Predictive Distance-based Road Pricing — Designing Tolling Zones through Unsupervised Learning

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Abstract

Congestion pricing is a standard approach to mitigate traffic congestion in a number of urban networks around the world. The advancement of satellite technology has spurred interest in distance-based congestion pricing schemes, which obviate the need for fixed infrastructure such as gantries that are used in area- and cordon-based pricing. Moreover, distance-based pricing has the potential to more effectively manage traffic congestion. In the context of distance-based congestion pricing, we propose the use of sparse subspace clustering methods employing Elastic Net optimization (SSCEL) and Orthogonal Matching Pursuit (SSCOMP), as well as two hierarchical density-based clustering methods, (OPTICS, HDBSCAN^{*}) for the derivation of tolling zones. These tolling zone derivations are then used within a simulation-based framework for real-time predictive distance-based toll optimization to examine network congestion and performance of the tolling schemes. Within this framework, for a given derivation of tolling zones, tolling function parameters are optimized in real-time using a simulation-based Dynamic Traffic Assignment (DTA) model. Guidance information generation is integrated into the predictive optimization framework and behavioral responses to the information and tolls along dimensions of departure time, route, mode, and trip cancellation are explicitly modeled. For the evaluation of network performance we make use of Travel Speed Index (TSI) data from the real-world Boston Central Business District urban network and demonstrate that tolling zones derived from the sparse subspace cluster-

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ing are effective means of operationalizing real-time distance-based toll optimization schemes and can positively impact overall network performance, showing improvements in average travel time and social welfare relative to the baseline.

Keywords: Distance-based Toll Optimization, Sparse Subspace Clustering, Density-based Clustering

1 1. Introduction

Traffic congestion is a serious issue world-wide, which results in large costs to travelers, the envi-2 ronment and economy. Congestion was estimated to result in a total of 5.5 billion hours of time delay 3 and 2.9 billion gallons of fuel expenditure in urban areas in the United States between 2000 and 2010 4 (Litman, 2019) and the costs of congestion were projected to increase from \$121 billion in 2011 to \$199 5 billion in 2020. Mitigating congestion is always a high-priority and also impacts transportation network 6 reliability, driver's comfort and traffic safety. Congestion pricing is a standard approach for congestion 7 mitigation that influences traveler behavior along several dimensions: trip making and frequency, mode, 8 destination, time of day, route, and so on. Traditional approaches to congestion pricing include facility-9 based and area-based schemes (de Palma and Lindsey, 2011) that rely on physical infrastructure such 10 as gantries or gates for vehicle detection. Unfortunately, the reliance on fixed physical infrastructure 11 makes it difficult to modify or relocate the charging areas or zones. Moreover, these schemes can result 12 in inefficiency in terms of congestion mitigation since they do not differentiate toll charges based on 13 the associated externalities or congestion caused due to differing distances traveled or time spent in 14 congestion. The aforementioned disadvantages of area- and facility-based pricing and the advancement 15 of Global Navigation Satellite Systems (GNSS) have focused attention on usage-based tolling wherein 16 toll charges depend on the distance-traveled or the time spent in congestion (see Smith et al. (1994) 17 and Bonsall and Palmer (1997) for a detailed discussion on the comparative performance of distance-18 and time-based schemes). Singapore is in the process of transitioning to such a GNSS-based electronic 19 road-pricing scheme (ERP2) (LTA, 2016, 2021). Distance-based schemes may be operationalized by 20 dividing the urban area into zones and charging a distance-based toll such that the tariff varies across 21 zones and by time-of-day. The motivation for the use of tolling zones (instead of a single distance-based 22 scheme over the entire network) is that it provides the flexibility to adjust the tolling rates based on 23 road-type and congestion levels, thereby improving overall efficiency gains. 24

Past research on area and cordon-based real-time toll optimization has typically applied reactive approaches (where the optimization of tolls is not based on forecasts of future traffic conditions, but

rather on prevailing traffic conditions) for small corridor networks and there are few studies that adopt 27 a predictive approach in the context of large networks (Gupta et al., 2016, 2020). A more detailed 28 discussion of cordon and area-based real-time toll optimization may be found in Gupta et al. (2020). 29 As noted previously, in contrast with cordon- and area-based schemes, distance-based tolling schemes 30 involve partitioning the network into zones, and levying a toll within each zone that is a function of 31 distance traveled (linear toll functions are considered in Gu et al. (2018); Yang et al. (2012); Zhu and 32 Ukkusuri (2015), and piece-wise linear functions are used in Liu et al. (2014); Meng et al. (2012); Sun 33 et al. (2016)). Distance-based toll optimization problems have largely been formulated as simulation-34 based optimization problems (Gu and Saberi, 2019b; Gu et al., 2018; Lentzakis et al., 2020), non-linear 35 programs (Yang et al., 2012) and mathematical programs with equilibrium constraints or MPEC (Liu 36 et al., 2014; Meng et al., 2012), which are solved by global optimization approaches (Liu et al., 2014), 37 meta heuristics (Lentzakis et al., 2020; Meng et al., 2012), reinforcement learning (Zhu and Ukkusuri, 38 2015) and feedback controllers (Gu and Saberi, 2019b; Gu et al., 2018). With the exception of Lentzakis 39 et al. (2020), these approaches are based on prevailing network conditions (i.e., they are reactive as 40 opposed to proactive), and do not consider elastic demand or the integration of guidance information 41 generation. 42

Several studies have also examined the partitioning of networks utilizing flow, speed and density 43 data (Ji and Geroliminis, 2012; Lentzakis et al., 2014; Saeedmanesh and Geroliminis, 2017) for the 44 design of traffic management schemes utilizing the Network Fundamental Diagram (NFD) concept. 45 Although area- and cordon-based pricing has been studied in great detail (Geroliminis and Levinson, 46 2009; Simoni et al., 2015; Zheng et al., 2016, 2012), distance-based pricing in particular has only recently 47 received attention on idealized networks (Daganzo and Lehe, 2015), using nested regions (Gu et al., 48 2018) and at the link-level (Simoni et al., 2019). With the exception of Lentzakis et al. (2020), there 49 has been limited research on systematic approaches for the derivation of tolling zones within distance-50 based toll optimization strategies. Due to the increasing significance of distance-based road pricing in 51 traffic network management and operations, this paper addresses the problem of how to define tolling 52 zones and proposes the application of sparse subspace clustering methods to define parsimonious sets 53

⁵⁴ of tolling zones. The performance of these methods is evaluated within a framework for real-time ⁵⁵ toll optimization which generates predictive optimized distance-based toll strategies combined with ⁵⁶ guidance information. This paper contributes to the existing literature in the following respects:

1. We apply sparse subspace and hierarchical density-based clustering methods for the derivation of 57 tolling zones that utilize location coordinates and travel speed indices (TSI) as features. The key 58 advantage of using sparse subspace clustering techniques is that they enable the effective use of 59 high-dimensional temporal network performance data (for example, travel speeds at a resolution of 60 five minutes) directly in the clustering algorithm. This provides a potentially promising alternative 61 to the procedure proposed in Lentzakis et al. (2020) where the clustering algorithm is applied to 62 a single aggregate measure of network performance (over the entire peak period) for each link. In 63 this paper, we focus specifically at the performance of the different clustering algorithms and the 64 implications for toll design/policy. 65

2. The proposed clustering methods are evaluated using a framework for real-time distance-based
 predictive toll optimization on the Boston CBD network and yield insights into their performance
 and suitability for deployment wherein one of our primary goals is minimization of computational
 effort.

70 2. Framework for Predictive Distance-based Toll Optimization

In this section, we summarize the real-time distance-based predictive toll optimization framework (more details may be found in Lentzakis et al. (2020)), the optimization problem formulation, the proposed clustering methods for tolling zone derivation and the algorithmic solution for the optimization problem.

75 2.1. Framework

The framework, shown in Figure 1, uses DynaMIT2.0 - a simulation-based Dynamic Traffic Assignment (DTA) system developed at the MIT Intelligent Transportation Systems Lab (Ben-Akiva et al.,



Figure 1: Real-time distance-based predictive toll optimization framework

2010; Lu et al., 2015b). DynaMIT2.0 employs a rolling horizon approach involving two key modules, 78 state estimation and state prediction. The state estimation process uses a combination of historical data, 79 real-time traffic surveillance data, and prevailing network control strategies (such as distance-based toll 80 optimization) to estimate the current state of the network. It used detailed models of demand (pre-trip 81 models of departure time, route and mode choice), supply (mesoscopic traffic simulator that com-82 bines speed-density relationships and a deterministic queuing model) and their interactions. Following 83 this, the state prediction module generates forecasts of traffic conditions for a pre-specified prediction 84 horizon (origin-destination demands and supply parameters are forecasted for the future using an au-85 toregressive process). The strategy optimization and guidance generation modules in conjunction use 86 the state predictions to first, optimize control strategies for the prediction horizon and second, generate 87 guidance information (traveler information) for the prediction horizon. The evaluation of candidate 88 control strategies makes use of network predictions and guidance information that are consistent, i.e., 89

the guidance information is as close as possible to actual predicted network travel times (see Figure 1 and Ben-Akiva et al. (2010) for more on this aspect of consistency).

92 3. Problem Formulation and Solution

In this section, we describe the optimization problem formulation (based on the framework described in Section 2) including details of the demand model within the DTA system, and the solution approach.

95 3.1. Context and Tolling Function Definition

We represent the transportation network of interest as a directed graph $\mathcal{G} = (\mathcal{N}, \mathcal{A})$, where \mathcal{N} denotes the set of n network nodes and \mathcal{A} denotes the set of m links. The network is partitioned into l = 1...L tolling zones, where every zone l is defined by a subset of network links $\mathcal{A}_l \subseteq \mathcal{A}$. For each zone l, we define a tolling function $\phi_l(\boldsymbol{\theta}_l^t, D_l)$ that maps distance traveled within the zone l, D_l to the toll amount; $\boldsymbol{\theta}_l^t$ is a vector of parameters that defines the tolling function in time interval t. Further, it is assumed that the toll payable in a zone is bounded, i.e $\tau_{LB} \leq \phi_l(\boldsymbol{\theta}_l^t, D_l) \leq \tau_{UB}, \forall l = 1, 2..., L \; \forall t =$ 1, 2, ..., T.

Denote the length of the state estimation interval in DynaMIT2.0 by Δ (usually 5 minutes) and 103 assume that the prediction horizon is composed of H such intervals so that the size of the prediction 104 horizon is $H\Delta$. We assume that the prediction horizon and the optimization horizon are identical. 105 Further, the tolling function parameters do not vary within a given time interval of size Δ and these 106 tolling intervals coincide with DynaMIT2.0 estimation intervals. For an arbitrary estimation interval 107 $[t_0 - \Delta, t_0]$, let $\theta^h = (\theta^h_1, \theta^h_2 \dots \theta^h_L)$ represent the vector of tolling function parameters for the time 108 period $[t_0 + (h-1)\Delta, t_0 + h\Delta]$ where h = 1, ..., H. Accordingly, for the current optimization horizon, 109 the decision variables are $\boldsymbol{\theta} = (\boldsymbol{\theta}^1, \boldsymbol{\theta}^2, ..., \boldsymbol{\theta}^H)$. 110

Implementing a system with complex zone-based tariffs that vary every five minutes is likely to impose unreasonable burdens on drivers that may compromise acceptability of the system. An added issue is that drivers may not have a viable alternative if for example they suddenly find themselves entering a zone where the tariff has increased substantially. Hence, we assume that drivers are charged the predicted toll that the system provides to them at the point of departure (more precisely, the point at which they make their decision, which may be up to 15 minutes prior to their actual departure). The underlying premise – justifiable given our rolling horizon design – is that the predictions of the toll in the future do not deviate appreciably from the actual implemented tolls. The rolling horizon framework is demonstrated in Figure 2



Figure 2: Rolling Horizon Approach for Tolling Function Optimization

Consider the set of vehicles v = 1, ..., V that are on the network during the prediction horizon $[t_0, t_0 + H\Delta]$. For each vehicle v, we denote the experienced trip travel on its chosen route by tt^v and the predictive guidance information by $\mathbf{tt}^g = (\mathbf{tt}_i^g; \forall i \in A)$, where \mathbf{tt}_i^g represents a vector of time dependent travel times for link i. Note that the vehicle travel times $\mathbf{tt} = (tt^v; v = 1, ..., V)$ are obtained from the state prediction module of DynaMIT2.0, which we characterize through a single constraint that represents the coupled demand and supply simulators as:

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$$G(\mathbf{x}^{\mathbf{p}}, \gamma^{\mathbf{p}}, \mathbf{t}\mathbf{t}^{\mathbf{g}}, \boldsymbol{\theta}) = \mathbf{t}\mathbf{t}$$
(1)

127

¹²⁸ Where $\mathbf{x}^{\mathbf{p}}$, $\gamma^{\mathbf{p}}$ represent the forecasted demand and supply parameters for the prediction horizon, and



Figure 3: Pre-trip Behavior Model

 θ is the vector of tolling function parameters. As noted previously, the state prediction module ensures consistency between tt^g and tt.

131 3.2. Pre-trip Behavioral Model with Elastic Demand

The pre-trip response of users to the travel time guidance and distance-based tolls is modeled using a path-size nested logit model with heterogeneous value of time (illustrated in Figure 3) that captures decisions of mode choice, trip cancellation, departure time and path (notation is provided in Table 1). We provide a brief description of the model here, for completeness (more details may be found in Lentzakis et al. (2020)).

In response to pre-trip information and tolls, a traveler may alter his/her habitual travel pattern, which may include changing mode, canceling trip, changing departure time or path, or changing departure time and path. This results in elastic total demand w.r.t. traffic congestion. The options of mode modeled are private car (drive alone) and public transit. The utility of change to transit for vehicle vis given by:

Abbreviation	Variable		
β_{CM}	Alternative Specific Constant (ASC) for change of mode to transit		
β_{CT}	ASC for canceling trip		
β_{CDT_d}	ASC for departure in time interval d		
c_m^v	monetary cost for traveling with non-private (transit) mode		
c^v_{dp}	toll charge for departure via path p in interval d		
c_p^v	toll for switching to path p		
t_m^v	travel time associated with non-private (transit) mode		
t_{dp}^g	travel time (guidance) for departure via path p in interval d		
t_p^g	travel time (guidance) for switching to path p		
$at^{hab}_{d'p'}$	arrival time (habitual)		
at_{dp}^{g}	arrival time (predicted) for departure via path p in time interval d		
β_c^v	monetary cost coefficient		
β_t^v	travel time coefficient		
β_E	schedule delay early coefficient		
β_L	schedule delay late coefficient		
PS_p	path size variable		
C_*	utility relating to number of left turns/signalized intersections and path		
	length		
ε_*	error component		

Table 1: Pre-trip Model - Abbreviations

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$$U^{v}(CM) = \beta_{CM} + \beta_{c}^{v} c_{m}^{v} + \beta_{t}^{v} t_{m}^{v} + \varepsilon_{m}$$

$$\tag{2}$$

143

The utility of departing at time interval d and choosing path p for vehicle v is given by:

$$U_{dp}^{v} = \beta_{CDT_{dp}} + \beta_{c}^{v} c_{dp}^{v} + \beta_{t}^{v} t_{dp}^{g}$$
$$+ \beta_{E} \max(at_{d'p'}^{hab} - at_{dp}^{g}, 0) + \beta_{L} \max(at_{dp}^{g} - at_{d'p'}^{hab}, 0)$$
$$+ \log(PS_{p}) + C_{dp} + \varepsilon_{dp}$$
(3)

where:

$$c_{dp}^{v} = \sum_{l=1}^{L} \phi_l(\boldsymbol{\theta}_l^{\boldsymbol{t}_{v,l}}, D_l^{v}),$$

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and $t_{v,l}$, D_l^v denote the predicted time of entry of vehicle v into zone l and the total distance traveled by vehicle v in zone l, respectively. Note that if there are a total of N combinations of path and departure time choices in the choice set, the alternative specific constant β_{CDT_d} can only appear in (N-1)utilities. The utility of canceling trip altogether is given by:

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$$U^{v}(CT) = \beta_{CT} + \varepsilon_{CT} \tag{4}$$

151

Thus, the probability of vehicle v choosing alternative c within the choice set C is given by: 153

$$P^{v}(c|C) = \frac{e^{\mu V_{c}^{v}}}{\sum_{a \in C} e^{\mu V_{a}^{v}}}$$
(5)

154

where V_c^v is the systematic utility given by $V_c^v = U_c^v - \varepsilon_c$ and μ is a scale parameter. The en-route choice model defines response of users in terms of path-choice to the toll and predictive travel time guidance. It is also formulated as a multinomial path size logit model where the utility of switching to ¹⁵⁸ path p is given by:

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$$\cup_{p}^{v} = \beta_{c}^{v}(tc_{p}^{v}) + \beta_{t}^{v}(tt_{p}^{g}) + log(PS_{p}) + C_{p} + \varepsilon_{p}$$
where :
$$tc_{p}^{v} = \sum_{l=1}^{L} \phi_{l}(\boldsymbol{\theta}_{l}^{t_{v,l}}, D_{l}^{v})$$
(6)

160

Note that owing to the design of the distance-based tolls, which require that users are charged upfront at the beginning of a trip, we assume that en-route changes to the path are not made.

163 3.3. Optimization Formulation

The objective function for the toll optimization problem, formulated from the standpoint of the traffic regulator, is total social welfare (SW), which is the sum of the consumer surplus and the producer surplus. In this context, the consumer surplus (CS) is defined as the sum of the experienced utilities across all travelers, derived at the end of each simulation run, and the producer surplus is the net revenue, denoted by TP, which is simply the toll revenue minus variable costs (fixed costs are ignored), TP = TR - VC. We assume that the variable costs are a proportion of the toll revenue (the proportionality factor is denoted by $\alpha < 1$). Thus, the social welfare is given by:

$$SW = CS + TP$$

= $CS + (TR - VC)$
= $\sum_{v=1}^{V} \frac{U^v}{|\beta_c^v|} + \left[(1 - \alpha) \times \sum_{v=1}^{V} c^v \right]$ (7)

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The absolute value of β_c^v is used to translate CS into dollar equivalents. The distance-based toll optimization problem is formulated as a simulation-based optimization problem in Equation 8, where the objective is social welfare, the decision variables are the vector of tolling function parameters for the current optimization horizon, and the constraints are toll bounds and the DTA model system. 176

$$\max_{\boldsymbol{\theta}} \left[\sum_{v=1}^{V} \frac{U^{v}}{|\beta_{c}^{v}|} + (1-\alpha) \times \sum_{v=1}^{V} c^{v} \right]$$

s.t.
$$G(\mathbf{x}^{\mathbf{p}}, \gamma^{\mathbf{p}}, \mathbf{t}\mathbf{t}^{\mathbf{g}}, \boldsymbol{\theta}) = \mathbf{t}\mathbf{t}$$

$$\tau_{LB} \leq \phi_{l}(\boldsymbol{\theta}_{l}^{h}, D_{l}^{v}) \leq \tau_{UB}, \forall v = 1, 2, ..., V; l = 1, 2..., L; h = 1, 2, ..., H$$

(8)

The upper and lower bounds τ_{LB} , τ_{LB} are imposed to allow for tolling function values within a safe and acceptable range, suitable for real-life implementations.

179 3.4. Solution Algorithm

Due to the highly non-convex nature of the objective function in 8, we apply a real-coded Genetic Algorithm (GA) to solve the optimization problem in 8. More details on the GA algorithm may be found in Lentzakis et al. (2020). Computational performance is enhanced by utilizing parallelization wherein the evaluations of different candidate solutions within an iteration of the GA are performed in parallel.

¹⁸⁵ 4. Tolling Zone Design through Unsupervised Learning

For most tolling-related implementation decisions, at least in the USA, tolling zone boundaries are 186 subject to extreme political scrutiny, Environmental Justice reviews, exemptions for residents of certain 187 areas, etc. Unsupervised machine learning utilizes historical data to reveal patterns, similarities or hid-188 den structure and can contribute to changing the current state-of-affairs, with regards to tolling zone 189 design. In this paper, we posit that it would be beneficial for a city or highway operator to rely on un-190 supervised learning approach in any sort of real-world setting, for expeditious implementation. Even in 191 the case that stakeholder involvement is mandatory, tolling zone derivation through unsupervised learn-192 ing can significantly augment the decision-making process. Unsupervised learning can be approached 193 through different techniques such as clustering, association rules, and dimensionality reduction. Our 194

focus will be on clustering. One of the inputs with significant impact on our distance-based tolling sys-195 tem performance is the tolling zone derivation. This input specifies which links belong to each tolling 196 zone and the number of zones. Each tolling function $\phi_l(\theta_l^h, D_l^v)$ corresponds to one tolling zone. Past 197 literature for partitioning urban traffic networks used datasets based on speed, flow, density (Gu and 198 Saberi (2019a); Ji and Geroliminis (2012); Lentzakis et al. (2014); Saeedmanesh and Geroliminis (2017)) 199 and, more recently, marginal cost toll data (Lentzakis et al., 2020). In our case, the travel speed index 200 (TSI) is used, a widely used quantitative indicator that employs link speed normalization (Li and Xiao, 201 2020), given the fact that identical link speed levels might reflect different traffic conditions. Speed 202 information for toll setting is currently used in a similar fashion as in Singapore's ERP system, (Lehe, 203 2019). It should be noted that the decision to use travel speed indices, rather than marginal cost tolls 204 (MCT) used in Lentzakis et al. (2020), has to do with the fact that, in this work, one of our main goals 205 was to reduce computational effort, both during data preprocessing and the predictive distance-based 206 toll optimization framework implementation, placing real-world applicability at the forefront. Should 207 circumstances allow it, the possibility of using MCT as a feature should definitely be explored. 208

209 4.1. Clustering Approaches

Elhamifar and Vidal (2009), inspired by compressed sensing (Lee et al., 2007), introduced Sparse 210 Subspace Clustering (SSC), which makes use of the self-expressiveness property to construct the affin-211 ity matrix (which quantifies the extent of pairwise similarity between a set of data points). Self-212 expressiveness (Elhamifar and Vidal, 2013) describes the fact that a data point found in a union of 213 subspaces can be represented as the linear combination of other data points. Based on the com-214 puted affinity matrix, spectral clustering is applied to derive the underlying subspaces. While subspace 215 clustering methods have been used extensively for, among others, temporal video segmentation and 216 switched system identification (Bako, 2011; Rao et al., 2009), only recently, has this technique come to 217 the attention of the transportation research community. Zhang et al. (2019) employed SSC to classify 218 spatiotemporal taxi patterns with regards to their passenger searching behavior. For our experiments 219 we selected to compare two Sparse Subspace Clustering variants, SSCEL and SSCOMP, employing 220

Elastic Net optimization (You et al., 2016a) and Orthogonal Matching Pursuit (You et al., 2016b) respectively, against two well-known hierarchical density-based clustering methods, OPTICS (Ankerst et al., 1999), (Ordering Points To Identify the Clustering Structure), and HDBSCAN* (Campello et al., 2013), (Hierarchical Density-Based Spatial Clustering of Applications with Noise).

225 4.1.1. Sparse Subspace Clustering Methods

For the Sparse Subspace Clustering application, we selected two variants,SSCEL and SSCOMP. We exploited the property of self-representation to learn the affinity matrix, to be subsequently used in our implementation of spectral clustering. As noted previously, data self-expressiveness (Elhamifar and Vidal, 2013) describes the fact that a data point found in a union of subspaces can be represented as the linear combination of other data points, expressed through the following optimization problem:

$$\min_{C} \|\mathbf{C}\|_{1}$$
s.t.
(9)
$$\mathbf{X} = \mathbf{X}\mathbf{C}$$

$$diag(\mathbf{C}) = 0$$

231

Where $\mathbf{X} \in \mathbf{R}^{D \times N}$ is the data point matrix and $\mathbf{C} \in \mathbf{R}^{N \times N}$ is the self-expression coefficient matrix. In practice, however, solving N such problems over N variables may be computationally expensive for large N. Instead, the optimization problem is expressed as follows:

$$\min_{c_j} \|\mathbf{x}_j - \mathbf{X} \mathbf{c}_j\|_2^2$$
s.t.
$$\|\mathbf{c}_j\|_0 \le \mathbf{k}$$

$$diag(\mathbf{C}) = 0$$
(10)

We can now efficiently solve the above problem using the Orthogonal Matching Pursuit algorithm, as described in You et al. (2016b). Orthogonal Matching Pursuit selects a single column of X each time, \mathbf{x}_{j} , such that the absolute value of the dot product with the residual \mathbf{c}_{j} is maximized and the coefficients are computed until k columns are selected. Subsequently, we learn the affinity matrix \mathbf{W} through data self-representation as: $\mathbf{W} = |\mathbf{C}| + |\mathbf{C}^{T}|$. Alternatively, we may employ Elastic Net regularization for scalable subspace clustering. Following You et al. (2016a), we used an active set algorithm that efficiently solves the elastic net regularization subproblem, which follows below, by capitalizing on the geometric structure of the elastic net solution:

$$\min_{\mathbf{c}_j} \lambda \|\mathbf{c}_j\|_1 + \frac{1-\lambda}{2} \|\mathbf{c}_j\|_2^2 + \frac{\gamma}{2} \|\mathbf{x}_j - \mathbf{X}\mathbf{c}_j\|_2^2$$
(11)

Where $\lambda \in (0,1]$ and $\gamma > 0$. In the majority of solution approaches for the Subspace Clustering problem, after learning the affinity matrix, spectral clustering is applied to the resulting matrix to derive the final clustering.

246 4.1.2. Hierarchical Density-based Clustering Methods

Hierarchical density-based clustering methods are gaining traction among the research community, exhibiting robustness during parameter selection and being able to cope with clusters characterized by large inter-cluster density variability, unlike their non-hierarchical predecessor, DBSCAN (Schubert et al., 2017).

OPTICS utilizes hyperparameters ϵ and κ , representing the maximum ball radius with each data point at 251 its center and the minimum density threshold, respectively. Assuming a metric space (X, d) comprising 252 of a set of data points $X = \{x_1, x_2, ..., x_n\}$, a data point x is considered to be a core point with respect 253 to ϵ and κ if its ϵ -neighborhood $N_{\epsilon}(x)$ contains a minimum of κ data points. Two core points x_i, x_j 254 are ϵ -reachable with respect to ϵ and κ if they are both contained within each others ϵ -neighborhood. 255 Two core points x_i, x_j are density-connected with respect to ϵ and κ if they are directly or transitively 256 ϵ -reachable. A cluster is the largest possible group of data points, where each two points are considered 257 connected in terms of density. In OPTICS data points are assigned a core distance $d_{\text{core}}^{\epsilon,\kappa}(x)$ to the κ -th 258 nearest neighbor, for varying degrees of density. The reachability-distance $d_{\text{reach}}^{\epsilon,\kappa}(x_i,x_j)$ is the maximum 259 between the core distance of x_i and the distance between data points x_i, x_j . A single global ϵ' value is 260

²⁶¹ used to extract a flat clustering.

HDBSCAN* is similar to OPTICS with parameter $\epsilon = \infty$ and a different technique, based on cluster stability, is utilized for flat clustering. In the case of HDBSCAN*, we have $d_{\text{core}}^{\kappa}(x_i)$ representing the κ -th nearest neighbor distance. For a fixed κ and a range of possible ϵ values, the mutual reachability distance $d_{\text{mreach}}^{\kappa}(x_i, x_j)$ is used to generate a complete hierarchy of clusterings. Thus, for any fixed ϵ value, the clustering produced by DBSCAN at a given level in the hierarchy is the clustering obtained for the corresponding ϵ value.

The selected hierarchical density-based clustering methods result in clusterings where some data points are considered noise. A feasible derivation of tolling zones, however, must involve the assignment of all data points to clusters. In order to address this issue, we perform a secondary assignment where all noise data points are assigned to the closest clusters (using Euclidean distance).

272 4.2. Clustering Performance Metrics

As clustering performance metrics, the Silhouette Coefficient (SC) (Rousseeuw, 1987) and the Davies-Bouldin index (DB) (Davies and Bouldin, 1979) were selected. SC is the average for the entire dataset of the silhouette, which measures cohesion and separation for each cluster and ranges from [-1,1], where -1 represents an inappropriate clustering (within-cluster variability is large and between cluster variability is small), 0 represents overlapping clusters and 1 represents highly dense clustering. DB is a function of the ratio of intra-cluster scatter to inter-cluster separation. DB values closer to 0 indicate a better clustering result.

280 4.3. Clustering Results

It would be preferable that the selected clustering methods produce clustering results that are of high quality, according to our previously presented internal evaluation indices, but also do not preclude any sort of practical application, due to high computational cost, incurred on the distance-based toll optimization framework. This translates into a static tolling zone derivation (non-varying during the simulation), with a reasonably low number of tolling zones. For our dataset, besides spatial coordinates, we decided to use the travel speed index (TSI) for each link as an additional feature, calculated as follows:

$$TSI_i = 1 - \frac{\nu_i}{\nu_i^f} \tag{12}$$

Where ν_i, ν_i^f the link speed and free flow speed for link *i* respectively. Simulated speed data at the 287 segment and link level, obtained from a calibrated DynaMIT2.0 model of the Boston CBD (Lu et al., 288 2015a), were used to derive the tolling zone derivations. In the case of static partitioning schemes 289 derived offline, a preferable alternative to using the average of TSI across specific intervals, as is the 290 case for our hierarchical density-based clustering approaches, would be to use the TSI values for all time 291 intervals, i.e., the entirety of our dataset, since self-representation, an integral part of sparse subspace 292 clustering, is amenable for use of datasets with spatiotemporal attributes (Hashemi and Vikalo, 2018; 293 Pham et al., 2012). The Boston CBD network, shown in Figure 4, has 846 nodes, 1746 links, 3085 294 segments, 5057 lanes and 13080 Origin-Destination pairs. 295



Figure 4: Boston CBD Network





(b) 2 zones derived using SSCOMP for feature TSI, with SC=0.198, DB=1.276

Figure 5: Clustering results and tolling zones (Sparse Subspace Clustering)



(b) 5 zones derived using HDBSCAN* for feature TSI, with SC=0.400, DB=0.776

Figure 6: Clustering results and Tolling zones (Hierarchical Density-based Clustering)

296 5. Experiments: Boston CBD Network

297 5.1. Experimental Design

In order to investigate the impact tolling zone derivations –which are derived from unsupervised 298 learning methods- have on the performance of adaptive distance-based congestion pricing schemes, 299 when applied on an urban network, experiments are conducted on the Boston CBD network illustrated 300 in Figure 4. A linear tolling function is considered with lower and upper bounds on the toll charged 301 in each zone (i.e $\phi_l(\boldsymbol{\theta}_l^t, D_l) = \theta_{l1}^t + \theta_{l2}^t D_l$; and $0 \leq \phi_l(\boldsymbol{\theta}_l^t, D_l) \leq 1.5$). The simulation period is from 302 06:00-09:00 covering the morning peak. As noted earlier, historical demand and supply parameters 303 are obtained from prior offline calibrations of DynaMIT2.0 for the Boston Central Business District 304 network (Azevedo et al., 2018). The estimation interval is 5 minutes and the prediction horizon is 30 305 minutes. The Boston network we consider contains 846 nodes, 1746 links, 3085 segments, 5057 lanes 306 and 13080 origin-destination pairs. 307

The performance measures are calculated for the population of vehicles with habitual departure time within 06:00-09:00 (these drivers may later change the departure time in response to the traffic conditions). A *warm-up* period of 15 min is used and the last 15 min of the simulation is a *cooldown* period without toll optimization to ensure that all the vehicles with habitual departure time in 06:00-09:00 finish their trips.

The mean and standard deviation of the value of time are S\$23.5 and S\$5.75 respectively. The cost coefficient for each vehicle is calculated from the lognormally distributed sampled value of time. The parameters of the pre-trip choice model are summarized in Table 2.

A total of six scenarios are considered, which are summarized in Table 3. All scenarios involve dynamic tolls computed using the framework described in Section 2, with the exception of the base scenario (**B0**) which is the *No Toll* case. Recall that the state estimation interval is 5 minutes implying that in the case of distance-based pricing schemes the tolling function parameters vary every 5 minutes. The simulations were run using Ubuntu Linux on an HPC Cluster, with 5x60 cores and 5x250GB RAM. The base scenario **B0** was calibrated to replicate prevailing traffic conditions in the Boston CBD

Parameter	Value		
β_{CM}	-0.5		
β_{CT}	-12		
β_{CDT_1}	-0.12		
β_{CDT_2}	-0.79		
β_{CDT_3}	-1.15		
β_{CDT_4}	- 1.65		
eta^v_t	-0.008		
β_E	-0.004		
β_L	-0.016		

Table 2: Pre-trip Behavioral Model - Parameters

(refer to Azevedo et al. (2018) for more details). However, given the fact that a No Toll base scenario 322 may not provide specific information regarding what portion of the performance uplift stems from these 323 novel distance-based tolling schemes, rather than the inherent effects of using tolling to internalize the 324 congestion externality, we are also considering a comparison scenario **B1**, (termed **UNIREG-TSI**), 325 which employs predictive distance-based tolling on the Boston CBD network as a unitary region. 326 Scenarios **B2**, **B3**, **B4**, **B5** employ predictive distance-based tolling and differ only in the derivation 327 of the tolling zones. In scenario **B2** (termed **SSCEL-TSI**), tolling zones are defined based on TSI 328 data using SSCEL. In scenario **B3** (termed **SSCOMP-TSI**), tolling zones are defined based on TSI 329 data using SSCOMP. In scenario **B4** (termed **OPTICS-TSI**), tolling zones are defined based on TSI 330 data using OPTICS, and finally, in scenario **B5** (termed **HDBSCAN*-TSI**) they are based on TSI 331 data using HDBSCAN^{*}. Scenarios **B0-B5** are evaluated on three performance measures, total social 332 welfare (SW), consumer surplus (CS) and average travel time (TT) to capture overall societal benefits, 333 together with the impact on individual travelers. 334

Table 3: Simulation scenarios

Scenario	Tolling Scheme	Description		
B0	No Toll	No tolling scheme in place		
B1	Predictive distance-based	Tolling zone encompassing entire network: UNIREG-TSI		
B2	Predictive distance-based	Tolling zones derived from: SSCEL-TSI		
B3	Predictive distance-based	Tolling zones derived from: SSCOMP-TSI		
B4	Predictive distance-based	Tolling zones derived from: OPTICS-TSI		
B5	Predictive distance-based	Tolling zones derived from: HDBSCAN*-TSI		

335 5.2. Results

The performance measures for all simulation scenarios are summarized in Table 4, the differences 336 in SW and CS (in \$ amounts) of scenarios B1-B5 relative to the base scenario B0 are presented in 337 Figure 7a, and the relative performance in terms of average travel time (% improvement) over the base 338 scenario B0 is illustrated in Figure 7b. From Table 4, **B1-B5** exhibit an increase between \$182623.5 339 - \$206866.5 and \$64814.9 - \$127062.4, for SW and CS respectively, relative to **B0**. The average SW 340 gain per traveller, relative to the No Toll case is found to be around \$1.69 for those acquired via sparse 341 subspace clustering and around \$2.15 for tolling zone derivations acquired via hierarchical density-based 342 clustering. 343

Observe that all the scenarios yield a positive consumer surplus indicating that net user benefits 344 are positive even prior to any use of the toll revenues. This is a surprising finding and in contrast with 345 several past studies that have estimated negative user benefits (for example Eliasson and Mattsson 346 (2006) and De Palma et al. (2005)). We conjecture that this is a result of several factors. First, as 347 noted by Van Den Berg and Verhoef (2011)), in the case when there is heterogeneity in the value of time 348 (and values of schedule delay), the net user benefits may depend in large part on the extent and nature 349 of heterogeneity. In experiments on a variant of the standard bottleneck model including departure 350 time choice and a transit alternative (with heterogeneity in value of time, schedule delay, early and 351

late), Chen (2022) find that when the coefficient of variation in the value of time exceeds around 0.5, 352 the net user benefits start to become positive (even before accounting for distribution of toll revenues). 353 Second, our system integrates the provision of consistent guidance information with the optimization 354 of tolls. These two factors coupled with the high levels of initial congestion may be the reason why we 355 observe positive net user benefits even prior to a redistribution of toll revenues. Similar tests across 356 different network topologies and spatio-temporal congestion patterns are required to determine whether 357 this finding is a peculiarity of our context and network. The significant variation of differences in both 358 welfare and CS across the five schemes confirms that the performance of distance-based tolling schemes 359 is appreciably affected by the definition of the tolling zones. First, observe that the two sparse subspace 360 clustering approaches yield quite different clusters and varying outcomes in terms of both CS and 361 welfare. Scenario **B2** (SCCEL) yields the second lowest overall welfare, which is only marginally higher 362 than scenario **B1** where the entire network is treated as a single zone. The reason for the relatively poor 363 performance is two-fold. First, as is apparent in Figure 5a, SCCEL results in clusters that lack spatial 364 compactness. In other words, zones are 'non-contiguous' and links in different parts of the network 365 belong to the same zone (links belonging to the red cluster or zone in particular). This clearly poses an 366 issue in the toll optimization, since the toll design includes a two-part tariff where the fixed component 367 is charged during each entry into a new zone (in other words each time a zone boundary is traversed). 368 Overall, it results in the fixed part of the tariff being optimized at a much lower level than in the case 369 when the zones are spatially compact (SSCOMP in Scenario **B3** and Scenarios **B4**, **B5**). Interestingly, 370 the low tolls charged result in a high consumer surplus, comparable with the best performing scenario 371 since the travel time gains and reductions in schedule delay costs are still significant. 372

The second reason for the poor performance of SCCEL in Scenario **B2** may be attributed to the clusters themselves. Observe that the key difference in the clusters or zones between Scenario **B2** and Scenario **B3** (which yields a significantly larger welfare) is that Scenario **B3** clearly demarcates the Back Bay region from the rest of Boston (Figure 4) whereas this is not the case in Scenario B2. The Back Bay region contains the Prudential center, which is a major attractor of trips in the morning peak and hence, arguably, the zone definitions in Scenario **B3** are more meaningful. This is also evident from the clustering performance metrics which clearly indicate that the clusters are more homogeneous in the case of Scenario **B3** than **B2** (SC of 0.198 versus 0.114).

Turning to the hierarchical density-based clustering approaches, we observe that both OPTICS 381 (Scenario B4) and HDBSCAN* (Scenario B5) yield meaningful clusters/zone definitions. Both dis-382 tinguish the densely residential South Boston region (red cluster in Figure 6a and orange cluster in 383 Figure 6b; see also Figure 4) from the commercial South Boston Waterfront (pink cluster in Figure 6a 384 and blue cluster in Figure 6b). In Scenario B4, the commercial downtown region (dark green cluster 385 in Figure 6a) is separated from the more residential North End and West End regions (light green 386 cluster in Figure 6a). These three regions are all combined into a single zone in Scenario B5 (green 387 cluster in Figure 6b). The most notable difference in the clusters between B4 and B5 and one that 388 most likely leads to the significant performance difference is that Scenario B5 clearly demarcates the 389 Back Bay region from the residential South End region (red and purple clusters in Figure 6b) unlike 390 Scenario B4. As discussed earlier, this appears to be the reason for Scenario B5 yielding the largest 391 gains in social welfare and consumer surplus. Scenario B5 also yields the clusters with links that are 392 internally homogeneous (SC of 0.4). Note that when using speed for clustering as we have done, the 393 more homogeneity within the clusters in an of itself does not appear to guarantee superior performance 394 in terms of welfare. This is evident when comparing Scenarios B3 and B4: B4 yields superior metrics 395 in terms of clustering performance but yields lower overall welfare. This underscores the importance 396 of checking the reasonableness of the clusters themselves using context specific knowledge of demand 397 patterns, land-use etc. 398

Notably, the TT performance improvement illustrated in Figure 7b, relative to the base case **B0** is substantial in all schemes. It would appear that the Boston CBD area would benefit from an application of a predictive distance-based tolling scheme, with average travel time TT improvements of up to 52% (relative to **B0**). However, we do caution that the large travel time improvements may also be, in part, due to a large number of short 'crossing' trips that are an artifact of modeling only the CBD area.

While it should be stated that while all the predictive distance-based tolling schemes yield substantial network performance benefits when compared to the No Toll scenario, scenario **B5** with HDBSCAN*- ⁴⁰⁶ based tolling zone derivation yields the largest welfare gains. The observed welfare increase comes from ⁴⁰⁷ the reduction in schedule delay costs and low travel times, which may be attributed to the efficient ⁴⁰⁸ internalization of travel externality-associated costs through distance-based tolling. This in fact applies ⁴⁰⁹ to all distance-based schemes considered in the experiments.

Scenario **B3** with only 2 tolling zones derived from SSCOMP resulted in comparable levels of 410 performance to the Scenario **B5**, and in cases where computational effort poses a significant hurdle 411 for practical implementation, it would be preferable to use SSCOMP. Although the HDBSCAN*-based 412 tolling zone derivation leads to the best results, it is also more computationally intensive, due to the 413 large number of tolling function parameters that require optimization. The overall computational time 414 for scenarios B1-B3 were around 4 hours. Given we are simulating the 6-9 AM peak period, this does not 415 yet achieve real-time performance for a 5-minute horizon. However, this could be attained by increasing 416 the parallelization or marginally reducing the number of GA generations during the optimization. In 417 case of scenarios B4, B5 where the number of zones are larger, the run times were significantly higher 418 at 12 hours. In this case, to achieve real-time performance we would need to switch to a 15-minute roll 419 period. For more details on computational considerations we refer the reader to Gupta et al. (2020). 420

	Scenarios						
Metrics	B1	B2	B3	B4	B5		
SW (\$)	181792.0	182623.5	205345.1	194744.3	206866.5		
CS (\$)	64814.9	126194.4	110504.2	84083.7	127062.4		
TT (s)	168.0	172.2	152.3	156.3	147.9		

Table 4: Performance measures

In Figure 8a, the Empirical Cumulative Distribution Function (ECDF) of the total toll charge (for the population of vehicles) for scenarios **B1**, **B2**, **B3**, **B4**, **B5** is presented. It is evident that the majority of the traveler population (almost 90%) pay total tolls no higher than \$3 for any of the distance-based pricing schemes. Further, the overall magnitude of toll charges in the case of scenario



Figure 7: Performance results for scenarios B1, B2, B3, B4, B5 relative to B0

B4 is consistently higher than that of scenarios **B3**, **B5**, which happen to be the best performing 425 scenarios. On the other hand, the overall magnitude of toll charges in scenario **B2** is consistently lower 426 than that of scenarios **B3**, **B5**, which could be explained by the fact that the corresponding tolling zone 427 derivation suffers in terms of spatial compactness, thus leading to lower tolling efficiency. For scenario 428 **B1**, where the entire BCBD network is treated as a single tolling zone, we can observe that more than 429 60% of the population is charged the toll upper bound (1.5\$), which leads to inequitable charging, but 430 also higher revenue. The reason for this lies in the fact that, unlike the case of scenarios **B2-B5**, there 431 is only one zone for the vehicles to traverse. 432

As is evident from Figure 8b, demonstrating the ECDF of travel time improvement per OD-pair, for less than 10% of the traveler population, travel times are equal or lower for scenario **B0**, as compared to scenarios **B1-B5**. Up to 90% of the traveler population benefits from lower travel times, in scenarios **B1-B5** employing distance-based tolling methods, compared to base scenario **B0**. It is also evident that the largest proportion of the traveler population subset that benefits from lower travel times corresponds to **B2**, though followed very closely by **B1**.



(a) ECDF of total Toll Charge values for scenariosB1, B2, B3, B4, B5



(b) ECDF of TT improvement per OD-pair over **B0** for scenarios **B1, B2, B3, B4, B5**



439 5.3. Iterating between toll zone definition and toll optimization

Recall that the motivation behind using unsupervised learning for the toll zone definition is to 440 decouple the problems of toll definition and toll value optimization. This avoids having to solve a 441 complex mixed-integer programming problem for the design of the distance-based scheme. Second, 442 and more importantly, the decoupling of the two problems also serves to provide a useful separation 443 between what is performed offline and what is performed online. Specifically, the proposed framework 444 involves setting the tolling zones offline and then optimizing the toll values in real-time every five or 445 fifteen minutes (within for example, a traffic management system). In this context, it may be desirable 446 to re-evaluate the zone definitions periodically, say every month or every quarter (as is done in the 447 current ERP system in Singapore for the setting of the toll rates). In this setting, a loop from the toll 448 optimization and the toll design would be beneficial. 449

In order to do so, we redo the clustering exercise in two ways. First, we compute an implied perdistance toll rate for each link and time interval from the optimized tolling function parameters obtained via the predictive distance-based toll optimization framework. We then use the resulting toll values from each scenario as a feature and perform the clustering once again with SSCEL,SSCOMP,OPTICS and HDBSCAN*, respectively. Note that clearly, since tolling function parameters are identical for all links in the same zone by construction, this can only yield an aggregation of the original zone definitions. Nevertheless, it serves to examine robustness of the original zone definitions. Second, we redo the clustering using the travel speed indices obtained after the application of the optimized tolls. Interestingly, in both cases we observe that the original clustering results and metrics are quite robust (see Figures 9–12). However, in the case that they are not, this procedure could in principle be performed iteratively and the zone definitions could be updated.



(a) 2 zones derived using SCCEL for feature TSI, with SC=0.118, DB=3.716 $$\rm SSCOMP-TOLL$$



(b) 2 zones derived using SSCOMP for feature TSI, with SC=0.194, DB=1.252

Figure 9: Clustering results and tolling zones (Sparse Subspace Clustering)



(b) 5 zones derived using HDBSCAN* for feature TSI, with SC=0.400, DB=0.776

Figure 10: Clustering results and Tolling zones (Hierarchical Density-based Clustering)



(b) 2 zones derived using SSCOMP for feature TSI, with SC=0.102, DB=4.009 $\,$

Figure 11: Clustering results and tolling zones (Sparse Subspace Clustering)



(b) 5 zones derived using HDBSCAN* for feature TSI, with SC=0.400, DB=0.776

Figure 12: Clustering results and Tolling zones (Hierarchical Density-based Clustering)

461 6. Conclusions and Future Work

In this paper we investigated the use of sparse subspace clustering methods to define tolling zones 462 for distance-based tolling schemes, and their impact on traffic network performance using a predictive 463 real-time distance-based toll optimization framework. Experiments were conducted on the real-world 464 urban network of the Boston Central Business District. We determined that the best network perfor-465 mance comes from the use of distance-based tolling zones derived from HDBSCAN*, when using Travel 466 Speed Index data. Performance using only 2 tolling zones acquired via the SSCOMP sparse subspace 467 clustering variant was found to be comparable to that of a 5-zone, HDBSCAN*-based derivation, so, in 468 cases where minimizing computational effort is one of the primary objectives, as is the goal of this work, 469 it should be considered as a viable alternative. Despite the fact that all clustering approaches produced 470 tolling zone derivations which, as part of our framework, contributed to significant performance gains, 471 when compared to the No Toll case, we observed large differences in performance between tolling zone 472 derivations acquired via the sparse subspace clustering variants. Specifically, for this particular dataset, 473 the SSCEL variant of sparse subspace clustering produced low quality clustering, due to the low degree 474 of spatial compactness. This warrants further investigation, however, overall, tolling zone derivations 475 acquired from both types of clustering methods, yielded significant benefits on network performance 476 and even outperformed a predictive distance-based tolling scheme that treated the network as a single 477 zone. Finally, the results also underscore the importance of relying not solely on clustering perfor-478 mance metrics but also the reasonableness of the clusters themselves using context-specific knowledge 479 of demand patterns, land-use etc. 480

In future work, we aim to evaluate alternate clustering methods for systematic tolling zone derivation as part of the distance-based tolling optimization framework. Compared to our No Toll base case, social welfare and network performance results suggest that the clustering can produce distance-based tolling zones with considerable positive impact. We are also in the process of investigating alternative solution approaches, including Bayesian and Surrogate Optimization, and comparing toll optimization framework performance to that of our currently used solution approach.

487 Author statement

⁴⁸⁸ The authors confirm contribution to the paper as follows:

Antonis F. Lentzakis: Conceptualization, methodology, visualization, investigation, formal analy sis, writing-Original draft preparation, writing-Review & Editing Ravi Seshadri: Conceptualization,
 methodology, writing-Original draft preparation, writing-Review & Editing Moshe Ben-Akiva: Con ceptualization, methodology, supervision.

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