New links between Fourier analysis and combinatorial optimization: from instances to rankings

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Starting date: 1st of December, 2022

Expected defense date: 15th of December, 2026

Abstract. The Fourier transform on the real domain allows us to decompose a given function into the superposition of sine and cosine waves representing its different frequency components. This decomposition was first studied in the 19th century and has since become widely used across many fields, including signal analysis, image processing, and data compression. Equally interesting, but much less known, is the finite group extension of the Fourier transform. Just as in the real domain, the Fourier transform on finite groups decomposes discrete functions into a sum of basic components, each capturing a different piece of information from the original function. Motivated by this perspective, the literature has long tried to exploit the Fourier transform to address optimization problems on such discrete domains. A central challenge in this line of research is the limited interpretability of the Fourier space, particularly when working with complex structures such as permutations. The primary objective of this thesis is therefore to advance the understanding of the Fourier transform in combinatorial optimization from two complementary points of view: the instances of the problems and the analysis of the rankings induced by their objective functions. We approach this task through the lens of metaheuristic optimization, seeking to bring the abstract nature of Fourier analysis into a concrete and interpretable framework.

Keywords: Fourier transform, combinatorial optimization, instances, rankings, binary vectors, permutations.

1 Introduction

It is known that any real-valued signal can be represented as an infinite superposition of sine and cosine waves at different frequencies [1, 2]. This transformation from the time domain to the frequency domain enables a wide range of analyses and applications that would otherwise be difficult or impossible to perform. For instance, consider a sound signal produced by three piano notes played simultaneously. From the signal alone, it is not straightforward to detect which notes are present. However, by applying the Fourier transform, the signal can be decomposed into its frequency components, which in turn can be used to identify the individual notes that compose the sound.

Decomposing a complex object into a set of more manageable pieces is also the heart of many classical algorithms in computer science. For example, one can think of the case of sorting algorithms such a quick sort and merge sort, which use divide and conquer strategies to effectively sort a large array by repeatedly sorting a set of smaller sub-arrays [3]. The field of optimization is also familiar with the idea of divide and conquer. A notable example is multi-objectivization [4–6], a well-studied approach in which a single objective function is reformulated into several distinct functions, each of which is handled separately during the optimization process. Thus, it seems natural to wonder: is it possible to apply the Fourier transform as a tool for optimization?

In this thesis, we are particularly interested in the case of combinatorial optimization problems (COPs). In combinatorial optimization, the solutions are not collections of real values, but a discrete set of finite (or countably infinite) elements that is called the search space of the problem. In many cases, the search space forms what is known as a finite group [7], a special kind of mathematical object with particular algebraic properties. The Fourier transform is also defined for functions on finite groups [8], so it is possible to apply this technique for the decomposition of the objective function of COPs.

The idea of using the Fourier transform to decompose objective functions of COPs is not new. It has been studied for at least 30 years, dating back to the 1990s, where multiple works laid the foundations for analyzing fitness landscapes through the lens of Fourier analysis [9–12]. However, one of the first proposals for an explicit practical application in combinatorial optimization appeared a decade later, when Kondor [13] introduced a branch-and-bound approach for the quadratic assignment problem. This method uses the Fourier transform on the symmetric group (i.e., the permutation domain) to compute better bounds for the problem in some particular cases.

The work by [13] hinted the beginning of a prolific line of research concerning the application of the Fourier transform for solving COPs, a research line that, however, has not yet fully materialize. Over the 2010s decade, the use of Fourier analysis in combinatorial optimization largely remained confined to constructing efficient surrogate functions for expensive or black-box objectives [14–16]. Other studies also employed Fourier transforms to enable theoretical comparisons between different problems within a unified representation space [17–19], but comparatively little progress was made toward practical optimization meth-

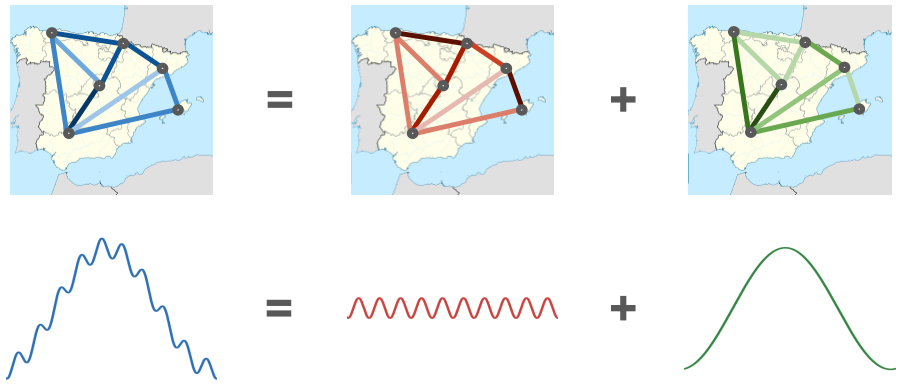


Fig. 1. Analogue to the Fourier transform in the function domain, the proposed instance-based framework aims to decompose COP instances into sub-instances that isolate specific types of interactions.

ods for solving COPs using these techniques. Some exceptions can be found in the binary domain, where spectral information has been used to identify epistatic interactions for the effective application of crossover operators [20], as well as to detect potentially improving movements in local search algorithms [21]. In contrast, progress in the permutation domain has been considerably slower. As an example, the algorithm by [13] was not generalized to higher-order assignment problems until 2022, by Clausen [22].

The thesis presented in this document is developed within this context. It addresses the limited use of the Fourier transform in combinatorial optimization from two complementary perspectives. The first concerns the instance space of COPs, particularly those defined in the permutation domain. In certain settings, information from individual Fourier components can be fully captured by problem instances with fixed structural properties. Motivated by this observation, we seek a systematic method for decomposing a given COP instance into a collection of sub-instances of the same problem and dimension, each corresponding to a single term in the Fourier transform of the objective function (Figure 1). Importantly, this decomposition is constructed without explicitly operating in the Fourier domain. We refer to this alternative methodology as the *Fourier transform-based instance decomposition*, and its purpose is to make the information encoded by the Fourier transform more accessible and practically usable in optimization.

Unlike the classical Fourier transform, the instance-based framework depends strongly on the specific characteristics of the problem at hand. Consequently, to the best of our knowledge, it is not possible to define a generic Fourier transform-

based instance decomposition that applies universally to any permutation-based problem. Instead, we concentrate on a particular class of related problems, namely the k-adic assignment problems (k-APs) [23]. This class encompasses many of the most well-known permutation-based problems from the literature, such as the linear ordering problem [24], the quadratic assignment problem [25], and the traveling salesperson problem [26], as well as many other higher-order problems such as the bi-quadratic assignment problem [27]. Therefore, although our analysis is restricted to a particular subset of permutation-based COPs, it remains sufficiently general and is applicable to some of the most studied scenarios in the literature.

Additionally, as an illustration of the potential applications of the proposed framework, we explore several research directions, all of them built on the idea that, similar to the Fourier transform on the real domain, each component in the Fourier transform of a permutation-based function exhibits distinct landscape characteristics. This ability could be leveraged both to design more effective neighborhood-based metaheuristics and to generate artificial instances with adjustable levels of difficulty, among other potentials usages.

The second perspective analyzed in this thesis focuses on a different aspect of COPs: the ranking of solutions induced by the objective function [28, 29]. A ranking in combinatorial optimization is a function that assigns to each feasible solution its position relative to all other solutions in the search space, ordered according to the corresponding fitness value. Although there are infinitely many possible objective functions, they induce only finitely many distinct rankings. Consequently, these objective functions can be partitioned into a finite set of equivalence classes, where each class corresponds to a unique ranking over the solutions. This partition of the space of objective functions results of theoretical interest due to the fact that many classical optimization algorithms work by comparing which solutions are better or worse, without actually paying attention to the exact objective function values. This is the case, for example, of many classical metaheuristic algorithms such as iterated local search [30], tabu search [31] or variable neighborhood search [32], as well as many evolutionary algorithms that use tournament or rank selection strategies [33].

The literature has recently linked the study of rankings with the Fourier analysis of combinatorial objective functions. A particularly notable example can be found in [34], where the authors tried to find the minimum Fourier support needed to generate a given ranking in the binary domain, focusing on small instances ($n = 3$). Expanding this analysis, and extending it to the permutation domain, constitutes another research direction within the scope of this thesis.

2 Objectives

This thesis aims to advance the understanding of the Fourier transform within the combinatorial optimization field. In particular, it investigates the instance and ranking spaces of COPs through the framework of Fourier analysis. The specific objectives addressed in this thesis are presented below.

$O1$ **Develop a Fourier transform-based instance decomposition for the linear ordering problem.** The linear ordering problem (LOP) is a well-known COP whose objective is to determine an optimal ordering (permutation) of a set of elements, given a matrix encoding pairwise preferences among them. It arises in a wide range of application domains, including archaeology [35], economics [36], voting theory [37], and mathematical psychology [38].
The LOP has been extensively investigated in the literature about Fourier analysis. In particular, it is known that the Fourier transform of its objective function contains only two non-trivial coefficients: one corresponding to first-order information and another capturing second-order interactions [18]. Elorza et al. [39] showed that, under certain conditions on the problem instance, either of these two components can be nullified. The authors wondered whether these conditions allow any LOP instance to be split into two parts, each linked to one of the Fourier coefficients. We aim to address the previous question by designing an easy to implement polynomial-time algorithm to perform the instance decomposition of the LOP without explicitly computing the Fourier transform. We also discuss the relationship between the proposed framework and other related approaches in voting theory applications [40].

$O2$ **Generalize the decomposition for the general case of k-adic assignment problems.** Once the Fourier transform–based instance decomposition for the LOP has been established in $O1$, the next step is to extend this approach to the more general setting of k-APs. A k-AP consists of finding the best matching between two hypergraphs of order k, in such a way that the sum of the the products between the weights of overlapping hyperedges gets maximized. A solution to the problem consits of a permutation that tells us how to map the vertices of one hypergraph to the vertices of the other.
In contrast to the LOP, a general k-AP involves a variable number of non-trivial Fourier coefficients, which depends on the parameter k. For example, when $k = 2$, the problem has three non-trivial coefficients [12]. This number increases to six when $k = 3$ and to eleven when $k = 4$. In general, larger values of k give rise to higher-order non-trivial coefficients [22].
Given this increased complexity, extending the decomposition framework from the LOP to general k-APs requires careful algorithmic design. In particular, the decomposition algorithm must be sufficiently optimized to ensure that the resulting framework remains computationally feasible and practically applicable, at least for small values of k. The objective is to achieve this by manipulating the instance values directly, without explicitly computing the Fourier transform.

$O3$ **Design metaheuristic algorithms that exploit the information provided by the Fourier transform.** As mentioned in the introduction, one of the main gaps identified in the literature is the design of optimization algorithms based on the Fourier transform, with particular emphasis on metaheuristic approaches. A metaheuristic algorithm is an optimization method that does not guarantee finding the global optimum of a problem, but instead balances solution quality and computational cost to obtain sufficiently

good solutions within a reasonable amount of time [41]. We argue that the information provided by the Fourier transform can be highly beneficial for the design of such algorithms.

This idea is illustrated by developing a metaheuristic algorithm that intelligently exploits the Fourier transform–based instance decomposition in the context of the LOP. We focus on this more constrained scenario compared to the general k-AP as it provides a natural starting point for experimentation. This choice is motivated by the fact that, according to [39], one of the Fourier components characterizing the objective function can be solved exactly in polynomial time. Consequently, the Fourier transform-based instance decomposition allows any LOP instance to be expressed as the sum of two different LOPs, one of which defines a P-complexity problem. This framework provides a particularly suitable setting for the design of metaheuristic algorithms, particularly local search-based methods that intentionally perturb the problem instance to obtain easier to navigate landscapes [42, 43].

$O4$ **Design instance generation procedures based on the Fourier transform.** Generating challenging artificial instances is an important task for evaluating algorithmic developments. Ideally, one would rely on a large collection of real-world instances that provide a realistic and representative benchmark for comparing different methods. In practice, however, this is often infeasible, as collecting such data can be both difficult and expensive. As a result, considerable research has focused on developing techniques for constructing artificial instances with controllable properties [44–46].

The strong connection between Fourier transform components and measures of ruggedness in fitness landscapes [47] provides a promising foundation for generating artificial instances of the k-AP. In particular, the Fourier transform-based instance decomposition introduced in this thesis offers a natural framework for directly tuning the spectral properties of k-AP problems at the instance level.

$O5$ **Expand the analysis on rankings of combinatorial optimization problems.** The ranking of solutions within the search space of a COP is a key feature, as it has a strong impact on the behavior of classical metaheuristic algorithms. Yet, compared to other properties, this aspect has received relatively little attention in the literature. Although some studies have examined the rankings of pseudo-boolean functions (i.e., functions defined on binary vectors) [29, 34], analyses in permutation-based settings remain limited [28].

In response, the final objective of this thesis is to deepen the study of rankings through the framework of the Fourier transform. We start with the more established setting of pseudo-boolean functions and then extend our results to permutations.

3 Methodology

In this section, we present the methodology and work plan designed to achieve the main objectives of the thesis. At the time of writing, the thesis is in its final year of development. Consequently, the first four objectives have already been addressed, and only the final objective remains under development.

- $O1$ **Develop a Fourier transform-based instance decomposition for the linear ordering problem.**
  - $T1.1$ Review the literature on Fourier analysis for combinatorial optimization problems.
  - $T1.2$ Building on the study in [39], check if the instance decomposition of the LOP is actually feasible.
  - $T1.3$ Develop a formal methodology for the decomposition process.
- $O2$ **Generalize the decomposition for the general case of k-adic assignment problems.**
  - $T2.1$ Review the literature on higher-order assignment problems.
  - $T2.2$ Characterize the conditions on the instance values that ensure that a k-AP has exactly one non-zero Fourier coefficient.
  - $T2.3$ Extend the instance decomposition methodology introduced in $T1.3$ by incorporating the conditions defined in $T2.2$.
- $O3$ **Design metaheuristic algorithms that exploit the information provided by the Fourier transform.**
  - $T3.1$ Examine and compare approaches for incorporating the Fourier transform–based instance decomposition within established metaheuristic frameworks.
  - $T3.2$ Identify the most promising strategy and propose a concrete metaheuristic algorithm based on it.
  - $T3.3$ Evaluate the proposed metaheuristic and statistically validate that the integration of the Fourier-domain knowledge is beneficial for the search process in the particular case of the LOP.
- $O4$ **Design instance generation procedures based on the Fourier transform.**
  - $T4.1$ Investigate how the characteristics of the Fourier components affect the difficulty of the k-AP for local search methods, considering both landscape ruggedness measures and empirical performance of metaheuristic algorithms.
  - $T4.2$ Develop an efficient method for controlling the contribution of the Fourier components to the variance of the objective function.
  - $T4.3$ Define a tunable instance generation procedure for the k-AP that combines the sub-instances obtained from the Fourier transform-based instance decomposition.
- $O5$ **Expand the analysis on rankings of combinatorial optimization problems.**
  - $T5.1$ Review existing literature on the relationship between Fourier analysis and the rankings induced by functions on finite groups, with particular focus on the well-studied binary setting.

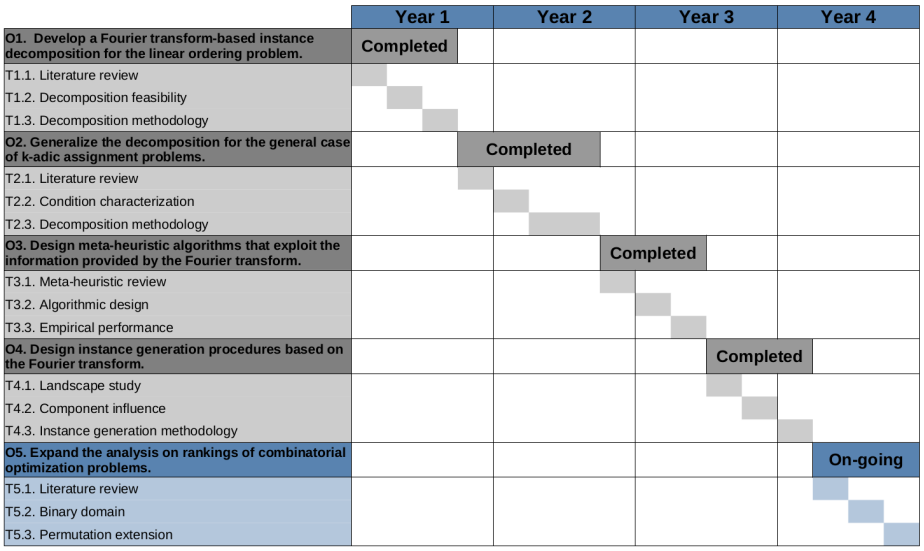


Fig. 2. Approximate timeline of the thesis project.

$T5.2$ Search for new connections in the Fourier characterization of pseudo-boolean functions sharing the same ranking.

$T5.3$ Generalize results from the binary domain to the permutation domain.

The approximate timeline of the work plan over the four years of the thesis project is presented in Figure 2.

4 Relevance

The Fourier transform has proven to be a powerful tool for the analysis of functions defined on finite groups. Its relationship with the structural properties of such functions indicates that the information encoded in the Fourier domain could substantially benefit optimization algorithms. Nevertheless, practical applications of these ideas remain relatively scarce. This thesis seeks to contribute to this area by examining two aspects of COPs through Fourier analysis: the problem instances and the rankings of solutions induced by their objective functions.

In this line, our first contribution consists in defining an easier to interpret instance-based analogue of the Fourier transform. First, we provide an explicit decomposition methodology for a wide class of permutation-based problems that does not require operating in the Fourier domain. Then, we demonstrate practical applications of the proposed methodology, focusing on metaheuristic algorithm design and artificial instance generation. Overall, this thesis opens a new perspective that, we hope, will help new researchers incorporate Fourier-domain

knowledge into their algorithmic developments. In this way, the Fourier transform may move beyond a primarily theoretical context and become a common tool for combinatorial optimization.

In addition to the study of instances, the thesis also explores the role of the Fourier transform in the analysis of rankings of COPs. We delve deeper into the study of rankings of pseudo-boolean functions, and attempt to extend the obtained results to the permutation domain. This line of research has interesting implications not only for the study of already existing metaheuristics, but for the proposition of new, more effective approaches. For example, consider the case of optimization methods that directly model interactions between variables, such as estimation of distribution algorithms [48]. These approaches usually aim to capture all interactions affecting the fitness function through complex probabilistic models. However, if the ranking of solutions is primarily characterized by low-order interactions (encoded by low-order Fourier coefficients), then simpler models may still capture the information regarding the relative quality of the solutions in the search space. Thus, for a given problem instance, developing methods to measure which types of interactions have the strongest influence on the ranking of solutions could be a promising research direction.

5 Scientific outputs

Over the first three years of the thesis project, several research outputs have been developed as part of the overall research pipeline. This section provides a brief overview of each of them and relates each item to the objectives defined in Section 2.

5.1 Journal publications

1. *P-NP instance decomposition based on the Fourier transform for solving the Linear Ordering Problem (Evolutionary Computation Journal, MIT Press) [49]*: Paper that introduces the Fourier transform-based instance decomposition of the LOP ($O1$), as well as a metaheuristic algorithm based on it ($O3$).
2. *Fourier transform-based instance decomposition for k-adic Assignment problems (Transactions on Evolutionary Computation, IEEE) [50]*: Paper that generalizes the Fourier transform-based instance decomposition to the k-AP class of problems ($O2$). It also introduces an instance generation method based on this framework ($O4$).
3. *Spectral characterization of rankings in combinatorial optimization by means of the Chow's theorem (Under review)*: Paper that studies the rankings of pseudo-boolean and permutation-based functions using Fourier analysis, with particular focus on the connections to threshold logic ($O5$).

The source code associated with the different publications has been made publicly available as supplementary material, either by direct download or through GitHub repositories.

5.2 Conference presentations

1. *XVI Congreso Español de Metaheurísticas, Algoritmos Evolutivos y Bioinspirados (28/05/2025-30/05/2025, San Sebastian, Spain):* Talk on the Fourier transform-based instance decomposition of the LOP and its application to the design of metaheuristic algorithms ($O1$, $O3$).
2. *XLI Congreso Nacional de Estadística e Investigación Operativa (10/06/2025-13/06/2025, Lleida, Spain):* Talk on the generalization of the Fourier transform-based instance decomposition to the k-AP class of problems ($O2$, $O4$).

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