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Acceleration of Solving the Dynamic Multi-Objective Network Design Problem Using Response Surface Methods

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Optimization of externalities and accessibility using dynamic traffic management measures on a strategic level is a specific example of solving a multi-objective network design problem. Solving this optimization problem is time consuming, because heuristics like evolutionary multi objective algorithms are needed and solving the lower level requires solving the dynamic user equilibrium problem. Using function approximation like response surface methods (RSM) in combination with evolutionary algorithms could accelerate the determination of the Pareto optimal set. Three algorithms in which RSM are used in different ways in combination with the Strength Pareto Evolutionary Algorithm 2+ (SPEA2+) are compared with employing the SPEA2+ without the use of these methods. The results show that the algorithms using RSM methods accelerate the search considerably at the start, but tend to converge more quickly, possibly to a local optimum, and therefore loose their head start. Therefore, usage of function approximation is mainly of interest if a limited number of exact evaluations can be done or this can be used as a pre phase in a hybrid approach.

Keywords Dynamic Multi-Objective Network Design Problem; Dynamic Traffic Management Measures; Evolutionary Algorithm; Externalities; Pareto Optimal Set; Response Surface Methods

INTRODUCTION

Although a significant portion of research on optimization in traffic and transport considers a single objective related to accessibility (Gao, Wu, & Sun, 2005; Zhang & Lu, 2007), it may no longer suffice to neglect externalities of traffic. This is also the case for optimization of networks through dynamic traffic management (DTM) measures. Optimization using DTM measures on a strategic level (i.e., implementation of measures optimizing long-term effects) incorporating objectives on externalities is a specific example of a multi-objective network design problem (MO-NDP) in which the implementation of DTM measures can influence the supply of infrastructure dynamically (e.g. traffic signals and rush hour lanes). The presence of multiple conflicting objectives makes the optimization problem interesting but difficult to solve. Since in general no single solution can be termed an optimum solution, the resulting multi-objective (MO) optimization problem resorts to a number of trade-off optimal solutions, known as Pareto optimal solutions.

Mathematical modeling of such a highly complex sociotechnical system provides insight in the extent to which objectives are conflicting or not and the consequences related to weights used concerning the trade-offs, which may be very useful in the decision-making process. The NDP is usually formulated as a bilevel problem in which the lower level describes the behavior of road users who optimize their own objectives (travel time and travel costs), modeled by solving the user equilibrium problem. Because DTM measures are the decision variables and traffic dynamics are important explanatory variables assessing the effects on externalities, a dynamic traffic assignment (DTA) to solve the lower level is preferred. The upper level consists of the objectives that have to be optimized for solving the NDP.

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Because of the nonconvexity of the problem (Chiou, 2005; Gao et al., 2005), often heuristics are used to optimize the total system. In multi-objective bilevel optimization studies, the solution approach using (population-based) evolutionary algorithms (EA) has been proven successful (Wismans, van Berkum, & Bliemer, 2012).

Because the evaluation of any possible solution requires solving the lower level using a DTA model and heuristics are needed to search the Pareto optimal solutions, computation time can become extremely large, especially for large-scale real-world applications. A possible solution for accelerating the search is combining an EA with function approximation methods. Function approximation methods are methods in which a surrogate model is estimated using exact evaluations of solutions (e.g., by fitting a model using regression). This estimated surrogate model can be used in different ways within the optimization process. Genetic algorithms (GA), which are part of the class of EA, are the most widely used heuristic also for NDP, and in the available studies comparing heuristics, GA has been proven to perform best. Earlier research (Fikse, 2010) has shown that response surface methods (RSM) in which a full quadratic function is estimated show promising results. A comparison of different GA has shown that the Strength Pareto Evolutionary Algorithm 2+ (SPEA2+) performs well for the dynamic MO-NDP (Wismans et al., 2012). Because the SPEA2+ shows more diversity in solution and objective space than other tested GAs and diversity is relevant for the estimation of the surrogate model, this algorithm is used as a starting point. However, the RSM methods can also be used in conjunction with other heuristics like swarm intelligence systems. In this research we compared three possible algorithms in which RSM are used, with employing the SPEA2+ algorithm without using these methods.

The use of a surrogate model in conjunction with a heuristic to accelerate the optimization of MO-NDPs has to the best of the authors' knowledge not been addressed earlier. The contribution of this article is a comparison of possible methods to use RSM methods as an accelerator for often-used solution approaches. Although not the main focus of this article, solving this highly complex dynamic MO-NDP using a DTA model that we connected with externality models that take traffic dynamics into account is also rarely addressed.

The outline of this article is as follows. In the second section we provide background information on MO-NDP problems. Then possible approximation methods are discussed in the third section, methods that can be found in the literature to accelerate expensive optimization problems in general. The fourth section describes the optimization problem and framework of the dynamic MO-NDP in which DTM measures are the decision variables. The SPEA2+ solution approach is presented in the fifth section, as well as the approaches using RSM. This section also describes the performance measures used for the comparison. The sixth section describes the case used to compare the algorithms and the results of the comparison is described in the seventh section. Finally, the eighth section closes with the conclusions and directions for further research.

MULTI-OBJECTIVE NETWORK DESIGN PROBLEM

The NDPs are typically grouped into discrete problems (DNDP), in which the decision variable is a discrete variable (Gao et al., 2005; Poorzahedy & Turnquist, 1982); continuous problems (CNDP), in which it is assumed that the decision variable is a continuous variable (Chiou, 2005; Dantzig, Harvey, Lansdowne, Robinson, & Maier, 1978; Friesz et al., 1993; Meng, Yang, & Bell, 2001; Xu, Wei, & Wang, 2009; Zhang & Lu, 2007); and mixed problems, which are a combination of both (Cantarella, Pavone, & Vitetta, 2006). Based on demand, NDPs can be grouped into fixed demand (Meng et al. 2001), stochastic demand (Chen, Kim, Lee, & Kim, 2010; Waller & Ziliaskopoulos, 2001), and (stochastic) elastic demand (Ukkusuri & Patil, 2009). Based on the way time is considered, NDPs can be classified into static, in which stationary travel demand and infrastructure supply is assumed (used in all but one of the already-mentioned studies), or dynamic, which is rarely used (Brands, van Berkum, & van Amelsfort, 2009; Waller & Ziliaskopoulos, 2001). Traditionally, the NDP is associated with the minimization of the total travel time using infrastructural investment decisions under a budget constraint. Additionally, technical constraints (e.g., possible extensions) and outcome constraints (e.g., related to equity) can be formulated. Most of the previous works consider fixed demand, and use a static user equilibrium to model the lower level.

There are also other design variables of networks that can be considered as an NDP. Minimizing delay in signal timing control (e.g., Cantarella & Vitetta, 2006; Cantarella et al., 2006; D'Acierno, Gallo, & Montello, 2012; Sadabadi, Zokaei-Aashtiani, & Haghani, 2008) is such an example. Most of this research is on calculating mutual consistent signal settings by formulating them as a asymmetrical equilibrium assignment problem in which the signal settings are locally optimized and static traffic assignment (STA) is used. However, it is shown that the resulting settings are in general not optimal and therefore perform less than solving a Stackleberg game in which the upper level anticipates the behavior of the lower level (Ceylan & Bell, 2004; Chen & Ben-Akiva, 1998). In addition, Chen and Ben-Akiva (1998) also showed that incorporation of traffic dynamics (i.e., using DTA) results in better solutions than a control strategy based on average traffic flow (i.e., using STA). However, almost all research on this subject when global optimization is also considered still uses STA to model the lower level.

In most cases, single-objective NDPs are studied in which accessibility is optimized, where accessibility is expressed as the total travel time in the traffic network (Gao et al., 2005; Zhang & Lu, 2007). Different studies incorporated the investment costs within the objective function. Chiou (2005), Meng et al. (2001), and Xu et al. (2009) optimized total travel time in which the investment was translated in time using a conversion factor, and in others travel time is translated into cost (Drezner & Wesolowsky, 2003; Poorzahedy & Turnquist, 1982). Occasionally other costs, like environmental costs (expressed in money), are added to the travel cost (Cantarella et al., 2006; Mathew & Sharma, 2006).

In fewer cases, multiple-objective functions are used in the upper level. Chen et al. (2010) use travel time and construction costs as two separate objective functions and used a GA. Friesz et al. (1993) focused on minimizing the transport costs, construction costs, vehicle miles traveled, and dwelling units taken for rights-of-way and used a weighted sum approach in combination with simulated annealing. Sharma, Ukkusuri, and Mathew (2009) used a GA to minimize total travel time and the higher moment for total travel time, that is, variance. Cantarella and Vitetta (2006) considered travel time, walking time, and CO emissions in their optimization using a GA. Most MO-NDP studies consider the minimization of investment cost as a second objective, as reported in Sharma et al. (2009).

For solving the NDP, different approaches are possible. Solving the NDP is normally difficult, because it is nonconvex and nondifferentiable and has been proved to be NP-hard (Johnson, Lenstra, & Rinooy Kan, 1978). Studies that did not reformulate the problem therefore all use heuristics to solve it. Various studies are available in which heuristics are compared for solving NDPs. In almost all studies GA outperformed other approaches like hill climbing or descent algorithms, simulated annealing, tabu search, add plus interchange algorithm, variable neighborhood search algorithm, random search, and path relinking (Cantarella et al., 2006; Drezner & Wesolowsky, 2003; Karoonsoontawong & Waller, 2006; Santos, Antunes, & Miller, 2009; Xu et al., 2009). Reformulating the NDP in such a way that it can be solved efficiently is also an active research topic. By reformulating is meant the adjustment or approximation of the original optimization problem based on additional assumptions. Within Chen and Bernstein (2004), Chiou (2005), and Cho and Lo (1999), the original bilevel optimization CNDP is, for example, converted into a single-level standard nonlinear optimization problem by using sensitivity methods to be able to calculate derivatives, which can be used to linearize the equilibrium constraints. Although these methods are of interest, reformulating the original problem generally results in finding less performing solutions and thus far is only possible in realistic cases when STA is used. This is also shown in Meng et al. (2001), Chiou (2005), Luathep, Sumalee, Lam, Li, and Lo (2011), and Ban, Lui, Lu, and Ferris (2006), in which heuristic approaches find better results in most cases.

In this research, the optimization problem is also formulated as an MO-NDP, assuming a Stackleberg game in which DTM measures are used to influence supply of infrastructure and the externalities of traffic the objectives. The DTM measures considered are control measures that directly influence supply (e.g., rush-hour lanes, variable speed limit, ramp metering, and traffic signals). Because traffic dynamics are important explanatory variables for the externalities of traffic and DTM measures are modeled as time dependent measures, a DTA model is used to operationalize the lower level. However, as mentioned earlier, solving this optimization problem is computationally expensive, especially because a DTA model is used to solve the lower level. This MO-NDP is used to compare the three algorithms.

APPROXIMATION METHODS

The upper level of the bilevel optimization problem is often solved by using heuristics. Heuristics like Evolutionary Multi-Objective Algorithms (EMOA) usually require a large number of function evaluations (i.e., evaluation of objective functions of possible solutions) that can become computationally expensive, especially in large-scale, real-world applications using DTA models. Because of the usage of a time-consuming DTA model as in the presented MO-NDP to solve the lower level optimization problem, it is often essential to use approximation methods to reduce the time needed to evaluate solutions or the number of solutions being evaluated exact. Approximation methods estimate the outcome of a function evaluation on the basis of previously observed objective functions of exact evaluated (neighboring) individuals.

Different approximation methods are available, such as functional approximation using kriging, radial basis functions (RBF), RSM, and evolutionary approximation using clusters and fitness inheritance (Fikse, 2010; Santana-Quintero, Ariaas Motano, & Coello Coello, 2010; Shi & Rasheed, 2010). Fitness inheritance and clusters are evolutionary approximation methods, which are specific for EA. The outcome of the function evaluations of the different assessed solutions and mutual comparison determine the fitness of the solutions within an EMOA. The method of fitness inheritance assigns fitness to a solution by the average (or weighted average) of the fitnesses of its parents. Clearly, also exact fitness function values are required to obtain enough information. Ducheney, De Daets, and de Wulf (2008) concluded that fitness inheritance methods can be used for convex and continuous problems, which is not the case in our MO-NDP. There is no generic approach that uses clustering, but this evolutionary approximation method refers to the use of clustering techniques. In the adaptive fuzzy fitness granulation (AFFG) it is, for example, used to assign fitness to a solution based on the fitness of solutions that are assigned to the same cluster in solution space (Davarynejad, Ahn, Vrancken, Van den Berg, & Coello Coello, 2010). The kriging, RBF, and RSM methods are functional approximation methods in which a new expression is constructed for the objective functions based on previous data obtained from exact evaluations. These models are also known as meta-models or surrogates. Based on research by Fikse (2010) in which kriging, RBF, and RSM are compared for MO-NDP, the RSM was selected as approximation method for this research, because of its performance, simplicity, and computational cost, and it does not require any tuning of parameters. This was also concluded in other research (Shi & Rasheed, 2010).

Two of the rare studies in which function approximation is used within traffic and transport optimization problems are research by Osorio (2011) and Chow (2010). Osorio used the trust region optimization method, which uses RSM methods, and which can be used for single-objective optimizations, to optimize the fixed-time signal control problem. Chow developed and applied the multi-objective radial basis function algorithm for traditional NDP.

OPTIMIZATION PROBLEM AND FRAMEWORK

The MO optimization problem is formulated as the following MO mathematical problem with equilibrium constraints (MPEC):

$$\min_{S\in F} \begin{pmatrix} z_1(S) \\ z_2(S) \\ \vdots \\ z_I(S) \end{pmatrix}, \text{ subject to}$$

$$(q(S), v(S), k(S)) \in \Gamma^{DTA}\left(G\left(N, A\left(C(S)\right)\right), D\right), \qquad (1)$$

in which S is a set of applications of strategic DTM measures to be selected from a set of feasible applications F, and $z_i(S)$, $i = 1, \ldots, I$, is the ith objective function of the link flows $q(S)$, the link speeds $v(S)$, and the link densities, $k(S)$, expressed as $z_i(S) = f_i\left(q(S), v(S), k(S)\right)$. These objectives in our case concern efficiency, climate, air quality, traffic safety, and noise. Furthermore, the link flows, speeds, and densities are assumed to follow from solving a dynamic user equilibrium problem, indicated by Γ^{DTA}, for which the supply of infrastructure is given by network G with nodes N and links A (with corresponding characteristics C), and the (dynamic) travel demand D. The link characteristics without any DTM measures, which we denote by C_0, include the outflow capacity, the number of lanes, the free-flow speed, the speed at capacity, and the jam density, and are all captured in a fundamental diagram. The DTA model Streamline (Raadsen, Mein, Schilpzand, & Brandt, 2010), which is a multiclass model with physical queuing and spillback, is used to solve for this dynamic user equilibrium.

The DTM measures defined in S are modeled as measures that influence the characteristics C of the links where the measures are implemented. This means for example that if a variable message sign (VMS) is used to change the speed limit, the free-flow speed and capacity of the links connected with this measure is changed. The characteristics C of links can therefore vary over time depending on the settings of the DTM measures, S. The impact of a measure depends on the actual settings, for example, the green time for a certain direction on a signalized intersection. Activation times and settings of the DTM measures are discretized, so the upper level then becomes a discrete optimization problem where for each time period a certain DTM measure with a certain setting is implemented or not. The set of feasible solutions, F, is assumed to be a discrete set of possible applications of strategic DTM measures. If we assume that there are B different DTM measures available in the network, the application of the DTM measures in time step t is defined by $S(t) = (s_1(t), ..., s_B(t))$, where each $s_b(t)$, $b = 1, \ldots, B$, can have M_b different settings, which we simply number from 1 to M_b. The set of feasible solutions can therefore be written as $F = \{S | s_b(t) \in \{1, \ldots, M_b\}, \forall t = 1, \ldots, T\}$, such that there are $\left(\prod_b M_b\right)^T$ possible solutions. The set of applications of the DTM measures for all time periods is defined by $S = (S(1), ..., S(T))$ and forms a possible solution for the optimization problem.

The set of solutions $X^* = \left\{S_1^*, .., S_n^*\right\}$, is the outcome of our MO MPEC problem (1) and consists of all solutions for which the corresponding objectives cannot be improved for any objective without degradation of another and is known as the Pareto optimal set. However, MO-NDP is an NP-hard problem, for which heuristics are needed to find a (near) optimal solution within acceptable computation time. In this research, the exact Pareto optimal set is not known; hence we aim at finding such a subset. Mathematically, the concept of Pareto optimality is as follows. If we assume two solutions $S_1, S_2 \in F$, then S_1 is said to strongly dominate S_2 (also written as $S_1 \succ S_2$) if $z_i(S_1) < z_i(S_2)$ for all i. Additionally, S_1 is said to cover or weakly dominate S_2 (written as $S_1 \succeq S_2$) if $z_i(S_1) \leq z_i(S_2)$ for all i.

SOLUTION APPROACHES

Multi-Objective Genetic Algorithm SPEA2+

The used SPEA2+ is a multi-objective GA developed by Kim, Hiroyasu, and Miki (2004). This algorithm is based on the SPEA2 approach, which was originally developed by Zitzler, Laumans, and Thiele (2001). Within the algorithm, the fitness assignment depends on the level of dominance and fitness sharing based on density to maintain population diversity and carried out in three steps. First, the strength of each solution is determined, representing the number of solutions it dominates. Second, the raw fitness of each solution is determined by summation of the strengths of its dominators. Third is determination of the fitness by incorporation of density information in the raw fitness value, which assigns a lower fitness to solutions in a highly populated area. The density of a solution is measured in the objective space as a decreasing function of the distance to the kth nearest neighbor. This density information forms the way fitness sharing is designed. SPEA2+ contains elitism by the preservation of good solutions in the environmental selection step. This is a deterministic step in which an archive is maintained containing the best solutions, based on their fitness, considered so far. Within the SPEA2+ approach, two archives are maintained. In one archive the distances between solutions within the solution space, while in the other archive the distances between solution within the objective space are used to truncate the Pareto optimal set if its size exceeds the predefined maximum size. These archives contain solutions used for the mating selection, which is done using neighborhood crossover, which crosses over solutions close to each other in the objective space.

Here is the algorithm in steps; for more information, we refer to Kim et al. (2004):

Step 1: *Initialization*: Set population size N_p, which is equal to the archive size N_a, the maximum number of generations G, and generate an initial population OA_0. Set $g = 0$, $DA_0 = \emptyset$ and $Q_0 = \emptyset$.
Step 2: *Fitness assignment*: Combine archive OA_g, DA_g, and children Q_g, forming $R_g = OA_g \cup DA_g \cup Q_g$, and calculate fitness values of solutions by strength values and density information.
Step 3: *Environmental selection*: Copy all nondominated solutions in R_g to new archives OA_{g+1} and DA_{g+1}. If size of OA_{g+1} and DA_{g+1} exceeds N_a, then reduce OA_{g+1} by truncation using distances in the objective space and DA_{g+1} by truncation using distances in the solution space; otherwise if less than N_a, then fill OA_{g+1} and DA_{g+1} with best solutions out of R_g based on their fitnesses.
Step 4: *Termination*: If $g \geq G$ or another stopping criteria is satisfied, then set X^* to the set of solutions part of DA_{g+1} with fitness value smaller than 1 (nondominated solutions) and determine the size of nondominated solutions N; note that $N \leq N_a$.
Step 5: *Mating selection*: If truncation procedure is used, select DA_{g+1} as mating pool of parents P_{g+1}, and otherwise if not, select OA_{g+1} as mating pool of parents P_{g+1}.
Step 6: *Variation*: Apply neighborhood crossover and mutation operators to the mating pool P_{g+1} to create offspring Q_{g+1}. Set $g = g + 1$ and go to Step 2.

Response Surface Methods

The RSM is introduced by Box and Wilson (1951) and was originally intended as a guideline to design experiments. In this case we fit a regression model using a pure quadratic polynomial (single and quadratic terms), which is also recommended in other studies (Fikse, 2010; Osorio, 2011; Shi & Rasheed, 2010):

$$\widetilde{z}_i(S) = \alpha_0 + \sum_{j=1}^{T}\sum_{k=1}^{B} \alpha_{(j-1)*T+k} S_k^j + \sum_{j=1}^{T}\sum_{k=1}^{B} \alpha_{TB+(j-1)*T+k} S_k^{j2}$$

By fitting a regression model, a least-squares problem is solved using the exact evaluated solutions as input and results in the estimates for the parameters α. To be able to solve the least-squares problem (finding a unique solution), the number of exact evaluated solutions that form the input should be at least equal to the number of parameters α to estimate. However, to avoid overfitting, the number of exact evaluated solutions should be larger. In addition, because the MO-NDP is not specifically interested in one part of solution space, the model is used for global approximation, and to avoid fast convergence to local optima, diversity of exact evaluated solutions that are used for fitting the regression model is relevant. This type of model use is easy to understand and can be estimated rapidly even with a large number of exact evaluated solutions.

Algorithms Using RSM

The surrogate model estimated by RSM methods can be used in different ways in combination with EMOA. The main differences depend on the level of confidence in the estimated surrogate model. The surrogate model can be used as a preevaluation to determine the solutions that should be evaluated exactly, as fitness evaluation in which the estimates are used as exact values, or as design of experiments in which the surrogate model is used to define solutions that should be exactly evaluated. These possible options are part of the algorithms compared.

Within the first approach (SPEA2+ pre evaluation FA), the surrogate model is used as a preevaluation within the SPEA2+ algorithm to determine which “children” are interesting to evaluate exactly. In addition, the children that are situated in less dense areas are also included to evaluate exactly because these solutions can improve the surrogate model and because the error of the approximation of these solutions is relatively high. If the algorithm tends to converge the preevaluation is neglected, which means that the algorithm becomes a regular SPEA2+ algorithm. The advantage of this approach is that it still uses the full characteristics of the original heuristic and is not fully dependent on the quality of the surrogate model. However, it is possible that only a limited number of solutions are not exactly evaluated and therefore the acceleration is limited. Within the second approach (FA optimized SPEA2+), the surrogate model itself is optimized using a SPEA2+ algorithm and the resulting solutions are exactly evaluated to determine the Pareto optimal set and used to update the approximation set. The advantage of this algorithm is that the surrogate model is fully used, which in theory can result in the largest acceleration possible. However, this also means that the quality of the surrogate model is determinative for the Pareto optimal set found and can result in erroneously not considering solutions in certain parts of the solution space. Within the third approach (FA seeded SPEA2+) the algorithm of the second approach is only used in the first h steps, after which the algorithm continues as a regular SPEA2+ algorithm. In this algorithm the surrogate model is used to obtain a seeded starting population. The advantage is that it combines the second approach with the original heuristic assuming that the largest acceleration is found in the first steps and therefore avoids fast convergence to suboptimal solutions. However, this also means that only in the first steps is acceleration possible.

All algorithms use a Latin hypercube sample (LHS) optimized for correlation as a starting population. This LHS is used as input (approximation set) for estimating the surrogate model. In all algorithms this approximation set is updated based on new solutions exactly evaluated. Within the SPEA2+

SPEA2+ pre evaluation FA

Step 1:*Initialization*: Set population size N_p, which is equal to the archive size N_a, the maximum number of generations *G*, and generate an initial population OA_0. Set $g = 0$, $DA_0 = \varnothing$ and $Q_0 = \varnothing$.

Step 2:*Fitness assignment*: Combine archive OA_g, DA_g, and children Q_g, forming $R_g = OA_g \cup DA_g \cup Q_g$, and calculate fitness values of solutions by strength values and density information.

Step 3:*Environmental selection*: Copy al non-dominated solutions in R_g to new archives OA_{g+1} and DA_{g+1}. If size of OA_{g+1} and DA_{g+1} exceeds N_a, then reduce OA_{g+1} by truncation using distances in the objective space and DA_{g+1} by truncation using distances in the solution space, otherwise if less than N_a, then fill OA_{g+1} and DA_{g+1} with best solutions out of R_g based on their fitnesses.

Step 4:*Update training set*: If $g = 0$ set approximation set $Y_{g+1} = OA_0$, otherwise update approximation set Y_{g+1} with solutions of offspring Q_g which are situated in less dense areas based on distance k-th nearest neighbor in solution space. Combine approximation set Y_{g+1} and DA_{g+1} if truncation procedure is used, otherwise combine Y_{g+1} and OA_{g+1} forming the training set $U_{g+1} = Y_{g+1} \cup DA_{g+1}$, or $U_{g+1} = Y_{g+1} \cup OA_{g+1}$.

Step 5:*Function approximation*: Estimate surrogate objective functions $\tilde{z}_i = f(S)$ based on training set U_{g+1}

Step 6:*Termination*: If $g \geq G$ or another stopping criteria is satisfied, then set X^* to the set of solutions part of DA_{g+1} with fitness value smaller than 1 (non-dominated solutions) and determine the size of non-dominated solutions *N*, note that $N \leq N_a$.

Step 7:*Mating selection*: If truncation procedure is used, select DA_{g+1} as mating pool of parents P_{g+1}, otherwise if not, select OA_{g+1} as mating pool of parents P_{g+1}.

Step 8:*Variation*: Apply neighborhood crossover and mutation operators to the mating pool P_{g+1} to create offspring Q_{g+1}.

Step 9:*Pre-evaluation:* Skip pre-evaluation if results tend to converge (based on C-metric), otherwise evaluate offspring Q_{g+1} using surrogate objective functions and update Q_{g+1} by removing children which will not be part of the Pareto optimal set. Add children to Q_{g+1} which are situated in less dense areas in solution space. Set $g = g+1$ and go to step 2.

FA optimized SPEA2+

Step 1:*Initialization*: Set population size N_p, which is equal to the archive size N_a, the maximum number of generations *G*, and generate an initial population OA_0. Set $g = 0$, $DA_0 = \varnothing$ and $Q_0 = \varnothing$.

Step 2:*Fitness assignment*: Combine archive OA_g, DA_g, and children Q_g, forming $R_g = OA_g \cup DA_g \cup Q_g$, and calculate fitness values of solutions by strength values and density information.

Step 3:*Environmental selection*: Copy al non-dominated solutions in R_g to new archives OA_{g+1} and DA_{g+1}. If size of OA_{g+1} and DA_{g+1} exceeds N_a, then reduce OA_{g+1} by truncation using distances in the objective space and DA_{g+1} by truncation using distances in the solution space, otherwise if less than N_a, then fill OA_{g+1} and DA_{g+1} with best solutions out of R_g based on their fitnesses.

Step 4:*Update training set*: If $g = 0$ set training set $U_{g+1} = OA_0$, otherwise combine training set U_g and solutions of offspring Q_g to update training set $U_{g+1} = U_g \cup Q_g$.

Step 5:*Function approximation*: Estimate surrogate objective functions $\tilde{z}_i = f(S)$ based on training set U_{g+1}

Step 6:*Termination*: If $g \geq G$ or another stopping criteria is satisfied, then set X^* to the set of solutions part of DA_{g+1} with fitness value smaller than 1 (non-dominated solutions) and determine the size of non-dominated solutions *N*, note that $N \leq N_a$.

Step 7:*Optimize surrogate model:* Optimize surrogate objective functions using regular SPEA2+ algorithm. Set resulting Pareto optimal set as offspring Q_{g+1}. Set $g = g+1$ and go to step 2.

FA seeded SPEA2+

Step 1:*Initialization*: Set population size N_p, which is equal to the archive size N_a, the maximum number of generations *G*, and create seeded initial population using FA optimized SPEA2+ algorithm for *m* generations. Set resulting Pareto optimal set as initial population OA_0. Set $g = 0$, $DA_0 = \varnothing$ and $Q_0 = \varnothing$.

Step 2:*Fitness assignment*: Combine archive OA_g, DA_g, and children Q_g, forming $R_g = OA_g \cup DA_g \cup Q_g$, and calculate fitness values of solutions by strength values and density information.

Step 3:*Environmental selection*: Copy al non-dominated solutions in R_g to new archives OA_{g+1} and DA_{g+1}. If size of OA_{g+1} and DA_{g+1} exceeds N_a, then reduce OA_{g+1} by truncation using distances in the objective space and DA_{g+1} by truncation using distances in the solution space, otherwise if less than N_a, then fill OA_{g+1} and DA_{g+1} with best solutions out of R_g based on their fitnesses.

Step 4:*Termination*: If $g \geq G$ or another stopping criteria is satisfied, then set X^* to the set of solutions part of DA_{g+1} with fitness value smaller than 1 (non-dominated solutions) and determine the size of non-dominated solutions *N*, note that $N \leq N_a$.

Step 5:*Mating selection*: If truncation procedure is used, select DA_{g+1} as mating pool of parents P_{g+1}, otherwise if not, select OA_{g+1} as mating pool of parents P_{g+1}.

Step 6:*Variation*: Apply neighborhood crossover and mutation operators to the mating pool P_{g+1} to create offspring Q_{g+1}. Set $g = g+1$ and go to step 2.

Figure 1 Developed and tested algorithms combining GA and RSM.

preevaluation FA and seeded SPEA2+ new solutions are added if these provide information for low dense areas in the solution space. Within the FA optimized SPEA2+ the approximation set consists of all exact evaluated solutions. This approximation set is combined with the Pareto optimal set known thus far, forming the training set to estimate the surrogate model (Figure 1).

Performance Measures

In order to compare the three algorithms, we used different complementary performance measures presented in Table 1 and illustrated for the bi-objective case in Figure 2. These measures are the S-metric, size of dominated space, the C-metric, coverage of two sets, and the spacing metric (Wismans et al.

Table 1 Overview of performance measures used.

Performance measure	Explanation
Spacing metric	Let $X' = (S'_1, S'_2, ..., S'_N) \subset X$ be a set of solutions. The function $SMO(X')$ determines how evenly the solutions of set X' are distributed in the objective space. Because also the distribution in the solution space is of interest, we also define $SMS(X')$. $SMO(X') = \frac{1}{\bar{d}}\sqrt{\frac{1}{N}\sum_{n=1}^{N}(d_n - \bar{d})^2}$, with $\bar{d} = \frac{1}{N}\sum_{n=1}^{N} d_n$. d_n is the Euclidean distance between each solution and its nearest solution. In function $SMO(X')$ this distance is measured in the objective space, while in function $SMS(X')$ this distance is measured in the solution space. The smaller the value of $SMO(X')$, the better the distribution of the solutions in X' in the objective space and the smaller the value of $SMS(X')$, the better the distribution of the solutions in X' in the solution space. The spacing metric only focuses on the spread across the solutions part of the considered set, which means that a certain set which is not near the true Pareto optimal set or only contains a specific part of this set still performs well on this metric.
C-metric	Let $X', X'' \subset X$ be two sets of solutions. The function $CTS(X', X'')$ determines the coverage of two sets of the ordered pair (X', X''), which means the level in which the solutions X' weakly dominates X''. $CTS(X', X'') = \frac{\lvert\{S'' \in X''; \exists S' \in X' : S' \succeq S''\}\rvert}{\lvert X'' \rvert}$ The value $CTS(X', X'') = 1$ means that all solutions in X'' are covered by the solutions in X'. The opposite, $CTS(X', X'') = 0$ represents the situation where none of the solutions in X'' are covered. The C-metric focuses on the ability to attain the global trade-offs, which means that a set of solutions which dominates most of the solutions of another set found better solutions. However, this measure does not incorporate to what extent these solutions are better (i.e. are an improvement for all objectives).
S-metric	Let $X' = (S'_1, S'_2, \ldots, S'_N) \subset X$ be a set of solutions. $SSC(X')$ equals the size of the space coverage. It is formed by the (hyper)volume enclosed by the union of the polytopes formed by the intersection of the following hyperplanes arising out of every single solution along with the axis in the objective space. For the minimization problem, the origin and therefore the axis are moved to a point representing the opposite of a utopian point, defined by $w(z_1^{\max}(S_i), z_2^{\max}(S_j))$, which means the upper bound of each objective. Because the true maximum values of the objective functions are not known, we choose a conservative point, based on the evaluated solutions. In the two-dimensional case, each polytope represents a rectangle defined by this point $w(z_1^{\max}(S_i), z_2^{\max}(S_j))$ and $(z_1(S_i), z_2(S_i))$. The hypervolumes are calculated based on the Hypervolume by slicing objectives (HSO) algorithm introduced by While et al. (2006). The larger the value of $SSC(X')$, the better the space coverage. The S-metric also focuses on the ability to attain the global trade-offs, which means a set of solutions performs better if its space coverage is larger. This measure does not take into account the number of solutions which are dominated. Therefore it is possible that a certain set of solutions performs better on the S-metric although most of its solutions are dominated by the other set of solutions.

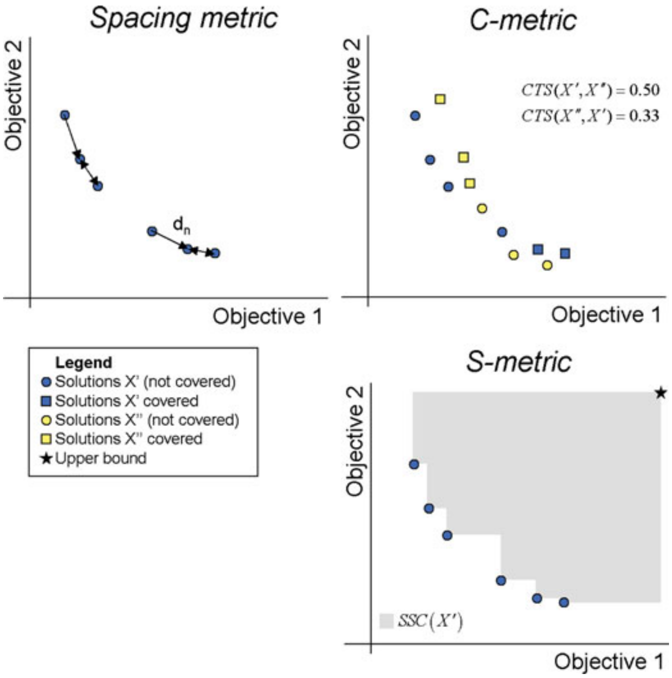

Figure 2 Performance measures.

2012; Zitzler, Thiele, Launmanss, Fonseca, & Grunert da Fonseca, 2003).

CASE

Description of Case

A case study is used to compare the algorithms using the formulated performance metrics and the results of these approaches concerning the found Pareto optimal solutions for the multi-objective optimization of externalities. For providing a clear demonstration, a simple transport network is hypothesized, consisting of a single origin–destination relation with three alternative routes. One route runs straight through a city with urban roads (speed limit of 50 km/h); the second route is via a ring road using a rural road (speed limit of 80 km/h); the third route is an outer ring road via a highway (speed limit of 120 km/h). Travel demand varies with time over the simulation period. A 3-hour morning peak was simulated between 6 a.m. and 9 a.m. The travel demand (maximum of 6,300 pcu/h in the morning peak; see Figure 3 for profile) consists of passenger cars and trucks (10% of total demand).

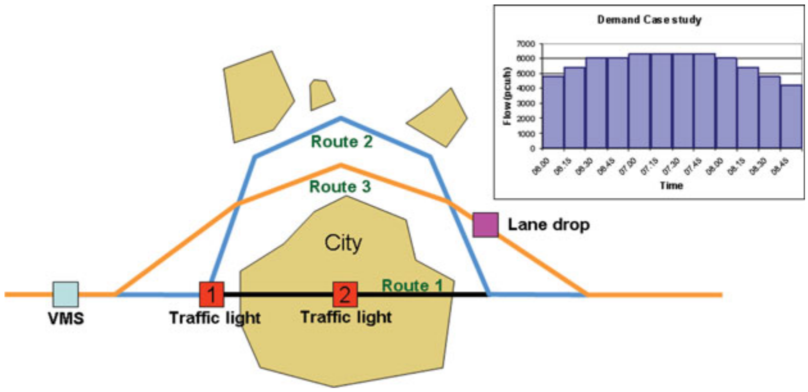

Figure 3 Representation of network.

Within the network, there are three measures available, namely, two traffic lights and a VMS used to change speed limits. The first traffic light is split into two measures because the two signaled directions are in this case independent. In total, six time intervals for the DTM measures are distinguished, equally divided into 30-minute slices, which means $t \in \{1, ..., 6\}$. The possible settings, and ways these are modeled by changing link characteristics, are given in Table 2. The representation of a solution in the GA is a vector of all $s_b(t)$. The constraints concerning the possible applications are therefore incorporated in the representation.

Although the network is small, it incorporates important elements like urban and nonurban routes when using DTM measures to optimize the externalities. Moreover, these objectives were modeled in a realistic manner incorporating traffic dynamics. In addition, these possible settings in this case study already result in 4.05×10^{21} possible solutions. Because the evaluation of one solution means solving the lower level DTA problem, which requires approximately one minute of CPU time, it would take 7.7×10^{15} years in order to assess all possible solutions.

Parameter Settings

In the comparison of the approaches, the total number of solutions exactly evaluated is a fixed number of 5,100 solutions (initialization inclusive). The analysis is therefore focusing on how well the algorithms perform given the same available computation time (approximately 85 hours on a single computer), because the exact evaluation of a solution is by far the most computationally expensive step in all approaches. For all algorithms we used the same genetic operators, namely, uniform crossover and mutation in which the initial mutation rate is 0.2 and decreases with 95% within the first 10 generations. Only small mutations occur, as we assume that mutation results in shifting the DTM application one up or down; that is, if $s_b(t)$is selected for mutation, its value after mutation becomes either $s_b(t) - 1$ or $s_b(t) + 1$. All approaches are repeated eight times, and the archive size was set to be equal to the population size of 100 solutions. In all algorithms the deterministic environmental selection procedure of the SPEA2+ algorithm was used in every iteration to select the 100 Pareto optimal solutions.

Objective Functions

Based on an extensive literature review (Wismans, van Berkum, & Bliemer, 2011), for each objective i an objective function f_i is defined, where the input stems from the DTA model. Efficiency is defined in terms of the total travel time in the network. Climate is represented by the total emission of CO_2. The emission calculations are based on the ARTEMIS traffic situation-based emission model (INFRAS, 2007), which means dependent on the level of service of traffic flows. Finally, noise is calculated as the average weighted sound power level, in which emissions are based on a load- and speed-dependent emission function (RMV, 2006). The weights of noise emissions depend on the level of urbanization. The objective functions used, which all should be minimized, are listed in Table 3.

RESULTS

The results of the comparison are discussed in this section. First, we discuss to what extent the algorithms are missing

Table 2 Overview modeling DTM measures.

	$s_b(t)$	Characteristic	$C\ (s_b(t))$	C_0
Traffic light 1	$s_1(t) \in \{1, ..., 11\}$	Outflow capacity	$C\ (s_1(t)) \in \{500, 600, ..., 1400, 1500\}$	$C = 1000$
	$s_2(t) \in \{1, ..., 11\}$	Outflow capacity	$C\ (s_2(t)) \in \{500, 600, ..., 1400, 1500\}$	$C = 1000$
Traffic light 2	$s_3(t) \in \{1, ..., 11\}$	Outflow capacity	$C\ (s_3(t)) \in \{500, 600, ..., 1400, 1500\}$	$C = 1000$
VMS	$s_4(t) \in \{1, ..., 3\}$	Free-flow speed, capacity increase	$C\ (s_4(t)) \in \left\{ \begin{pmatrix} 80 \\ 0.05 \end{pmatrix}, \begin{pmatrix} 100 \\ 0.025 \end{pmatrix}, \begin{pmatrix} 120 \\ 0 \end{pmatrix} \right\}$	$C = \begin{pmatrix} 120 \\ 0 \end{pmatrix}$

Table 3 Overview of measures and objective functions used.

Objective	Measure	Remark
Efficiency	Total travel time (h)	Because fixed demand is assumed, minimizing total travel time is equal to minimizing vehicle lost hours.
$z_1 = \sum_a \sum_t \sum_m \frac{q_{am}(t)\ell_a}{v_{am}(t)}$ (2)		
Climate	Total amount of CO_2 emissions (grams)	Calculation based on traffic situation based emission model ARTEMIS.
$z_3 = \sum_a \sum_t \sum_m \sum_d q_{am}(t)\delta_{ad} E_{md}^{CO2}(v_{am}(t))\, \ell_a$ (3)		
Noise	Weighted average sound power level at the source (dB(A))	Calculation based on the standard calculation method (RMV, 2006) used in The Netherlands.
$z_5 = 10\log\left(\frac{\sum_a \sum_w \delta_{aw}\ell_a 10^{\frac{\bar{L}_w - \eta_w}{10}}}{\sum_a \sum_w \delta_{aw}\ell_a}\right)$, with $\bar{L}_w = 10\log\left(\frac{\sum_a \sum_t \delta_{aw}\ell_a \Delta t \sum_m 10^{\frac{L_m(v_{am}(t))}{10}}}{T\sum_a \delta_{aw}\ell_a}\right)$,		
where $L_m(v_{am}(t)) = \alpha_m + \beta_m \log\left(\frac{v_{am}(t)}{v_m^{\text{ref}}}\right) + 10\log\left(\frac{q_{am}(t)}{v_{am}(t)}\right)$ (4)		
with		

Variable	Explanation
z_1	Objective function efficiency (= total travel time) (h)
z_3	Objective function climate (= total amount of CO_2 emissions) (grams)
z_5	Objective function noise (= weighted average sound power level at source) (dB(A))
$q_{am}(t)$	Vehicle type m inflow to link a at time t (vehicles)
$v_{am}(t)$	Average speed of vehicle type m on link a at time t (km/h)
$E_{md}^{CO2}(\cdot)$	CO_2 emission factor of vehicle type m, depending on average speed (grams/(vehicles-km))
$L_m(\cdot)$	Average sound power level for vehicle type m, depending on the average speed (dB(A))
$\bar{L}_w$	Weighted average sound power level on network part with urbanization level w (dB(A))
ℓ_a	Length of link a (km)
δ_{ad}	Road type indicator, equals 1 if link a is of road type d, and 0 otherwise
δ_{aw}	Urbanization level indicator, equals 1 if link a has urbanization level w, and 0 otherwise
η_w	Correction factor for urbanization level w (dB(A)))
w_a	Level of urbanization around link a
α_m, β_m	Parameters dependent of vehicle category for noise calculations
v_m^{ref}	Reference speed dependent of vehicle category

relevant parts of the efficient frontier. Then the performance of the algorithms is discussed using the performance measures presented earlier, in the fifth section.

Figure 4 shows the Pareto optimal solutions of one randomly chosen application for each algorithm. The results show that the algorithms find similar Pareto optimal fronts and objectives efficiency and climate in this case are strongly aligned. However, both objectives are opposed to the objective noise. Optimizing efficiency aims at avoiding congestion using full capacity of the available routes, which is also good for minimizing CO_2 emissions. Optimizing noise aims at lowering the driving speeds as much as possible and also avoiding traffic using the urban routes.

Figure 4 also shows that the different algorithms do find solutions in similar parts of the objective space. Analyzing the found minima (i.e., absolute minima and average minima of repetitions) of the three objective functions concerning efficiency, climate, and noise shows that the differences compared to the regular SPEA2+ algorithm are less than 1%. The differences in found maxima for climate and noise are also less than 1%. For efficiency the differences for SPEA2+ preevaluation FA is less than 1%, for FA seeded SPEA2+ less than 1.5%, and for FA optimized SPEA2+ less than 1.6%. Therefore, the use of approximation methods within the proposed algorithms does not result in missing relevant parts of the Pareto optimal set. To compare the algorithms in more detail the different performance measures are analyzed.

The average performance of the algorithms after the algorithms are terminated (after 5,100 exactly evaluated solutions), is presented in Table 4. The results show that the differences between the algorithms are small. The SPEA2+ preevaluation FA performs slightly better than the SPEA2+ algorithm and the other algorithms slightly less well. The similar performance also means that the use of approximation methods does not result in bad performance, because of wrong decisions based on the estimated surrogate model.

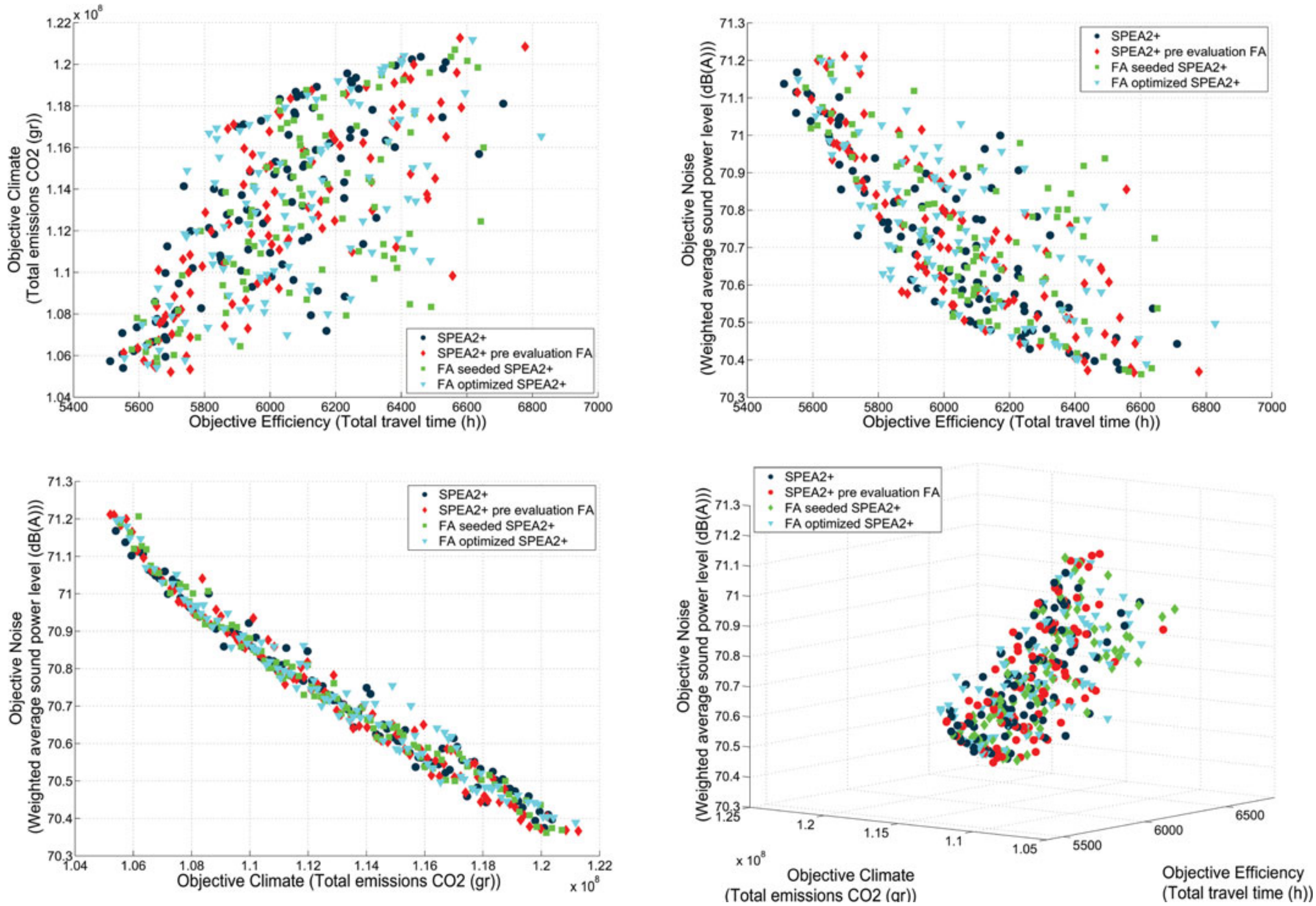

Figure 4 Pareto optimal solutions.

One of the reasons the algorithms perform similarly is because the results are converging, meaning that all algorithms, and also the regular SPEA2+ algorithm, do not find new solutions resulting in major improvements in the last generations. The time given in this test case is enough for all algorithms to find a reasonably good performing set of solutions. Therefore, it is also of interest how the performance of the algorithms develops over the number of solutions exactly evaluated. In Figure 5 the development of the S-metric and C-metric is shown. In these figures the performance is presented dependent on the exact evaluated solutions. For the C-metric the regular SPEA2+ is used as the reference case—for example, after 500 exact evaluated solutions the SPEA2+ preevaluation FA dominates on average 59% of the solutions of regular SPEA2+ and regular SPEA2+ dominates on average 8% of the solutions of SPEA2+ preevaluation FA. The development of both performance measures shows that all three algorithms using function approximation show better results at least till 1,500 solutions are exactly evaluated. This means that with less exact evaluated solutions the algorithms using RSM methods already found good solutions. However, the algorithms are not capable of maintaining their head start. This can be explained because the quality of the surrogate model determines the quality of the decisions taken based on this surrogate model. The surrogate model does push the search in good directions at the start, but after a certain number of generations the contribution of the surrogate model in guiding the search diminishes. In addition, after some generations the quality of this surrogate model does not improve anymore, although more solutions are exactly evaluated and used as training set. The results show that when using these RSM methods, the

Table 4 Overview of performance algorithms.

	S-metric	C-metric* X′,X″	X″,X′	Spacing metric (obj)	Spacing metric (sol)
SPEA2+	2.03E+11	0.00	0.00	0.37	0.20
SPEA2+ pre evaluation FA	2.03E+11	0.19	0.10	0.36	0.20
FA seeded SPEA2+	2.00E+11	0.14	0.17	0.44	0.22
FA optimized SPEA2+	2.01E+11	0.14	0.18	0.55	0.16

*X'' is set of solutions SPEA2+.

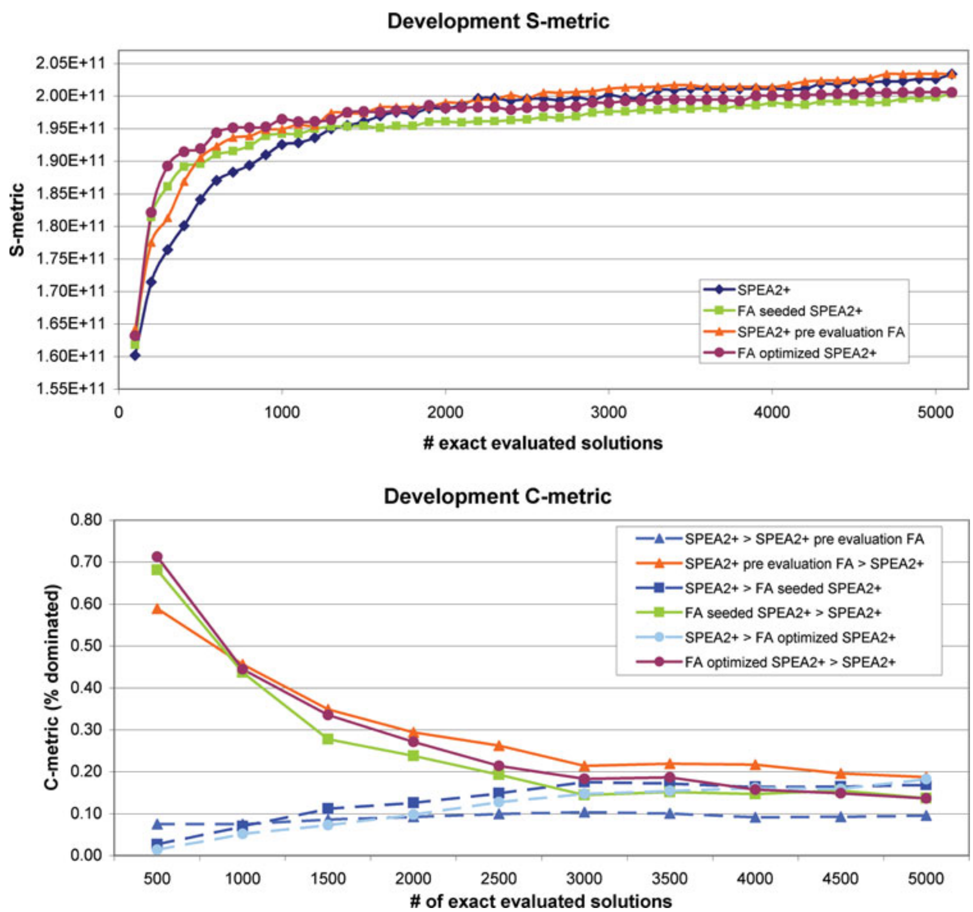

Figure 5 Development C-metric and S-metric.

optimization tends to converge more quickly, possibly to a local optimum or a less performing set of solutions. This also depends on the level of confidence in the estimated surrogate model in the various algorithms. Therefore, these methods are mainly of interest if a limited number of exact evaluations can be done or can be used as a prephase in a hybrid approach. To avoid premature convergence, two algorithms proceed with regular SPEA2+ in which the FA seeded SPEA2+ has difficulties to find further improvements, whereas the SPEA2+ preevaluation FA performs at least similarly in these generations to the regular SPEA2+ algorithm. This results in a slightly better performance of the SPEA2+ preevaluation FA than the regular SPEA2+ algorithm after the final generation.

CONCLUSIONS AND FURTHER RESEARCH

DTM measures are traditionally used to optimize efficiency, but can also be used to optimize externalities, which are objectives that can no longer be neglected. These DTM measures can be used on a strategic level to influence a transport system optimizing the objectives over the long term. This optimization problem can be formulated as the dynamic MO-NDP in which DTM measures are used to influence supply of infrastructure and efficiency and externalities are the objectives. The dynamic MO-NDP is solved as a bilevel optimization problem in which in the upper level the objectives concerning efficiency and externalities are optimized and in the lower level the road users optimize their own objectives (i.e., minimizing travel times). Solving this dynamic MO-NDP is challenging to solve and computationally expensive because it requires the use of heuristics and a DTA model. A possible solution for accelerating the search is combining function approximation methods with heuristics. In this research three different algorithms using RSM in combination with the SPEA2+ are compared with regular SPEA2+ to determine whether these are viable. The algorithms proposed are especially of interest for larger real-scale networks, because in that case solving the lower level optimization (i.e., application of DTA model) needs large computation times. Being able to reduce the number of exact evaluations can result in significantly lower computation times. However, the number of decision variables influences the possibilities because the training set needs to be large enough to estimate the surrogate model. Further research on using these algorithms for larger networks is therefore needed.

The comparison of the algorithms shows that the use of RSM methods does find solutions in similar parts of the objective space as regular SPEA2+ and therefore does not result in missing relevant parts of the Pareto optimal set. The average performance of the algorithms after the algorithms are terminated on the performance measures is similar in that the SPEA2+ pre evaluation FA performs slightly better than regular SPEA2+. The development of the performance measures shows that the algorithms using RSM methods accelerates the search at the start considerably. With less exact evaluated solutions, already good solutions are found. However, the algorithms using these RSM methods tend to converge more quickly, possibly to a local optimum, and therefore loose their head start, because these algorithms depend largely on the quality of the surrogate model. Therefore, these methods are of interest if a limited number exact evaluations can be done and a reasonable performing set of solutions is already satisfactory or can be used as a prephase in a hybrid approach as proposed in the SPEA2+ preevaluation FA. Although the algorithms using RSM methods all used SPEA2+ as a base case, the methods can also be used for other EA as well with possibly similar advantages and deficiencies, depending of the quality of the solutions proposed by these algorithms. Further research on comparing and testing the approaches with other algorithms is therefore of interest.

Because the quality of the surrogate model is determinative for the acceleration of the search, research is needed on this subject. Further acceleration can possibly be established by incorporating further knowledge of road transport systems within the solution approach (e.g., intelligent reduction of solution space or incorporation of this knowledge into the surrogate model). Another option, not investigated here, is using neighborhood search as in Chow (2010) when the algorithm tends to converge or using other approximation methods like fitness granulation (Davarynejad et al., 2010). Finally, because the algorithms are tested on a single case, further research is needed using other and more complex networks.

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