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Generation of the exact Pareto set in multi-objective traveling salesman and set covering problems

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Abstract: The calculation of the exact set in Multi-Objective Combinatorial Optimization (MOCO) problems is one of the most computationally demanding tasks as most of the problems are NP-hard. In the present work we use AUGMECON2 a Multi-Objective Mathematical Programming (MOMP) method which is capable of generating the exact Pareto set in Multi-Objective Integer Programming (MOIP) problems for producing all the Pareto optimal solutions in two popular MOCO problems: The Multi-Objective Traveling Salesman Problem (MOTSP) and the Multi-Objective Set Covering problem (MOSCP). The computational experiment is confined to two-objective problems that are found in the literature. The performance of the algorithm is slightly better to what is already found from previous works and it goes one step further generating the exact Pareto set to till now unsolved problems. The results are provided in a dedicated site and can be useful for benchmarking with other MOMP methods or even Multi-Objective Meta-Heuristics (MOMH) that can check the performance of their approximate solution against the exact solution in MOTSP and MOSCP problems.

Keywords: multi-objective, traveling salesman problem, set covering problem, ε-constraint, exact Pareto set

Table of Abbreviations

Abbreviation	Meaning
2PPLS	Two-Phase Pareto Local Search
2P-SAECON	Two Phase Simulated Annealing Epsilon Constraint method
AM	Approximate Method
AUGMECON	Augmented Epsilon Constraint
AUGMECON2	Augmented Epsilon Constraint 2
B&C	Branch and Cut algorithm
BCH	Branch and Cut and Heuristic
BCHTSP	Branch and Cut and Heuristic algorithm for Traveling Salesman Problem
BOSCP	Bi-Objective Set Covering Problem
BOTSP	Bi-Objective Traveling Salesman Problem
CONCORDE	The relevant CONCORDE solver for TSP
EPS	Exact Pareto Set
GAMS	General Algebraic Modeling System
HV	Hypervolume metric
IP	Integer Programming
LKH	Lin-Kernighan algorithm of Helsgaun
MCO	Multi-Criteria Optimization
MOCO	Multi-Objective Combinatorial Optimization

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MOIP	Multi-Objective Integer Programming
MOMH	Multi-Objective Meta-Heuristics
MOMP	Multi-Objective Mathematical Programming
MOSCP	Multi-Objective Set Covering Problem
MOTSP	Multi-Objective Traveling Salesman Problem
MS	Models Solved
MTZ	Miller-Tucker-Zemlin formulation for the TSP
PE	Potentially Efficient solutions
*PF**	exact Pareto Front
PMA	Pareto Memetic Algorithm
POS	Pareto Optimal Solution(s)
R	Reference Set
RHS	Right Hand Side
SCP	Set Covering Problem
SE	Supported Efficient solutions
SLS	Stochastic Local Search
TSP	Traveling Salesman Problem

1. Introduction

Multi-Criteria Optimization (MCO) attracts all the more interest mainly due to two reasons: (1) the multiple points of view (expressed as criteria or objective functions) that allow the decision maker to make more balanced decisions through a Multi-Objective Decision Making approach (2) MCO is a computational intensive task that can take advantage of the vast improvement in computational systems and algorithms. Usually there is no unique optimal solution (optimizing simultaneously all the criteria) but a set of Pareto optimal solutions which are mathematically equivalent (Pareto set). The decision maker must be involved in order to express his preferences in order to find the most preferred among the Pareto optimal solutions [1]. Therefore, MCO methods have to combine optimization with decision support.

Multi-Objective Mathematical Programming (MOMP) deals with the MCO problem when it is formulated as a Mathematical Programming problem with more than one objective functions. Hwang and Masud [2] classified the MOMP methods into three classes according to the phase in which the decision maker was involved in the decision making process: The a priori methods, the interactive methods and the a posteriori or generation methods. The a posteriori methods were given lower priority at these days as they were the most computationally demanding and the solution of even medium-sized problems was impossible.

From the beginning of the 21st century MOMP entered the area of Multi-Objective Combinatorial Optimization (MOCO) problems (Ehrgott and Gandibleux [3]). The basic characteristic of MOCO problems is that the decision variables are integer (mostly binary) and the relevant problems are most of the time NP-complete even in their single objective version. In addition, the discrete feasible region allows for the calculation of all the Pareto optimal solutions, at least theoretically. The difficulty of calculating the exact Pareto set i.e. all the Pareto optimal solutions, gave rise to approximate methods mainly based on metaheuristic algorithms (Coello et al. [4]).

The aim of this paper is to apply the recently proposed improved version of the augmented ε-constraint method (AUGMECON2, Mavrotas and Florios [5]), which is suitable for general MOIP problems, to two popular MOCO problems, namely, the Multi-Objective Traveling Salesman Problem (MOTSP) and the Multi-Objective Set Covering Problem (MOSCP). Although AUGMECON2 is designed for the general case, here it is applied to bi-objective problems confined by benchmark-data availability. We test the AUGMECON2 method, a MOMP method which is capable of producing the exact Pareto set in Multi-Objective Integer Programming (MOIP) problems, in some of the well known benchmarks. After some experimentation with available formulations, the proposed method was eventually a combination of a general purpose MOIP model (AUGMECON2), with a Branch-and-Cut-and-Heuristic model (BCHTSP) available in General Algebraic Modeling System (GAMS) model library.

Our proposed method solves exactly for first time, 16 specific benchmarks of symmetric MOTSP with 2 objectives and 100 cities which were previously only heuristically solved. The same is done for 44 MOSCP benchmark problems found in the literature, some of them never solved exactly. We publish the exact Pareto Fronts in a website (https://sites.google.com/site/kflorios/motsp), in order to promote benchmarking of Multi-Objective Metaheuristics (MOMHs). In other words, having the exact Pareto set for MOTSP or MOSCP benchmarks, the MOCO community is able to assess the effectiveness of state-of-the-art Multi-Objective Metaheuristics (MOMHs).

In addition, we stress our approach to produce the exact Pareto front (1) to a bigger bi-objective TSP problem with 150 cities and (2) to a three objective TSP problem aiming at exploring the limits of our approach. For bi-objective TSP problems with more than 150 cities, a combination of simulated annealing and ε-constraint that produces an approximate (not the exact) Pareto front is also developed and compared with relevant available algorithms. It must be noted that even in the cases that an approximation of the Pareto set in MOCO problems is sought; all the solutions that are obtained with AUGMECON2 are confirmed to be true Pareto Optimal solutions (e.g. there are no other undiscovered solutions that dominate them).

The structure of the paper is as follows: In Section 2 we review the literature in MOTSP and MOSCP and present the corresponding problem formulations. Section 3 describes the methodology, mainly the AUGMECON2 method, the Branch and Cut and Heuristic (BCH) model for the TSP and their coupling for the solution of MOTSP problems. MOSCP solution is more straightforward since its MOIP formulation is simpler. In Section 4, the computational experiment is described, mainly presenting the specific benchmarks that we solve. The results are discussed in Section 5, focusing on run-time analysis for our proposed approach and on comparison with existing state-of-the-art metaheuristic approaches (mainly multi-objective local search methods) and exact methods (mainly adaptive epsilon constraint). Finally, in Section 6 the basic concluding remarks are discussed.

2. Related literature

In Section 2.1 we present a non exhaustive literature review for the Multiobjective Traveling Salesman Problem (MOTSP). In Section 2.2 we present a non exhaustive literature review for the Multiobjective Set Covering Problem (MOSCP).

2.1 Multi-Objective Traveling Salesman Problem literature review

The Multi-Objective Traveling Salesman Problem (MOTSP) is conceptually defined as in Lust and Teghem [6]: given N cities and p costs $c_{i,j}^{k}$, k=1,…,p associated with traveling from city i to city j, the MOTSP is aiming at finding a tour, i.e. a cyclic permutation π of the N cities, minimizing

$$\min \ z_k(\pi) = \sum_{i=1}^{N-1} c_{\pi(i),\pi(i+1)}^{k} + c_{\pi(N),\pi(1)}^{k} \tag{1}$$

A solution π' is Pareto optimal (nondominated, efficient) if and only if it is feasible and there is no other feasible π such that $z_k(\pi) \leq z_k(\pi')$ for k=1,…,p with at least one strict inequality. The set of the Pareto optimal solutions is coined as the Pareto set (in the decision variable space). In the MOTSP it is actually the set of the nondominated permutations π whose corresponding images $z_k(\pi)$, k=1,…,p into $\mathbb{R}^p$ comprise the *Pareto front* (in the criteria space).

A non-exhaustive literature review on MOTSP is presented, focusing on early contributions, mathematical programming approaches, survey papers, and the main heuristic approaches. Probably, the first paper on MOTSP was in 1982 by Fischer and Richter [7] who proposed a dynamic programming solution method for MOTSP. The interest in MOTSP is revived after Borges and Hansen [8], Hansen [9] and Jaszkiewicz [10]. Since then, a continuously increasing number of papers on MOTSP has been published focusing mainly on local search methods, evolutionary methods and ant colony optimization methods. Paquete and Stützle [11, 12] proposed two local search methods for MOTSP, namely two-phase local search and stochastic local search, respectively. Lust and Teghem [13] proposed the Two-Phase Pareto Local Search (2PPLS) for MOTSP with two objectives and 100, 300 and 500 cities. Lust and Jaszkiewicz [14] developed speed-up techniques for large scale biobjective TSP with up to 1000 cities. Jaszkiewicz and Zielniewicz [15] suggested the Pareto memetic algorithm (PMA) with path relinking for biobjective TSP. Genetic algorithms have been tested on MOTSP by Peng et al. [16] and Samanlioglu et al. [17]. The Ant colony optimization algorithm was proposed by García-Martínez et al. [18] , Cheng et al. [19] and López-Ibáñez and Stüzle [20] for the bi-criteria TSP. Very recently, Liefooghe et al. [21] used the dominance-based multiobjective local search on traveling salesman (and scheduling) problems. Two excellent PhD theses on MOTSP are Paquete [22] and Lust [23]. A survey on MOTSP has been presented by Lust and Teghem [6] focusing on metaheuristic methods.

The mathematical programming approaches to MOTSP are rather scarce. Approaches are either restricted to specific cases of MOTSP which are polynomially solvable (see Özpeynirci and Köksalan [24, 25]) or to regular symmetric instances of rather small size (with up to 50 cities and p=2 objectives, see Stanojević, et al. [26]). An interesting variant of MOTSP is the so called traveling salesman problem with profits. The work of Bérubé et al. [27] used an exact ε-constraint method with CPLEX for the solution of the problem, but the details of their ε-constraint method are different from our approach (i.e. AUGMECON2) and also the problem is a selective TSP (the salesman is not obliged to visit all cities, he can skip some). Another interesting paper on TSP with profits is Jozefowiez et al. [28] employing a metaheuristics approach as a main solution method. A more theoretical paper, from a computer science perspective, is Manthey and Shankar Ram [29] which explores approximation algorithms for multi-criteria TSP.

Regarding the single objective TSP, the interested reader is referred to the classic papers of Laporte [30], Papadimitriou [31], Applegate et al. [32] and Volgenant [33]. Regarding general Multiobjective Programming, a recent work on Multiobjective Integer Programming problems is Jahanshahloo et al. [34], on Multiobjective Mixed 0-1 Linear Programming, Mavrotas and Diakoulaki [35], while a general survey can be found in Chinchuluun and Pardalos [36]. Additionally, we note that the AUGMECON method has already been used in several applications e.g. Khalili-Damghani et al. [37].

2.2 Multi-Objective Set Covering Problem literature review

As most of the work in the literature is for the bi-objective version of the MOSCP (denoted as BOSCP for Bi-Objective Set Covering Problem), we also restrict ourselves to BOSCP. The formulation of BOSCP is as follows (Lust et al. [38], Jaszkiewicz [39] and Prins et al. [40]):

$$
\begin{aligned}
&\min \ \sum_{j=1}^{n} c_j^{(1)} x_j \\
&\min \ \sum_{j=1}^{n} c_j^{(2)} x_j \qquad st \\
&\sum_{j=1}^{n} t_{ij} x_j \geq 1 \qquad i = 1,\ldots,m \\
&x_j \in \{0,1\} \qquad j = 1,\ldots,n
\end{aligned}
\tag{2}
$$

The number of constraints is m, the number of variables is n, the first objective function's coefficients are $c^{(1)}$, the second objective function's coefficients are $c^{(2)}$ and the matrix t_{ij} is as follows. For each constraint $i=1,\ldots,m$ in matrix t, it is $t_{ij}=1$ if variable $j=1,\ldots,n$ is involved in the $i=1,\ldots,m$ constraint. Else, $t_{ij}=0$. Matrix t is a sparse matrix, containing 0-1 elements t_{ij}. The maximum number of 1s in row i of the matrix t_{ij} is the parameter *max-one*. Also, note that the RHS of the ≥ constraints in model (2) is 1 (set covering constraints) and this is a vector minimization problem (BOSCP).

Recently, in the literature there are efforts to solve BOSCP instances. Lust et al. [38] implement the adaptive ε-constraint in a collection of 44 benchmarks for the BOSCP. These problems are also solved approximately in Jaszkiewicz [39], Prins et al. [40] and are available in the MOCOlib library at http://xgandibleux.free.fr/MOCOlib/MOSCP.html. The BOSCP is less studied in the literature compared with the MOTSP. Nevertheless, the single objective set covering problem has been extensively studied (Nemhauser and Wolsey [41]).

3. Methodological part

3.1 The improved version of the augmented ε-constraint (AUGMECON2)

AUGMECON2 (Mavrotas and Florios, [5]) is an improvement of the original AUGMECON method (Mavrotas, [42]) which was an attempt to effectively apply the well known ε-constraint method for generating the Pareto Optimal Solutions (POS) in Multi-Objective Programming models. For the integrality of the paper we briefly describe the characteristics of AUGMECON2 for Multi-Objective Integer Programming (MOIP) problems where all the decision variables are discrete (integer or binary).

AUGMECON2 follows the main concept of ε-constraint i.e. it keeps one objective function and appropriately transforms the remaining objective functions to constraints. By systematically varying the right hand side of these constraints, the relevant POS are generated. The proposed version achieves computational economy by applying early exit from the loops where infeasibilities are met (Mavrotas [42]) and "jumping" over several grid points when specific conditions are met (Mavrotas and Florios [5]).

It must be noted that the ε-constraint method is preferable than the weighting method especially in MOIP problems as it is the MOTSP. The weighting method cannot produce unsupported efficient solutions in MOIP problems, while the ε-constraint method does not suffer from this pitfall (Mavrotas, [42]; Steuer, [1]; Miettinen, [43]). The flowchart of the AUGMECON2 is shown in Figure 1.

As it is described in Mavrotas and Florios [5] AUGMECON2 can achieve great computational economy by applying "jumps" based on the bypass coefficient that is calculated at each iteration. This is particularly useful in MOIP problems where the feasible region is discrete and the number of POS is finite. The algorithm actually allocates equidistant grid points at the range of the objective functions and afterwards scans the grid points solving one Integer Programming problem per grid point. The number of grid points per objective function determines the density of the produced Pareto front.

In the case of integer coefficients in the objective functions of the MOIP problems the values of the objective functions are also integer. Therefore, by fixing the number of grid points equal to the objective function range it is assured that no Pareto optimal solution can be located in between the grid points. Consequently AUGMECON2 can be used to produce the exact (or complete) Pareto set in MOIP problems and therefore in MOTSP. Moreover if the objective function coefficients are not integer we can easily transform the problem to have integer objective function coefficients by multiplying with the appropriate power of 10.

In the present study we deal with bi-objective problems (BOTSP and BOSCP). Although the computational experiments deal with the bi-objective versions the method can be extended to MOTSP and MOSCP. The computational strategy for calculating the exact Pareto set in these problems with integer objective function coefficients is the following (without loss of generality, assume that all the objective functions are to be minimized):

1. Calculate the objective function ranges of the $p-1$ objective functions. This means that we have to calculate or estimate upper bounds for the nadir points. If the nadir points are not straightforward (e.g. when more than two objective functions are considered), an appropriate method may be applied (see Mavrotas and Florios [5]).
2. Assume that the objective function range for the k-th objective function is r_k (integer). We select for each objective function a unity step so that for each one of them the number of grid points is exactly r_k+1
3. We apply AUGMECON2 and obtain the exact Pareto set. The unity step size and the calculation of the nadir point guarantee that no POS is left undiscovered.

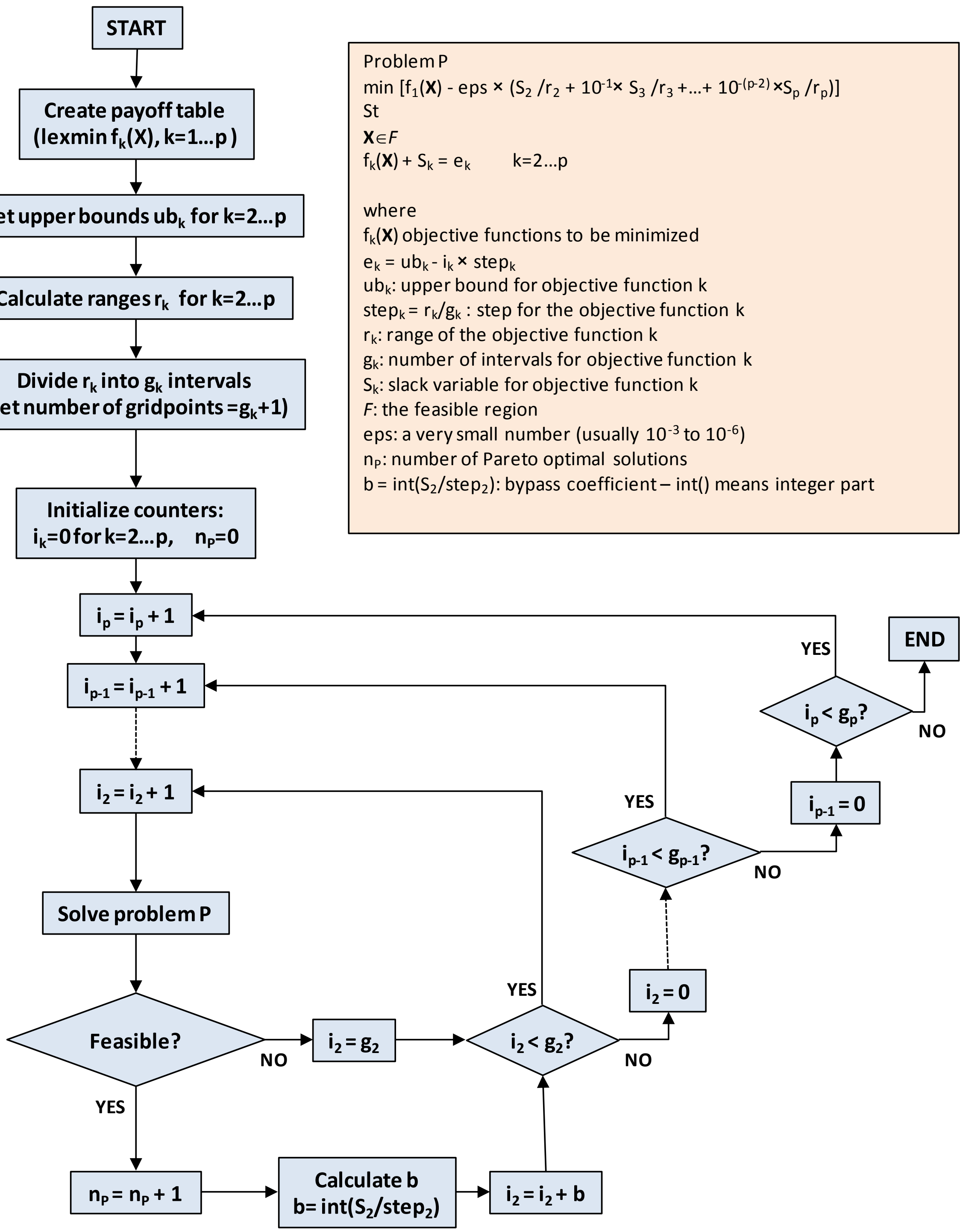


Figure 1. *Flowchart of the AUGMECON2 method*

3.2 The branch-and-cut-and-heuristic facility for the TSP (BCHTSP)

In the two following sub-sections we focus on the TSP. The most efficient way to solve TSP using Mathematical Programming in a Modeling Language is to use the Branch-and-Cut-and-Heuristic Facility

(BCH) available in GAMS. For a general MIP problem the BCH is documented in http://www.gams.com/docs/bch.htm (see Bussieck [44]).

It is well known that solving difficult MIP problems can be enhanced by using user supplied routines that generate cutting planes and good integer feasible solutions. Modellers traditionally supply cutting planes and an integer feasible point as part of the model given to the solver, by adding a set of constraints indicating likely to be violated cuts and a feasible solution. A truly dynamic interaction between a branch-and-cut (B&C) solver like CPLEX and user supplied routines was not possible until recently. The Branch-and-Cut-and-Heuristic (BCH) facility serves this purpose. More details about the GAMS coding of BCH facility can be retrieved at [44].

The specific implementation of the BCH facility we have used is the one for the TSP problem, which is model ‘bchtsp’ available in the GAMS Model Library with No.348 [45, 46]. The model is titled ‘Traveling salesman problem instance with BCH’ and accepts format “.tsp” for input files, as defined by the maintainers of the TSPLIB (Reinelt, [47, 48]). The subtour elimination constraints are supplied dynamically while GAMS/CPLEX is running. The incumbent checking BCH call checks if the integer solution contains subtours, stores the corresponding cuts, and rejects the solution. The cut BCH call supplies the cuts produced by the previous call. Model ‘bchtsp’ can handle asymmetric TSP problems and therefore symmetric as well. The coupling of AUGMECON2 method and BCHTSP model ensures the efficient treatment of MOTSP in a flexible Modeling Language environment (e.g. GAMS [49]). The exact Pareto Front, PF*, is effectively generated with our approach, for the first time, for 16 MOTSP instances with 100 cities, two objectives, and symmetric cost matrices of various types (Euclidean, random matrix, mixed-type of the previous two).

3.3 Coupling of AUGMECON2 and BCHTSP for solution of MOTSP

In order to couple AUGMECON2 method with BCHTSP model, the BCHTSP model is altered in order to solve the augmented ε-constraint sub-problem described in Eq. (3).

$$
\begin{aligned}
&\min\ \mathrm{z}_1 = \sum_{i=1}^{N}\sum_{j=1}^{N} c_{ij}^{1} x_{ij} \ - \delta \frac{s_2}{r_2} \ \text{ st} \\
&z_2 = \sum_{i=1}^{N}\sum_{j=1}^{N} c_{ij}^{2} x_{ij} \\
&z_2 + s_2 = \varepsilon_2 \\
&\varepsilon_2 = z_2^{\max} - \eta \cdot (z_2^{\max} - z_2^{\min}) \\
&x \in S
\end{aligned}
\tag{3}
$$

The first objective function is kept, and the second is turned into a ‘≤’ constraint (corresponding to a ‘minimization’ objective). The ε-constraint problem accepts a dimensionless parameter $\eta \in [0,1]$. The parameter δ is a small number typically 10^{-3} to 10^{-6}. Consequently, in the GAMS model ‘bchtsp’ the following operations are added:

a) Input of the cost matrix c^2 for the 2nd objective function

b) Input the nadir value $z_2^{\max}$ and the ideal value $z_2^{\min}$ of the 2nd objective function as obtained from the individual optimization of both objective functions.

c) Solve bchtsp(η) for specific $\eta \in [0,1]$ externally defined from the AUGMECON2 procedure.

d) Return the counter of the Pareto Optimal Solution (c_{POS}), the values of the objective functions (z_1, z_2), the Right Hand Side (ε_2), the bypass coefficient (b), the counter of the grid point (i), the CPU time in seconds (runtime) and the resulting tour π for every time procedure bchtsp(η) is called from AUGMECON2.

The pseudo-code of the computational procedure is the following:

AUGMECON2-BCHTSP($N, C^{(1)}, C^{(2)}$)

1 $\pi = \text{argmin } z_1 = \sum_{i=1}^{N-1} c^1_{\pi(i),\pi(i+1)} + c^1_{\pi(N),\pi(1)}$

2 $z_2^{\max} = z_2(\pi)$

3 $\pi = \text{argmin } z_2 = \sum_{i=1}^{N-1} c^2_{\pi(i),\pi(i+1)} + c^2_{\pi(N),\pi(1)}$

4 $z_2^{\min} = z_2(\pi)$

5 // calculate range of objective function 2

6 $r_2 = z_2^{\max} - z_2^{\min}$

7 // do some initializations

8 i= -1

9 stepsize=1

10 $\eta_{stepsize}$=stepsize/float(r_2)

11 c_{POS}=0

12 // the main loop

13 while ($i \leq r_2$)

14   i=i+1

15     $\eta = i \cdot \eta_{stepsize}$

16   // Run procedure bchtsp(η) which solves Eq. (3) in GAMS returning the bypass coefficient $b=s_2$

17   bchtsp($\eta, z_1, z_2, b, \varepsilon_2$, runtime, π)

18   i=i+b

19     $c_{POS} = c_{POS} + 1$

20   write c_{POS}, z_1, z_2, i, b, ε_2, runtime, π // write useful info in a diary file

The above procedure implements AUGMECON2 for MOTSP with p=2 objectives and has been coded in Fortran with Intel Visual Fortran Compiler 11.1. For $\eta = i/r_2 = 0$ (i.e. i=0) the Eq. (3) is solved with RHS, $\varepsilon_2 = z_2^{\max}$. On the other hand, for $\eta = i/r_2 = 1$ (i.e. $i = r_2$) the Eq. (3) is solved with RHS, $\varepsilon_2 = z_2^{\min}$. So, as the value of i increases from 0 to r_2 through the relations $i=i+1$ and $i=i+b$, we solve progressively more constrained problems with respect to the constraint which is derived from the second objective. Furthermore, we parallelize the computational process by splitting the while loop in 3 parts, with each one corresponding to a different thread of the CPU. Specifically, in thread 1 we have the iterations for i=1 to int($0.60 \times r_2$) where int() denotes the integer part of a number. For thread 2 we have the iterations for i=int($0.60 \times r_2$)+1 to int($0.85 \times r_2$) and finally for thread 3 we have the iterations for i=int($0.85 \times r_2$)+1 to r_2. This is easily done by only altering lines 8 and 13 of the algorithm. The split points 0.60 and 0.85 were found after some experimentation in order to have the three loops with almost equal computational time.

The computational time depends mainly on the number of solver calls which is not proportional to the number of grid points in r_2. For example, in the first iterations AUGMECON2 is making greater "jumps" so the number of solver calls in the interval $[z_2^{max}, z_2^{max} - 0.6 \times r_2]$ is almost equal to the number of solver calls in the interval $[z_2^{max} - 0.6 \times r_2, z_2^{max} - 0.85 \times r_2]$. The flowchart of the AUGMECON2-BCHTSP algorithm is shown in Figure 2.

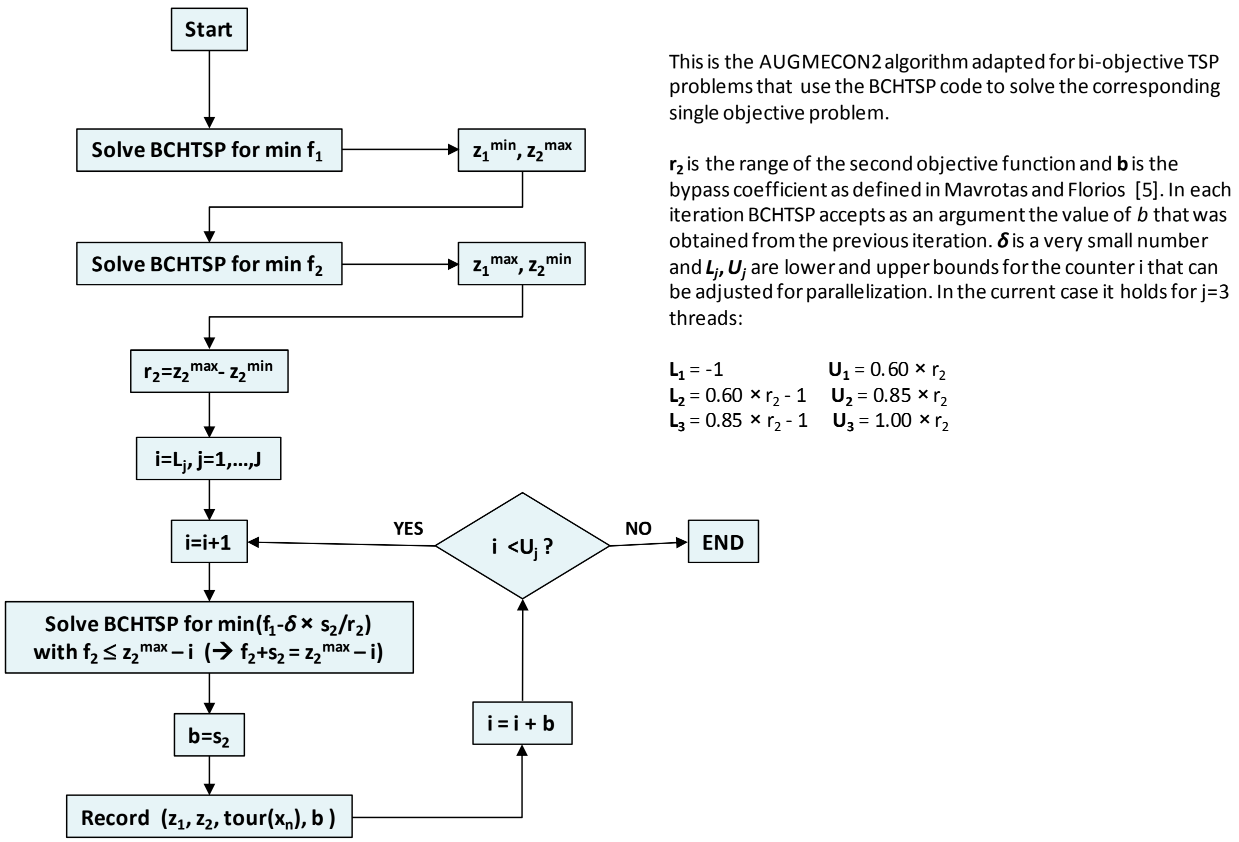


Figure 2. *Flowchart of the AUGMECON2 – BCHTSP method*

We have compiled three applications, called thread1.exe, thread2.exe and thread3.exe for the AUGMECON2-BCHTSP algorithm and we have run them always in parallel in a 4 thread personal computer, in order to perform as much calculations as possible in parallel. The sub-problems bchtsp(η) with $\eta \in [0,1]$ are independent so the split works fine. Special care needs to be paid to the fact that η must be defined as a double precision variable (we always printed and read 12 significant digits for η among GAMS/Fortran and text files) since truncation errors may lead to non-discovered Pareto Optimal Solutions if only 7-8 significant digits are used (with single precision for η). It must be noted that the BCHTSP model (due to its implementation) cannot take advantage of the parallel mode of CPLEX, so parallelization is only possible the way we have implemented it, by splitting the while loop for counter i in three parts, for $L_1 \leq i \leq U_1$, $L_2 \leq i \leq U_2$, $L_3 \leq i \leq U_3$, and assigning each part in a different thread of a multi-core PC. In this way, parallelization of AUGMECON2-BCHTSP has been accomplished which can be generalized to more than 3 threads (if available) and so improve computational performance for larger

MOTSP problems. From a technical point of view, step 17 is performed calling GAMS from the Operating System with an environment variable (called *EtaValue*) equal to the given number of η defined inside the loop. The GAMS call is easily written in a batch file (for variable η values) within Fortran. Any modern computer language can be used to code the aforementioned algorithm, and only I/O in text files is assumed and ability for system calls.

4. Computational experiment

4.1 Bi-Objective TSP (BOTSP)

AUGMECON2 using the branch-and-cut-and-heuristics facility for the solution of the ε-constraint sub-problem of type TSP (BCHTSP) is used in order to compute the exact Pareto Front, PF*, of 16 datasets available in the literature. The structure of these datasets is illustrated in Table 1.

Table 1. The test bed of 16 datasets for the bi-objective TSP

Lust's Instances	*Name*	*Paquete's Instances*	*Name*
L1	kroAB100	*P1*	euclAB100
L2	kroAC100	*P2*	euclCD100
L3	kroAD100	*P3*	euclEF100
L4	kroBC100	*P4*	randAB100
L5	kroBD100	*P5*	randCD100
L6	kroCD100	*P6*	randEF100
L7	euclAB100	*P7*	mixdGG100
L8	clusAB100	*P8*	mixdHH100
L9	randAB100	*P9*	mixdII100
L10	mixdGG100		

Lust's datasets have been used in his PhD thesis [23], in Lust and Teghem ([6]) (instances L7-L10, also called the DIMACS instances) and in Lust and Teghem ([13]) (instances L1-L6, also called the Krolak/Felts/Nelson instances - with prefix kro in TSPLIB). The data are downloadable from [50]. Paquete's datasets have been used in his PhD thesis [22] as well as in Paquete and Stützle ([12]). The data are downloadable from [51]. Note that L7 is the same as P1, L9 is the same as P4 and finally L10 is the same as P7. So, we have in total 16 different datasets to solve. Especially the Krolak instances of Table 1 have been solved approximately in numerous papers in the past, especially with metaheuristic approaches e.g. genetic algorithms, ant colony optimization and multi-objective local search methods (see Jaszkiewicz [10] and references therein).

4.2 Bi-Objective SCP (BOSCP)

AUGMECON2 will be used in a collection of 44 benchmarks for the BOSCP available at the MOCO library (MOCOlib) and are downloadable from [52]. These benchmarks are solved approximately in Jaszkiewicz [39], Prins et al. [40] and Lust et al. [38]. Especially, Lust et al. [38] implemented the adaptive ε-constraint (Laumanns et al. [53]) in order to solve exactly several instances of MOSCP from MOCOlib. Also, Prins et al. [40] have solved the smallest benchmarks of MOSCP from MOCOlib exactly in the past. For every model ranging from 1 to 11, there exist 4 instances, namely A,B,C,D so there are totally 11×4=44 instances.

Table 2. The benchmarks for the BOSCP

No	Model name	# Constraints	# Variables
1	*11*	10	100
2	*41*	40	200
3	*42*	40	400
4	*43*	40	200
5	*61*	60	600
6	*62*	60	600
7	*81*	80	800
8	*82*	80	800
9	*101*	100	1000
10	*102*	100	1000
11	*201*	200	1000

From Jaszkiewicz, [39], Prins et al., [40], Lust et al., [38]

5. Results and Discussion

The MOTSP model and the AUGMECON2-BCHTSP method proposed in this paper have been created and solved in GAMS 23.5 environment using CPLEX 12.2 solver. The OS is Windows 7 64-bit and the hardware is an Intel Q9650 core 2 quad CPU at 3.00 GHz with 4GB RAM. The time limit was set up to 60 hours wall clock time.

5.1 Bi-Objective TSP results with 100 cities

5.1.1 Lust et al. benchmarks

Table 3 presents the results for the exact solution of Lust instances.

Table 3. AUGMECON2 results using the BCHTSP model for the bi-objective TSP (Lust, 10 datasets, [13, 6])

Dataset	Pareto front size |PF*|	Models Solved (MS)	CPU time (h) in Parallel Processing Thread 1 (h)	Thread 2 (h)	Thread 3 (h)
L1	3332	3372	39	37	58
L2	2458	2509	30	26	18
L3	2351	2370	12	16	21
L4	2752	2790	24	25	28
L5	2657	2705	21	23	22
L6	2044	2078	7	11	21
L7	1812	1839	16	9	16
L8	3036	3110	12	13	27
L9	1707	1718	6	7	21
L10	1848	1863	12	9	17

(*) Hardware is a core 2 quad CPU capable of running 4 threads with Windows 7 64bit.

The critical information in Table 3 is the cardinality of the exact Pareto Front, expressed as |PF*|. Thus, there are exactly 3332 POS for *L1* (=kroAB100) problem, 2458 POS for *L2* (=kroAC100) problem, and so on. The Models Solved number (MS) is the number of augmented ε-constraint subproblems solved (essentially problems of Eq. (3), see Section 3.3). We see that MS is very close to |PF*| (slightly larger of course) which indicates that our proposed approach is very economic in the calls to the single objective solver it makes. The last three columns of Table 3 indicate the CPU time in hours of every one of the three applications thread1.exe, thread2.exe and thread3.exe described in Section 3.3, which essentially implement the parallel AUGMECON2-BCHTSP algorithm. The wall clock time, *w*, of our approach is $w=\max(t_1, t_2, t_3)$, where t_i, $i=1,2,3$ is the CPU time of thread *i*. The wall clock time is illustrated with grey cells in Table 3, and can be lowered by splitting the while loop of Section 3.3 in more than 3 parts, apparently 6 or more parts if a machine with more threads (e.g. 8 threads) is available for computations. It is noticed that the third part of the second objective function range $[0.85\ r_2, r_2]$ is in most cases the most computational demanding part (due to the increased number of Models Solved). The graphical illustrations of the Pareto fronts for instances kroAB100 (*L1*) and euclAB100 (*L7*) are shown in Figure 3.

5.1.2 Paquete et al. benchmarks

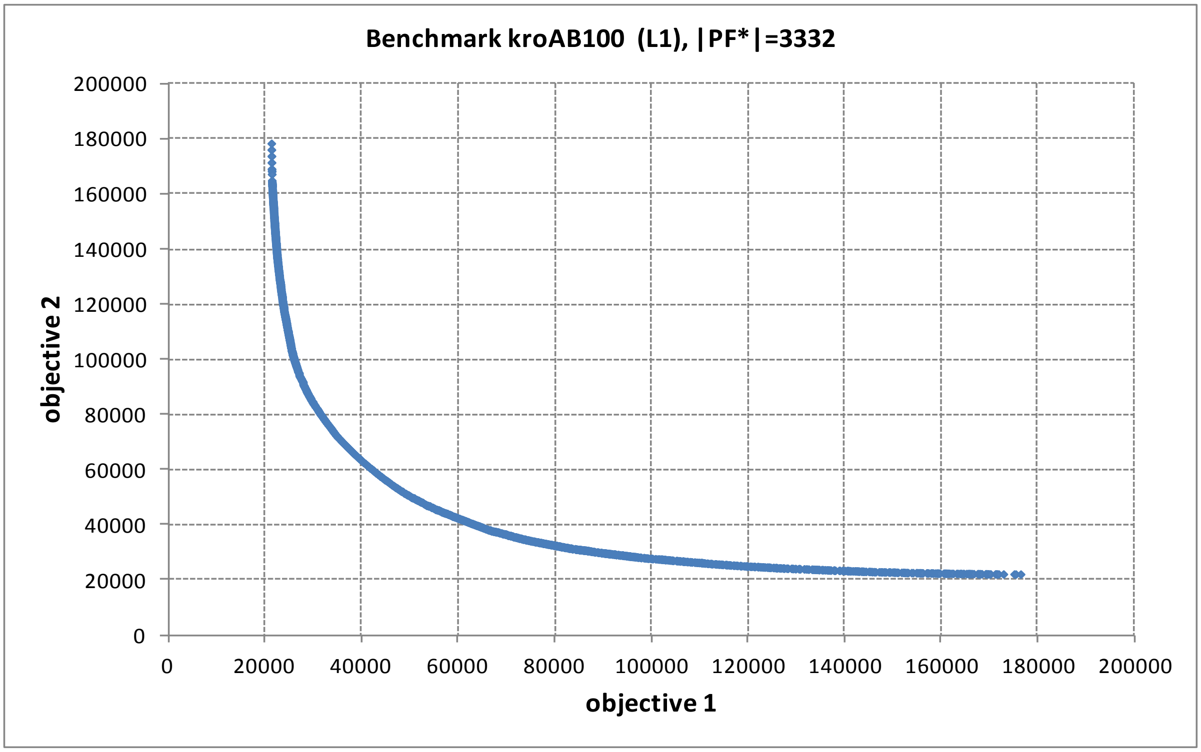
Table 4 presents the results for the exact solution of Paquete instances (9 DIMACS of various types, Paquete and Stützle [12])

Table 4. AUGMECON2 results using the BCHTSP model for the bi-objective TSP (Paquete, 9 datasets, [12])

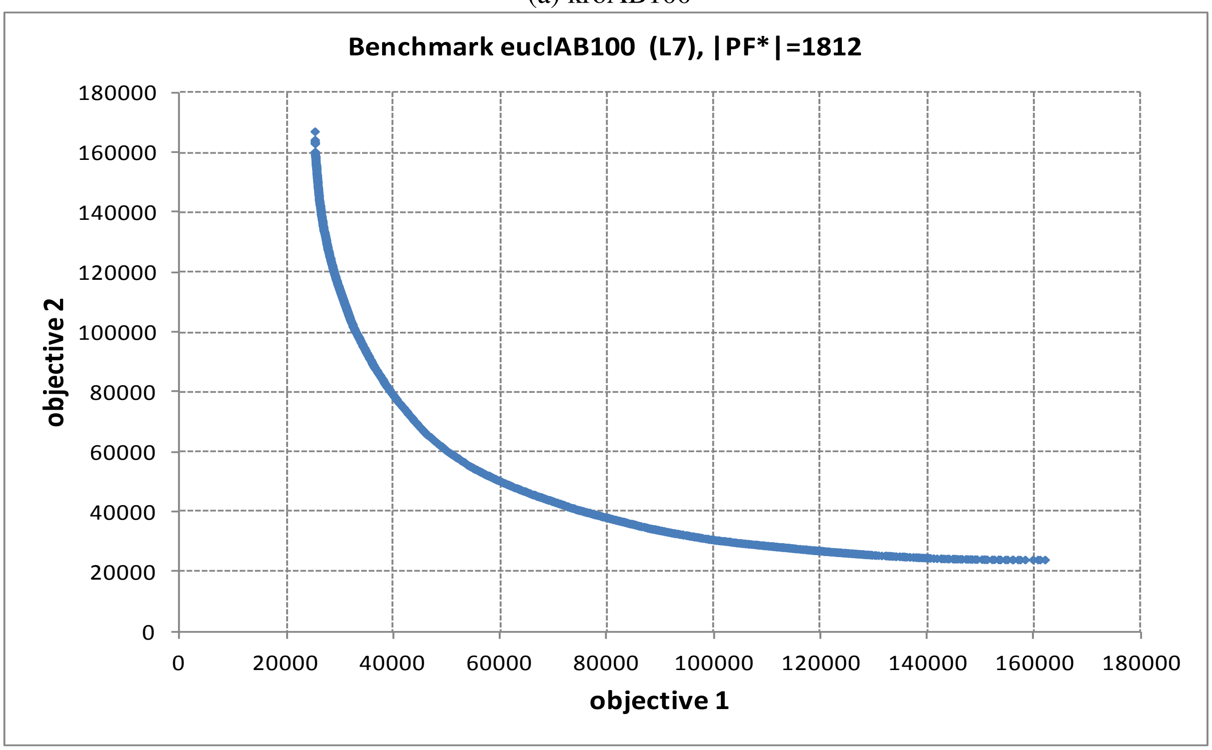
Dataset	|PF*|	MS	CPU time (h) in Parallel Processing		
			Thread 1 (h)	Thread 2 (h)	Thread 3 (h)
P1	1812	1839	16	9	16
P2	2268	2294	19	14	34
P3	2530	2559	11	18	23
P4	1707	1718	6	7	21
P5	1850	1868	11	12	16
P6	1882	1902	9	14	21
P7	1848	1863	12	9	17
P8	2108	2137	8	9	18
P9	1883	1906	11	13	16

(*) Hardware is a core 2 quad CPU capable of running 4 threads with Windows 7 64bit.

In Table 4, the cardinality of the exact Pareto Front is displayed as |PF*|. For instance, there are 1812 POS in problem *P1* (=euclAB100), 2268 POS in problem *P2* (=euclCD100), and so on. Again, the Models Solved number (MS) is the number of augmented ε-constraint subproblems of Eq. (3) solved in the AUGMECON2-BCHTSP approach. We see that, like before, MS is very close to |PF*| (MS is obviously always slightly larger than |PF*|) which is very advantageous for our proposed approach. The last three columns of Table 4 indicate the CPU time of every one of the three thread applications for AUGMECON2-BCHTSP we used in parallel. The wall clock time for every dataset is shown in grey color. The Pareto fronts for instances randAB100 (*P4*) and mixedGG100 (*P7*) are shown in Figure 4.

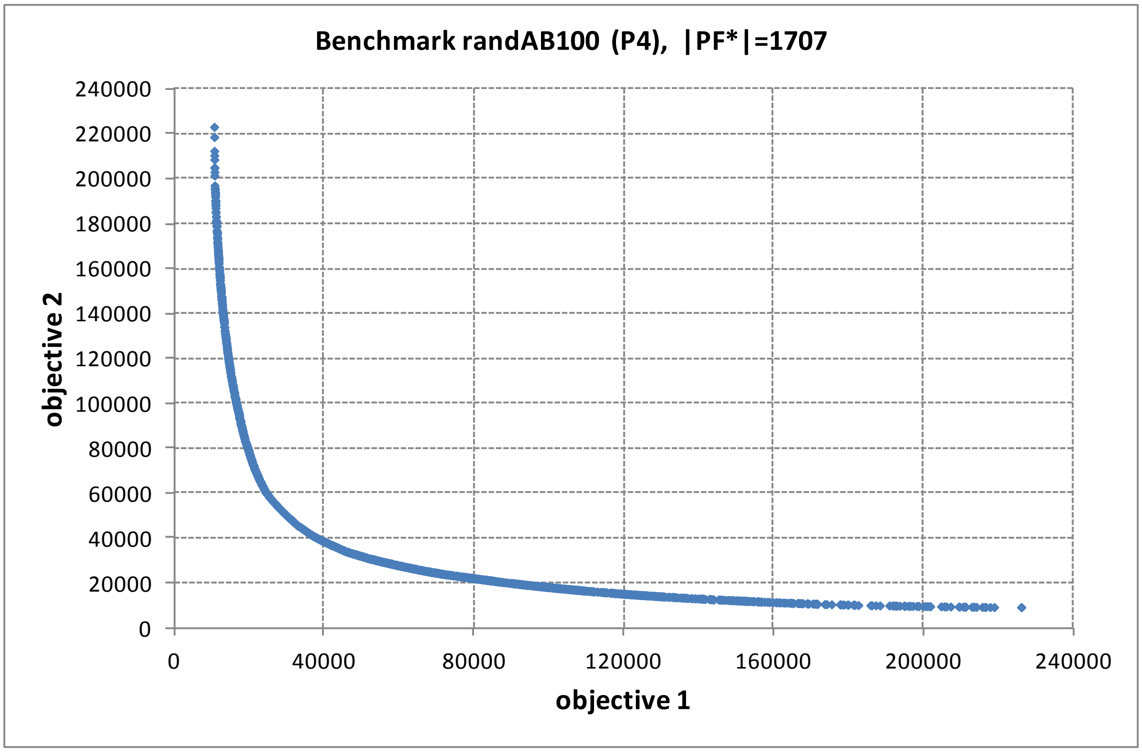


(a) kroAB100

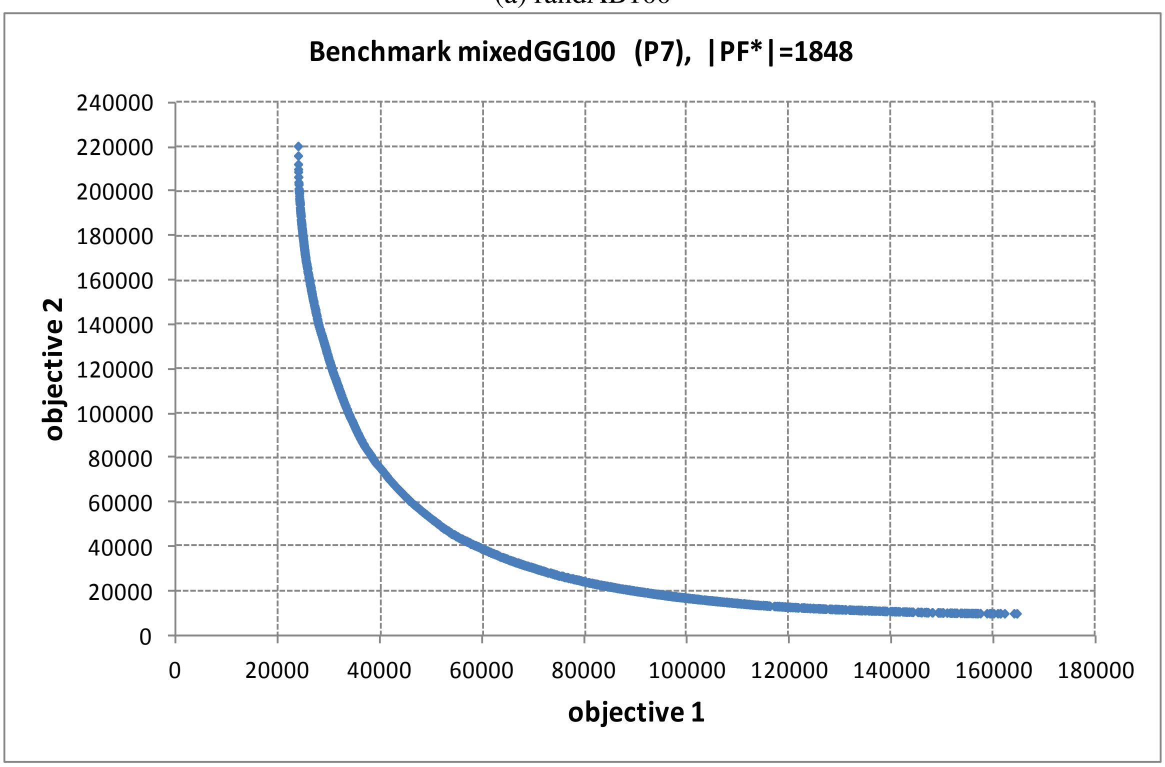


(b) euclAB100

Figure 3. *Visualization of exact Pareto front for kroAB100 and euclAB100 datasets for biobjective TSP from Lust and Teghem [13, 6].*



(a) randAB100



(b) mixedGG100

Figure 4. *Exact Pareto front for randAB100 and mixedGG100 datasets from Paquete and Stützle [12].*

5.1.3 Comparison with state-of-the-art approximate methods

In the following, we will evaluate state-of-the-art metaheuristic methods which have already been used for the approximation of the Pareto Fronts in MOTSP problems. Since we have solved the same datasets exactly with our approach, the evaluation of the metaheuristic approaches can be made taking into consideration the information on the Exact Pareto Set (EPS), which is for first time available in our work.

First, we define the coverage metric *C*(A,B). The coverage metric, in our case, presents the percentage of Pareto optimal solutions in set B, which are weakly dominated by a solution discovered by the approximate algorithm in set A. The term "weakly" is used to facilitate the cases of identical solutions in the two sets (Deb, [54], p. 325).

$$C(A,B) = \frac{\left|\left\{b \in B \mid \exists a \in A : a \leq^{w} b\right\}\right|}{|B|} \tag{4}$$

the symbol $\leq^{w}$ represents weak dominance (for minimization problems), that also holds true if f(*a*) = f(*b*). Therefore, the coverage metric *C*(AM, EPS) indicates how many solutions from the Approximate Method (AM) are also found in the Exact Pareto Set (EPS). It actually reports the % of discovered Pareto optimal solutions by the Approximate Method and the closer to 1 is the coverage metric *C*(AM, EPS) the better is the approximation.

Table 5 presents the coverage metric values for the method two-phase Pareto Local Search developed in Lust and Teghem [13] for Lust-1 to Lust-6 datasets and Lust and Teghem [6] for Lust-7 to Lust-10 datasets.The second column of Table 5 denotes the exact Pareto Front, |PF*|, obtained by AUGMECON2. The third column denotes the Potentially Efficient solutions, |PE|, by 2PPLS over 20 runs. The fourth column describes the dominated part, |D|, of |PE| for 2PPLS. In the fifth column, the non-dominated part, |ND|, of |PE| for 2PPLS is given. Finally, *C*(2ppls,EPS) is coverage of 2ppls over EPS.

Additionally, in Table 5 the convergence metric (Khare et al., p.379 [55]) of 2PPLS in relation to the full Pareto front is presented for the ten problems. The 'convergence' metric gives the average Euclidean distance of the solutions of the obtained approximation to the true Pareto front.

Table 5. Coverage and Convergence metrics for two phase Pareto Local Search (2PPLS) (Lust and Teghem [13, 6])

dataset	|PF*| exact	|PE| 2ppls	|D| 2ppls	|ND| 2ppls	C(2ppls,EPS) = |ND|/|PF*|	Convergence (2ppls,EPS)
L1	3332	2640	988	1652	0.4958	1.6105e-4
L2	2458	2007	679	1328	0.5403	1.2093e-4
L3	2351	1885	730	1155	0.4913	1.8511e-4
L4	2752	2200	740	1460	0.5305	1.1034e-4
L5	2657	2058	579	1479	0.5566	1.0208e-4
L6	2044	1673	610	1063	0.5201	1.8434e-4
L7	1812	1397	502	895	0.4939	1.8457e-4
L8	3036	2557	878	1679	0.5530	1.1048e-4
L9	1707	663	266	397	0.2326	2.5694e-4
L10	1848	1011	376	635	0.3436	2.3069e-4

The main conclusion is that even if we gather the elite solutions after 20 runs of 2PPLS, the method 2PPLS has a coverage of approximately 50% compared to the exact Pareto set for Krolak instances (L1-L6). Also, regarding DIMACS instances, the coverage for 2PPLS is as low as 25%-35% for Random Matrix (L9) and Mixed instances (L10). The first two DIMACS instances (L7 and L8) are also x-y coordinate based and achieve a coverage near 50% just like the other x-y coordinate based Krolak instances.

Moreover, with respect to the 'convergence' metric, we see that the approximation of 2PPLS elite solutions in relation to the full Pareto front is of high quality since in all cases the convergence metric is of the order 10^{-4}.

With respect to the 'coverage' metric, we have indications that 2PPLS performs better in x-y coordinate based datasets (L1-L6, L7, L8), rather worse in mixed datasets (L10) and is least effective in random matrix datasets (L9). Nevertheless, the coverage metric values are at most 50%-55%.

Table 6 presents the coverage and convergence metric values for an ensemble of methods titled 'best non-dominated set found' used in Paquete and Stützle [11], Paquete [22]. The same datasets have been solved in Paquete and Stützle [12], with Stochastic Local Search (SLS), also approximately.

Table 6. Coverage and Convergence metrics for an ensemble of methods 'best non-dominated set found' of Paquete and Stützle [11] and Paquete [22]. Datasets are approximately solved in Paquete and Stützle [12], also.

dataset	|PF*| exact	|PE| best known	|D| best known	|ND| best known	C(best,EPS) = |ND|/|PF*|	Convergence (best,EPS)
P1	1812	1719	76	1643	0.9067	1.5090e-5
P2	2268	2123	121	2002	0.8827	1.5538e-5
P3	2530	2387	68	2319	0.9166	8.3322e-6
P4	1707	1247	497	750	0.4394	2.1464e-4
P5	1850	1424	402	1022	0.5524	1.5730e-4
P6	1882	1287	611	676	0.3592	2.5196e-4
P7	1848	1644	145	1499	0.8111	4.1347e-5
P8	2108	1892	225	1667	0.7908	5.8902e-5
P9	1883	1724	132	1592	0.8455	4.1221e-5

The second column of Table 6 denotes the exact Pareto Front, |PF*|, obtained by AUGMECON2. The third column denotes the Potentially Efficient solutions, |PE|, which are the solutions of the 'best non-dominated set found' available at [51]. The fourth column describes the dominated part, |D|, of |PE| for 'best non-dominated set found'. In the fifth column, the non-dominated part, |ND|, of |PE| for 'best non-dominated set found' is given. Finally, C(Best Known,EPS) is coverage of 'Best Known' over EPS.

We note that P1-P3 are Euclidean instances, P4-P6 are random matrix instances and P7-P9 are mixed instances. The coverage metric of 'best known' by Paquete for the Euclidean instances is very high, around 90%, which means a very good approximation of the EPS. Nevertheless, for random matrix datasets the coverage metric of 'best known' by Paquete drops to 35%-55% which is low enough. The coverage metric for mixed datasets (i.e. one objective Euclidean, one objective random matrix type) is between the two previously found values, close to 80%-85%.

Moreover, with respect to the 'convergence' metric, we see that the approximation of 'best Nondominated set found' at [51] in relation to the full Pareto front is of even higher quality since in most cases the convergence metric is of the order 10^{-5}.

We conclude that the Pareto Front approximations supplied by Paquete at his webpage are of better quality than the approximations supplied by Lust at his website. This is confirmed for the datasets which are present in both testbeds (P1-P9) and (L1-L10).

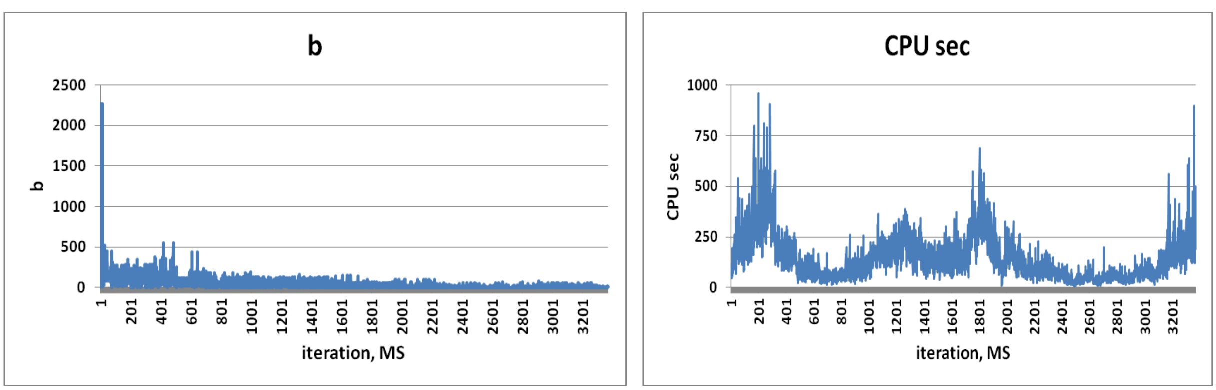
- For L7=P1, Paquete finds 90.67% of the POS, and Lust's method only 49.39% of the POS.
- For L9=P4, Paquete finds 43.94% of the POS, and Lust's method only 23.26% of the POS.
- For L10=P7, Paquete finds 81.11% of the POS, and Lust's method only 34.36% of the POS.

Overall, both methods perform rather well, having a significant coverage of the Exact Pareto Set. Especially, Lust and Teghem method (2PPLS) finds considerably fewer POS, than the ensemble of methods called 'best non-dominated set found' of Paquete.

All the generated exact Pareto fronts (the objective function values along with the corresponding tours) are published in https://sites.google.com/site/kflorios/motsp. We also publish the corresponding Fortran code and the GAMS models that combine AUGMECON2 with BCHTSP.

5.1.4 Detailed analysis of AUGMECON2 approach featuring BCHTSP

We present the working of our approach especially for one representative dataset, namely *L1* (or kroAB100). Specifically for kroAB100, we present the bypass coefficient values for all Models Solved as well as the run-time for every Models Solved (i.e. of Eq. (3)). Figure 5 presents this detailed information on AUGMECON2 featuring BCHTSP for kroAB100.



(a) bypass coefficient, b (b) CPU sec

Figure 5. *Visualization of bypass coefficient, b, and CPU sec per iteration 'Models Soved' (MS) of our approach for the solution of kroAB100.*

We see that for kroAB100, which is actually the hardest dataset to solve, the bypass coefficient is almost always below 500, (note that the range of the second objective function is r_2=156,305) and it takes 3372 calls to the BCHTSP solver to span this range. The CPU time for every iteration is always below 1000 seconds, and often below 500 seconds which is affordable for 3372 iterations.

In order to perform the 3372 iterations concurrently we have made three executables, called thread1.exe, thread2.exe and thread3.exe as described in Section 3.3. The split of the computational load has been made according to Figure 6. Figure 6 presents the way that thread1 takes η values in [0, 0.60], thread2 takes η values in [0.60, 0.85] and thread3 takes η values in [0.85, 1.00]. Every thread discovers a separate part of the Pareto Front as presented in Figure 6.

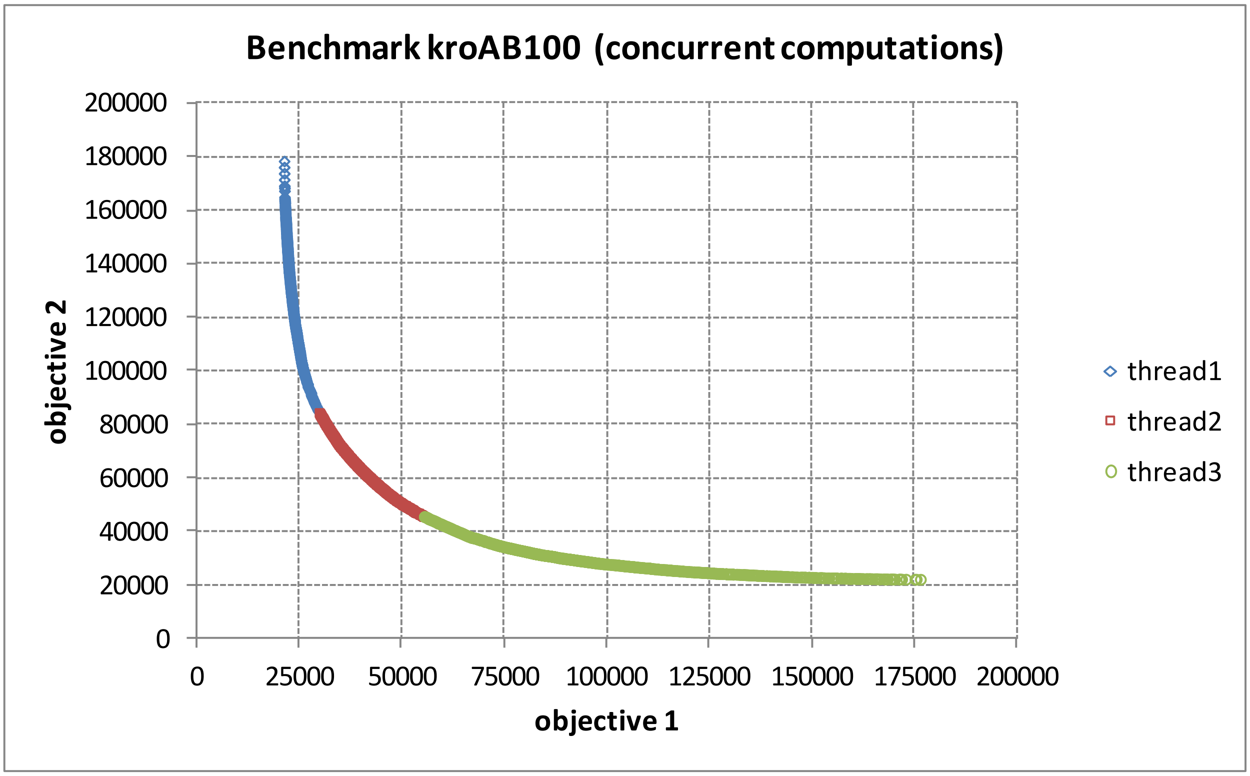


Figure 6. *AUGMECON2 concurrent computations in 3 threads for the solution of kroAB100*

Also, a video (created by MATLAB R2011a code) illustrating the conflicting nature of objectives for tour1 (kroA100) and tour2 (kroB100) is available at: https://sites.google.com/site/kflorios/motsp.

5.1.5 Supported and unsupported Pareto Optimal Solutions

In addition to the above work, it is very interesting to study the proportion of the supported POS in the total number of the generated POS. We remind that the supported POS are those that can be obtained from a convex combination of the objective functions. As a consequence, the weighting method when used in MOIP problems produces only the supported POS, while the ε-constraint method does not suffer from this pitfall. Regarding the 16 benchmark problems the results concerning the ratio of supported POS to the total number of generated POS are shown in Table 7. The supported POS are calculated ex post from the exact set of POS using an ad hoc slope increasing algorithm.

It is impressive that, on average, only 4.39% of the POS are supported. This actually means that when someone uses the weighting sum method for generating the POS in a MOTSP problem with N=100 cities, more than 95% of the true POS are left undiscovered. These results are in accordance with the conclusions from Visée et al. [56], Ehrgott and Gandibleux [3], Przybylski et al. ([57, 58]) which state that the number of supported POS is a small proportion among the generated POS.

Table 7. Percentage of Supported Efficient solutions over all POS in 16 datasets

	dataset	|PF*| exact	|SE| weighted sum	|SE|/|PF*| ratio
1	*L1*	3332	111	3.33%
2	*L2*	2458	106	4.31%
3	*L3*	2351	90	3.83%
4	*L4*	2752	114	4.14%
5	*L5*	2657	112	4.22%
6	*L6*	2044	98	4.79%
7	*L7*	1812	95	5.24%
8	*L8*	3036	109	3.59%
9	*L9*	1707	77	4.51%
10	*L10*	1848	98	5.30%
11	*P2*	2268	96	4.23%
12	*P3*	2530	100	3.95%
13	*P5*	1850	85	4.59%
14	*P6*	1882	89	4.73%
15	*P8*	2108	96	4.55%
16	*P9*	1883	92	4.89%
			Average	4.39%

|PF*|: cardinality of exact Pareto Front obtained by AUGMECON2

|SE| : Number of Supported Efficient solutions as obtained from a weighting sum approach

5.2 Larger bi-objective TSP results

5.2.1 Exact solution of a bi-objective TSP instance with 150 cities

In order to test the scalability of our approach, we solved a larger bi-objective instance that has been generated with the DIMACS generator 'portgen' available in the website http://dimacs.rutgers.edu/Challenges/TSP/codes.zip with parameter MAXCOORD=1000 and seed 1977 for objective 1 x-y coordinates and seed 1978 for objective 2 coordinates. The result is a bi-objective Euclidean DIMACS dataset like the ones of Section 5.1, but with N=150 cities and x-y coordinates in the range 1 – 1000. We call this problem '2tsp-150'. The range of the 2nd objective function is r_2=73,085. This dataset is computationally very difficult to solve and it took several days of computations to generate the Exact Pareto Set. It was solved exactly with AUGMECON2-BCHTSP, and it has a Pareto Front with |PF*|=4701 Pareto Optimal Solutions which was computed after MS=4934 Models Solved i.e. problems of Eq. (3). The Pareto Front is shown in Figure 7. So, we conclude that problems with N=150 cities and range of coordinates equal to 1-1000 is the limit of our exact approach with current hardware technology.

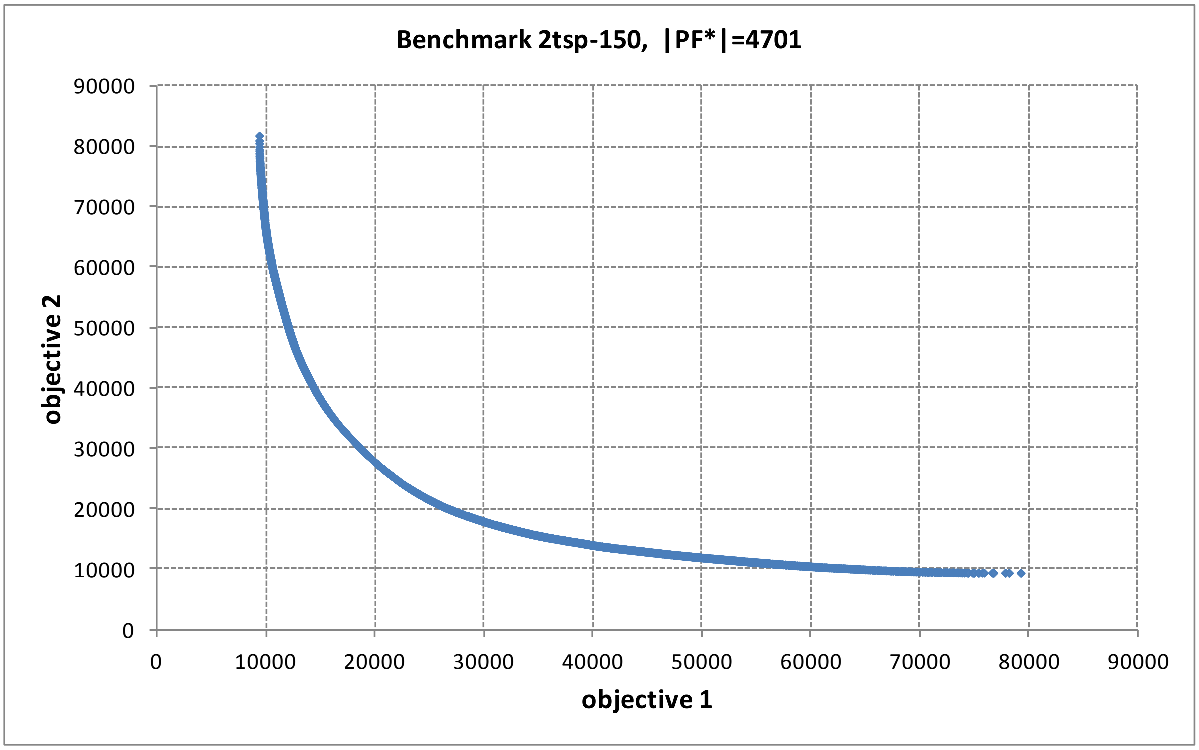
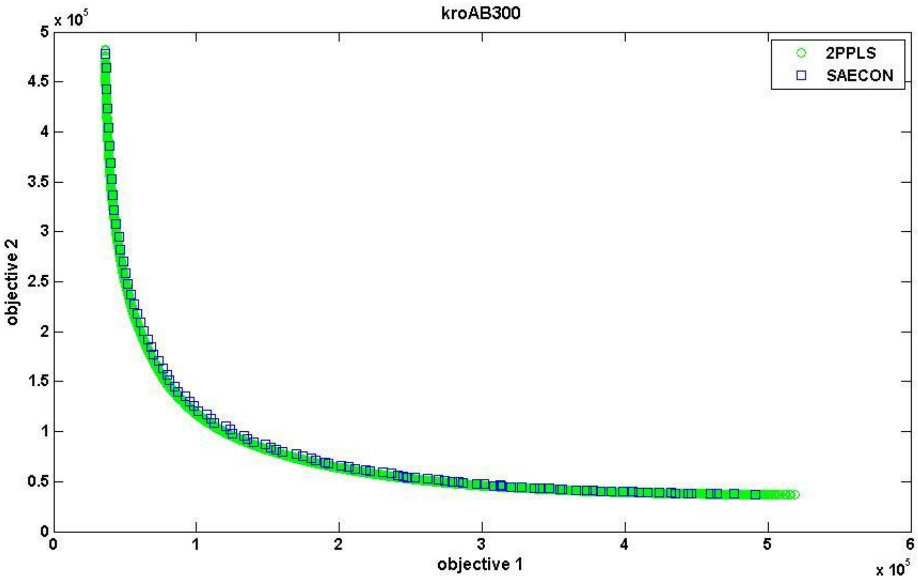


Figure 7. *Visualization of exact Pareto front for 2tsp-150 dataset for biobjective TSP generated by 'portgen'.*

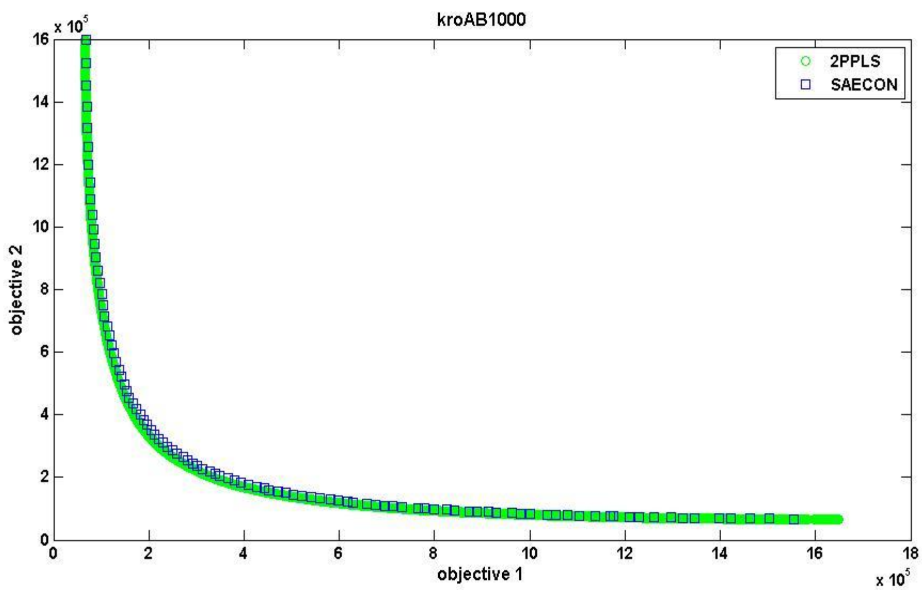
5.2.2 Approximate solution of bi-objective TSP instances with 300 up to 1000 cities

Although the subject of this paper is the exact solution of multi-objective TSP problems, we tried an approximate method based on ε-constraint for problems with more than 150 cities. For this reason we developed a variant of Simulated Annealing which solves ε-constraint sub-problems in order to generate approximately the POS. This approach uses reversal and transport moves as described in [59] (p.366-374) and also a pre-processing phase with the Lin-Kernighan algorithm of Helsgaun (LKH) [60]. Using this heuristic approach, we were able to compute good approximations to the problems kroAB300, kroAB500, kroAB750 and kroAB1000 available in [50].The relevant approximations are shown in Figure 8 for 300 and 1000 city problems. Also, Table 8 reports the convergence [55], hypervolume ratio [54] and spread [54] metrics for the simulated annealing algorithm vs. 2PPLS. The convergence metric for method 'two phase simulated annealing ε-constraint' (2P-SAECON) has been computed for 100 grid points of the ε-constraint method. Phase one was conducted with the LKH heuristic and 40 grid points for the weights. Phase two was conducted with ε-constraint/simulated annealing and 100 grid points for the RHS of the constraint objective 2. As is well known, phase one aims at discovering the supported POS through a weighted sum approach, and phase two finds the unsupported POS (e.g. in our case with ε-constraint).

By observing Figure 8 and Table 8, we see that the simulated annealing algorithm scales up well with the problem size and the approximation obtained with 100 grid points for 2P-SAECON is satisfactory in relation to state-of-the-art 2PPLS. The convergence metric of 2P-SAECON in relation to 2PPLS is of the order of 10^{-3} for all problem sizes. The hypervolume ratio is over 0.99 with maximum desired value equal to 1. Finally, the spread is well below the value of 1, and relatively close to 0 (always well below 0.50) which indicates a well distributed Nondominated front. The run time of 2P-SAECON is much shorter than AUGMECON2-BCHTSP but also significantly larger than the run time of 2PPLS.



(a) kroAB300



(b) kroAB1000

Figure 8. *Two phase simulated annealing ε-constraint algorithm (2P-SAECON) compared to 2PPLS approximate results in BOTSP problems with (a) 300 cities and(b) 1000 cities*

Table 8. Convergence, Hypervolume Ratio and Spread metrics for two phase Simulated Annealing ε-Constraint (2P-SAECON) with respect to two phase Pareto Local Search (2PPLS) of Lust and Teghem ([13, 6]) in larger scale datasets of BOTSP with up to 1000 points of interest.

dataset	Reference Set, R	Convergence (2p-saecon, R)	HV(2p-saecon) / HV(R)	Spread(2p-saecon)
kroAB100	3332*	0.0026620	0.992829	0.44071
kroAB300	14867	0.0038793	0.991295	0.37600
kroAB500	33929	0.0040101	0.991519	0.36756
kroAB750	61184	0.0042229	0.991772	0.36412
kroAB1000	98151	0.0042333	0.992035	0.38035

In kroAB100, R=PF, and in other larger datasets, R=2PPLS run 1 out of 20.

5.3 Three objective TSP results

Finally, in order to test the AUGMECON2 algorithm in more than two objectives, we constructed a dataset which we called '3tsp-15' with the 'portgen' generator available in the website http://dimacs.rutgers.edu/Challenges/TSP/codes.zip with parameter MAXCOORD=1000 and ncities=15 with seeds 1977, 1978 and 1979 for coordinates of objectives 1, 2 and 3, respectively. This is a three objective TSP problem that was solved with our proposed approach AUGMECON2 using the Miller, Tucker and Zemlin [61] formulation of the TSP (MTZ). It was solved in 5 hours of CPU providing a Pareto Front of |PF*|=630 POS which was computed with *MS*=16886 models solved. This is an exact solution, which shows that the AUGMECON2 approach can handle three objective TSP problems, but obviously the number of cities is very small (*N*=15) in accordance to the literature [62, 63]. Therefore, it is obvious from these results that in 3-objective problems the number of the Models Solved is much higher than the number of Pareto Optimal Solutions, especially in relation to the 2-objective cases that we studied. Conclusively, the generation of the exact Pareto front for 3-objective TSP problems, even of small size (20-30 cities), is rather an utopian task and the use of approximate algorithms seems to be our only choice. Our website contains information on the solutions of problems described in Sections 5.2-5.3 as well as on the well-known instances from Section 5.1.

5.4 Two objective SCP results

The AUGMECON2 method was applied to the 44 instances of BOSCP that are described in section 4.2. The formulation of the problem is the one presented in section 2.2, properly adjusted for the AUGMECON2 method. The results for the benchmarks with 1 to 11, and types A-D are presented in Table 9. Where an asterisk (*) is noted, which is the case for 9C, 10C, 10D, 11A, 11B datasets, it means that 4 threads of CPLEX have been used for the IP sub-problems. Otherwise only one thread of CPLEX has been used. In their work, Prins et al. [40] present the results for the 4/11 or 16/44 smaller datasets of Table 9 with up to 40 constraints and 400 variables.

Table 9. AUGMECON2 performance for BOSCP benchmarks No 1-11.

No	File	Type	# constraints	# variables	CPU sec	|PF*|	Models Solved
1	*11*	*A*	10	100	8.64	39	39
		B			6.26	43	44
		C			2.78	10	11
		D			1.45	5	7
2	*41*	*A*	40	200	18.01	107	108
		B			16.63	108	109
		C			7.96	24	25
		D			23.87	43	44
3	*42*	*A*	40	400	35.83	208	210
		B			52.04	276	280
		C			31.79	87	91
		D			7.14	15	16
4	*43*	*A*	40	200	12.80	46	47
		B			7.51	28	30
		C			3.78	13	14
		D			3.48	13	14
5	*61*	*A*	60	600	83.66	257	261
		B			114.01	338	344
		C			18.49	28	31
		D			167.29	67	68
6	*62*	*A*	60	600	58.10	98	99
		B			60.20	99	100
		C			211.26	6	7
		D			134.17	38	45
7	*81*	*A*	80	800	148.66	424	430
		B			130.26	354	363
		C			7.76	14	17
		D			9.33	12	13
8	*82*	*A*	80	800	116.51	132	135
		B			38.16	88	94
		C			671.76	8	9
		D			1511.86	44	47
9	*101*	*A*	100	1000	375.84	157	270
		B			225.50	141	142
		C			20933*	13	14
		D			3812	24	25
10	*102*	*A*	100	1000	104.76	83	87
		B			211.48	86	91
		C			2464*	14	15
		D			16724*	16	23
11	*201*	*A*	200	1000	6850*	274	282
		B			4278*	282	288
		C			dnt	dnt	dnt
		D			dnt	dnt	dnt

* 4 threads of CPLEX have been used

For these smaller datasets, the |PF*| we have found with AUGMECON2 conforms with Prins et al. results. Furthermore, Lust et al. [38] (p. 265) report that in their work the datasets 201a and 201b (1000×200) could not be exactly solved. In our paper, we were able to compute the Exact Pareto Set for 201a and 201b in no more than 2hours each. Nevertheless, the 201c and 201d variants (with plateaus at the objective function coefficients for BOSCP) did not terminate within 24h.

As in the case of the MOTSP we can also observe that the number of models solved is very close to the cardinality of the Pareto set. This means that AUGMECON2 is very effective in avoiding redundant iterations that do not result in new POS. This is mainly attributed to the "jumps" caused by the bypass coefficient *b* (see section 3.1 and section 3.3) that greatly accelerate the process.

6. Concluding remarks

The aim of this paper is to apply the recently proposed improved version of the augmented ε-constraint method (AUGMECON2), which is suitable for general MOIP problems, to two popular MOCO problems, namely, the Multi-Objective Traveling Salesman Problem (MOTSP) and the Multi-Objective Set Covering Problem (MOSCP). Although AUGMECON2 is designed for the general case, here it is applied to bi-objective problems confined by benchmark-data availability.

For the MOTSP case the proposed method was a combination of a general purpose MOIP model (AUGMECON2), with a Branch-and-Cut-and-Heuristic model (BCHTSP) available in GAMS model library. It was found that the ε-constraint sub-problem is solved almost as many times as the cardinality of the Exact Pareto Set, which is a very favourable characteristic for a generation approach (no redundant iterations). Obviously, the BCHTSP model is appropriately modified in order to solve the ε-constraint sub-problem. Relying on the efficiency of the modified BCHTSP which is used as a subroutine, the AUGMECON2 method is able to effectively calculate the Exact Pareto Set in 24-60h wall clock time for every instance of our test bed. A novel feature of our implementation is the parallelization of the AUGMECON2 loop into indicatively three threads. In general, the AUGMECON2 method is appropriate for parallelization as the main loop can be divided into independent segments.

In our work it was reaffirmed that MOTSP is among the hardest MOCO problems. Even bi-objective instances with 100 cities have not been solved exactly in the literature. To the best of our knowledge our work is the first one that generates the exact Pareto set for 16 popular MOTSP instances with 2 objectives and 100 cities, studied intensively in the literature. In general, our approach is among the few implementations able to solve the MOTSP exactly (i.e. produce the exact Pareto set). We also created and solve exactly a bi-objective problem with 150 cities but probably this is the upper limit for the exact solution of bi-objective problems with our method and the current hardware. Moving to three objective functions, the difficulty of generation of the exact Pareto front escalates dramatically and the upper limit seems to be 15-20 cities, which make the use of exact algorithms prohibitive even for small size multi-objective TSP problems. We think that a great contribution of our work is that the data sets and the results are available in https://sites.google.com/site/kflorios/motsp for the interested readers.

Having the exact Pareto set for the BOTSP we were able to assess the effectiveness of state-of-the-art Multi-Objective Metaheuristics (MOMHs) previously utilized to approximately solve the same 16 datasets. The MOMHs are evaluated, using the two set coverage and convergence metrics exploiting the information of the Exact Pareto Set. In our case the coverage metric is actually the percentage of POS found by the MOMH. The coverage metric in the MOTSP problems varied from 25% to 90% depending on the type of instances. Euclidean instances were better approximated by MOMH techniques. Random matrix instances showed poor performance for MOMHs. The mixed type instances yielded approximations better than random matrix but worse than Euclidean instances, as expected. With respect to the convergence metric, we found that, in general, state-of-the-art MOMHs approximate very well the Exact Pareto Set. The magnitude of the convergence metric with respect to the true Pareto Front found by our work, was either of the order of 10^{-4} or 10^{-5}, depending on the MOMH type and the instance type.

Another important finding which is in accordance with similar results from other researchers in MOCO, is that the number of supported POS is only a small proportion among the generated POS. Consequently, the POS produced using the weighting method (that produces only supported POS) is a remarkable underestimation of the true Pareto set for the MOTSP.

Regarding the BOSCP, AUGMECON2 succeeded in solving the previously unsolved benchmarks (instances 201a and 201b) of the MOCOlib for the MOSCP problem. In total, 42 out of 44 benchmarks were exactly solved, leaving only 2 datasets unsolved (in a 24 hours time limit).

In general, for both kinds of problems, namely MOTSP and MOSCP, the effectiveness of the AUGMECON2 method is reflected on the fact that for each benchmark the number of model solved is very close to the cardinality of the Pareto set, indicating good performance and computational economy.

In order to contribute to the testing of relevant algorithms (MOMH or exact algorithms) for the MOTSP and the MOSCP a web site was created that gathers all the datasets and the results, as well as source code in Fortran implementing AUGMECON2 and GAMS implementing modified BCHTSP for the ε-constraint sub-problem.

Extension of our approach, AUGMECON2-BCHTSP to three objective TSPs and massive parallelization (using more than 3 threads for computations) is studied. The optimal allocation of computational load for many processors in the bi-objective case is an interesting problem. Also, parallelization of AUGMECON2 for three objective problems is more delicate, since only the outer loop can be parallelized safely. Perhaps, the research stream with the most potential for the exact solution of MOTSP is to substitute the BCHTSP part of the AUGMECON2-BCHTSP algorithm with a fast dedicated exact solver like CONCORDE [64] or TSP1 [33] but this needs nontrivial programming. The ε-constraint sub-problem has to be programmed inside CONCORDE or TSP1 which requires effort but would be worthwhile. Also, comparison of the AUGMECON2 method with other exact schemes for general MOIP problems as well as the specific MOTSP seems promising (e.g. methods of Lemesre et al. [65] and Dächert et al. [66]).

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