A computationally efficient simulation-based optimization algorithm for large-scale urban transportation problems

Carolina Osorio, Linsen Chong
Civil and Environmental Engineering Department, Massachusetts Institute of Technology, Office 1-232, Cambridge, Massachusetts 02139, USA, osorioc@mit.edu, linsenc@mit.edu,

This paper proposes a computationally efficient simulation-based optimization (SO) algorithm suitable to address large-scale generally constrained urban transportation problems. The algorithm is based on a novel metamodel formulation. We embed the metamodel within a derivative-free trust region algorithm and evaluate the performance of this SO approach considering tight computational budgets. We address a network-wide traffic signal control problem using a calibrated microscopic simulation model of evening peak period traffic of the full city of Lausanne (Switzerland), which consists of more than 600 links and 200 intersections. We control 99 signal phases of 17 intersections distributed throughout the entire network. This SO problem is a high-dimensional nonlinear constrained problem. It is considered large-scale and complex in the fields of derivative-free optimization, traffic signal optimization and simulation-based optimization. We compare the performance of the proposed metamodel method to that of a traditional metamodel method and that of a widely used commercial signal control software. The proposed method systematically and efficiently identifies signal plans with improved average city-wide travel times.

Key words: simulation-based optimization, metamodel, large-scale urban transportation problems

1. Introduction

The massive amount and variety of mobility data that can now be collected through, for instance, ubiquitous mobile devices, is enhancing our fundamental understanding of individual mobility. For instance, it improves our understanding of the intricate behavior of travelers, e.g., how they make activity and thereby travel decisions, and how these decisions are motivated by an underlying objective to enhance their well-being.

State-of-the-art microscopic traffic simulation models embed such disaggregate models of traveler behavior (e.g., departure time choice, multi-modal route choice, access and response to en-route traffic information), and account for behavior heterogeneity. They represent individual vehicles, and can therefore be coupled with vehicle-specific simulators (e.g., propulsion simulators) to yield detailed estimates of the performance of vehicles (e.g., energy consumption or emissions estimates) in networks with complex topologies and complex traffic dynamics. Additionally, microscopic simulators provide a detailed representation of the underlying supply (e.g., variable message signs, public transport priorities).

Microscopic traffic simulators describe in detail the interactions between (i) vehicle performance, (ii) traveler behavior and (iii) the underlying transportation infrastructure, and yield an elaborate description of traffic dynamics in urban networks. They are therefore suitable tools to address transportation problems where a detailed representation of either of these three components should be accounted for.

Microscopic simulators are popular tools used in practice to evaluate the performance of a set of predetermined transportation strategies. Cities such as Toronto, New York, Boston, Stockholm and Hong Kong have used these tools to inform their planning and operations decisions (Traffic Technology International 2012a,b, Papayannoulis et al. 2011, Toledo et al. 2003, Hasan 1999).

For a given strategy, these simulators can provide accurate and detailed performance estimates. Their use is mostly limited to what-if analysis (also called scenario-based analysis) or sensitivity analysis. That is, they are used to evaluate the performance of a set of predetermined transportation alternatives (e.g., traffic management or network design alternatives), such as in Bullock et al. (2004), Ben-Akiva et al. (2003), Hasan et al. (2002), Stallard and Owen (1998),Gartner and Hou (1992) and Rathi and Lieberman (1989). See further references in Ben-Akiva et al. (2003).

The numerous models of disaggregate traveler behavior, vehicle-performance and supply components lead to detailed performance estimates, yet also to models which are expensive to develop and calibrate, and computationally expensive to evaluate. Thus, an accurate estimation of performance is computationally costly to obtain. Additionally, these

simulators derive stochastic nonlinear, and typically nonconvex, performance measures with no closed-form available. For these reasons, the use of these simulators to address optimization problems is a challenge.

Currently, the use of these simulation tools is mostly limited to what-if analysis. With the ubiquity of access to real-time traffic information, and the increasing number of prevailing and interacting traffic control strategies, traffic dynamics of congested networks are becoming more and more intricate. Thus, determining a priori a set of alternatives with good local and network-wide performance is no longer feasible. Thus, there is a need to embed these detailed simulators within optimization frameworks in order to systematically identify alternatives with improved local and network-wide performance. Additionally, given the high cost of developing large-scale simulation tools, transportation projects would benefit from computationally efficient methods that allow the use of simulators to go beyond a what-if analysis.

This paper proposes a simulation-based optimization (SO) method that allows large-scale urban transportation problems to be addressed with detailed microscopic traffic simulators. We focus on problems where the objective function is derived from the simulator and, thus, no closed-form analytical expression is available. The problems have general (e.g., nonconvex) constraints. Closed-form analytical and differentiable expressions are available for all constraints (i.e., the constraints are not simulation-based).

These urban transportation problems can be formulated as:

$$\min_{x\in\Omega} f(x,z;p) \equiv E[F(x,z;p)], \tag{1}$$

where the purpose is to minimize the expected value of a given stochastic performance measure F, x denotes the deterministic continuous decision vector, z denotes other endogenous variables, and p denotes the deterministic exogenous parameters. For instance, in this paper we use the proposed SO approach to solve a traffic signal control problem where F denotes trip travel time, x represents the green times of the signal phases, z accounts, for instance, for signalized link capacities, route choice decisions, and p accounts, for instance, for the network topology, the total traffic demand, and fixed lane attributes (e.g., length, grade, maximum speed). The feasible space Ω consists of a set of general, typically nonconvex, deterministic, analytical and differentiable constraints.

This paper proposes a technique that can efficiently address generally constrained large-scale simulation-based urban transportation problems. The performance of the technique is evaluated by considering a network-wide traffic signal control problem. This problem is considered large-scale and complex for derivative-free algorithms, signal control algorithms and simulation-based optimization algorithms.

Additionally, the paper focuses on SO techniques with good short-term performance, i.e., computationally efficient methods that can identify alternatives with improved performance within a tight computational budget. The computational budget can be defined as a limited number of simulation runs or a limited simulation run time. Such techniques respond to the needs of transportation practitioners by allowing them to address problems in a practical manner.

We present a review of past work in this field in Section 2. In Section 3 of this paper, we present the methodology. We then present the traffic signal control problem which is used to evaluate the scalability and short-term performance of this approach (Section 4). Empirical results are detailed in Section 5, followed by conclusions (Section 6).

2. Literature Review

Few SO methods that embed microscopic simulators have been developed (Li et al. 2010, Stevanovic et al. 2008, Branke et al. 2007, Yun and Park 2006, Hale 2005, Joshi et al. 1995). The most common approach is the use of heuristic algorithms and, in particular, the use of genetic algorithms (see Yun and Park (2006) for a review). These methods embed microscopic simulators within general-purpose optimization algorithms. They treat the simulator as a black-box, using no a priori structural information about the underlying transportation problem (e.g., network structure). They therefore require a large number of simulated observations in order to identify transportation strategies (i.e., trial points) with improved performance.

This paper proposes an SO technique with good short-term performance suitable for microscopic traffic simulators to be used to address complex high-dimensional problems. In order to derive computationally efficient methods that embed inefficient simulators, information from other more efficient (i.e., tractable) models that provide analytical structural information to the algorithm should be used throughout the optimization process.

In general, methods to address SO problems can be classified as direct-search methods, stochastic gradient methods and metamodel methods. For reviews of SO methods see Hachicha et al. (2010), Barton and Meckesheimer (2006), Fu et al. (2005). This paper focuses on metamodel methods. For a description of why metamodel techniques are a suitable approach to address complex simulation-based transportation problems, see Osorio and Bierlaire (forthcoming).

Metamodel methods build an analytical approximation of the simulation-based components of the optimization problem (e.g., objective function, constraints). In this paper,

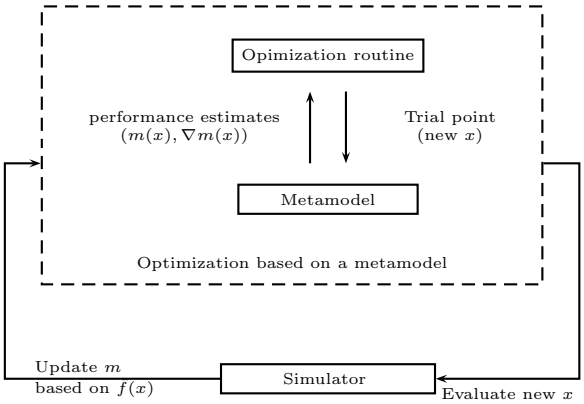


Figure 1 Metamodel simulation-based optimization methods. Adapted from Alexandrov et al. (1999).

the objective function is simulation-based. Thus, the metamodel provides an analytical approximation of the objective function. By resorting to a metamodel approach, the stochastic response of the simulation is replaced by an analytical response function (the metamodel), such that deterministic optimization techniques can be used. Metamodel techniques use an indirect-gradient approach, i.e., they compute the gradient of the metamodel, which is a deterministic function. Thus, traditional deterministic gradient-based optimization algorithms for generally constrained problems can be used.

Metamodel SO methods are iterative methods based on two main steps depicted in Figure 1 (for more details see Osorio and Bierlaire (forthcoming)). Step 1 fits the metamodel based on the current sample of simulated observations. Step 2 uses the fitted metamodel to perform optimization and derive a trial point (e.g., a suitable traffic management or network design alternative). The performance of the trial point is then evaluated by the simulator, which leads to new observations. As new observations become available, the metamodel is fitted again (step 1) leading to more accurate metamodels and ultimately to trial points with improved performance (step 2).

Reviews of metamodels are given by Conn et al. (2009b), Barton and Meckesheimer (2006) and Søndergaard (2003). Metamodels can be classified as either physical or functional metamodels (Søndergaard 2003). Physical metamodels are application or problem-specific metamodels. Their functional form and parameters have a physical interpretation. Functional metamodels are general-purpose (i.e., generic) functions chosen based on their analytical tractability. The most common general-purpose metamodel is the use of low-order polynomials, and particularly of quadratic polynomials (Conn et al. 2009b, Kleijnen 2008, Marti 2008). Other general-purpose metamodels include spline models, radial basis functions and Kriging models (Kleijnen et al. 2010, Wild et al. 2008, Barton and Meckesheimer 2006).

The existing metamodels consist of either physical or functional components. Recent work has proposed a metamodel that is a combination of a functional and a physical metamodel (Osorio and Bierlaire forthcoming). The functional component ensures asymptotic metamodel properties necessary for convergence analysis (such as full linearity (Conn et al. 2009a)). The physical component is an analytical and differentiable macroscopic traffic model. It provides a problem-specific analytical approximation of the objective function, unlike the generic approximation provided by the functional component. The physical component therefore yields structural information about the problem at hand, which enables the identification of well performing alternatives (i.e., trial points) with very small samples (i.e., good short-term algorithmic performance). The physical component used here is an analytical differentiable queueing network model. This macroscopic traffic model is less detailed and accurate than the simulator, yet is computationally efficient to evaluate.

This combined use of functional and physical metamodels allows information from the detailed, yet inefficient, microscopic simulator to be combined with analytical information from a more efficient macroscopic model. This leads to an algorithm with a good detail-tractability trade-off and good short-term performance.

This physical and functional metamodel approach has been used to efficiently address complex urban transportation problems, such as signal control problems that account for detailed (also called microscopic) vehicle-specific energy consumption patterns (Osorio and Nanduri 2012), emissions patterns (Osorio and Nanduri 2013), and reliable signal control problems that used detailed full distributional travel time estimates provided by the simulator to improve both average travel times and travel time reliability (Chen et al. 2012).

This approach has been successfully used to control networks with approximately 50 roads, yet is not suitable to address problems for much larger scale networks. This paper builds upon this existing metamodel SO technique (hereafter referred to as the *initial* method), and proposes a metamodel that can efficiently address high-dimensional simulation-based problems.

3. Methodology

3.1. Metamodel functional form

Recall the general form of the urban transportation problems that we address (Equation (1)). Since there is no closed-form available for the objective function, f, we use a metamodel to approximate it. The functional form of the metamodel used in this paper

is that proposed by Osorio and Bierlaire (forthcoming). It combines a physical and a functional component. Its functional form is given by:

$$m(x, y; \alpha, \beta, q) = \alpha T(x, y; q) + \phi(x; \beta), \tag{2}$$

where ϕ (the functional component) is a quadratic polynomial in x with diagonal second-derivative matrix, T (the physical component) represents the approximation of the objective function proposed by the analytical macroscopic traffic model, y are endogenous macroscopic model variables (e.g., queue length distributions), q are exogenous macroscopic parameters (e.g., total demand), α and β are parameters of the metamodel. The metamodel m can be interpreted as a macroscopic approximation of the objective function provided by T, which is corrected parametrically by both a scaling factor α and a separable error term $\phi(x; \beta)$. For details regarding the choice of this functional form, we refer the reader to Osorio and Bierlaire (forthcoming).

In this paper, we use the same functional component as in Osorio and Bierlaire (forthcoming) (i.e., the quadratic polynomial ϕ). We propose a novel scalable physical component. In Section 3.2 we recall the formulation of the physical component of the initial metamodel and describe its limitations. We then present the new formulation of the physical component in Section 3.3.

3.2. Initial queueing network model

The physical component of the initial metamodel is an urban traffic model based on queueing network theory. It combines ideas from existing traffic models, various national urban transportation norms, and queueing models. The detailed formulation of the model is given in Osorio and Bierlaire (2009b) (which is based on the more general queueing network model of Osorio and Bierlaire (2009a)). We outline here the main ideas of its formulation.

Each lane of an urban road network is modeled as a queue (and in some cases as a set of queues). In order to account for the limited physical space that a queue of vehicles may occupy we resort to *finite capacity queueing theory*, where there is a finite upper bound on the length of each queue. Each lane is modeled as a finite capacity M/M/1/k queue. The network model analytically approximates the queue interactions among adjacent lanes. Congestion and spillbacks are modeled by what is known in queueing theory as *blocking*. This occurs when a queue is full, and thus blocks arrivals from upstream queues at their current location. This blocking process is described by endogenous variables such as blocking probabilities and unblocking rates. The model consists of a set of nonlinear equations that capture these between-queue interactions.

In the following notation the index i refers to a given queue.

γ_i	external arrival rate;
λ_i	total arrival rate;
μ_i	service rate;
$\tilde{\mu}_i$	unblocking rate;
μ_i^{eff}	effective service rate (accounts for both service and eventual blocking);
ρ_i	traffic intensity;
P_i^f	probability of being blocked at queue i;
k_i	upper bound of the queue length;
N_i	total number of vehicles in queue i;
$P(N_i = k_i)$	probability of queue i being full, also known as the blocking or spillback probability;
p_{ij}	transition probability from queue i to queue j;
$\mathscr{D}_i$	set of downstream queues of queue i.

The queueing network model is formulated as follows.

$$
\begin{cases}
\lambda_i = \gamma_i + \dfrac{\sum_j p_{ji}\lambda_j(1 - P(N_j = k_j))}{(1 - P(N_i = k_i))}, & \text{(3a)} \\
\dfrac{1}{\tilde{\mu}_i} = \displaystyle\sum_{j \in \mathscr{D}_i} \frac{\lambda_j(1 - P(N_j = k_j))}{\lambda_i(1 - P(N_i = k_i))\mu_j^{\text{eff}}}, & \text{(3b)} \\
\dfrac{1}{\mu_i^{\text{eff}}} = \dfrac{1}{\mu_i} + P_i^f \dfrac{1}{\tilde{\mu}_i}, & \text{(3c)} \\
P(N_i = k_i) = \dfrac{1 - \rho_i}{1 - \rho_i^{k_i+1}}\rho_i^{k_i}, & \text{(3d)} \\
P_i^f = \displaystyle\sum_j p_{ij} P(N_j = k_j), & \text{(3e)} \\
\rho_i = \dfrac{\lambda_i}{\mu_i^{\text{eff}}}. & \text{(3f)}
\end{cases}
$$

Equation (3a) is a flow conservation equation, it relates flow transmission between upstream and downstream queues. The factor $(1 - P(N_i = k_i))$ represents the probability that queue i is not full (i.e., the queue can receive flow from its upstream queues). If the queue is full, it cannot receive flow from upstream queues, which may lead to spillbacks. Equation (3b) defines the rate at which spillbacks at queue i dissipate, $\tilde{\mu}_i$. Equation (3c) defines the rate at which queue i dissipates accounting for both spillback and non-spillback states, μ_i^{eff}. It is defined as a function of the service rate of the queue, μ_i. The latter is determined by combining ideas from national transportation norms, and is a function, for instance, of the free flow capacity of the underlying lane. Equation (3d) defines the probability that a queue is full, i.e., the spillback probability of the underlying lane. This expression is derived from finite capacity queueing theory (Bocharov et al. 2004). Equation (3e) defines the probability of a vehicle being blocked while at queue i, i.e., the probability that a vehicle at the underlying lane is affected by spillback from a downstream lane. Equation (3f) defines the traffic intensity of a queue, it is also derived from traditional finite capacity queueing formulae.

In this model, the exogenous parameters of a given queue are γ_i, μ_i, p_{ij} and k_i. All other parameters are endogenous. When used to solve a signal control problem, the flow capacity of the signalized lanes become endogenous, which makes the corresponding service rates, μ_i, endogenous. In that case, the exogenous parameters are γ_i, p_{ij} and k_i. This is a stationary model with exogenous traffic assignment (the turning probabilities p_{ij} are exogenous). As described in Section 6, analytical tractable formulations that describe both traffic dynamics and endogenous assignment are being developed as part of ongoing work.

As described in Section 2, this model has been used to solve signal control problems for medium-scale networks. However, it is not sufficiently tractable to address large-scale network problems. For instance, in the case of the Lausanne city network (with over 600 links and 200 intersections), the time needed by a standard nonlinear optimization algorithm to solve the trust region (TR) subproblem (detailed in Section 4.2) exceeds 20 minutes. Since this TR subproblem is solved at every iteration of the SO algorithm, it is critical to solve it efficiently.

In this paper, we propose a more tractable and scalable physical component of the metamodel. It is an approximation of this initial queueing network model. It consists of a simple system of one linear and two nonlinear equations. In particular, as is detailed in Section 5.2, the TR subproblem is now solved on average within less than 2 minutes. This significantly enhances the computational efficiency of the SO algorithm, and allows to efficiently address more complex high-dimensional constrained transportation problems.

3.3. Highly-tractable queueing network model

We introduce the following two variables:

$$\begin{array}{ll} \lambda_i^{\text{eff}} & \text{effective arrival rate;} \\ \rho_i^{\text{eff}} & \text{effective traffic intensity.} \end{array}$$

These two new variables are defined by:

$$\lambda_i^{\text{eff}} = \lambda_i(1 - P(N_i = k_i)) \tag{4}$$

$$\rho_i^{\text{eff}} = \frac{\lambda_i^{\text{eff}}}{\mu_i^{\text{eff}}}. \tag{5}$$

The highly tractable queueing network model is given by:

$$\begin{cases} \lambda_i^{\text{eff}} = \gamma_i(1 - P(N_i = k_i)) + \sum_j p_{ji}\lambda_j^{\text{eff}} & \text{(6a)} \\ \rho_i^{\text{eff}} = \dfrac{\lambda_i^{\text{eff}}}{\mu_i} + \left(\sum_{j \in \mathscr{D}_i} p_{ij} P(N_j = k_j)\right)\left(\sum_{j \in \mathscr{D}_i} \rho_j^{\text{eff}}\right) & \text{(6b)} \\ P(N_i = k_i) = \dfrac{1 - \rho_i^{\text{eff}}}{1 - (\rho_i^{\text{eff}})^{k_i+1}}(\rho_i^{\text{eff}})^{k_i}. & \text{(6c)} \end{cases}$$

Equation (6a) is obtained directly by inserting Equation (4) into Equation (3a). Equation (6b) is obtained as follows. Multiply Equation (3b) and (3c), respectively, by λ_i^{eff} to obtain:

$$\frac{\lambda_i^{\text{eff}}}{\tilde{\mu}_i} = \sum_{j \in \mathscr{D}_i} \frac{\lambda_j^{\text{eff}}}{\mu_j^{\text{eff}}}, \tag{7}$$

$$\rho_i^{\text{eff}} = \frac{\lambda_i^{\text{eff}}}{\mu_i} + P_i^f \frac{\lambda_i^{\text{eff}}}{\tilde{\mu}_i}. \tag{8}$$

Insert Equation (7) into (8) to obtain:

$$\rho_i^{\text{eff}} = \frac{\lambda_i^{\text{eff}}}{\mu_i} + P_i^f \Big(\sum_{j \in \mathscr{D}_i} \rho_j^{\text{eff}}\Big). \tag{9}$$

Insert the expression of P_i^f given by Equation (3e), and Equation (6b) results.

Equation (6c) is an approximation of Equation (3d) which is obtained by replacing the traffic intensity ρ, by the effective traffic intensity ρ^{eff}. That is, we use the expression of the blocking probability of a finite capacity queue, yet approximate the traffic intensity with the effective traffic intensity.

Equation (5) defines ρ^{eff} and shows that it may underestimate ρ. For queues with light traffic, we have $\rho^{\text{eff}} \approx \rho$, and the two models will yield similar network performance estimates. For congested links, the scalable approximation may underestimate link congestion.

The proposed model consists of three endogenous variables per queue ($\lambda_i^{\text{eff}}, \rho_i^{\text{eff}}, P(N_i = k_i)$). When using this model to address signal control problems, μ_i also becomes endogenous. This model is defined by one linear and two nonlinear equations. This formulation results in increased computational efficiency, enabling us to address a full city-scale microscopic simulation-based optimization problem.

3.4. Example of functional form of T

As described in Section 2, one of the advantages of using a physical component in the metamodel is to have problem-specific approximations of the objective function. In this section, we give an example of the functional form of the analytical approximation of the objective function provided by the queueing model, $T(x, y; q)$. In Section 4, we address a signal control problem, where the objective is to minimize the expected trip travel time. The queueing approximation of this expectation is obtained by applying Little's law (Little 2011, 1961) to the entire network. It is given by:

$$\frac{\sum_i E[N_i]}{\sum_i \gamma_i (1 - P(N_i = k_i))}, \tag{10}$$

where $E[N_i]$ represents the expected number of vehicles in lane i, γ_i is the rate of vehicles entering the network via lane i (i.e., the external arrival rate), and $P(N_i = k_i)$ is the

probability that lane i is full (i.e., spillback or blocking probability). The numerator of Equation (10) represents the expected number of vehicles in the network, whereas the denominator represents the effective arrival rate to the network. Their ratio yields the expected time in the network.

The expected number of vehicles on lane i, $E[N_i]$, is given by:

$$E[N_i] = \rho_i \left(\frac{1}{1-\rho_i} - \frac{(k_i+1)\rho_i^{k_i}}{1-\rho_i^{k_i+1}} \right). \tag{11}$$

This expression is derived in Appendix A. In the scalable model proposed in this paper, ρ_i is approximated by ρ_i^{eff} in Equation (11).

3.5. SO algorithm

The SO algorithm used in this paper is that of Osorio and Bierlaire (forthcoming). It is given in Appendix B. It is based on the derivative-free trust region (TR) algorithm proposed by Conn et al. (2009a). For an introduction to trust region (TR) methods, we refer the reader to Conn et al. (2000). They summarize the main steps of a TR method in the *Basic trust region algorithm*. The derivative-free method proposed by Conn et al. (2009a) builds upon the *Basic trust region algorithm* by adding two additional steps: a model improvement step and a criticality step. This algorithm allows for arbitrary metamodels to be used and, unlike traditional TR algorithms, it makes no assumptions on how these metamodels are fitted (interpolation or regression). It is therefore particularly appealing for the simulation-based context where derivatives are costly to estimate and where metamodels fitted via regression are more suitable than their interpolated versions.

At a given iteration k of the SO algorithm, it solves a trust region subproblem and approximates the objective function by the current metamodel m_k (defined in Equation (2)). The metamodel parameters (α_k and β_k) are fitted via regression based on the simulated observations collected so far. For a detailed description of the algorithm, see Osorio and Bierlaire (forthcoming).

4. Traffic signal control problem

This methodology is suitable to address a variety of simulation-based urban transportation optimization problems. In this section, we evaluate the performance of the methodology by considering a large-scale network-wide traffic signal control problem.

4.1. Problem formulation

A detailed review of traffic signal control formulations is given in Appendix A of Osorio (2010). In this paper, we consider a fixed-time strategy. Fixed-time (also called time of day or pre-timed) strategies are pre-determined based on historical traffic patterns. They yield

one traffic signal setting for the considered time of day. The traffic signal optimization problem is solved offline.

In this paper, the signal plans of several intersections are determined jointly. For a given intersection and a given time interval (e.g., evening peak period), a fixed-time signal plan is a cyclic (i.e., periodic) plan that is repeated throughout the time interval. The duration of the cycle is the time required to complete one sequence of signals. The cycle times of the intersections controlled in the Lausanne network (used in the case study of this paper) are 80, 90 or 100 seconds.

A phase is defined as a set of traffic streams that are mutually compatible and that receive identical control. The cycle of a signal plan is divided into a sequence of periods called stages. Each stage consists of a set of mutually compatible phases that all have green. The stage sequence is defined such as to separate conflicting traffic movements at intersections. The cycle may also contain all-red periods, where all streams have red indications, as well as stages with fixed durations (e.g., for safety reasons). The sum of the all-red periods and the fixed periods is called the fixed cycle time.

Cycle times, green splits and offsets are the three main signal timing control variables. The green split corresponds to the ratio of green times (i.e., total duration of a phase) to cycle time. Offsets are defined as the difference in time between the start of cycles for a pair of intersections. Offset settings are especially important in coordinating the signals of adjacent intersections (e.g., to create green waves along arterials or corridors).

In this paper cycle times, offsets and all-red durations are kept constant. The stage structure is also given, i.e., the set of lanes associated with each stage as well as the sequence of stages are both known. This is known as a stage-based approach. The decision variables consist of the endogenous green splits of the different intersections.

To formulate this problem we introduce the following notation:

c_i	cycle time of intersection i;
d_i	fixed cycle time of intersection i;
e_ℓ	ratio of fixed green time to cycle time of signalized lane ℓ;
s	saturation flow rate [veh/h];
$x(j)$	green split of phase j;
x_L	vector of minimal green splits;
$\mathscr{I}$	set of intersection indices;
$\mathcal{L}$	set of indices of the signalized lanes;
$\mathscr{P}_I(i)$	set of endogenous phase indices of intersection i;
$\mathscr{P}_L(\ell)$	set of endogenous phase indices of lane ℓ.

The problem is traditionally formulated as follows:

$$\min_x f(x;p) \equiv E[F(x;p)] \tag{12}$$

subject to

$$\sum_{j \in \mathscr{P}_I(i)} x(j) = \frac{c_i - d_i}{c_i}, \ \forall i \in \mathscr{I} \tag{13}$$

$$x \geq x_L. \tag{14}$$

The decision vector x consists of the green splits for each phase. The objective is to minimize the expected trip travel time (Equation (12)). The linear constraints (13) link the green times of the phases with the available (i.e., non-fixed) cycle time for each intersection. Equation (14) ensures lower bounds for the green splits. These bounds are determined based on the prevailing transportation norms.

4.2. Trust region subproblem

This section presents the trust region (TR) subproblem that is solved at each iteration of the SO algorithm. It is a variation of the signal control problem defined in Section 4.1. At a given iteration k, the SO algorithm considers a metamodel $m_k(x, y; \alpha_k, \beta_k, q)$, an iterate x_k (point considered to have best performance so far) and a TR radius Δ_k. The TR subproblem is formulated as follows:

$$\min_{x,y} \ m_k = \alpha_k T(x, y; q) + \phi(x; \beta_k) \tag{15}$$

subject to

$$\sum_{j \in \mathscr{P}_I(i)} x(j) = \frac{c_i - d_i}{c_i} \ \forall i \in \mathscr{I} \tag{16}$$

$$h(x, y; q) = 0 \tag{17}$$

$$\mu_\ell - \sum_{j \in \mathscr{P}_L(\ell)} x_j s = e_\ell s, \ \forall \ell \in \mathcal{L} \tag{18}$$

$$\|x - x_k\|_2 \leq \Delta_k \tag{19}$$

$$y \geq 0 \tag{20}$$

$$x \geq x_L. \tag{21}$$

The TR subproblem approximates the objective functions by the metamodel at iteration k, m_k. It contains the constraints of the signal control problem, and includes three additional constraints. Equations (16) and (21) are the signal control constraints, they correspond to Equations (13) and (14). The function h of Equation (17) represents the queueing network model (Equations (6a)-(6c)). Equation (18) relates the green splits of a phase to the flow capacity of the underlying lanes (i.e., the service rate of the queues). Constraint (19) is the trust region constraint. The endogenous variables of the queueing model are subject to positivity constraints (Equation (20)). Thus, the TR subproblem consists of a nonlinear objective function subject to nonlinear and linear equalities, a nonlinear inequality and bound constraints.

Implementation notes This problem is solved with the Matlab routine for constrained nonlinear problems, *fmincon*, and its sequential quadratic programming method (Coleman and Li 1996, 1994). We set the tolerance for relative change in the objective function to 10^{-3} and the tolerance for the maximum constraint violation to 10^{-2}. For further details on the TR subproblem formulation and its implementation, see Osorio and Bierlaire (forthcoming).

We implement the lower bound constraints of Equation (21) as nonlinear equations by introducing a new variable g and implementing Equation (21) as:

$$x = x_L + g^2. \tag{22}$$

We do not enforce the positivity of all endogenous variables (Equation (20)) yet check a posteriori that all endogenous variables are positive. In our numerous experiments, we have not encountered a case with a negative value. We insert Equation (18) into Equation (6b), and implement the two constraints as a single constraint.

For a problem with n endogenous phases, ℓ lanes, b signalized intersections, where each lane is modeled by a single queue (i.e., we have ℓ queues), there are $3\ell + n$ endogenous variables, which consist of 3 endogenous queueing variables per lane, and the green splits for each phase. There are ℓ linear equations, $2\ell + b$ nonlinear equations and 1 nonlinear inequality (trust-region constraint).

5. Empirical Analysis

5.1. Lausanne city network

We evaluate the scalability and short-term algorithmic performance of this framework by solving a large-scale signal control problem. We solve a problem for the entire Swiss city of Lausanne. The map is displayed in Figure 2, the considered area is delimited in white.

We use a microscopic traffic simulation model of the Lausanne city center developed by Dumont and Bert (2006). It is implemented with the Aimsun simulator (TSS 2008), and is calibrated for evening peak period demand. Details regarding this Lausanne network are given in Osorio and Bierlaire (2009b). In this paper, the considered demand scenario consists of the first hour of peak period traffic, 17h-18h.

The road network consists of 603 links and 231 intersections. The signals of 17 intersections are controlled in this problem. The modeled road network is displayed in Figure 3, where the 17 intersections are depicted as filled squares. This leads to a total of 99 endogenous phase variables (i.e., the dimension of decision vector is 99).

The queueing model consists of 902 queues. The TR subproblem consists of 2805 endogenous variables with 1821 nonlinear equality constraints, 902 linear equality constraints.

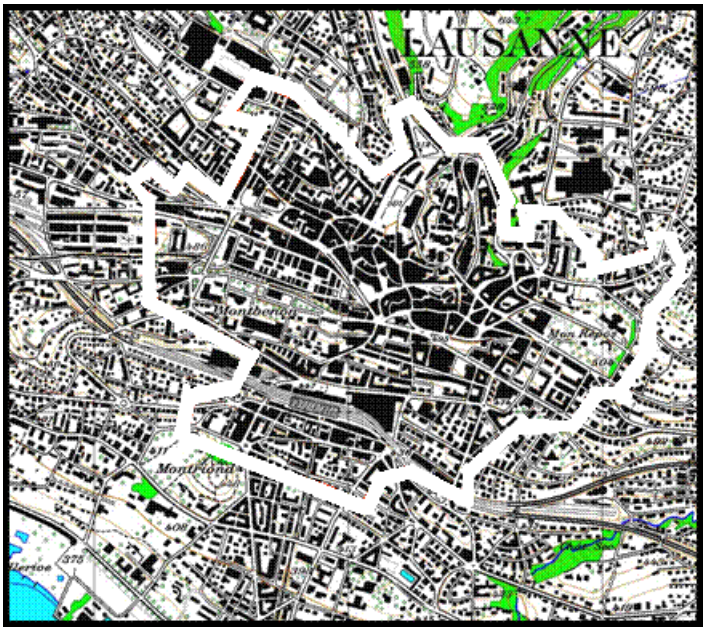


Figure 2 **Lausanne city road network (adapted from Dumont and Bert (2006))**

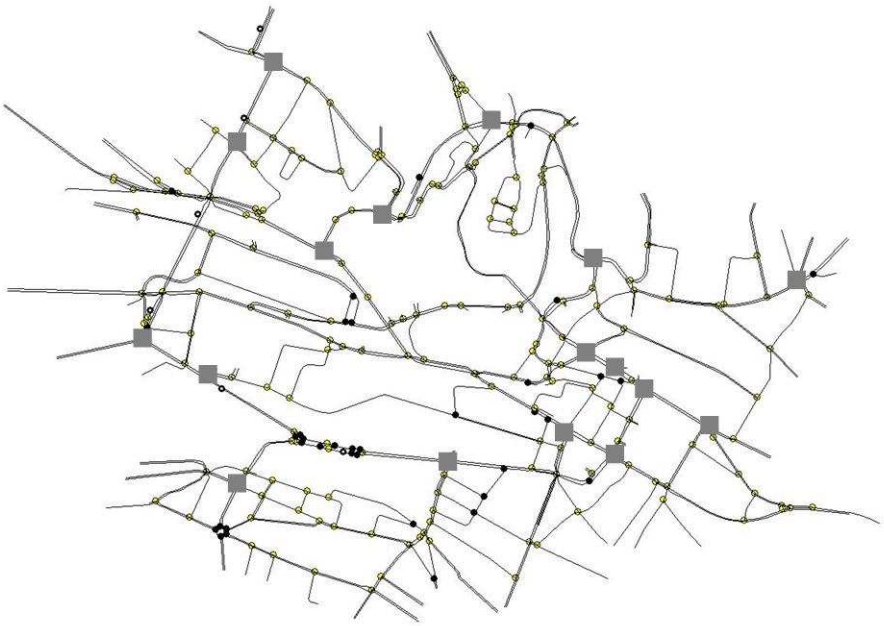


Figure 3 **Lausanne network model**

The lower bounds of the green splits (Equation (14)) are set to 4 seconds according to the Swiss transportation norm (VSS 1992).

Performing network-wide signal control of networks with around 70 links and 16 intersections is currently considered large-scale in the field of signal control, as illustrated by recent studies (Aboudolas et al. 2010, 2007). Thus, the simulation-based signal control

problem of this paper is a challenging large-scale network-wide signal control problem that considers a congested network with a complex topology.

This problem is considered large-scale for existing unconstrained derivative-free algorithms, where the most recent methods are limited to problems with around 200 variables (Conn et al. 2009b), not to mention the added complexity of nonlinear constraints and stochasticity. Given the complexity of the underlying simulator, this problem is also considered complex for simulation-based optimization algorithms.

5.2. Numerical results

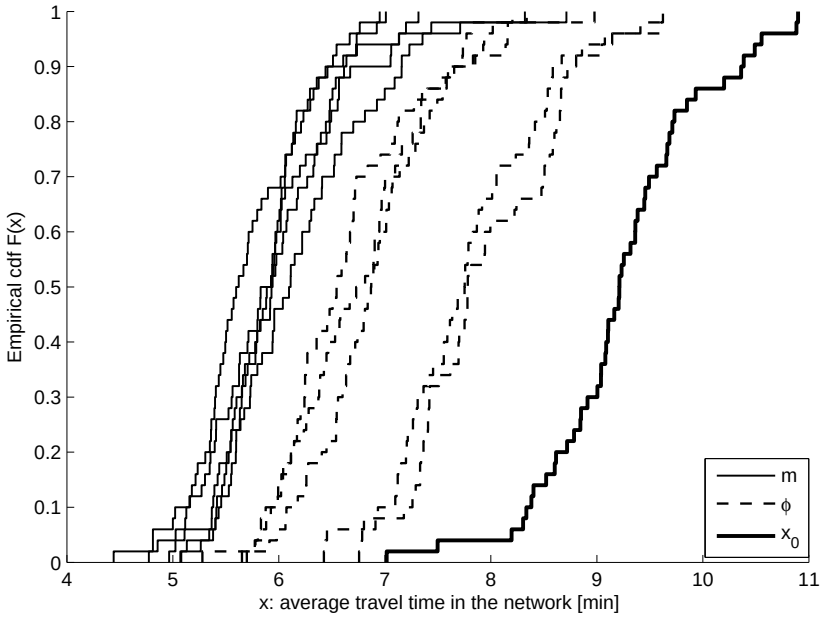
We compare the performance of the proposed metamodel with a traditional metamodel method that consists only of a functional component, which is a quadratic polynomial with diagonal second derivative matrix (i.e., the metamodel consists of ϕ, defined in Equation (2)). In order to compare the two methods, we consider a tight computational budget, which is defined as a maximum of 150 simulation runs that can be carried out.

We consider three different initial points (i.e., signal plans). These points are uniformly drawn from the feasible space defined by Equations (13) and (14). For each initial point, we run the SO algorithm five times, each time allowing for 150 simulation runs. Thus, for each method and each initial point, we derive five "optimal" (or proposed) signal plans. We then use the simulator to evaluate in detail the performance of the proposed signal plans. For each proposed plan signal, we run 50 replications. We compare the empirical cumulative distribution function (cdf) of the average travel times obtained from these 50 replications.

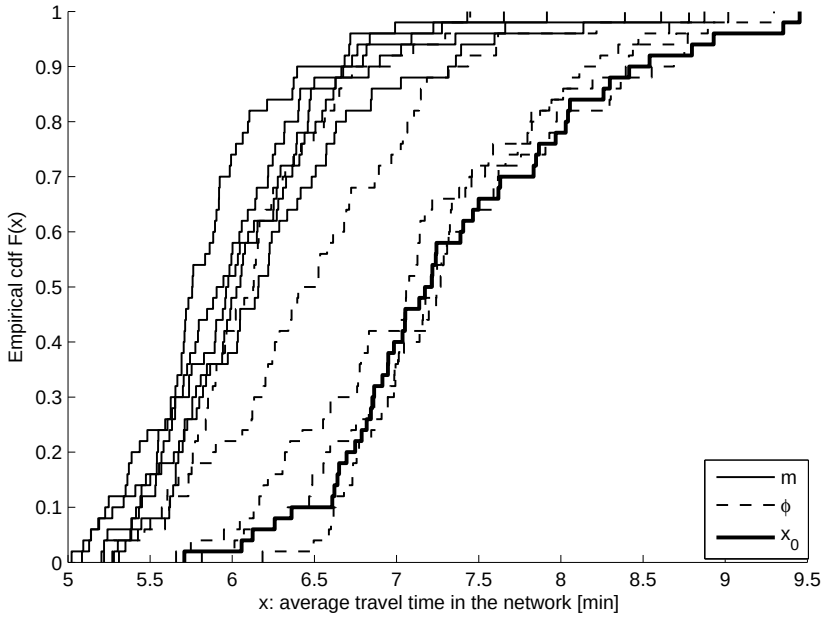
Each plot of Figure 4 considers a different randomly drawn initial point. Each curve of each plot displays the empirical cdf's of a given signal plan. The solid thick curve corresponds to the empirical cdf of the initial signal plan (denoted x_0), the dashed curves (resp. solid thin curves) are the empirical cdf's of signal plans proposed by the traditional metamodel, i.e., the polynomial ϕ, (resp. the proposed metamodel, m).

Figure 4(a) indicates that all five plans derived by both the proposed metamodel and the traditional metamodel yield improved performance when compared to the initial signal plan. All five plans derived by the proposed metamodel also have better performance compared to those proposed by the traditional metamodel.

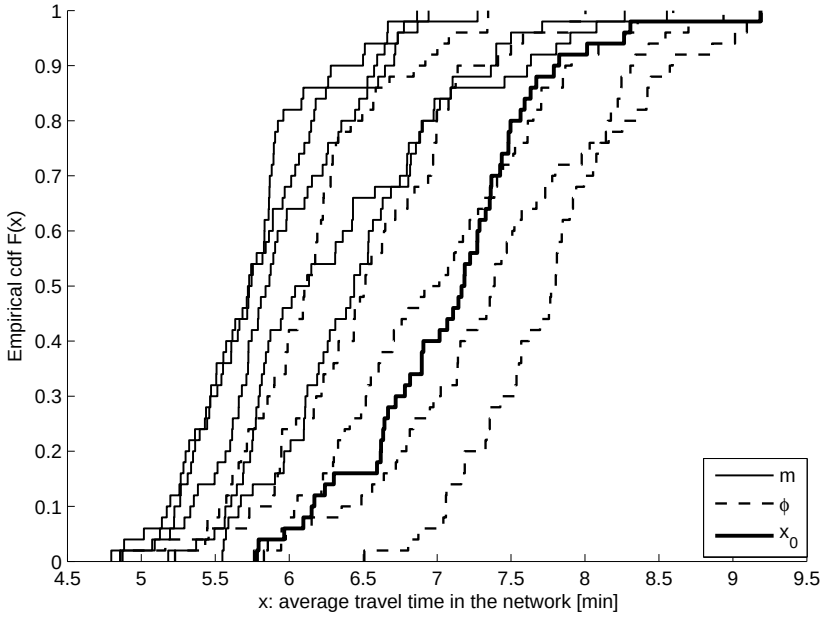
Figure 4(b) indicates that all five signal plans derived by the proposed metamodel yield improved performance when compared to the initial plan. Four of them outperform all five plans derived by the traditional metamodel. Two of the signal plans derived by the traditional metamodel outperform the initial plan and the other three have similar performance as the initial plan.



(a)



(b)



(c)

Figure 4: Empirical cdf's of the average travel times considering initial random signal plans and allowing for 150 simulation runs

In Figure 4(c), all five plans derived by the proposed metamodel yield improvement compared to the initial plan, three of them outperform all five signal plans proposed by the traditional metamodel. Two of the signal plans proposed by the traditional metamodel have worse performance than the initial signal plan, one has similar performance and two have improved performance.

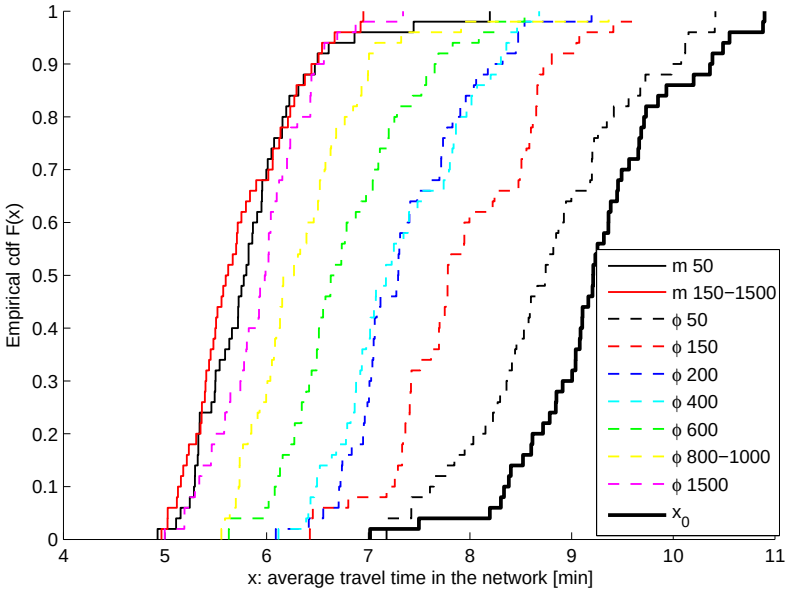
For all three initial points, the proposed method systematically derives signal plans with improved performance when compared to the initial plan, and most often, when compared to the plans obtained from the traditional metamodel. Additionally, the plans derived by the proposed method have good and very similar performance across all SO runs and all initial points, whereas the performance of the plans proposed by the traditional metamodel varies depending on both the initial point and the SO run. This illustrates the robustness of the proposed method to both initial points and to the stochastics of the simulator.

We evaluate the performance of the proposed approach for larger sample sizes. We run the SO algorithm once, and allow for a total of 1500 simulation runs. We choose two random initial signal plans. We evaluate the performance of the signal plans proposed at sample sizes 50, 150, 200, 400, 600, 800, 1000 and 1500. We evaluate their performance just as before, i.e., for a given proposed plan we run 50 replications of the simulator and plot the empirical cdf (over these 50 replications) of the average travel times.

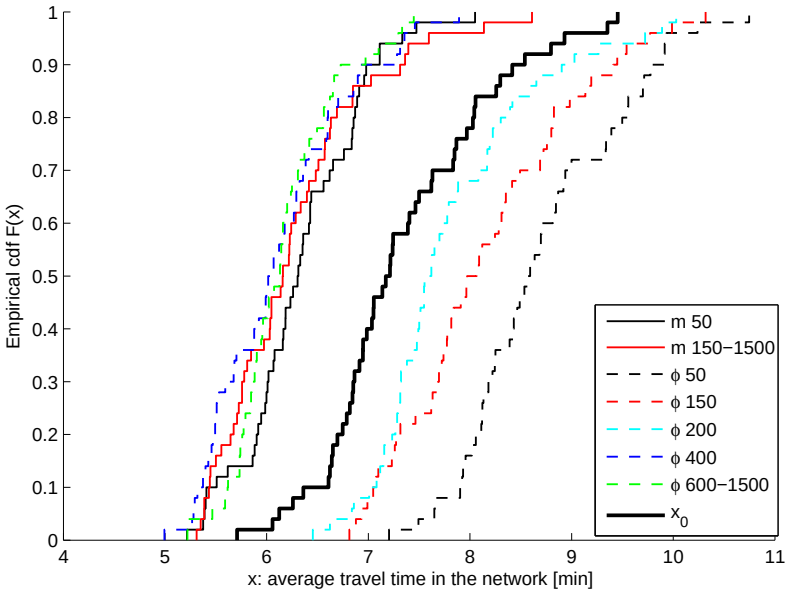
Figure 5(a) displays the corresponding cdf's of the initial signal plan used in Figure 4(a). The proposed approach identifies a signal plan with excellent performance already at sample size 50 (cdf labeled m 50). The signal plan identified as of sample size 150 remains the best up to sample size 1500. It has slightly improved performance, and in particular reduced variability, compared to that of sample size 50.

The performance of the signal plans proposed by the traditional metamodel (dashed curves) improves as the sample size increases. The traditional metamodel requires a much larger sample size to identify signal plans with good performance.

We carry out a paired t-test to evaluate whether the difference in performance of the signal plans proposed by each method at sample size 1500 is statistically significant. We assume that the observed average travel times arise from a normal distribution with common but unknown variance. The null hypothesis assumes that the expected travel time is the same for both methods, whereas the alternative hypothesis assumes that they differ. The confidence level is 0.05, and there are 49 degrees of freedom. The sample average and sample standard deviation of our proposed signal plan (resp. that proposed by the polynomial metamodel) are 5.73 minutes and 0.51 minutes (resp. 5.95 minutes and 0.47 minutes). The critical value of the test is 1.96. The difference is statistically significant (t-statistic of -2.38, p-value of 0.02).



(a)



(b)

Figure 5 **Empirical cdf's of the average travel times considering initial random signal plans and allowing for 1500 simulation runs**

Thus, at sample size 1500 the proposed method still outperforms its traditional counterpart. That is, the signal plan identified by the proposed method as of sample size 150 outperforms that identified by the traditional method at sample size 1500.

Figure 5(b) displays the results considering the initial plan used in Figure 4(b). Similarly, the proposed approach identifies a signal plan with an excellent performance even at sample size 50. The signal plan with best performance derived by the proposed metamodel

is obtained at sample size 150 and remains the same until sample size 1500. It has similar performance to that of sample size 50.

For sample sizes smaller than 400 the traditional metamodel yields signal plans with worse performance than the initial plan. Their performance significantly improve with increasing sample size until size 400. The performance of the derived signal plans with samples larger than 400 are similar. The signal plans proposed by the traditional metamodel method for sample sizes 600 to 1500 are the same.

We carry out the same paired t-test as before in order to evaluate whether the difference in performance of the signal plans proposed by each method at sample size 1500 is statistically significant. The sample average and sample standard deviation of our proposed signal plan (resp. that proposed by the polynomial metamodel) are 6.25 minutes and 0.73 minutes (resp. 6.16 minutes and 0.50 minutes). The difference is not statistically significant (t-statistic of 0.72, p-value of 0.48).

Figure 6 displays two instances of the Lausanne city map. The links are colored based on average link travel times (averaged over the 50 replications). The left (resp. right) map considers the average link travel times for the initial (resp. proposed) signal plan. Here the proposed plan is that obtained with the initial plan and sample size of 150 of Figure 5(a). Green links have average travel times below 40 seconds, yellow links have travel times between 40 and 80 seconds, while red links have travel times greater than 80 seconds. This figure shows how the proposed plan yields city-wide travel time improvements.

At each iteration of the SO algorithm, the two most computationally expensive tasks are the evaluation of the simulator as well as the solution of the trust-region subproblem (i.e., call of the fmincon routine). We consider the first initial plan (used in Figures 4(a) and 5(a)), and account for all 5 runs. Figure 7 displays the cdf of the simulation runs, and the TR subproblem runs. On average one simulation run takes 1.3 minutes, it takes 1.9 minutes to solve the TR subproblem. The experiments were run on a standard laptop (processor: 2.70GHz and 4 GB of RAM). Thus, the metamodel can be used to efficiently solve the TR subproblem at each iteration of the SO algorithm. Additionally, the structural information that it provides through the queueing network model allows the SO algorithm to identify signal plans with excellent performance under very tight computational budgets.

5.3. Synchro comparison

In this section we compare the performance of the signal plans derived by our approach to those derived by the mainstream, commercial, and widely used, traffic signal control software Synchro (Trafficware 2011, Synchro 8). Synchro is a traffic signal control optimization software based on a macroscopic, deterministic and local traffic model. It is widely used

Figure 6: Average link travel times using the initial signal plan (left map) and the signal plan proposed by the SO approach (right map). The averages (in seconds) are taken over 50 simulation replications.

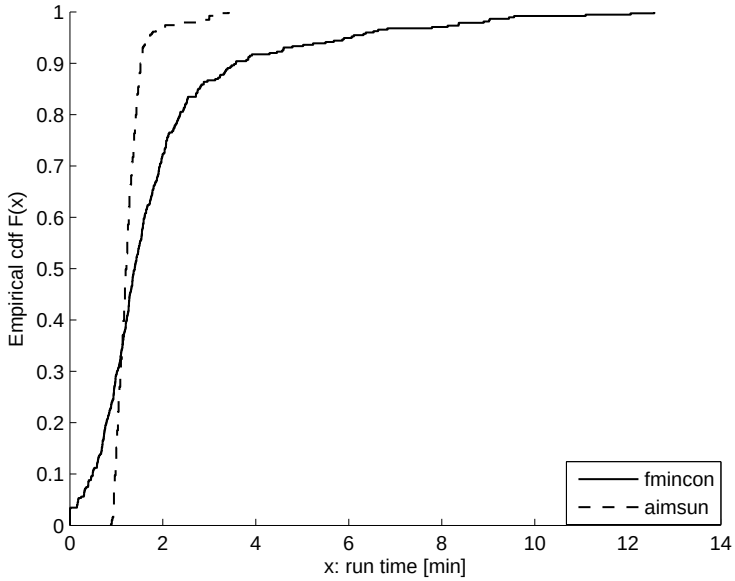


Figure 7 Simulation and trust region subproblem run times

across the US (NYCDOT 2012, Riniker et al. 2009, Abdel-Rahim and Dixon 2007, ATAC 2003). For details on the split optimization technique within Synchro, we refer the reader to Chapter 14 of Trafficware (2011).

The Synchro version used does not allow for any fixed (i.e., exogenous) phase durations. Hence, we solve a signal control problem without fixed phases. For each intersection we take as cycle time its available (i.e., non-fixed) cycle time, $c_i - d_i$. The problem formulation is given by Equations (12)-(14) and by replacing the right-hand side of Equation (13) by $(c_i - d_i)/(c_i - d_i)$, which equals 1. Synchro and our proposed SO method address this same problem. The corresponding TR subproblem is given by Equations (15)-(21), and replacing the right-hand side of (16) by 1 and the right-hand side of (18) by zero.

The Lausanne network is coded in Synchro. All signal plan information needed for Synchro (e.g., phase structure) is obtained from the existing Lausanne signal plan. The minimum splits are set to 4 seconds as in Section 5.1. Lane saturation flows (denoted s in Section 4.1) are set to 1800 vehicles per hour, following Swiss transportation norms. Synchro also needs, as inputs, estimates of prevailing movement flows. This was also needed when calibrating the analytical queueing model (e.g., to obtain turning probabilities). Hence, we use the same estimates as those provided to the queueing model. These are obtained from the simulator using the existing Lausanne signal plan.

To initialize the proposed SO approach, we consider the same three random initial signal plans as used in Figure 4. For each initial plan, we run the SO algorithm once, each time allowing for 150 simulation runs. To evaluate the performance of a plan, we use the simulator and proceed as described in Section 5.2.

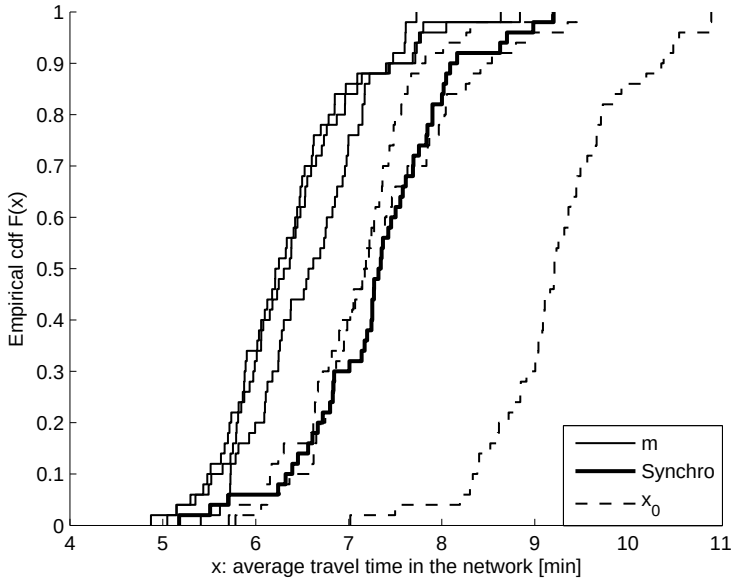


Figure 8 **Emprical cdf's of the average travel times of the signal plans proposed by the SO approach and by Synchro.**

Figure 8 presents the corresponding cdf curves. The three solid thin curves correspond to the plans derived by our proposed metamodel approach (denoted m). The dashed curves correspond to the three random initial signal plans (denoted x_0). The solid thick curve corresponds to the Synchro plan. All three plans derived by the purposed metamodel approach yield improved performance when compared to all three initial plans. All three plans derived by the SO approach also outperform the plan proposed by Synchro. The Synchro plan has similar performance to two of the three randomly drawn signal plans.

6. Conclusions

This paper proposes a metamodel for large-scale simulation-based urban transportation optimization problems. It is a computationally efficient technique that identifies trial points (e.g., signal plans) with improved performance under tight computational budgets. This metamodel SO technique is based on the use of a highly tractable metamodel that combines a general-purpose component (a quadratic polynomial) with a physical component (a highly-tractable analytical queueing network model).

We evaluate the performance of this approach by addressing a large-scale network-wide signal control problem for the Swiss city of Lausanne. This problem considers a congested network (evening peak period demand) with an intricate topology. We compare the performance of the proposed metamodel to that of a traditional metamodel. The proposed method identifies signal plans that improve the distribution of average travel times compared to both the initial signal plans, and most often, to the signal plans derived

by the traditional method. This network-wide signal control problem is considered high-dimensional for SO algorithms, for derivative-free algorithms as well as for signal control algorithms. We also compare the performance of the proposed approach to that of a widely-used signal control software, Synchro. All proposed signal plans outperform the plan derived by Synchro.

In this paper, random uniformly drawn signal plans are used as initial points for the SO algorithm. The results illustrate the robustness of the proposed metamodel method to initial points. This allows practitioners to use the method to address a variety of signal control problems without requiring any field-knowledge to initialize the method.

As part of ongoing research, we are investigating the use of the proposed method to address a variety of generally constrained simulation-based transportation problems, including microscopic model calibration, multi-modal traffic management, and multi-modal network design problems. We are also developing SO algorithms with improved short-term performance by using information from analytical probabilistic traffic models, such as the queueing network model used in this paper, to inform both sampling strategies and statistical tests.

We are also investigating novel analytical traffic model formulations with increased accuracy. The model used in this manuscript is a stationary model, we are currently working on a time-dependent formulation based on the use of transient finite capacity queueing theory. Ongoing work is also developing a formulation with endogenous analytical traffic assignment. The main challenge in this analytical work is to derive a differentiable and highly tractable formulation suitable for large-scale simulation-based optimization.

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References

Abdel-Rahim, Ahmed, Michael Dixon. 2007. Guidelines for designing and implementing traffic control systems for small- and medium-sized cities in Idaho. Tech. Rep. N06-18, Idaho Department of Transportation.

Aboudolas, K., M. Papageorgiou, E. Kosmatopoulos. 2007. Control and optimization methods for traffic signal control in large-scale congested urban road networks. *American Control Conference*. 3132–3138.

Aboudolas, K., M. Papageorgiou, A. Kouvelas, E. Kosmatopoulos. 2010. A rolling-horizon quadratic-programming approach to the signal control problem in large-scale congested urban road networks. *Transportation Research Part C: Emerging Technologies* **18**(5) 680 – 694. doi:10.1016/j.trc.2009.06.003.

Alexandrov, N M, R M Lewis, C R Gumbert, L L Green, P A Newman. 1999. Optimization with variable-fidelity models applied to wing design. Tech. Rep. CR-1999-209826, NASA Langley Research Center, Hampoton, VA, USA.

ATAC. 2003. Signal coordination strategies final report. Tech. rep., Advanced Traffic Analysis Center, Upper Great Plains Transportation Institute, North Dakota State University.

Barton, R R, M Meckesheimer. 2006. Metamodel-based simulation optimization. S G Henderson, B L Nelson, eds., *Handbooks in operations research and management science: Simulation*, vol. 13, chap. 18. Elsevier, Amsterdam, 535–574.

Ben-Akiva, Moshe, David Cuneo, Masroor Hasan, Mithilesh Jha, Qi Yang. 2003. Evaluation of freeway control using a microscopic simulation laboratory. *Transportation Research Part C* **11** 29–50.

Bocharov, P P, C D'Apice, A V Pechinkin, S Salerno. 2004. *Queueing theory*, chap. 3. Modern Probability and Statistics, Brill Academic Publishers, Zeist, The Netherlands, 96–98.

Branke, J, P Goldate, H Prothmann. 2007. Actuated traffic signal optimization using evolutionary algorithms. *Proceedings of the 6th European Congress and Exhibition on Intelligent Transport Systems and Services*.

Bullock, Darcy, Brian Johnson, Richard B. Wells, Michael Kyte, Zhen Li. 2004. Hardware-in-the-loop simulation. *Transportation Research Part C* **12**(1) 73 – 89.

Chen, X, C Osorio, B F Santos. 2012. A simulation-based approach to reliable signal control. *Proceedings of the International Symposium on Transportation Network Reliability (INSTR)*. Submitted. Available at: http://web.mit.edu/osorioc/www/papers/osoCheSanReliableSO.pdf.

Coleman, T F, Y Li. 1994. On the convergence of reflective newton methods for large-scale nonlinear minimization subject to bounds. *Mathematical Programming* **67**(2) 189–224.

Coleman, T F, Y Li. 1996. An interior, trust region approach for nonlinear minimization subject to bounds. *SIAM Journal on Optimization* **6** 418–445.

Conn, Andrew R, Nicholas I M Gould, Philippe L Toint. 2000. *Trust-region methods*. MPS/SIAM Series on Optimization, Society for Industrial and Applied Mathematics and Mathematical Programming Society, Philadelphia, PA, USA.

Conn, Andrew R, Katya Scheinberg, Luis N Vicente. 2009a. Global convergence of general derivative-free trust-region algorithms to first- and second-order critical points. *SIAM Journal on Optimization* **20**(1) 387–415.

Conn, Andrew R, Katya Scheinberg, Luis N Vicente. 2009b. *Introduction to derivative-free optimization*. MPS/SIAM Series on Optimization, Society for Industrial and Applied Mathematics and Mathematical Programming Society, Philadelphia, PA, USA.

Dumont, A G, E Bert. 2006. Simulation de l'agglomération Lausannoise SIMLO. Tech. rep., Laboratoire des voies de circulation, ENAC, Ecole Polytechnique Fédérale de Lausanne.

Fu, M C, F W Glover, J April. 2005. Simulation optimization: a review, new developments, and applications. M E Kuhl, N M Steiger, F B Armstrong, J A Joines, eds., *Proceedings of the 2005 Winter Simulation Conference*. Piscataway, New Jersey, USA, 83–95.

Gartner, N H, D L Hou. 1992. Comparative evaluation of alternative traffic control strategies. *Transportation Research Record* **1360** 66–73.

Hachicha, W, A Ammeri, F Masmoudi, H Chachoub. 2010. A comprehensive literature classification of simulation optimisation methods. *Proceedings of the International Conference on Multiple Objective Programming and Goal Programming MOPGP10*. Sousse, Tunisia.

Hale, D. 2005. Traffic network study tool TRANSYT-7F. Tech. rep., McTrans Center in the University of Florida, Gainesville, Florida.

Hasan, M. 1999. Evaluation of ramp control algorithms using a microscopic traffic simulation laboratory, MITSIM. Master's thesis, Massachusetts Institute of Technology.

Hasan, Masroor, Mithilesh Jha, Moshe Ben-Akiva. 2002. Evaluation of ramp control algorithms using microscopic traffic simulation. *Transportation Research Part C* **10**(3) 229–256.

Joshi, S, A Rathi, J Tew. 1995. An improved response surface methodology algorithm with an application to traffic signal optimization for urban networks. C Alexopoulos, K Kang, W R Lilegdon, D Goldsman, eds., *Proceedings of the 1995 Winter Simulation Conference*. 1104–1109.

Kleijnen, Jack P C. 2008. Response surface methodology for constrained simulation optimization: An overview. *Simulation Modelling Practice and Theory* **16**(1) 50–64.

Kleijnen, Jack P C, Wim van Beers, Inneke van Nieuwenhuyse. 2010. Constrained optimization in expensive simulation: Novel approach. *European Journal of Operational Research* **202**(1) 164–174.

Li, P, M Abbas, R Pasupathy, L Head. 2010. Simulation-based optimization of maximum green setting under retrospective approximation framework. *Transportation Research Record* **2192** 1–10.

Little, John D C. 1961. A proof for the queuing formula: L= λ W. *Operations Research* **9**(3) 383–387.

Little, John D C. 2011. Littles law as viewed on its 50th anniversary. *Operations Research* **59**(3) 536–549.

Marti, K. 2008. *Stochastic optimization methods*. Springer, Berlin, Germany.

NYCDOT. 2012. Downtown Flushing, mobility and safety improvement project. Tech. rep., New York City Department of Transportation.

Osorio, C. 2010. Mitigating network congestion: analytical models, optimization methods and their applications. Ph.D. thesis, Ecole Polytechnique Fédérale de Lausanne.

Osorio, C, M Bierlaire. 2009a. An analytic finite capacity queueing network model capturing the propagation of congestion and blocking. *European Journal of Operational Research* **196**(3) 996–1007.

Osorio, C, M Bierlaire. 2009b. A surrogate model for traffic optimization of congested networks: an analytic queueing network approach. Tech. Rep. 090825, Transport and Mobility Laboratory, ENAC, Ecole Polytechnique Fédérale de Lausanne. Available at: http://web.mit.edu/osorioc/www/papers/osorBier09TechRepQgTraf.pdf.

Osorio, C, M Bierlaire. forthcoming. A simulation-based optimization framework for urban transportation problems. *Operations Research* Available at: http://web.mit.edu/osorioc/Public/Papers/osoBie10so.pdf.

Osorio, C, K Nanduri. 2012. Energy-efficient traffic management: a microscopic simulation-based approach. *International Symposium on Dynamic Traffic Assignment (DTA)*. Martha's Vineyard, USA. Submitted. Available at http://web.mit.edu/osorioc/www/papers/osoNanEnergySO.pdf.

Osorio, C, K Nanduri. 2013. Emissions mitigation: coupling microscopic emissions and urban traffic models for signal control. Tech. Rep. 19082013, Massachusetts Institute of Technology. Submitted. Available at: http://web.mit.edu/osorioc/www/papers/osoNanEmissionsSO.pdf.

Papayannoulis, V, M Marsico, T Maguire, J Strasser, S Scalici. 2011. An integrated travel demand, mesoscopic and miroscopic modeling platform to assess traffic operations for Manhattan, New York. *Proceedings of the Transportation Research Board (TRB) Conference*. Washington DC, USA.

Rathi, A K, E B Lieberman. 1989. Effectiveness of traffic restraint for a congested urban network: a simulation study. *Transportation Research Record* **1232** 95–102.

Riniker, Keith, Perry Eisenach, Thomas Hannan. 2009. City of Winchester, VA traffic signal upgrade project. Tech. rep.

Søndergaard, J. 2003. Optimization using surrogate models - by the Space Mapping technique. Ph.D. thesis, Technical University of Denmark.

Stallard, Charlie, Larry Owen. 1998. Evaluating adaptive signal control using CORSIM. D Medeiros, E Watson, J Carson, M Manivannan, eds., *Proceedings of the 1998 Winter Simulation Conference*.

Stevanovic, Jelka, Aleksandar Stevanovic, Peter T. Martin, Thomas Bauer. 2008. Stochastic optimization of traffic control and transit priority settings in VISSIM. *Transportation Research Part C* **16**(3) 332 – 349.

Toledo, Tomer, Haris N Koutsopoulos, Angus Davol, Moshe E. Ben-Akiva, Wilco Burghout, Ingmar Andreasson, Tobias Johansson, Christen Lundin. 2003. Calibration and validation of microscopic traffic simulation tools: Stockholm case study. *Transportation Research Record* **1831** 65–75.

Traffic Technology International. 2012a. *Admirable Solution*. Traffic Technology International. February/March.

Traffic Technology International. 2012b. *In the Frame*. Traffic Technology International. April/-May.

Trafficware. 2011. *Synchro Studio 8 User Guide*. Trafficware, Sugar Land, TX.

TSS. 2008. *AIMSUN NG and AIMSUN Micro Version 5.1*. Transport Simulation Systems.

VSS. 1992. *Norme Suisse SN 640837 Installations de feux de circulation; temps transitoires et temps minimaux*. Union des professionnels suisses de la route, VSS, Zurich.

Wild, Stefan M, Rommel G Regis, Christine A Shoemaker. 2008. ORBIT: Optimization by radial basis function interpolation in trust-regions. *SIAM Journal on Scientific Computing* **30** 3197–3219.

Yun, I, B Park. 2006. Application of stochastic optimization method for an urban corridor. *Proceedings of the Winter Simulation Conference*. 1493–1499.

Appendix A: Derivation of $E[N]$

In this section we omit the index i that refers to a given queue. $E[N]$ is defined as:

$$E[N] = \sum_{n=0}^{k} nP(N=n). \tag{23}$$

The stationary probabilities for each queue, $P(N=n)$, are given in Bocharov et al. (2004) by:

$$P(N=n) = \frac{1-\rho}{1-\rho^{k+1}}\rho^n. \tag{24}$$

Inserting Equation (24) into (23), and then rearranging the terms yields

$$E[N] = \sum_{n=0}^{k} n\frac{1-\rho}{1-\rho^{k+1}}\rho^n, \tag{25}$$

$$= \sum_{n=1}^{k} n\frac{1-\rho}{1-\rho^{k+1}}\rho^n, \tag{26}$$

$$= \frac{1-\rho}{1-\rho^{k+1}}\sum_{n=1}^{k} n\rho^n, \tag{27}$$

$$= \frac{1-\rho}{1-\rho^{k+1}}\rho\sum_{n=1}^{k} n\rho^{n-1}. \tag{28}$$

We then derive an expression for the last summation as follows. For a geometric series, such that $\rho \neq 1$, we have:

$$\sum_{n=0}^{k} \rho^n = \frac{\rho^{k+1}-1}{\rho-1}. \tag{29}$$

We differentiate this formula with respect to ρ and obtain:

$$\sum_{n=1}^{k} n\rho^{n-1} = \frac{1-\rho^{k+1}}{(1-\rho)^2} - \frac{(k+1)\rho^k}{1-\rho}. \tag{30}$$

Inserting the expression of Equation (30) into Equation (28), and rearranging the terms gives:

$$E[N] = \frac{1-\rho}{1-\rho^{k+1}}\rho\left(\frac{1-\rho^{k+1}}{(1-\rho)^2} - \frac{(k+1)\rho^k}{1-\rho}\right) \tag{31}$$

$$= \rho\left(\frac{1}{1-\rho} - \frac{(k+1)\rho^k}{1-\rho^{k+1}}\right). \tag{32}$$

Appendix B: SO algorithm

This SO algorithm is formulated in detail in Osorio and Bierlaire (forthcoming) and is based on the derivative-free trust region algorithm of Conn et al. (2009a). The parameters of the algorithm are set according to the values in Osorio and Bierlaire (forthcoming).

0. **Initialization.**

Define for a given iteration k: $m_k(x,y;\alpha_k,\beta_k,q)$ as the metamodel (denoted hereafter as $m_k(x)$), x_k as the iterate, Δ_k as the trust region radius, $\nu_k=(\alpha_k,\beta_k)$ as the vector of parameters of m_k, n_k as the total number of simulation runs carried out up until and including iteration k, u_k as the number of successive trial points rejected, ε_k as the measure of stationarity (norm of the derivative of the Lagrangian function of the trust region (TR) subproblem with regards to the endogenous variables) evaluated at x_k.

The constants $\eta_1,\gamma,\gamma_{inc},\varepsilon_c,\bar{\tau},\bar{d},\bar{u},\Delta_{max}$ are given such that: $0<\eta_1<1$, $0<\gamma<1<\gamma_{inc}$, $\varepsilon_c>0$, $0<\bar{\tau}<1$, $0<\bar{d}<\Delta_{max}$, $\bar{u}\in\mathbb{N}^*$. Set the total number of simulation runs permitted (across all points) n_{max}, this determines the computational budget. Set the number of simulation replications per point $\tilde{r}$ (here we use $\tilde{r}=1$).

Set $k=0, n_0=1, u_0=0$. Determine x_0 and Δ_0 ($\Delta_0\in(0,\Delta_{max}]$).

Given the initial point x_0, compute $f_A(x_0)$ (analytical approximation of Equation (12)) and $\hat{f}(x_0)$ (simulated estimate of Equation (12)), fit an initial model m_0 (i.e., compute ν_0).

1. **Criticality step.** If $\varepsilon_k\leq\varepsilon_c$, then switch to *conservative mode*.

2. **Step calculation.** Compute a step s_k that reduces the model m_k and such that x_k+s_k (the trial point) is in the trust region (i.e. approximately solve the TR subproblem).

3. **Acceptance of the trial point.** Compute $\hat{f}(x_k+s_k)$ and

$$\rho_k = \frac{\hat{f}(x_k)-\hat{f}(x_k+s_k)}{m_k(x_k)-m_k(x_k+s_k)}.$$

- If $\rho_k\geq\eta_1$, then accept the trial point: $x_{k+1}=x_k+s_k,\ u_k=0$.
- Otherwise, reject the trial point: $x_{k+1}=x_k,\ u_k=u_k+1$.

Include the new observation in the set of sampled points ($n_k=n_k+\tilde{r}$), and fit the new model m_{k+1}.

4. **Model improvement.** Compute $\tau_{k+1}=\frac{\|\nu_{k+1}-\nu_k\|}{\|\nu_k\|}$. If $\tau_{k+1}<\bar{\tau}$, then improve the model by simulating the performance of a new point x, which is uniformly drawn from the feasible space. Evaluate f_A and $\hat{f}$ at x. Include this new observation in the set of sampled points ($n_k=n_k+\tilde{r}$). Update m_{k+1}.

5. **Trust region radius update.**

$$\Delta_{k+1} = \begin{cases} \min\{\gamma_{inc}\Delta_k, \Delta_{max}\} & \text{if } \rho_k > \eta_1 \\ \max\{\gamma\Delta_k, \bar{d}\} & \text{if } \rho_k \leq \eta_1 \text{ and } u_k \geq \bar{u} \\ \Delta_k & \text{otherwise.} \end{cases}$$

If $\rho_k \leq \eta_1$ and $u_k \geq \bar{u}$, then set $u_k = 0$.

If $\Delta_{k+1} \leq \bar{d}$, then switch to *conservative mode*.

Set $n_{k+1} = n_k, u_{k+1} = u_k$, $k = k+1$.

If $n_k < n_{max}$, then go to Step 1. Otherwise, stop.