Proceedings of the 10th International Conference on Civil Structural and Transportation Engineering (ICCSTE 2025)
July, 2025 | Imperial College London Conference Center, London, United Kingdom
Paper No. 191
DOI: 10.11159/iccste25.191

Investigation of the Applicability of Surrogate Models in Transportation Network Design Problems

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Abstract – The rapidly increasing rate of vehicle ownership causes significant transportation problems, especially in developing countries. The increase in travel costs and safety are among these issues. To solve this problem, transportation-related institutions generally plan to change the existing geometry of the roads or open alternative roads. These solutions are quite costly and time-consuming. In addition, existing conditions are not always sufficient for applying these solutions. At the same time, the results of these improvements are not known with certainty. Both travel costs and road and driving safety should be increased with these improvements. This study developed a bi-level optimization model considering these two objectives. According to the network design decisions taken in the lower-level problem of the developed bi-level model, the route choice of the transportation network users is determined by the deterministic user equilibrium assignment model. The assumptions made by Wardrop (1952) were considered in the assignment model. It has been observed that the user equilibrium conditions are ensured in the developed assignment model. The objective function of the upper-level optimization model is to minimize the expected number of accidents to increase road safety. The solution of optimization models developed to work on large-scale road networks takes quite a long time. Since the assignment problem solved in the lower-level optimization model contains continuous loops, the time spent on the solution of the model increases. Therefore, surrogate models were used to shorten this period in the study. Surrogate models can solve large-scale problems in less time by producing their data with actual data. As a result of the study, it has been determined that using surrogate models in a medium-sized network shortens the long processing time and gives the most accurate result in a short time. In this respect, surrogate models hope to obtain accurate and applicable results by conducting field studies in an entire transportation network with a short processing time.

***Keywords*:** Bi-level optimization, differential evaluation algorithm, surrogate models, transportation network design problem.

1. Introduction

Especially in developing countries, due to the increase in the rate of vehicle ownership, the existing roads cannot meet the increasing travel demand. In addition, when considering the unplanned growth, lack of adequate transportation infrastructure, increased time spent in traffic, insufficient capacity of existing roads, increasing traffic congestion and long queues, and the damage caused by all these problems to nature, decision-makers start to seek various alternatives to solve these problems. These alternatives are improving existing roads or constructing new routes for traffic.

Every road user wants to reduce travel time and reach their destinations safely. In addition, the increasing demand for transportation causes an increase in traffic accidents due to the inadequacy of the existing roads. For this reason, road safety has emerged as one of the leading transportation problems to be improved in recent years. Governments and transport agencies are willing to spend large sums on improving roads, reducing accidents and travel times, and eliminating congestion. Road safety may be affected in projects developed with congestion concerns, and travel times may be involved in projects designed to increase road safety. Therefore, the projects to be made by the institutions related to transportation should be chosen by considering road safety and travel times [1].

A linear programming model was developed that minimizes travel delays and accident-related costs by [2]. In this model, traffic flows are assumed to be constant. The effect of candidate domains is ignored at the network level.

Optimization problems for road safety improvement projects are solved as integer or complex integer linear problems. Optimization objectives should minimize the total accidents or the costs associated with these accidents or maximize the benefits of accident reduction. There must be at least one budget constraint [1].

Harwood and others aimed for a model that maximizes the net benefit calculated by reducing travel time and accident costs [3]. Mishra and others developed a max-min model that seeks to maximize the benefit obtained by reducing the number of accidents. It maximized a minor utility in the candidate areas [6]. Pal and Sinha investigated the effects of road improvements on traffic. The model is presented as a reflection of the constant growth factors of traffic growth for the project type and each improvement area [5] Khasnabis and others developed an evaluation procedure for road safety-related improvements [6].

Yang and others considered a security objective in addition to congestion and environmental goals in solving transportation network design problems. An optimization model has been developed to determine different speed limits on road networks [7].

Studies on the solution of transportation network design problems occupy a vast area in the literature. These studies deal with road users' reactions to the decision maker's decisions. The transportation network design problem includes many elements of transportation planning but also consists of all decision-making processes, including strategic, tactical, and operational decisions [8]. In another study, strategic decisions were defined as long-term decisions about the infrastructure of transportation networks. Tactical decisions make the most efficient use of transportation infrastructure and resources, and business decisions are primarily about traffic flow, demand management, and scheduling problems [9].

The transportation network design problem has been discussed in the literature as an optimization problem in which decision-makers try to reach the most appropriate planning for the transportation system, considering the behaviour of network users [10]. Therefore, it is modelled as a bi-level problem [11]. In the bi-level model, network design decisions are at the upper level, and the reactions of the network users to these decisions are at the lower level.

This study aims to develop a bi-level optimization model to minimize the travel cost in selected candidate links, increase road safety, and find the most accurate result in the shortest time in large-scale transportation networks. In this context, the route selection was made using the traditional assignment method, and accident modification factors were calculated to increase safety. Matlab program interfaces were used in the study.

2. Bi-Level Optimization Model

Bi-level optimization models are defined as non-convex NP-hard problems [12]. For this reason, heuristic algorithms are proposed to solve such issues, which cannot be proven to converge to the optimum solution but provide acceptable near-optimal solutions at proper times [9], [13].

Bi-level problems involve two overlapping levels of optimization. These levels are called upper and lower-level problems. The lower and upper-level problems have their objectives and constraints. In parallel, two classes of decision vectors depend on the upper and lower levels. The lower-level problem is a constraint for the upper-level problem. The lower-level optimization problem is parametric. In other words, while the upper-level decision vector is evaluated as a parameter in the lower-level problem, the upper-level problem is solved according to the lower-level decision vector. The optimal solutions obtained from the lower-level problem also constitute the constraints for the upper-level problem.

An uncertainty arises for any given lower-level decision vector if multiple lower-level optimal solutions exist. In the presence of multiple lower-level optimal solutions, the optimal solution obtained from the lower level will reveal some uncertainties at the upper level. These uncertainties can be eliminated by defining different positions [14].

$$\min_{u} Z(\mathbf{s}, \mathbf{v}(\mathbf{s})) \quad (1)$$

Constraints:

$$G(\mathbf{s}, \mathbf{v}(\mathbf{s})) \le 0 \quad (2)$$

$$\min_{v} z(\mathbf{s}, \mathbf{v}) \tag{3}$$

$$\mathbf{g}(\mathbf{s}, \mathbf{v}) \leq 0 \tag{4}$$

Where z and s are the decision maker's objective function and decision vector represented by the upper-level model, respectively, and G is the upper-level decision vector constraint set. z and v are the lower-level objective function and decision variable vector, respectively, and g is the lower-level decision variable constraint set. v(s) is the reaction function for s to determine the travel flows. The bi-level network design problem aims to determine the optimum decision variable s*, optimizing the high-level objective function Z, adhering to the given constraints [12].

2.1. Upper-Level Model

In the upper-level model, the aim is to improve road safety. In order to improve road safety, the expected number of accidents on the links on the existing network should be minimized crash modification factors were determined to calculate the expected number of accidents. Crash Modification Factors (CMF) are applied to estimate the effects of the geometric designs of roads and traffic control properties. If the crash frequency for any feature is greater than the standard conditions, the CMF will be greater than 1.00; if it is less crash ratio, the CMF will be less than 1.00 [15].

The expected annual number of accidents is solved with the help of the following equation.

$$minZ_2 = \sum_a N'_a \tag{5}$$

Here, N'_a appears as the expected number of accidents in the link a. If the expected accident number is shown as N''_a in a link designed under standard conditions, the formula for the expected accident number is given below.

$$N''_a = N'_a \times C_R \times \prod_{i=1}^{n^c_{t_a}} C_{a,i}(P_a) \tag{6}$$

Therefore, in the light of the information given, the safety objective function is below.

$$minZ_2 = \sum_{a \in A} N'_a \times C_R \times \prod_{i=1}^{n^c_{t_a}} C_{a,i}(P_a) \tag{7}$$

2.2. Lower-Level Model

The lower-level model in this study aims to minimize the travel cost. Therefore, a deterministic user equilibrium assignment has been made to solve the traffic assignment problem. An implementation of the Fank-Wolfe algorithm has been created. Beckman and others defined user equilibrium as an equivalent minimization problem [16]. However, link costs are considered to be dependent on link flows. The literature's most widely used cost function is the Bureau of Public Roads (BPR). Because the BPR cost function is a simple and powerful function representing real traffic network flows [17].

$$t_a = t_{0,a}\left[1 + \alpha_a (\frac{x_a}{C_a})^{\beta_a}\right] \tag{8}$$

Here, $t_{0,a}$ a is a link free flow travel time, xa is a link flow, K_a is link practical capacity. α and β are model parameters and take the values of 0.15 and 4, respectively. Based on this information, the objective function for the lower-level model is as follows. According to the network design decisions, the average travel cost will be calculated by traffic assignment.

$$minZ_1 = \frac{\sum_{a \in A} x_a \times t_a}{\sum_{w \in W} d_w} \tag{9}$$

Here, W represents the set of Origin-Destination (OD) pairs, d_w is the travel demand between w OD pair, x_a is the traffic flow through link a, and t_a is the trip cost on link a. In this study, two different surrogate models that give the expected annual number of accidents and average travel cost values for different values of t0 and c parameters of the candidate links for which design decisions will be made are used. AADT values are among the CMF parameters used to determine the annual number of accidents. Travel costs and network user travel preferences are affected by the decisions made.

3. Surrogate Models

Surrogate models are metamodels or surface models used instead of expensive simulation models during optimization [18]. A model is constructed based on the original problem's response to a limited number of smartly chosen data points. In surrogate models, there is no need to know the internal behavior of the problem. Only the input/output behavior related to the problem is essential. These models produce simpler surrogates that capture the relationships between input and output variables independent of the underlying process [19].

Surrogate models are created using data from models faithful to the original. New designs or solving a complex problem provide the desired result and model constraints to be reached in a much shorter time. Therefore, it makes it possible to obtain more precise results in such studies and optimize the solution of more complex problems in a shorter time [20]. Surrogate models and representation-based optimization are used in solving problems such as aerodynamic systems, design of aerodynamic structures, and propulsion engines. Today, it has started to be used in costly and time-consuming issues, such as designing and improving large-scale transportation networks. Surrogate models are used in optimization models, reducing long-cycle costs.

Recently, surrogate models have been used in transportation network design problems. It has been used in microscopic simulations and design tolling schemes, traffic management, and road expansion projects of transportation network design [21]-[29].

Surrogate models are also using to solve some transportation problems. Liu and Meidani proposed a data-driven neural network surrogate model to predict the drag force of the truck platoon system. They aim to generalize to truck platoons of various configurations and evaluate fuel consumption reduction of truck platoons using surrogate models [30]. Li and others examined bridges in traffic networks under earthquake conditions using surrogate models as simulation-free. They aimed to benefit the rapidity of surrogate models in traffic networks [31]. Yuan and others proposed a novel deep learning-based surrogate modeling method, leveraging the strength of edge-conditioned convolutional networks (EECNs) and deep belief networks (DBNs) in traffic networks [32].

This study used the most commonly used surrogate models in the literature on a medium-sized network. Surrogate models with the best results have been identified. The results from the bi-level model were compared with those obtained from the surrogate models.

4. Structure of Surrogate Models

The construction of surrogate models consists of four stages. When creating a surrogate model, the design of the experiments in which the data can be modelled is created first. The design of experiments involves using strategies for segregated samples within the design space. The choice to be made depends on the number of samples. In addition, this modelling technique will be used to create a new surrogate model. Although surrogate models usually use explicit formulas, they are calculated with a particular minimization problem. Each input variable in the input space is not random and has its own value. Therefore, surrogate models can be easily used in various problems. In the second stage, numerical simulations are made in the selected regions. Here, computationally expensive models are run for all values of the input variables determined in the design method of the experiments mentioned in the previous step. The model and parameters that best represent the problem are found in the third stage. In the last step, after the surrogate model is selected, the surrogate model is trained using the available data, and the results are evaluated [20].

4.1. Types of Surrogate Models

Various types of surrogate models are in the literature, and they have a wide range of applications. Interpolating models such as Kriging and radial basis function and polynomial regression models, which are non-interpolating, are among the models in the literature [33],[34].

4.1.1. Polynomial Regression Models

The response surface method uses statistical techniques for regression and analysis of variance to obtain the minimum variance of responses. The simplicity of polynomials makes them a good approximation for approximating most polynomial response surfaces. At this point, the essential step is to define the initial model. This model is constructed as an ordered regression. The second step is to update the iterative estimate according to the result of the previous iteration and continue this process according to the stopping criterion. The third step is to reach the maximum number of steps achieved in the loop [19].

4.1.2. Kriging Model

The response surface method, called Kriging, is a spatial estimation method belonging to the geostatistical methods group. It is based on minimizing the mean squared error and defines the spatial and temporal correlation between the model values [19]. It is a compact and inexpensive evaluation process [35]. To its nature, longer times are required for the Kriging method in problem-solving. However, this situation is compensated by the accuracy of the obtained a surrogate [36].

4.1.3. Support Vector Machine Model (SVM)

SVM is a set of related controlled learning methods that analyse data and recognize patterns [37]. It is inspired by statistical learning theory. SVM maps its inputs to a larger area; however, cross-products can be easily computed for variables in the original space, making the computational burden reasonable. Cross products in larger spaces are defined as kernel functions that can be selected by the problem [19].

5. Comparison of Surrogate Models and Results

It has been mentioned above that bi-level optimization models can solve transportation network design problems. The lower-level problem of the bi-level model is generally considered the assignment problem. While the lower-level problem is solved by traffic assignment, it creates many iterative loops. Therefore, this optimization takes much time, especially in large networks. This study used surrogate models trained at the lower level instead of the assignment problem.

On the other hand, surrogate models enable these long processes to be done in a shorter time. Therefore, surrogate models are used in this study. Five thousand data were created to solve the assignment problem. Surrogate models are trained with this generated data. The trained surrogate model is included in the optimization as a low-level model. The results obtained after the created bi-level optimization model were trained with surrogate models. The Kriging model and SVM are used for training. There are three different types of SVM. This study considers the results of the SVM-Quadratic model with the smallest RMSE value. This value allows us to predict the model's performance by training on new data. A low RMSE value indicates the model's accuracy.

The surrogate models calculate the time to solve this problem in minutes or even seconds. The results obtained from the selected surrogate models are given in Table 1. An assignment with the Kriging and Support Vector Machine model is completed in 0,071 and 0.0036 seconds, respectively. The duration of an assignment made without using surrogate models was determined as 2.33 minutes.

The dataset was completed in 6.02 minutes with Krigging and in 18 seconds with Support Vector Machines, one of the surrogate models. About five hours are required to calculate the selected network's assignment and safety-related parts. The assignment used at the lower level takes a long time, especially in large-scale networks and bi-level models used to solve transportation network design problems.

Table 1: Results of Surrogate Models

Surrogate Model	Travel Obj. Func.		Safety Obj. Func.	
	R squared	RMSE	R squared	RMSE
SVM-Quadratic	0,98	580,75	0,91	60,205
SVM-Cubic	0,98	605,82	0,91	63,786
SVM- Linear	0,98	808,95	0,91	67,352
Kriging	1	315,04	0,92	58,246

These models are used instead of low-level assignment, significantly reducing this time. Kriging and Support Vector Machine models gave the best results among the surrogate models used in the interfaces. Among these two models, the Krigging model provided the most accurate result. The travel time and expected accident number values for the Kriging model that gives the best results are given in Table 2.

Table 2: Comparison of Real Data and Kriging Model

%Error	Krigging Model	Total Travel Cost (veh/sec)	Expected Crash Number (Crash/year)	Krigging Model	%Error
1,00	119630,00	119590,00	4503	4575	1,59
1,00	115580,00	115550,00	4992	5066	1,01
1,00	119310,00	119160,00	4906	4862	0,99
0,99	113270,00	113480,00	4821	4806	0,99
0,99	114970,00	115000,00	4655	4653	0,99

The model output is given in Figure 1 for the trip cost. The R2 value of the Krigging model is 1.00. The estimation rate is about 4500 obs/second. The training time for 5000 data is 859.24 seconds. The RMSE value for the model was found to be 315.04. The MAE value was found to be 247.54. This value should always be positive and less than the RMSE value, which gives the mean exact error.

Figure 1 shows the graphs of the Kriging model for the travel objective function. As a result of the study, the Kriging model with the most extended training period gave the most accurate results. In this respect, this model eliminates its disadvantage in terms of time.

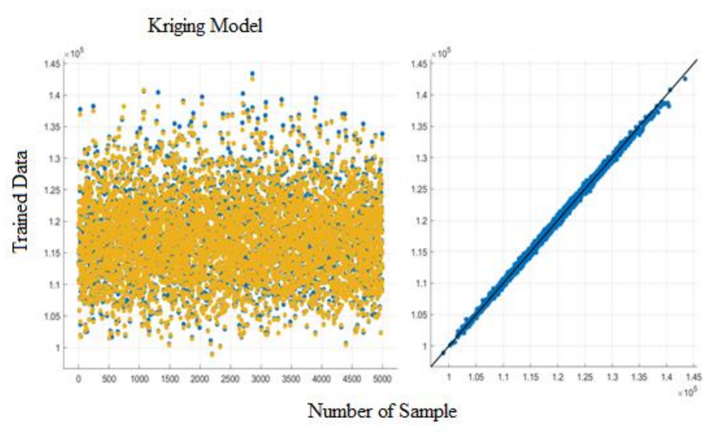

Fig.1: Kriging Model for Travel Objective Function

The R2 value of the Kriging Model for the safety objective function was found to be 0.92. Its RMSE value is 58.246. The training time of the model for 5000 training data is approximately 21.5 seconds. Training outputs for the expected number of accidents are given in Figure 2.

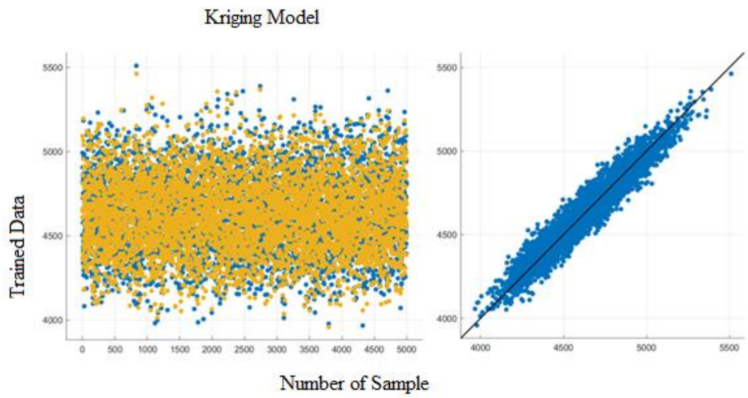

Fig.2: Kriging Model for Safety Objective Function

Using the assignment and expected accident numbers, the results were trained with the help of surrogate models. It has been determined that the assignment problem solved with surrogate models is 136 times faster than the assignment problem solved without using the surrogate models. However, it was observed that the error between the actual data and the data trained with the help of surrogate models did not exceed 1%. Heuristic methods are needed in optimizations made with surrogate models. Therefore, the differential improvement algorithm was used in the study. In the lower level of the bi-level model, unlike traditional methods, surrogate models trained with assignment data are used instead of the trip assignment model, and surrogate models trained with expected accident numbers are used instead of the safety objective function.

6. Conclusions

The study investigated the applicability of surrogate models in bi-level models used in transportation network design problems. The results of the literature's three most commonly used surrogate models were evaluated. The study investigated the applicability of surrogate models in bi-level models used in transportation network design problems. The results of the literature's three most commonly used surrogate models were evaluated.

A large part of the processing time in bi-level optimization models creates continuously repeated sublevel assignment models. When using simulation models, it is impossible to complete optimization models in large and real-scale networks, which require a long processing time at the lower level. Considering this problem, surrogate models should be used to shorten the processing time, especially in large-scale road networks. Surrogate models can be trained with real values in complex engineering problems, reducing computation time. Therefore, these models can calculate objective function values accurately in short processing times. Considering that the use of surrogate models in the solution of transportation network design problems is not very common and the advantages mentioned above are taken into account, two surrogate models in the literature are used in this study.

The study investigated Kriging, support vector machine, and polynomial regression surrogate models. All of the models gave perfect results. It has been observed that the Kriging model lags behind other models regarding computation time. Therefore, the disadvantage of this model in terms of time can be ignored. However, the most accurate results were obtained from this model.

As a result of the study, it has been determined that using surrogate models in a medium-sized network shortens the long processing time and gives the most accurate result in a short time. In this respect, surrogate models hope to obtain accurate and applicable results by conducting field studies in a real transportation network with a short processing time. Future field studies are planned to solve the transportation design problem of surrogate models in a real network.

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