheuristics with fixed neighborhood structure, while NDE works with varied neighborhood structure.

4.1. Non-Dominance Search (NDS)

Given a neighborhood definition in the solution space, a local search process iteratively evaluates the neighborhood of the current solution and moves to a better neighboring solution. Local search usually stops at a solution that is not worse than its neighbors but not necessarily all other solutions in the solution space, i.e. a local optimum. To escape from the local optimum, a possible strategy is to enlarge the neighborhood size. For example, in Variable Neighborhood Search (VNS), once the search is trapped in a local optimum, the neighborhood size is enlarged until a better solution in the enlarged neighborhood is found.

However, enlarging the neighborhood size can result in high computational complexity if all the solutions in the enlarged neighborhood are all to be evaluated. The proposed NDS can reduce the computational complexity by only selecting the neighboring solutions of the local optimum that are non-dominated to the current local optimum with regard to \((f_1, f_2)\) and only evaluating the neighborhood of the selected neighboring solutions.

Below we first give the definition of dominance and non-dominance in the multi-objective minimization case and then present the NDS procedure.

**Definition 4.1.** Dominance: A vector \(u = (u_1, \ldots, u_m)\) is said to dominate a vector \(v = (v_1, \ldots, v_m)\), if and only if \(u_k \leq v_k, \forall k \in \{1, \ldots, m\}\) \(\land\) \(\exists k \in \{1, \ldots, m\}: u_k < v_k\), denoted as \(u \prec v\).
Figure 4: Assume the local optimum $x_*$ has six neighboring solutions. The neighborhood of $x'_2$ are more likely to break through the contour of $f(x_*)/\sqrt{2}$ than the neighborhood of $x'_1$ since $x'_2$ is non-dominated to $x_*$. 

**Definition 4.2. Non-dominance:** If $u$ is not dominated by $v$ and $v$ is not dominated by $u$, we say that $u$ and $v$ are *non-dominated* to each other, denoted as $u \not\succ v$ or $v \not\succ u$.

The idea behind NDS is presented in Figure 4 in which we assume that a local optimum $x_*$ has six neighboring solutions for a minimization problem $f(x)$. All the neighboring solutions are located above the $f(x_*)/\sqrt{2}$ contour (red line in Figure 4) since $x_*$ is a local optimum. NDS intends to find a neighboring solution whose neighborhood can break through the contour of $f(x_*)/\sqrt{2}$. From Figure 4 we can see that the neighboring solution that are not dominated by $x_*$ (e.g. $x'_2$) are more likely to be close to the contour of $f(x_*)/\sqrt{2}$, compared to the solutions that are dominated by $x_*$ (e.g. $x'_1$). Hence the neighborhood of $x'_2$ are more likely to contain a solution that can break through the $f(x_*)/\sqrt{2}$ contour than the neighborhood of $x'_1$.

The detailed procedure of NDS in a minimization case is shown in Algorithm 1 in which the first-improvement strategy is used. The input of NDS is a local optimum $x_*$. If a solution $x'$ in the neighborhood of $x_*$ is non-dominated w.r.t. the decomposed sub-objectives (line 3), the neighborhood of $x'$ is to be explored. Once a better solution is found (line 5), NDS will immediately terminate and return the better solution (line 6). If no better solution can be found, NDS will return the original local optimum $x_*$. 

NDS cannot be used as a standalone COP solver. Rather, it can be embedded within a metaheuristic with fixed neighborhood structure. As a case study, we combine NDS with the basic Iterated Local Search (ILS) procedure and the resultant algorithm is called ILS+NDS. The procedures of
Algorithm 1: Non-Dominance Search (NDS)

\begin{algorithm}
\SetVline
\caption{Non-Dominance Search (NDS)}
\begin{algorithmic}[1]
\Input{$x_\ast, f, f_1, f_2$}
\State $x_{output} \leftarrow x_\ast$;
\For {each $x' \in \text{Neighborhood}(x_\ast)$}
\If {$(f_1(x'), f_2(x')) \not\succ (f_1(x_\ast), f_2(x_\ast))$}
\For {each $x'' \in \text{Neighborhood}(x')$}
\If {$f(x'') < f(x_\ast)$}
\State $x_{output} \leftarrow x''$;
\State \textbf{exit};
\EndIf
\EndFor
\EndIf
\EndFor
\State \Return $x_{output}$
\end{algorithmic}
\end{algorithm}

the original ILS and the proposed ILS+NDS are shown in Algorithm 2 and Algorithm 3, respectively. The key difference of ILS+NDS to ILS is that the perturbation process in ILS (line 5 in Algorithm 2) is replaced by the NDS process in ILS+NDS (line 6 in Algorithm 3) to obtain a better re-starting point. If the NDS procedure fails, ILS+NDS will conduct a perturbation process to escape from the current local optimum (line 8 in Algorithm 3).

Algorithm 2: Iterated Local Search (ILS)

\begin{algorithm}
\SetVline
\caption{Iterated Local Search (ILS)}
\begin{algorithmic}[1]
\State $x'_0 \leftarrow$ randomly or heuristically generated solution;
\State set $x_{best} \leftarrow x'_0$ and $j \leftarrow 0$;
\While {stopping criterion is not met}
\State $x_j \leftarrow \text{LocalSearch}(x'_j)$;
\State $x'_{j+1} \leftarrow \text{Perturbation}(x_j)$;
\State $j \leftarrow j + 1$;
\If {$f(x_{j+1}) < f(x_{best})$}
\State $x_{best} \leftarrow x_{j+1}$;
\EndIf
\EndWhile
\State \Return the historical best solution $x_{best}$
\end{algorithmic}
\end{algorithm}

We do not claim that ILS+NDS is competitive to the state-of-the-art metaheuristics for COPs. The aim of designing ILS+NDS is to show that the proposed multi-objectivization method is beneficial to metaheuristics like ILS.
Algorithm 3: ILS+NDS

1. Decompose $f$ into $f_1$ and $f_2$;
2. $x_0' \leftarrow$ random or heuristically generated solution;
3. set $x_{\text{best}} \leftarrow x_0'$ and $j \leftarrow 0$;
4. while stopping criterion is not met do
   5. $x_j \leftarrow \text{LocalSearch}(x_j')$;
   6. $x_{j+1}' \leftarrow \text{NDS}(x_j|f, f_1, f_2)$;
   7. if $x_{j+1}' == x_j$ then
      8. $x_{j+1}' \leftarrow \text{Perturbation}(x_j)$;
   9. if $f(x_{j+1}) < f(x_{\text{best}})$ then
      10. $x_{\text{best}} \leftarrow x_{j+1}$;
   11. $j \leftarrow j + 1$;
5. return the historical best solution $x_{\text{best}}$.

4.2. Non-Dominance Exploitation (NDE)

In the previous sub-section, we propose the NDS technique to enhance local search based metaheuristics. To apply NDS, the neighborhood structure in the local search method should be fixed during the search.

However, in some metaheuristics, the neighborhood structure is varying during the search. For example, in the LK local search for the TSP, a fine-grained edge exchange strategy is used at each move. The number of exchanged edges is not fixed among moves. The neighborhood structure is thus varied during the LK search.

Though NDS is not able to be embedded within the LK, this does not mean that the proposed decomposition-based multi-objectivization method cannot benefit the LK local search. In this section, we propose to embed the decomposition method within the Iterated Lin-Kernighan local search (ILK). The proposed algorithm is called ILK with Non-Dominated Exploitation (ILK+NDE). The ILK is also known as the Chained Lin-Kernighan algorithm \([5]\). It is a variant of ILS, in which a LK local search and a double bridge perturbation (please see Figure 5 for a demo) are iteratively executed.

Different to NDS who finds promising neighboring solutions in the neighborhood of local optima, ILK+NDE explores promising LK local optima based on the non-dominance relationship of $(f_1, f_2)$. The detailed procedure of ILK+NDE is shown in Algorithm 4. In Algorithm 4, the original problem
Figure 5: An example of the double bridge perturbation on the TSP

$f$ is first decomposed into two sub-objectives (line 1). A current best solution $x_{\text{best}}$ is found by applying the LK search (lines 2 to 3). At each iteration $j$, if the current solution $x_j$ is non-dominated to $x_{\text{best}}$ with regard to $(f_1, f_2)$, the region close to $x_\ast$ in the search space will be further exploited (line 8) and $x_{j+1}$ is returned. The exploitation procedure is summarized in Algorithm 5.

In ILK+NDE, if the exploitation procedure is failed (i.e. $x_{j+1} = x_j$), a perturbation method is applied (lines 9 to 11). The algorithm terminates until the stop criterion is met.

In the exploitation procedure (Algorithm 5), at each round of the exploitation, first $k$ edges are randomly selected from $x_\ast$ and a penalty cost $\tilde{c}$ will be added to the selected edges (line 4 in Algorithm 5) by $\text{AddRandomPenalty}(x_\ast, f, k, \tilde{c})$ (Algorithm 6). This will result in a new instance $f'$. An LK local search is started from $x_\ast$ on $f'$ and returns $x'$ (line 5 in Algorithm 5). A new LK local search then applies from $x'$ on the original problem $f$ and returns $x''$ (line 6 in Algorithm 5). If $f(x'') < f(x_\ast)$, then the exploitation procedure will immediately stop and output $x''$. Otherwise, a new round of random penalization will be executed on $x_\ast$ and $f$. If after $T$ rounds of penalization the procedure still cannot find a better $x''$ than $x_\ast$, Algorithm 5 terminates and returns $x_\ast$.

4.3. Discussions

The similarity between NDS and NDE is that they both use the non-dominance relationship introduced by the decomposed sub-objectives $(f_1, f_2)$ to judge whether a solution is “promising” (i.e. worth further exploitation). In NDS, the neighboring solutions of a local optimum are checked, while in NDE, the local optima encountered during the search are judged based on $(f_1, f_2)$. One may argue that a reasonable and easy way to judge the potential of the neighboring solutions is to set a threshold and exclude solutions that are with objective function values worse than the threshold. However, since different problem instances have different ranges of function values, it is not easy to find a general method to properly set the threshold for different
Algorithm 4: ILK+NDE

Input: $f$, $T$, $k$, $\tilde{c}$

1. Decompose $f$ into $f_1$ and $f_2$ such that $f(x) = f_1(x) + f_2(x)$;
2. $x_0' \leftarrow$ random or heuristically generated solution;
3. $x_0 \leftarrow \text{LK}(x_0' \mid f)$;
4. $x_{\text{best}} \leftarrow x_0$;
5. $j \leftarrow 0$;
6. while stopping criterion is not met do
7.     if $(f_1(x_j), f_2(x_j)) \neq (f_1(x_{\text{best}}), f_2(x_{\text{best}}))$ then
8.         $x_{j+1} \leftarrow \text{FurtherExploit}(x_j \mid T, k, \tilde{c})$;
9.         if $x_{j+1} == x_j$ then
10.            $x_{j+1}' \leftarrow \text{Perturbation}(x_j)$;
11.            $x_{j+1} \leftarrow \text{LK}(x_{j+1}' \mid f)$;
12.     else
13.         $x_{j+1}' \leftarrow \text{Perturbation}(x_j)$;
14.         $x_{j+1} \leftarrow \text{LK}(x_{j+1}' \mid f)$;
15.     if $f(x_{j+1}) < f(x_{\text{best}})$ then
16.         $x_{\text{best}} \leftarrow x_{j+1}$;
17.     $j \leftarrow j + 1$;
18. return the historical best solution $x_{\text{best}}$

Algorithm 5: FurtherExploit($x_\ast \mid T, k, \tilde{c}$)

1. $x_{\text{output}} \leftarrow x_\ast$;
2. $j \leftarrow 1$;
3. while $j \leq T$ do
4.     $f' \leftarrow \text{AddRandomPenalty}(x_\ast, f, k, \tilde{c})$;
5.     $x' \leftarrow \text{LK}(x_\ast \mid f')$;
6.     $x'' \leftarrow \text{LK}(x' \mid f)$;
7.     if $f(x'') < f(x_\ast)$ then
8.         $x_{\text{output}} \leftarrow x''$;
9.     exit;
10.    $j \leftarrow j + 1$;
11. return $x_{\text{output}}$
Algorithm 6: AddRandomPenalty($x_*, f, k, \tilde{c}$)

1. $\tilde{E} \leftarrow$ randomly select $k$ edges from $x_*$;
2. for each edge $(i, j)$ in the TSP $f$ do
   3. if edge $(i, j) \in \tilde{E}$ then
      4. $c'_{i,j} \leftarrow c_{i,j} + \tilde{c}$
   5. else
      6. $c'_{i,j} \leftarrow c_{i,j}$
7. return $f'$: the TSP based on $\{c'\}$

Problem instances. Using the sub-objectives ($f_1, f_2$) as the judging criterion is relatively less subjective since the decomposition is conducted in a stochastic way. In addition, the proposed objective decomposition method can be easily applied to different problem instances.

5. Experimental Studies and Results

In this section, we first investigate the neighborhood non-dominance hypothesis, then conduct systematic experiments to test the performance of ILS+NDS and ILK+NDE.

5.1. The Neighborhood Non-dominance Hypothesis

In the first experiments, we verify the hypothesis of NDS, i.e., the neighborhood of the non-dominated neighbors of a local optimum is more likely to contain a better solution. We select five TSP instances from the TSPLIB [46] and five UBQP instances form the OR-Library [47]. For the TSP instances, we use the 2-Opt neighborhood structure, i.e., a neighboring solution is obtained by replacing two edges of the current solution by another two edges, as illustrate in Figure 6. For an $n$-city TSP, the size of the 2-Opt neighborhood is $n(n-3)/2$ [48]. For the UBQP instances, we use the 1-bit-flip neighborhood structure, i.e., a neighboring solution is obtained by flipping a bit of the current solution. For an $n$-bit UBQP, the size of the 1-bit-flip neighborhood is $n$. Features of the selected TSP and UBQP instances are shown in Table 1.

To decompose the TSP instances, we first define a function $p'(t)$ in the
Figure 6: An example of the 2-Opt neighborhood in the TSP

Table 1: The selected TSP and UBQP instances

| TSP instance | eil51 | st70 | pr76 | rat99 | rd100 |
|--------------|-------|------|------|-------|-------|
| Problem size | 51    | 70   | 76   | 99    | 100   |
| 2-Opt neighborhood size | 1224 | 2345 | 2774 | 4752  | 4850  |

| UBQP instance | bqp1000.1 | bqp2500.1 | p3000.1 | p4000.1 | p5000.1 |
|---------------|------------|------------|----------|----------|----------|
| Problem size  | 1000       | 2500       | 3000     | 4000     | 5000     |
| 1-bit-flip neighborhood size | 1000 | 2500 | 3000 | 4000 | 5000 |

interval \((0, c_{i,j})\) for each edge \((i, j)\):

\[
p'(t) = \begin{cases} 
  t^a & \text{if } a \geq 0 \text{ and } 0 < t \leq \frac{c_{i,j}}{2}, \\
  (c_{i,j} - t)^a & \text{if } a \geq 0 \text{ and } \frac{c_{i,j}}{2} < t < c_{i,j}, \\
  (c_{i,j} - t)^a & \text{if } a < 0 \text{ and } 0 < t \leq \frac{c_{i,j}}{2}, \\
  t^a & \text{if } a < 0 \text{ and } \frac{c_{i,j}}{2} < t < c_{i,j},
\end{cases}
\]

(8)

where \(a\) is a pre-defined parameter. Then the probability distribution function \(p(t)\) for each edge \((i, j)\) is defined by

\[
p(t) = \frac{p'(t)}{\int_0^{c_{i,j}} p'(t) dt}.
\]

(9)

For example, if \(c_{i,j} = 1000\), Figure 7 shows the probability distribution function \(p(t)\) when \(a = -10, 0, 10\), respectively.

On each TSP instance, we test different \(a\) values ranging from \(-15\) to \(15\) and calculate the \(\rho\) values of the generated \((f_1, f_2)\) pairs. Then eight pairs of \((f_1, f_2)\) with the \(\rho\) value ranging from about -0.5 to about 0.9 are selected for the following experiments. The \(\rho\) values of the selected eight pairs of \((f_1, f_2)\) on each TSP instance are listed in Table 2. For the decomposition of the UBQP instances, the probability distribution function \(p(t)\) is defined in the interval \((\frac{q_{i,j}}{2} - q', \frac{q_{i,j}}{2} + q')\) (see Section 3.2). We set \(q' = 100\) and use the similar method to generate \(p(t)\) and decompose each UBQP instance into eight sub-objective pairs. Specially, if \(q_{i,j} = 0\) in the original UBQP \(f\),
then we directly let $q_{i,j}^{(1)} = 0$ in the sub-objective $f_1$ and $q_{i,j}^{(2)} = 0$ in $f_2$. The sub-objective pairs of the UBQP instances are listed in Table 3.

For each pair and each instance, we conduct 10,000 local search from random initial solutions. For each local optimum, we evaluate all the neighboring solutions and all the neighboring solutions' neighboring solutions based on the original objective function $f$ and the eight sub-objective function pairs.

Assume that $x'$ is a neighboring solution of a local optimum $x_*$, if $x'$ satisfies that $\exists x'' \in \text{Neighborhood}(x'), f(x'') < f(x_*)$ (in a maximization case, $f(x'') > f(x_*)$), then we denote that $x'$ is a promising neighboring solution (P) of the local optimum $x_*$. Otherwise, $x'$ is a non-promising neighboring solution (NP) of $x_*$. On the other hand, given a sub-objective pair $(f_1, f_2)$, if $(f_1(x'), f_2(x'))$ is dominated by $(f_1(x_*), f_2(x_*))$, then we denote that $x'$ is a dominated neighboring solution (D) of $x_*$. Otherwise, $x'$ is a non-dominated neighboring solution (ND) of $x_*$. In our experiment, for each local optimum, we count the proportions of P (NP) neighboring solutions and the proportions of of D (ND) neighboring solutions based on each pairs of $(f_1, f_2)$. Then we average the counting results of the 10,000 local optima. Table 2 and Table 3 lists the average proportion of each type of neighboring solution on the TSP instances and the UBQP instances, respectively. In Table 2 and Table 3, we also list the average proportion of the cross type of neighboring solutions, e.g., NP&D indicates the neighboring solutions that are both non-promising and dominated. The last two columns in Table 2 and Table 3 give the proportion of promising solutions in all the dominated neighboring solution $\left(\frac{P&D}{D}\right)$ and the proportion of promising solutions in all of the non-dominated neighboring solutions $\left(\frac{P&ND}{ND}\right)$. 

![Figure 7: Examples of probability distribution $p(t)$ when $c_{i,j} = 1000.$](image)
Table 2: Local Optimum Neighborhood Investigate Results on the test TSP Instances

| Instance | Sub-objective pairs | Correlation coefficient | Neighboring solution type | Cross neighboring solution type | Relative ratio |
|----------|---------------------|-------------------------|---------------------------|--------------------------------|----------------|
| eil51    | $(f_1, f_2)$        | $\rho = 0.857$         | [Table values]             |                                |                |
|          | $(f_1, f_3)$        | $\rho = 0.858$         | [Table values]             |                                |                |
|          | $(f_1, f_4)$        | $\rho = 0.2271$        | [Table values]             |                                |                |
|          | $(f_2, f_3)$        | $\rho = 0.1087$        | [Table values]             |                                |                |
|          | $(f_2, f_4)$        | $\rho = 0.3122$        | [Table values]             |                                |                |
|          | $(f_3, f_4)$        | $\rho = 0.0789$        | [Table values]             |                                |                |
|          | $(f_4, f_5)$        | $\rho = 0.7146$        | [Table values]             |                                |                |
| st70     | $(f_1, f_2)$        | $\rho = 0.7387$        | [Table values]             |                                |                |
|          | $(f_1, f_3)$        | $\rho = 0.5235$        | [Table values]             |                                |                |
|          | $(f_1, f_4)$        | $\rho = 0.1130$        | [Table values]             |                                |                |
|          | $(f_2, f_3)$        | $\rho = 0.3392$        | [Table values]             |                                |                |
|          | $(f_2, f_4)$        | $\rho = 0.4846$        | [Table values]             |                                |                |
|          | $(f_3, f_4)$        | $\rho = 0.7441$        | [Table values]             |                                |                |
|          | $(f_4, f_5)$        | $\rho = 0.9334$        | [Table values]             |                                |                |
| pr76     | $(f_1, f_2)$        | $\rho = 0.5412$        | [Table values]             |                                |                |
|          | $(f_1, f_3)$        | $\rho = 0.1811$        | [Table values]             |                                |                |
|          | $(f_1, f_4)$        | $\rho = 0.6223$        | [Table values]             |                                |                |
|          | $(f_2, f_3)$        | $\rho = 0.3545$        | [Table values]             |                                |                |
|          | $(f_2, f_4)$        | $\rho = 0.5442$        | [Table values]             |                                |                |
|          | $(f_3, f_4)$        | $\rho = 0.7753$        | [Table values]             |                                |                |
|          | $(f_4, f_5)$        | $\rho = 0.9371$        | [Table values]             |                                |                |
| rat99    | $(f_1, f_2)$        | $\rho = 0.5066$        | [Table values]             |                                |                |
|          | $(f_1, f_3)$        | $\rho = 0.2972$        | [Table values]             |                                |                |
|          | $(f_1, f_4)$        | $\rho = 0.1518$        | [Table values]             |                                |                |
|          | $(f_2, f_3)$        | $\rho = 0.0350$        | [Table values]             |                                |                |
|          | $(f_2, f_4)$        | $\rho = 0.3819$        | [Table values]             |                                |                |
|          | $(f_3, f_4)$        | $\rho = 0.5747$        | [Table values]             |                                |                |
|          | $(f_4, f_5)$        | $\rho = 0.9476$        | [Table values]             |                                |                |
| rd100    | $(f_1, f_2)$        | $\rho = 0.4940$        | [Table values]             |                                |                |
|          | $(f_1, f_3)$        | $\rho = 0.4017$        | [Table values]             |                                |                |
|          | $(f_1, f_4)$        | $\rho = 0.4770$        | [Table values]             |                                |                |
|          | $(f_2, f_3)$        | $\rho = 0.0821$        | [Table values]             |                                |                |
|          | $(f_2, f_4)$        | $\rho = 0.3106$        | [Table values]             |                                |                |
|          | $(f_3, f_4)$        | $\rho = 0.4873$        | [Table values]             |                                |                |
|          | $(f_4, f_5)$        | $\rho = 0.7526$        | [Table values]             |                                |                |
|          | $(f_5, f_6)$        | $\rho = 0.9374$        | [Table values]             |                                |                |
Table 3: Local Optimum Neighborhood Investigate Results on the test UBQP Instances

| Instance | Neighboring solution type | Cross neighboring solution type | Relative ratio |
|----------|---------------------------|---------------------------------|----------------|
|          | Correlation coefficient | Neighboring solution type | Cross neighboring solution type | |
| bqp1000.1 | p = -0.4162 | (f₁, f₂) | 51.89% | 0.05% | 0.02% | 0.73% | 0.06% | 1.40% |
|          | p = -0.2055 | (f₁, f₂) | 44.92% | 0.01% | 0.03% | 0.72% | 0.07% | 1.60% |
|          | p = -0.0112 | (f₁, f₂) | 36.10% | 0.02% | 0.04% | 0.71% | 0.07% | 1.60% |
|          | p = 0.1716 | (f₁, f₂) | 30.13% | 0.03% | 0.05% | 0.70% | 0.08% | 1.73% |
|          | p = 0.1914 | (f₁, f₂) | 24.13% | 0.04% | 0.05% | 0.70% | 0.08% | 1.73% |
|          | p = 0.2707 | (f₁, f₂) | 18.48% | 0.04% | 0.06% | 0.68% | 0.06% | 1.60% |
|          | p = 0.7417 | (f₁, f₂) | 11.05% | 0.03% | 0.06% | 0.64% | 0.10% | 1.57% |
|          | p = 0.9231 | (f₁, f₂) | 4.38% | 0.05% | 0.07% | 0.57% | 0.10% | 1.10% |
| bqp2500.1 | p = -0.4128 | (f₁, f₂) | 51.59% | 0.03% | 0.06% | 0.69% | 0.02% | 0.69% |
|          | p = -0.2086 | (f₁, f₂) | 42.83% | 0.04% | 0.06% | 0.67% | 0.02% | 0.67% |
|          | p = -0.0073 | (f₁, f₂) | 35.70% | 0.04% | 0.06% | 0.67% | 0.02% | 0.67% |
|          | p = 0.1726 | (f₁, f₂) | 29.51% | 0.04% | 0.06% | 0.67% | 0.02% | 0.67% |
|          | p = 0.3225 | (f₁, f₂) | 24.66% | 0.04% | 0.06% | 0.67% | 0.02% | 0.67% |
|          | p = 0.2890 | (f₁, f₂) | 17.48% | 0.05% | 0.06% | 0.67% | 0.02% | 0.67% |
|          | p = 0.7451 | (f₁, f₂) | 11.13% | 0.05% | 0.06% | 0.67% | 0.02% | 0.67% |
|          | p = 0.9241 | (f₁, f₂) | 6.18% | 0.05% | 0.06% | 0.67% | 0.02% | 0.67% |
| p3000.1 | p = -0.4897 | (f₁, f₂) | 51.70% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = -0.1957 | (f₁, f₂) | 43.65% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.0024 | (f₁, f₂) | 35.52% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.1797 | (f₁, f₂) | 29.98% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.3273 | (f₁, f₂) | 24.57% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.5328 | (f₁, f₂) | 17.53% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.7466 | (f₁, f₂) | 10.46% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.9248 | (f₁, f₂) | 8.66% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
| p4000.1 | p = -0.4897 | (f₁, f₂) | 51.61% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = -0.1955 | (f₁, f₂) | 41.84% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = -0.0024 | (f₁, f₂) | 35.52% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.1793 | (f₁, f₂) | 29.65% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.3264 | (f₁, f₂) | 24.19% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.5355 | (f₁, f₂) | 17.12% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.7466 | (f₁, f₂) | 10.46% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.9248 | (f₁, f₂) | 8.66% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
| p5000.1 | p = -0.4897 | (f₁, f₂) | 51.35% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = -0.1949 | (f₁, f₂) | 42.31% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = -0.0024 | (f₁, f₂) | 35.52% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.1801 | (f₁, f₂) | 29.72% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.3267 | (f₁, f₂) | 24.67% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.5330 | (f₁, f₂) | 17.50% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.7667 | (f₁, f₂) | 10.52% | 0.05% | 0.06% | 0.69% | 0.00% | 0.19% |
|          | p = 0.9247 | (f₁, f₂) | 8.54% | 0.06% | 0.06% | 0.69% | 0.00% | 0.19% |

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Based on the results in Table 2 and Table 3, we have the following observations.

First, by comparing column “NP” and column “P” in Table 2 and Table 3, we can see that, on all the TSP/UBQP instances, in all the neighboring solutions of a local optimum, the proportion of the promising neighboring solutions is quite low. The proportion decreases further as the problem size increases. This indicates that it is quite hard to find a promising neighboring solution.

Second, by observing column “D” and column “ND” in Table 2 and Table 3, we can see that, in most cases, the proportion of the non-dominated neighboring solutions is significantly lower than that of the dominated neighboring solutions, except when $\rho$ is very small (e.g. when $\rho = -0.4162$ for the UBQP instance bqp1000.1 in Table 3). In addition, with increasing $\rho$, the proportion of the non-dominated neighboring solutions further decreases. This is intuitive since when $\rho \to 1$, $(f_1(x), f_2(x)) \approx (f(x)/2, f(x)/2)$ for any solution in the solution space (as shown in Figure 3) and $(f(x')/2, f(x')/2) \prec (f(x*)/2, f(x*)/2)$ if $x_*$ is a local optimum and $x'$ is one of its neighboring solutions.

Third, by observing columns “NP&D”, “NP&ND”, “P&D” and “P&ND” in Table 2 and Table 3, we can see that, in most cases, the proportion of the both non-promising and dominated neighboring solutions (NP&D) is the highest among the four cross types of neighboring solutions. The proportion of the intersection of the promising and dominated neighboring solutions (P&D) is the lowest. This means that if a neighboring solution is dominated by the original local optimum, then it is very likely that this solution is non-promising.

Fourth, in the last two columns we list the ratios $\frac{P&D}{D}$ and $\frac{P&ND}{ND}$. The ratios reflect the probability to find a promising neighboring solution in the dominated neighboring solutions and in the non-dominated neighboring solutions, respectively. We can see that, the chance to find a promising neighboring solution in the non-dominated neighboring solutions is significant higher than that in the dominated neighboring solution. It also is higher than the probability to find a promising solution in all the neighboring solutions (column “P”). This supports the neighborhood non-dominance hypothesis that the non-dominated neighboring solutions of a local optimum are more likely to contain a neighboring solution that improves the local optimum.

Fifth, from Table 2 and Table 3, we see that the correlation between the
sub-objectives have a significant influence on the ratio \( \frac{P\&ND}{ND} \) (see Figure 8). On most test instances, we observed that the ratio increases as \( \rho \) increases. However, the correlation should not be too large, since when \( \rho = 1 \) the bi-objective problem \((f_1, f_2)\) will be degenerated into a single-objective problem (because \( f_1 = f_2 \)) and there will be no non-dominated neighboring solution. On the small size TSP instances eil51 and st70, we observed the decrease of the ratio \( \frac{P\&ND}{ND} \) when \( \rho \) increases from about 0.7 to about 0.9.

Particularly, in Table 3 an interesting phenomenon is that on the UBQP instances the proportions of the intersection of the promising and dominated neighboring solutions (P&D) are extremely low, especially on large UBQP instances. For example, on the UBQP instance p5000.1, the P&D proportion is 0 for all the eight sub-objective pairs.

To better illustrate the neighborhood investigate results, Figure 9 plots all the neighboring solutions of an example local optimum of the UBQP instance bp1000.1 in the eight bi-objective spaces with different levels of correlation. Note here that the UBQP is a maximization problem hence the dominance definition in the UBQP is opposite to that in the TSP. In Figure 9 the local optimum is marked by green dots, the dominated neighboring solutions are in red color while the non-dominated ones are in blue color; the promising neighboring solutions are marked by triangles while the non-promising ones are marked by dots. Hence, in Figure 9 a blue triangle means a solution is both non-dominated and promising. From Figure 9 we can see that most of the promising neighboring solutions are non-dominated to the original local optimum.
optimum.

5.2. The Performance of ILS+NDS

In this sub-section, we compare ILS+NDS against the origin ILS, and an ILS variant called ILS with Exhaustive Neighborhood Search (ILS+E NS). ILS+ENS is similar to ILS+NDS, except that in ILS+ENS the NDS procedure is replaced by the ENS procedure. The ENS procedure can be seen as a NDS procedure without the guidance of the sub-objectives \((f_1, f_2)\), which is shown in Algorithm 7. By comparing ILS+NDS against ILS+ENS, we should know whether the sub-objects can truly improve the performance of ILS.

The test instances in Table 1 are also used as benchmark. For the TSP instances, the 2-Opt neighborhood and the double bridge perturbation are applied in the implementations of ILS, ILS+E NS and ILS+NDS. For the UBQP instances, the 1-bit-flip neighborhood and a random flip perturbation strategy are applied. In the random flip perturbation, 25% of the total bits in the current solution are randomly selected and flipped. On each instance, the implementation of ILS+NDS uses the same eight sub-objective
Algorithm 7: Exhaustive Neighborhood Search (ENS)

Input: \( x^*, f \)

1. \( x_{output} \leftarrow x^*; \)
2. for each \( x' \in \text{Neighborhood}(x^*) \) do
   3. for each \( x'' \in \text{Neighborhood}(x') \) do
      4. if \( f(x'') < f(x^*) \) then
         5. \( x_{output} \leftarrow x''; \)
      6. exit;
3. return \( x_{output} \)

pairs in Table 2 and Table 3. Hence, on each test instance, we have ten test algorithms: ILS, ILS+ENS, ILS+NDS with \((f_1, f_2)_1\), ILS+NDS with \((f_1, f_2)_2\), …, ILS+NDS with \((f_1, f_2)_8\). Each algorithm is executed 50 times from different random initial solutions and stops when the globally optimal function value is reached or after \(10^{10}\) function evaluations. The globally optimal function values of the UBQP instances are available from [49]. The code is implemented in GNU C++ with O2 optimizing compilation. The computing platform is two 6-core 2.00GHz Intel Xeon E5-2620 CPUs (24 Logical Processors) under Ubuntu OS.

To measure the quality of the solutions found by different algorithms, we use the metric excess which is defined by

\[
\text{excess}(x) = \frac{|f(x) - f(x_{opt})|}{f(x_{opt})},
\]

where \( x_{opt} \) is the global optimum. The lower excess the better. Figure 10 shows the mean excess achieved by the compared algorithms against time. In Figure 10 the mean excess curves are in logarithmic to the base 10 scale. If a curve terminates before the final time it means that all the runs have found the global optimum before the final time.

From Figure 10 we can see that, on all the test instances, the best performance is achieved by ILS+NDS. In addition, at most setups of \( \rho \), ILS+NDS performs better than ILS and ILS+ENS. On some instances (e.g. UBQP instance bpq1000.1), ILS+ENS performs better than ILS. However, on most instances, ILS+ENS performs worse than ILS. This indicates that without the guidance of the sub-objectives, the search efficiency of ILS+ENS decreases significantly.
By comparing different ILS+NDS setups, we can observe that the sub-objective correlation significantly influences the performance of ILS+NDS. In the previous neighborhood exploration experiment, we observed that the higher correlation the better chance to find a promising neighboring solution. However, in this experiment, it shows that the sub-objective correlation is not the higher the better. For example on the TSP instance rd100, the ILS+NDS implementation with $\rho = 0.9374$ performs significantly worse than the ILS+NDS implementation with $\rho = 0.3106$. This shows that the performance of a neighborhood search algorithm is not only decided by the probability to find improving neighboring solutions. Many other factors could influence the algorithm performance. Although a much high correlation is not preferred, the results show that a positive correlation coefficient is better than a negative one on most test instances.

5.3. The Performance of ILK+NDE

In this section, we test the performance of ILK+NDE on six middle-size and large-size TSP instances. To verify the effect of the proposed NDE technique, we compare ILK+NDE against the original ILK and a variant of ILK+NDE in which the guidance of the sub-objectives is removed which is named as Iterated Lin-Kernighan algorithm with further Exploitation (ILK+E). ILK+E is summarized in Algorithm 8, in which we can see that ILK+E conducts further exploitation on all the encountered LK local optima. By comparing ILK+E against ILK+NDE, we can verify whether the sub-objectives ($f_1, f_2$) can truly improve the algorithm performance.

In the following experiment, we compare ILK+NDE against ILK and ILK+E on six middle-size and large-size TSP instances from the TSPLIB: {pcb3038, fnl4461, pla7397, rl11849, usa13509, d18512}. In the experiments, the implementation of the LK local search is from the Concorde software package\footnote{http://www.math.uwaterloo.ca/tsp/concorde/}. In the implementation of the LK local search, the edge exchange is restricted in a sub-graph of the original TSP graph $G$. In the sub-graph, each vertex (city) only connect with its 20 nearest vertexes (cities). The double bridge perturbation is used in the implementations of ILK, ILK+E and ILK+NDE. For the implementation of ILK+E and ILK+NDE, we set $T = 1000$, $k = 5$ and the penalty $\tilde{c}$ is equal to the largest edge cost in each test instance. In the ILK+NDE, first the original TSP is decomposed into two
Figure 10: Excess vs. function evaluations on 5 TSP instances and 5 UBQP instances
Algorithm 8: ILK+E

Input: $f$, $T$, $k$, $\tilde{c}$

1. Decompose $f$ into $f_1$ and $f_2$;
2. $x'_0 \leftarrow$ randomly or heuristically generated solution;
3. $x_0 \leftarrow$ LK($x'_0$ | $f$);
4. $x_{\text{best}} \leftarrow x_0$;
5. $j \leftarrow 0$;
6. while stopping criterion is not met do
   7. $x_{j+1} \leftarrow$ FurtherExploit($x_j$ | $T$, $k$, $\tilde{c}$);
   8. if $x_{j+1} = x_j$ then
      9. $x'_{j+1} \leftarrow$ Perturbation($x_j$);
   10. $x_{j+1} \leftarrow$ LK($x'_{j+1}$ | $f$);
   11. if $f(x_{j+1}) < f(x_{\text{best}})$ then
      12. $x_{\text{best}} \leftarrow x_{j+1}$;
      13. $j \leftarrow j + 1$;
7. return the historical best solution $x_{\text{best}}$

Sub-objectives ($f_1$, $f_2$) based on the decomposition introduced in Section 3.1. Since the LK local search only focuses on the edges in the nearest sub-graph of the TSP, we only decompose the edges in the sub-graph. Based on the previous experimental results, it is better to have a relative high - but not very high - sub-objective correlation.

With different probability distribution $p$ (see Eq. (9)), we decompose each test instance and choose the the following sub-objective correlation coefficients: $\{\text{pcb3038: 0.3534, fnl4461: 0.2736, pla7397: 0.3622, rl11849: 0.4552, usa13509: 0.5099, d18512: 0.4129}\}$. It is very hard to count the function evaluation number in the LK local search, hence we use the CPU runtime as the stopping criterion for the compared algorithms. The max runtime on the test instances are $\{\text{pcb3038: 600s, fnl4461: 900s, pla7397: 1500s, rl11849: 2400s, usa13509: 2700s, d18512: 3700s}\}$. In the ILK+E and ILK+NDE implementations, in the first 1/5 runtime the ILK procedure is applied; while in the last 4/5 runtime it is the ILK+E/ILK+NDE procedure. On each instance, each algorithm is run 50 times from different random initial solutions.

Figure 11 shows the mean excess achieved by different algorithms against time. Table 4 shows the obtained final excess values. From Figure 11 and
Table 4: Final Excess of Different Algorithms

| Instance | Final Excess (%) | P-value |
|----------|------------------|---------|
|          | ILK  | ILK+E | ILK+NDE | ILK+E vs. ILK+NDE |
| pcb3038  | 0.4334| 0.2712| **0.2349**| 0.0318 |
| fnl4461  | 0.5117| 0.2341| **0.2340**| 0.9945 |
| pla7397  | 0.4567| 0.4405| **0.3552**| 0.0093 |
| rl11849  | 0.8580| 0.8183| **0.5957**| 0.0011 |
| usa13509 | 0.6495| 0.4543| **0.3978**| 0.0005 |
| d18512   | 0.6560| 0.4244| **0.4012**| 0.0320 |

Table 4 we can see that, on five of the six test instances, ILK+NDE performs the best. On fnl4461, ILK+NDE and ILK+E perform the same. Since in the first 1/5 runtime ILK+NDE runs the ILK procedure, its behavior is same to the ILK implementation. After the first 1/5 runtime, the unique mechanism of ILK+NDE starts to take effect and the performance of ILK+NDE becomes obvious better than that of ILK and ILK+E on five of the six test instances. From the p-values of the Mann-Whitney U-test shown in the last column of Table 4, we may conclude that ILK+NDE performs significantly better than ILK+E on the used instances at a significance level of 0.05. This results show that the sub-objectives \( f_1, f_2 \) can indeed benefit the LK local search on middle-size and large-size TSP instances.

6. Conclusions

In this paper, we proposed a new objective decomposition method which is suitable for a certain subclass of COPs, which we called the sum-of-the-parts COPs. We gave the formalization of the sum-of-the-parts COP and showed that the TSP and the UBQP belong to this class. The proposed method decomposes the objective function of a sum-of-the-parts COP into two sub-objectives by splitting the unit costs following a certain probability distribution. It was shown that the correlation between the decomposed sub-objectives can be controlled by the use of the probability distribution.

Based on the non-dominance relationship introduced by the decomposed sub-objectives, we proposed two new multi-objectivization techniques. The first was called Non-Dominance Search (NDS). NDS can be used as an escaping scheme from local optima for metaheuristics with fixed neighborhood structure. NDS is based on our neighborhood non-
Figure 11: Excess vs time on 6 middle-size and large-size large TSP instances
dominance hypothesis which states that the neighborhood of a non-dominated neighboring solution of a local optimum is more likely to improve the local optimum. Empirical studies on some selected TSP and UBQP instances confirm that the hypothesis hold. NDS was combined within the Iterated Local Search, called ILS+NDS. Experimental results on the same TSP and UBQP instances showed that ILS+NDS outperform the original ILS and ILS+ENS.

The second is called Non-Dominance Exploitation (NDE), which is applicable for metaheuristics with varied neighborhood structure, such as the Lin-Kernighan (LK) heuristic for the TSP. NDE is proposed to exploit promising local optima based on the non-dominance relationship. NDE was combined with the Iterated Lin-Kernighan algorithm (ILK), called ILK+NDE. Experimental results on middle-size and large-size TSP instances showed that ILK+NDE significantly outperform the original ILK and ILK+E.

In the future, we intend to test the performance of the proposed objective decomposition method on other sum-of-the-parts COPs.

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