Optimal toll design problems under mixed traffic flow of human-driven vehicles and connected and autonomous vehicles

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\textbf{Abstract:} Compared to human-driven vehicles (HDVs), connected and autonomous vehicles (CAVs) can drive closer to each other to enhance link capacity. Thereby, they have great potential to mitigate traffic congestion. However, the presence of HDVs in mixed traffic can significantly reduce the effects of CAVs on link capacity, especially when the proportion of HDVs is high. To address this problem, this study seeks to control the HDV flow using the autonomous vehicle/toll (AVT) lanes introduced by Liu and Song (2019). The AVT lanes grant free access to CAVs while allowing HDVs to access by paying a toll. To find the optimal toll rates for the AVT lanes to improve the network performance, first, this study proposes a multiclass traffic assignment problem with elastic demand (MTA-ED problem) to estimate the impacts of link tolls on equilibrium flows. It not only enhances behavioral realism for modeling the route choices of HDV and CAV travelers by considering their knowledge level of traffic conditions but also captures the elasticity of both HDV and CAV demand in response to the changes in the level of service induced by the tolls on AVT lanes. Thereby, it better estimate the equilibrium network flows after the tolls are deployed. Then, two categories of optimal toll design problems are formulated according to whether the solution of the HDV route flows, CAV link flows and corresponding origin-destination demand of the proposed MTA-ED problem is unique or not. To solve these optimal toll design problems, this study proposes a revised method of feasible direction. It linearizes the anonymous terms in the upper-level problem by leveraging the analytical sensitivity analysis results of the lower-level MTA-ED problem. This algorithm is globally convergent on the condition that the MTA-ED problem has a unique solution. It can also be leveraged to solve optimal toll design problems when the MTA-ED problem has multiple solutions. Numerical application found that due to disruptive effects on link capacity, using HDVs may significantly reduce the network performance such as customer surplus and total travel demand. The proposed method can assist different stakeholders to find the optimal toll rates for HDVs on AVT lanes to maximize the network performance under mixed traffic environments.

\textbf{Keywords:} Connected and autonomous vehicles; Multiclass traffic assignment problem with elastic demand; Optimal toll design; Sensitivity analysis

1. Introduction

Connected and autonomous vehicle (CAV) is a transformative technology that will significantly improve the mobility of people and goods in the future. They equip with advanced sensors and high-performance computers which enable them to detect and react to the surrounding driving environments.

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much faster than humans. Compared to human-driven vehicles (HDVs), a CAV can follow the leading vehicle with a shorter distance. The spacing between vehicles can be further reduced if the CAVs form a platoon to drive cooperatively with each other, which significantly increases the link capacity (Wang et al., 2019a). Existing studies show that the link capacity can be increased by as large as four times if all vehicles are CAVs and drive cooperatively with each other in a platoon (Tientrakool et al., 2011). Thereby, the CAVs have great potential to mitigate the traffic congestion problem.

However, in the transition period when both HDVs and CAVs exist on a road, the road capacity is sensitive to the proportions of vehicle classes due to various time headways for each vehicle class (Xiao et al., 2018). The higher time headways and heterogeneous driving behavior of HDVs can significantly reduce the mobility of the mixed traffic. Further, a large proportion of HDVs in the flow will also reduce the occurrence and size of the CAV platoon. Thereby, the presence of HDVs in the mixed traffic will reduce the effects of CAVs on enhancing link capacity, especially when the proportion of HDVs is high. Recently, several analytical-based and simulation-based studies (e.g., Levin and Boyles, 2016; Xiao et al., 2018; Olia et al., 2018) have found that the link capacity is a superlinear function of the proportion of CAVs. It has no significant improvement if the proportion of CAVs in mixed traffic is less than 40% (e.g., the proportion of HDVs is over 60%). Thereby, how to exploit the potential of CAVs to enhance link capacity and reduce traffic congestion under mixed traffic environments is a great challenge for both engineers and researchers.

To address this problem, recently, two strategies have been proposed to amplify the effects of CAVs on link capacity, including the autonomous vehicle dedicated lanes (Chen et al. 2016; Chen et al. 2017) and the autonomous vehicle/toll (AVT) lanes (Liu and Song, 2019). The AV dedicated lanes enhance the link capacity by preventing HDVs to access. However, this strategy may underutilize the road resources when the market penetration rate of CAVs is low (Liu and Song, 2019). By comparison, the autonomous vehicle/toll (AVT) lanes, which grant free access to AVs while allowing HDVs to access the lanes by paying a toll, can provide more freedom for the operators to control the link capacity. The concept of AVT is similar to congestion pricing in inner cities where private vehicles need to pay a toll to access this area while the transit vehicles are toll-free due to its large capacity in transporting passengers. Note that CAVs can not only increase the link capacity to reduce traffic congestion, but also significantly save the valuable urban space for parking. Thereby, compared with HDVs, it is a more desirable modal to access the congestion areas in a city, especially the areas with dense land use.

To fully exploit the potential of CAVs for mitigating traffic congestion and encourage the adoption of CAVs in the transition period, this study seeks to optimize the toll rates for the AVT lanes to control the HDV flow to maximize the system objectives for both public- and private-sector stakeholders. In this study, we assume all autonomous vehicles are CAVs and have level 4 automation as defined by SAE International (2016), where little human intervention is needed during trips. Further, we assume each AVT lane is an independent link and will use the term AVT link to avoid confusion.

The concept to control the network flows to maximize network performance through road pricing has been extensively studied in the literature. Based on where the toll roads can be set, the toll design problems can be divided into two categories; the first-best toll pricing problem and the second-best toll pricing problem (Yang and Huang, 2005). The first-best toll pricing problem seeks to charge the users on all links to minimize the total travel cost (with fixed demand) or maximize the customer surplus (with elastic demand). Typically, the theory of first-best pricing is developed upon the fundamental economic
principle of marginal-cost pricing. Existing theoretical studies show that the social net benefit can be maximized by setting a toll on each road equivalent to the difference between the marginal social cost and the marginal private cost in the context of homogeneous users (Walters, 1961; Dafermos and Sparrow, 1969; Dafermos and Sparrow, 1971). Investigations are also conducted on how the marginal-cost pricing scheme would work in the context of multiple user classes with heterogeneous vehicle types (Dafermos, 1973; Xu et al., 2013), or the value of time (Yang and Zhang, 2002). The second-best toll pricing charges the users on only some of the links rather than on all links in the network to maximize the network performance. It is more practical and deployable compared to the first-best toll pricing (Han and Yang, 2009). Extensive studies have been conducted by leveraging the concept of the second-best toll pricing to find the optimal charging schemes to: maximize the revenue (Yang and Lam, 1996), maximize the customer surplus (Santos, 2004), and reduce the environmental impacts of traffic (Ferrari, 1995) considering different flow and toll-based constraints.

The above-mentioned studies address the toll design problems in the context of HDV flows. For optimal toll design problems under mixed traffic environments with HDVs and CAVs, Liu and Song (2019) proposed a bi-level programming problem to optimize the deployment of AVT links and corresponding toll rates simultaneously to minimize the social cost. However, they characterize the route choice behavior of both CAVs and HDVs using the user equilibrium (UE) model, which assumes the travelers have perfect information on the traffic conditions and can choose a route to minimize the actual travel cost. This assumption cannot hold for HDV travelers as human drivers typically have limited knowledge of traffic conditions (Wang et al., 2019b). Further, they assume the demand is fixed regardless of the tolls charged for HDVs on the AVT links. This assumption overlooks the travelers’ responses to the change of origin-destination (OD) travel cost. Several existing studies show that travelers’ travel decisions are very sensitive to travel costs including petrol prices and the tolls paid for driving (Goodwin, 1992; Oum et al., 1992). For example, a field study showed that the total trips by passenger vehicles to the toll zones in London, Stockholm, and Milan are reduced by 18%, 18%, and 14.2%, respectively, after the toll schemes are implemented, which the modal shift to public transport is the major contributor to this reduction (Hensher and Li, 2013). A state preference survey also shows that the number of passenger vehicle-based trips would be reduced by 4%-15% across different locations under different tolling schemes (Li and Hensher, 2012). Thereby, it is not hard to deduce that deploy AVT links will induce a significant change of OD demand for both HDVs and CAVs.

Note that the equilibrium model which captures the change in travel behavior (e.g., cancel or make the trip, or change route to avoid the toll) in response to the tolls on AVT links is critical to estimate the network flows. Therefore, it is necessary to endogenously model the route choice and elasticity of travel demand for both HDVs and CAVs to predict the future demand and flow distribution pattern more accurately to avoid the biased assessment of the effects of tolls on AVT links under mixed traffic environments. To address the gaps in the previous study, this study develops a new multiclass traffic assignment problem with elastic demand (label MTA-ED problem). The MTA-ED problem assumes that the HDV travelers choose routes according to the cross-nested logit (CNL) model with elastic demand (label CNL-ED model) while the CAV travelers choose routes according to the UE model with elastic demand (label UE-ED model). The CNL-ED model not only captures traveler’s perception error of the route travel cost but also models the change of trip rate in response to the change of level of service induced by tolls on AVT links. The UE-ED model characterizes the CAVs’ capability to acquire accurate
information on traffic conditions and their trip rate over OD travel cost simultaneously. Thereby, the proposed model enhances behavioral realism for both HDV and CAV travelers.

To find the optimal toll rates for the AVT links for both public- and private-sector stakeholders, this study proposes two categories of optimal toll design problems according to whether the solution of HDV route flows, CAV link flows and corresponding OD demand of the MTA-ED problem is unique or not. When the solution is unique, the upper-level problem is developed to find the optimal toll rates for the AVT links to maximize the performance indicator. When multiple solutions exist for the MTA-ED problem, the upper-level problem seeks to find the optimal toll rates for the AVT links to maximize the performance indicator in the worst case (i.e., the local equilibrium solution under which the performance indicator is minimum). The lower-level problem is the MTA-ED problem formulated to capture the impacts of link tolls on the distribution of both HDV and CAV flows. Three performance indicators are used in this study (i) the total revenue (i.e., total tolls collected), (ii) the customer surplus, and (iii) the total demand. It should be noted that the AVT links considered in this study are only a subset of the links in the network, i.e., there exist some other links which are not tollable. Thereby, the optimal toll design problems discussed in this study belong to the category of second-best toll pricing problem.

To solve the proposed bi-level programming problems when the MTA-ED problem has a unique solution, this study revises the norm-relaxed method of feasible direction (NRMFD) proposed by Cawood-Kostreva's (1994). It linearizes the anonymous terms (such as link capacity, equilibrium link flows, objective function, etc.) in the upper-level problem using first-order Taylor approximation method with corresponding derivatives obtained through sensitivity analysis of the lower-level MTA-ED problem. In each iteration, it solves a quadric programming problem developed upon the linearized system of the upper-level problem to find a feasible descent direction. A new method is then proposed to find the optimal step for the feasible descent direction. The solution algorithm can converge globally if the lower-level MTA-ED problem has a unique solution (Cawood and Kostreva, 1994; Chen and Kostreva, 2000). A solution algorithm is also presented by leveraging the revised NRMFD to find the optimal toll rates on AVT links to maximize the network performance in the worst case when the MTA-ED problem has multiple solutions.

The current study seeks to answer and address three interrelated and important questions related to optimal toll design in the transition period when both HDVs and CAVs exist. First, how to access the impact of link tolls on the distribution of the mixed flows? Second, how to find the optimal toll rates for the AVT links to maximize the design objectives for different stakeholders in cases when the MTA-ED problem has a unique solution and in cases when it has multiple solutions. Third, is it necessary to control the access of the HDVs on some links in the network under mixed traffic environments? The first question is addressed by proposing an MTA-ED problem that considers the travel behavior of both HDV and CAV users. The second question is addressed by the proposed solution algorithm which can solve different optimal toll design problems effectively and efficiently. The third question is analyzed by comparing the network performance indicators (e.g., customer surplus and total demand) before (i.e., no tolls) and after deploying the optimal toll rates.

The contributions of this study are threefold. First, we formulate a variational inequality (VI)-based MTA-ED traffic assignment problem. It not only enhances the behavioral realism for modeling the route choices of HDV travelers but also captures the elasticity of traffic demand of both HDVs and CAVs in response to the tolls on AVT links. Thereby, it enhances behavior realism and can better estimate the
impacts of link tolls on the equilibrium flow solution compared with the existing study (Liu and Song, 2019). Further, we formulate an equivalent fixed demand-based multiclass traffic assignment (MTA) problem to enable the application of the route-swapping-based solution algorithm (Wang et al., 2019b) to solve the proposed MTA-ED problem. Second, we revise the norm-relaxed method of feasible direction (label revised NRMFD) proposed by Cawood and Kostreva’s (1994) to solve the three optimal toll design problems when the low-level MTA-ED problem has a unique solution. This algorithm converges very fast and is globally convergent even if the bi-level optimal toll design problems are non-convex. To our knowledge, this is the first study in the literature applying this algorithm to solve a bi-level network design problem. We also propose a solution algorithm for optimal toll design problems when multiple solutions exist for the MTA-ED problem by leveraging the revised NRMFD. Third, to enable the application of the revised NRMFD, we analytically formulate the sensitivity analysis method for the MTA-ED problem. It aids in obtaining the derivatives of the equilibrium link flows, equilibrium capacity of AVT links, and the objective functions of the proposed optimal toll design problems with respect to the link toll rates. These derivatives can be leveraged to solve the optimal toll design problems as well as be used to approximate the equilibrium solutions of the MTA-ED problem when the network is subject to perturbations (e.g., capacity reduction due to road construction).

The structure of this study is as follows. Section 2 develops a VI-based MTA-ED problem in which the HDV travelers and CAV travelers are assumed to choose routes according to the CNL-ED model and the UE-ED model, respectively. A solution algorithm is then proposed for the MTA-ED problem. In Section 3, two categories of optimal toll design problems are formulated according to whether the MTA-ED problem has a unique solution or not. Section 4 presents the solution algorithm for the proposed optimal toll design problems. Section 5 discusses the results of numerical experiments for the proposed model and the convergence performances of the solution algorithms. Section 6 concludes with the main findings, insights, and potential future research directions.

2. Formulation and solution algorithm for the multiclass traffic assignment problem with elastic demand

The following notations will be used to formulate the equivalent VI-based MTA-ED problems and develop a corresponding solution algorithm. Let the subscript $H$ and $A$ denote the HDV and CAV, respectively. Let $z$ be a vehicle class and $Z = \{H, A\}$ be the set of all vehicle classes. Let $W_z$ be the set of all OD pairs and $R^w_z$ be the set of all routes connecting OD pair $w$, $w \in W_z$ for vehicle class $z$, $z \in Z$. Denote $q^w_{k,z}$ as the travel cost of route $k$ between OD pair $w$ for vehicle class $z$. Denote $q^w_{a,z}$ as the flow of vehicle class $z$ on route $k$ between OD pair $w$. Let $v_{a,z}$ be the flow of vehicles in vehicle class $z$ on link $a$. Denote $q^w_z$ as the demand between OD pair $w$, $w \in W_z$ for vehicle class $z$ and $q_z$ be the vector of all OD demand for vehicle class $z$, $z \in Z$. Dente $S^w_z$ as the expected perceived travel cost for OD pair $w$ and vehicle class $z$. Denote $D^w_z(S^w_z)$ as the elastic demand function for OD pair $w$, $w \in W_z$ and vehicle class $z$, $z \in Z$. $\Gamma_z$ denotes the set of all links for vehicle class $z$.

2.1 VI formulations for the MTA-ED problem

2.1.1 VI formulation for CNL-ED model

This section presents an equivalent VI problem for the CNL-ED model. It is constructed upon route
flows to facilitate formulating the MTA-ED problem and designing a corresponding solution algorithm. For simplicity, suppose the network only contains the HDVs. According to Prashker and Bekhor (1999), and Wang et al. (2019b), at equilibrium state of the CNL-ED model, the probability to choose route \( k \) between OD pair \( w \) (i.e., \( p^w_H(k) \)) can be formulated as

\[
p^w_H(k) = \sum_{m \in \Gamma_H} p^w_H(k|m)p^w_H(m)
\]

(1a)

where \( p^w_H(m) \) is the marginal probability that a traveler between OD pair \( w \) will choose the nest(link) \( m \); and \( p^w_H(k|m) \) is the conditional probability that a traveler between OD pair \( w \) will choose route \( k \) provided that he/she already choose the nest(link) \( m \).

\[
p^w(k|m) = \frac{\left[ \alpha^w_{m,k} \exp (-\theta c^w_{k,H}) \right]^{1/u}}{\sum_{l \in \Gamma_H} \left[ \alpha^w_{m,l} \exp (-\theta c^w_{l,H}) \right]^{1/u}}
\]

(1b)

\[
p^w(m) = \frac{\left( \sum_{k \in \Gamma_H} \left[ \alpha^w_{m,k} \exp (-\theta c^w_{k,H}) \right]^{1/u} \right)^u}{\sum_{b \in \Gamma_H} \left( \sum_{l \in \Gamma_H} \left[ \alpha^w_{b,l} \exp (-\theta c^w_{l,H}) \right]^{1/u} \right)^u}
\]

(1c)

where \( u \) is the degree of nesting, \( 0 < u \leq 1 \), \( \theta \) is the dispersion parameter, \( \alpha^w_{m,k} \) is the inclusion coefficient, formulated as

\[
\alpha^w_{m,k} = \left( \frac{l_m}{l^w_k} \right)^\gamma \delta^w_{m,k}
\]

(1d)

where \( l_m \) and \( l^w_k \) are the length of link \( m \) and route \( k \) between OD pair \( w \), respectively, and \( \delta^w_{m,k} = 1 \) if route \( k \) uses link \( m \) and 0 otherwise.

Further, according to Kitthamkesorn et al. (2016), the equilibrium OD demand should also be a function of the expected perceived travel cost between corresponding OD pair, i.e.,

\[
q^w_H = \sum_{k \in \Gamma_H} f^w_{k,H} = D^w_H(S^w_{H*})
\]

(2a)

where

\[
S^w_{H*} = -\frac{1}{\theta} \ln \sum_{b \in \Gamma_H} \left( \sum_{l \in \Gamma_H} \left[ \alpha^w_{b,l} \exp (-\theta c^w_{l,H}) \right]^{1/u} \right)^u
\]

(2b)

Or equivalently, the inverse of the elastic demand function (i.e., \( D^{-1}_H(q^w_H) \)) equals the expected perceived travel cost at the equilibrium state, namely,

\[
D^{-1}_H(q^w_H) = S^w_{H*}
\]

(2c)

where \( q^w_H \) is the equilibrium HDV demand between OD pair \( w \). \( f^w_{k,H} \) is the equilibrium HDV flow on route \( k \) between OD pair \( w \). \( D^{-1}_H(q^w_H) \) is the inverse of the demand function \( D^w_H(S^w_{H*}) \) in Eq. (2a). Eq. (2a) and Eq. (2b) show that charging HDVs on AVT links used by some routes for HDVs between OD pair \( w \) are likely to increase the expected perceived OD travel cost, resulting in fewer OD travel demand.

To formulate the equivalent traffic assignment problem for CNL-ED model, let \( G^w_{k,H} \) be the generalized travel cost of route \( k \) for HDVs between OD pair \( w \), formulated as
\[
G_{k,H}^w = \frac{1}{u} c_{k,H}^w - \frac{1}{\theta} H_{k,H}^w + \frac{1}{\theta} \ln \left( \frac{f_{k,H}^w}{q_H^w} \right)
\]

where
\[
H_{k,H}^w = \ln \left[ \sum_{m \in R_H} \left( \alpha_{m,k}^w \right)^{1/u} \left( \sum_{l \in R_H^w} [\alpha_{m,l}^w \exp (-\theta \tilde{c}_l^w)]^{1/u} \right) \right]^{u-1}
\]

It should be noted that the generalized travel cost is different from it is in Wang et al. (2019b). Note that the OD demand can be obtained by summing the flows of routes between the corresponding OD pair. Thereby, we only study the conditions for equilibrium route flows for CNL-ED. Recall that at the equilibrium state of the CNL-ED model, the route flows should satisfy Eq. (1) and Eq. (2) simultaneously, the following necessary and sufficient conditions are developed for the CNL-ED model.

**Proposition 1:** The CNL-ED route flows \( f_{k,H}^w \) are at equilibrium if and only if they satisfy
\[
G_k^w (f_{k,H}^w) - D_{k,H}^{-1,w} (q_{k,H}^w) = 0, \quad \text{if} \ f_{k,H}^w > 0; \quad \forall w \in W, \forall k \in R_H^w
\]

where \( \Lambda_H f_{k,H}^w = q_{k,H}^w, \quad f_{k,H}^w \geq 0. \) \( q_{k,H}^w \) is a vector of equilibrium demand of all OD pairs for HDVs.

**Proof:** We first prove the ‘if part’. Suppose the route flow vector \( f_{k,H}^* \) satisfies Eq. (5). As the probability to choose a route with zero flow is 0, we only consider the routes whose flows are positive. According to Eq. (3) and Eq. (5), we have
\[
\frac{1}{u} c_{k,H}^w - \frac{1}{\theta} H_{k,H}^w + \frac{1}{\theta} \ln \left( \frac{f_{k,H}^w}{q_H^w} \right) = D_{k,H}^{-1,w} (q_{k,H}^w)
\]

Then, the probability that a route \( k \) is chosen by a traveler for an OD pair \( w \) is:
\[
p_k^w = \frac{f_{k,H}^w}{q_H^w} = \exp \left( -\frac{\theta}{u} c_{k,H}^w + H_{k,H}^w + \theta D_{k,H}^{-1,w} (q_{k,H}^w) \right)
\]

Note that
\[
1 = \sum_{j \in R_H^w} p_j^w = \sum_{j \in R_H^w} \exp \left( -\frac{\theta}{u} c_{k,H}^w + H_{k,H}^w + \theta D_{k,H}^{-1,w} (q_{k,H}^w) \right)
\]

\[
= \exp \left( \theta D_{k,H}^{-1,w} (q_{k,H}^w) \right) \sum_{j \in R_H^w} \exp \left( -\frac{\theta}{u} c_{k,H}^w + H_{k,H}^w \right)
\]

Then, we have
\[
\exp \left( \theta \cdot D_{k,H}^{-1,w} (q_{k,H}^w) \right) = \frac{1}{\sum_{j \in R_H^w} \exp \left( -\frac{\theta}{u} c_{k,H}^w + H_{k,H}^w \right)}
\]

Therefore,
\[
p_k^w = \frac{\exp \left( -\frac{\theta}{u} c_{k,H}^w + H_{k,H}^w \right)}{\sum_{j \in R_H^w} \exp \left( -\frac{\theta}{u} c_{k,H}^w + H_{k,H}^w \right)}
\]

Submit Eq. (4) into Eq. (10), we have
\[
p_k^w = \frac{\sum_{m \in R_H} \left( \alpha_{m,k}^w \right)^{1/u} \left( \sum_{l \in R_H^w} [\alpha_{m,l}^w \exp (-\theta \tilde{c}_l^w)]^{1/u} \right) \left( \sum_{m \in R_H} \left( \alpha_{m,k}^w \right)^{1/u} \left( \sum_{l \in R_H^w} [\alpha_{m,l}^w \exp (-\theta \tilde{c}_l^w)]^{1/u} \right) \right)^{u-1}}{\sum_{b \in R_H} \left( \sum_{l \in R_H^w} [\alpha_{b,l}^w \exp (-\theta \tilde{c}_l^w)]^{1/u} \right)^u}
\]

Eq. (11) is consistent with the cross-nested logit (CNL) route choice model shown in Eqs. (1a-1c).
Now, we will show that if \( f_H^* \) satisfies Eq. (5), the inverse of the demand function equals the expected perceived OD travel cost at the equilibrium state.

Note that if \( f_H^* \) satisfies Eq. (5), then Eq. (11) holds. Submit Eq. (3), Eq. (4) and Eq. (11) into Eq. (5), we have

\[
G_{k,H}^w D_{H}^{-1,w}(q_{H}^w) = \frac{1}{u} c_{k,H}^w - \frac{1}{\theta} H_{k,H}^w + \frac{1}{\theta} \ln(p_{k}^w(k))
\]

\[
= \frac{1}{u} c_{k,H}^w + \frac{1}{\theta} \ln\left( \frac{p_{k}^w(k)}{\sum_{m \in R_H^w}(\alpha_{m,k}^w \frac{1}{u} \left( \sum_{i \in R_H^w} \alpha_{i,m}^w \exp(-\theta c_{i,l}^w) \right)^{1/u}} \right)
\]

\[
= \frac{1}{\theta} \ln\left( \frac{1}{\sum_{b \in R_H^w} \left( \sum_{i \in R_H^w} \alpha_{b,i}^w \exp(-\theta c_{i,l}^w) \right)^{1/u}} \right)
\]

\[
= -\frac{1}{\theta} \ln \sum_{b \in R_H^w} \left( \sum_{i \in R_H^w} \alpha_{b,i}^w \exp(-\theta c_{i,l}^w) \right)^{1/u}
\]

(12)

According to Eq. (12) and Eq. (2b), \( D_{H}^{-1,w}(q_{H}^w) = S_{H}^w \). The equilibrium condition for demand elasticity (i.e., Eq. (2c)) is satisfied.

The above proof shows that if \( f_H^* \) satisfies Proposition 1, then it is the equilibrium route flow of the CNL-ED model. The proof of ‘if part’ is done. Suppose \( f_H^* \) is the equilibrium route flow of the CNL-ED model. The proof of only if part follows the same steps by submitting \( q_{H}^w = D_{H}^w(S_{H}^w) \) and Eq. (11) into Eq. (5). The details of the proof are omitted to avoid duplication.

According to Proposition 1, the conditions in Proposition 1 can be formulated as the following VI-based CNL-ED model. The equivalence between Eq. (13) and Proposition 1 can be proved using the same method as shown in Wie et al. (1995).

\[
\sum_{k \in K_{H}^w} \sum_{w \in W} (G_{k,H}^w(f_H^*)) - D_{H}^{-1}(q_{H}^w) (f_{H}^w - f_{H}^w) \geq 0
\]

(13)

where \( f_H^* \in \Omega_{f_H^*} = \{f_H | \Lambda_H f_H = q_H, f_H^* \geq 0\}, \Omega_{f_H^*} \in \Omega_{f_H^*} \).

2.1.2 Equivalent VI-based MTA-ED problems

Note that the CAVs can obtain information on traffic conditions through vehicle-to-infrastructure communication. Thereby, we assume the CAVs have perfect information on the traffic state and make route choices according to the UE-ED model. Without loss of generality, let the generalized route travel cost for CAVs equals the actual route travel cost, i.e., \( G_{k,A}^w = c_{k,A}^w \). Suppose \( f_A^* = [f_{k,A}^*, \forall k \in R_A^w, \forall w \in W_A] \) is the equilibrium route flow solution for CAVs. Then, according to Nagurney (2013), \( G_{k,A}^w, \forall k \in R_A^w, \forall w \in W_A \) must satisfy:

\[
G_{k,A}^w - D_{A}^{-1,w}(q_{A}^w) = 0, \text{ if } f_{k,A}^* > 0, \forall k \in R_A^w, \forall w \in W_A
\]

(14)

where \( \Lambda_A f_A^* = q_A^*, f_A^* \geq 0 \). \( D_{A}^{-1,w}(q_{A}^w) \) is the inverse demand function for CAVs between OD pair \( w \), which equals the shortest travel cost of all the routes between OD pair \( w \) at the equilibrium state.

Denote \( G_{k,z}^w = G_{k,z}^w - D_{z}^{-1,w}(q_{z}^w) \) as the revised travel cost for route \( k \) between OD pair \( w \) for vehicle class \( z \). Let \( f_H^* \) and \( f_A^* \) be the vector of flows of all routes for HDVs and CAVs, respectively.
According to equilibrium conditions (5) and (14), it can be shown that the route flows \( \{f^*_H, f^*_A\} \) are at the equilibrium state of the CNL-ED model and the UE-ED model for HDVs and CAVs, respectively, if and only if they solve the following VI problem:

\[
\sum_{w \in W_H} \sum_{k \in R^W_H} C^w_{k,H}(f^*_{k,H}) (f^*_{k,H} - f^*_{k,H}) + \sum_{w \in W_A} \sum_{k \in R^W_A} C^w_{k,A}(f^*_k) (f^*_k - f^*_k) \geq 0,
\]

or equivalently, in a vector form

\[
C_H(f^*)^T (f_H - f^*_H) + C_A(f^*)^T (f_A - f^*_A) \geq 0
\]

where \([f^T_H, f^T_A] \in \Omega = \{[f^T_H, f^T_A] | \Lambda_H f_H = q^H_H; \Lambda_A f_A = q^A_H; f_H \geq 0; f_A \geq 0 \} \). \( f^* = [f^*_H, f^*_A] \). \( C_H(f^*) \) and \( C_A(f^*) \) are vectors of the revised travel costs of all routes for HDVs and CAVs, respectively. The equivalence between VI problem (15) and the two equilibrium conditions in Eq. (5) and Eq. (14) can be shown using the method in Nagurney (2000). To find the working routes that are likely to be used by both HDV and CAV travelers in VI problem (15), the link penalty approach proposed by De La Barra et al. (1993) will be used in this study.

Note that

\[
\sum_{w \in W_A} \sum_{k \in R^W_A} G^w_{k,A}(f^*_{k,A} - f^*_{k,A}) = t^*_A (v_A - v^*_A)
\]

\[
- \sum_{w \in W_A} \sum_{k \in R^W_A} D^{-1}_{A} (w)(f^*_{k,A} - f^*_{k,A}) = (-D^{-1}_{A}) (q^*_A - q^*_A)
\]

where \( t^*_A \) is the vector of travel costs of all links for CAVs at the CNL-ED equilibrium state \( f^* \); \( v_A \) is the vector of all CAV link flows and \( v^*_A \) is the equilibrium CAV link flows at the CNL-ED equilibrium state \( f^* \); \( D^{-1}_{A} = [D^{-1}_{A}(w), \forall w \in W_A] \); \( q^*_A = [q^w_{A}, \forall w \in W_A] \).

Let \( X = [f^T_H, v^T_A, q^T_A] \), and \( X^* = [f^*_H, v^*_A, q^*_A] \) be the equilibrium solution corresponding to \( f^* \). According to Eq. (16), the VI problem (15) can be written equivalently as

\[
C_H(f_H - f^*_H) + t_A(v_A - v^*_A) + (-D^{-1}_{A}) (q^*_A - q^*_A) \geq 0
\]

where \([f^T_H, v^T_A, q^T_A] \in \Omega_X = \{[f^T_H, v^T_A, q^T_A] | \Lambda_H f_H = q^H_H; \Lambda_A f_A = v^A_H; f_H \geq 0; v_A \geq 0 \} \).

It is important to know that the VI problem (17) contains three decision vector variables, i.e., the vector of all HDV route flows \( f_H \), the vector of all CAV link flows \( v_A \) and the vector of all OD demand of CAVs \( q_A \).

### 2.1.3 Link travel cost functions for HDVs and CAVs

To characterize the link travel time for mixed traffic, the following Bureau of Public Roads (BPR) function proposed by Wang et al. (2019b) will be used in this study

\[
\bar{t}_a(v_{a,H}, v_{a,A}) = \bar{t}_a^0 \left[ 1 + \left( \frac{v_{a,H} + v_{a,A}}{Q_a} \right)^4 \right]
\]

where \( \bar{t}_a(v_{a,H}, v_{a,A}) \) is the travel time of either a CAV or an HDV on link \( a \), and \( t_a^0 \) is the free-flow travel time of link \( a \). \( v_{a,H} \) and \( v_{a,A} \) are the HDV and CAV flows on link \( a \), respectively. \( Q_a \) is the capacity of link \( a \), computed as

\[
Q_a = \frac{1}{v_{a,H} + v_{a,A}} + \frac{1}{v_{a,H} + v_{a,A} Q_{a,h}} + \frac{1}{v_{a,H} + v_{a,A} Q_{a,a}}
\]
where $Q_{a,H}$ and $Q_{a,A}$ are link capacities when all vehicles are CAVs and HDVs, respectively. $P_{a,A}$ is the proportion of CAVs on link $a$. The denominator on the right-hand side of Eq. (19) denotes the average time headway of the mixed traffic. $Q_{a,A} \geq Q_{a,H}$ as the reaction times of CAVs are no larger than those of HDVs (Wang et al., 2019b).

![Figure 1. Link capacity under different proportions of CAVs](image)

It should be noted that the effects of CAVs on link capacity in mixed traffic are heterogeneous for different proportions of CAVs. To better illustrate this fact, suppose the capacity of a link with pure HDVs is 2000 (i.e., $Q_{a,H} = 2000$). Figure 1 shows the evolution of link capacity with respect to proportions of CAVs in the mixed traffic when $Q_{a,A} = 2Q_{a,H}$, $Q_{a,A} = 2.5Q_{a,H}$ and $Q_{a,A} = 3Q_{a,H}$, respectively. As can be seen, when the proportion of CAVs is low (less than 40%), they do not significantly affect link capacity. The effects of CAVs on increasing link capacity become salient when the proportion of CAVs in the mixed traffic is large. This is because link capacity is an inverse function of the average time headway of the mixed traffic, which decreases linearly with respect to the proportion of CAVs. This pattern shows that when the proportion of CAVs on a link is small, controlling the HDV flow can significantly increase the link capacity and reduce the link travel time of the mixed traffic.

Note that for HDVs, the travel cost not only includes the travel time but also includes the tolls paid to access the AVT links. Thereby, the following equivalent link travel time will be used to measure the link travel cost for HDVs and CAVs, respectively.

$$t_{a,H} = \bar{t}_a(v_{a,H}, v_{a,A}) + \tau_a \cdot E_a, a \in \Gamma_H$$  \hspace{1cm} (20a)

$$t_{a,A} = \bar{t}_a(v_{a,A}), a \in \Gamma_A$$  \hspace{1cm} (20b)

where $t_{a,H}$ and $t_{a,A}$ are link travel costs (measured by equivalent link travel time) for HDVs and CAVs, respectively. $\tau_a$ is the toll rate for HDVs on link $a$ ($\tau_a \equiv 0$ if link $a$ is not an AVT link). $E_a$ is the equivalent travel time for one unit of toll.

It is important to know that the link capacity function (19) is formulated based on the assumption of
heterogeneous time headways for CAVs and HDVs. It can be replaced by other models proposed in the literature (e.g., Lazar et al., 2017; Liu and Song., 2019), which considers the impacts of heterogeneous time headways for different vehicle pairs (i.e., an HDV follows a CAV, an HDV follows an HDV, a CAV follows an HDV, and a CAV follows a CAV). This will not impact the modeling framework and algorithm design for both the multiclass traffic assignment and the optimal toll problem as they all functions of the ratio of CAVs.

2.1.4 Existence and local uniqueness of the solution for the MTA-ED problem (17)

The following assumption will be made to discuss the existence and local uniqueness of the solution for the MTA-ED problem.

**Assumption 1:** The demand function $D_z^w(S_z^w)$ is a continuous, and a monotonically decreasing function of $S_z^w$, $\forall w, \forall z$.

Based on Assumption 1 and the link travel cost functions in Eq. (20), both $C_H(f)$ and $C_A(f)$ are continuous in $f$. As $\Omega_f$ is convex, compact, and non-empty, there must exist at least one solution for the VI problem (15), so do VI problem (17).

However, due to the complex term $H_{H,A}$, and the heterogeneous impacts of HDV flow and CAV flow on link travel cost, the Jacobian matrix of the vector-valued function $[C_H, t_A^T, (-D_A^{-1})^T]^T$ is asymmetric. It is very hard to show that this Jacobian matrix is positive definite throughout the feasible space of the decision variables (i.e., $\Omega_f$). Thereby, the MTA-ED problem (17) may be non-convex and have multiple solutions. Nevertheless, the equilibrium solution $[f_H^T, v_A^T, q_A^T]$ to the MTA-ED problem (17) is locally unique for given inputs of parameters $Q_{a,H}$ and $Q_{a,A}$.

To show this, let $\bar{\mathbf{C}} = [C_H, t_A^T, (-D_A^{-1})^T]^T$. Denote $\bar{\mathbf{c}}^*$ as the value of $\bar{\mathbf{C}}$ at an arbitrary local equilibrium state $x^*, x^* = [f_H^T, v_A^T, q_A^T]$. Then, the Jacobian matrix of the vector-valued function $[C_H, t_A^T, (-D_A^{-1})^T]^T$ at $x^*$ can be written as

$$
\frac{\partial \bar{\mathbf{C}}^*}{\partial \mathbf{x}} = \begin{bmatrix}
\frac{\partial C_H}{\partial f_H} & \frac{\partial t_A^*}{\partial v_A} & 0 \\
\frac{\partial C_H}{\partial f_H} & \frac{\partial t_A^*}{\partial v_A} & 0 \\
0 & 0 & -\frac{\partial D_A^{-1}}{\partial q_A}
\end{bmatrix}
$$

Using similar proof in Wang et al. (2019), it can show that the Jacobian matrix $\begin{bmatrix}
\frac{\partial C_H}{\partial f_H} & \frac{\partial t_A^*}{\partial v_A} \\
\frac{\partial C_H}{\partial f_H} & \frac{\partial t_A^*}{\partial v_A} \\
\frac{\partial C_H}{\partial f_H} & \frac{\partial t_A^*}{\partial v_A}
\end{bmatrix}$ is positive definite at the local equilibrium state $x^*$ (it is omitted here to avoid duplication). Under Assumption 1, $-\partial D_A^{-1}/\partial q_A$ is positive definite. Thereby, $\partial \bar{\mathbf{C}}^*/\partial \mathbf{x}$ is positive definite at $x^*$. This indicates that the equilibrium solution $x^*$ is locally unique.

Thereafter, other than specified, when we say the MTA-ED problem has a unique solution or its solution is locally unique we intend to say the solution of HDV route flows, CAV link flows and corresponding OD demand of the MTA-ED problem (17) (i.e., $x^*$) is unique or locally unique.
2.2. Solution algorithm for the MTA-ED problem

2.2.1 Equivalent fixed demand-based MTA problem

The MTA-ED problem is hard to be solved using the VI-based solution algorithms (e.g., projection method, Tikhonov regularization method, etc.) because they need to solve a subproblem to find a feasible descent direction in each iteration, which is computationally expensive due to the complex generalized route travel cost function for HDVs (Eq. (3)). To address this problem, Wang et al. (2019b) proposed a route-swapping-based solution algorithm, labelled RSRS-MSRA algorithm. It finds a descent direction based on an analytically model developed upon Smith’s route swapping model and updates the steps in each iteration using a modified self-regulated average method. Thereby, it circumvents solving the subproblems in VI-based solution algorithms which significantly reduce the computational complexity.

However, the RSRS-MSRA algorithm is only applicable to the fixed demand-based MTA problems. It cannot be applied to solve VI problem (15) due to the elastic demand function. To enable the application of the RSRS-MSRA solution algorithm, we will convert the MTA-ED problem into an equivalent fixed demand-based MTA problem similar to the method proposed in Sheffi (1985) which converts the UE-ED problem into an equivalent fixed-demand UE problem.

To do this, we add a dummy route to connect each OD pair directly. The dummy route can be used by both HDVs and CAVs (see Figure 2). We use the subscript ‘\(dmy\)’ to denote the dummy route between the corresponding OD pair.

The revised travel costs for all dummy routes are set as 0 (See Figure 2). To distinguish from the real network, define the real network combined with all dummy routes as the augmented network. By this definition, the real network is a subnetwork of the augmented network.

![Figure 2. Conceptual illustration of an augmented network for one OD pair](image)

Suppose the demand for each OD pair is fixed in the augmented network. Denote \(\tilde{q}^w_z\) as the fixed demand for OD pair \(w, w \in W\), and vehicle class \(z, z \in Z\) in the augmented network. \(\tilde{q}^w_z\) is set sufficiently large such that \(\tilde{q}^w_z > q^w_*= \sum_{k \in R^w_z} f^w_{k,z}\). Let \(\bar{\mathbf{q}}_z\) be the vector of all OD demand for vehicle class \(z\) in the augmented network. Denote \(f^w_{dmy,z}\) as the flow of vehicles in class \(z\) on the dummy route between OD pair \(w\), and \(f^w_{dmy,z} = \left[f^w_{dmy,z}, \forall z, w\right]\). Similar to Wang et al. (2019b), the fixed demand-based MTA problem for the augmented network can be written as

\[
\sum_{z \in Z} \sum_{w \in W} \sum_{k \in R^w_z} C^w_{k,z}(f^w)\left(f^w_{k,z} - f^w_*) + \sum_{z \in Z} \sum_{w \in W} C^w_{dmy,z}(f^w_{dmy,z} - f^w_*) \geq 0
\]

where

\[
[f^T_z, f^T_{dmy,z}, \forall z] \in \bar{\Omega}_f = \{(f^T_z, f^T_{dmy,z}, \forall z) | \Lambda_z f_z + f_{dmy,z} = \bar{\mathbf{q}}_z; f_z, f_{dmy,z} > 0, \forall z \in Z\}.
\]

The main difference between the VI problem (21) and the VI problem (15) is that the OD demand in VI problem (21) is fixed to enable the application of the RSRS-MSRA solution algorithm. Let \(f_{dmy} = \)
\([\tilde{f}_{dmy,H}^T, \tilde{f}_{dmy,A}^T]\). The following two Propositions will be used to show the consistency of the equilibrium flow solution on real routes between the VI problem (21) and the VI problem (15).

**Proposition 2.** For an arbitrary OD pair \(w\) and vehicle class \(z\), if \(\tilde{q}_z^w\) is sufficiently large, then at the equilibrium state of VI problem (21), \(f_{dmy,z}^w > 0\).

**Proof:** Let \([f^*, f_{dmy}^T]^T\) be the equilibrium route flow solution for the VI problem (21). Let \(f_{k,z}^w\) and \(f_{dmy,z}^w\) be the equilibrium route flow solution for vehicles in class \(z\) on a real route \(k\) and the dummy route between OD pair \(w\), respectively. According to Wang et al. (2019b), at the equilibrium state, the revised costs of all used routes are equal, i.e., \(C_{k,z}^w = G_{k,z}^w (f^*) - D^{-1}_z(q_z^w) = \eta\) for \(f_{k,z}^w > 0, \forall k \in R_z^w\), where \(\eta\) is a finite value. Note that \(q_z^w = \sum_{j \in R_z^w} f_{k,z}^w\). Then, we have \(q_z^w = D^{-1}_z(G_k^w (f^*) - \eta)\). Recall that \(D^w(G_k^w (f^*) - \eta)\) is positive and decreases in \(G_k^w (f^*)\). Thereby, \(D^w(G_k^w (f^*) - \eta)\) is bounded. Let \(\tilde{q}_z^w\) be the upper bound of the demand function \(D_z^w\). Note that \(f_{dmy,z}^w + \sum_{k \in R_z^w} f_{k,z}^w = f_{dmy,z}^w + q_z^w = \tilde{q}_z^w\). Thereby, if \(\tilde{q}_z^w > q_k^w\), we must have \(f_{dmy,z}^w = \tilde{q}_z^w - q_z^w > q_k^w - q_z^w \geq 0\). This completes the proof.

The following Proposition shows that the equilibrium flow solution of VI problem (21) on real routes in the augmented network also solves the VI model (15).

**Proposition 3:** Suppose \([f^*, f_{dmy}^T]^T\) is the equilibrium route flow solution for the VI problem (21), if \(f_{dmy,z}^w > 0, \forall z, w\), then \(f^*\) solves the VI problem (15).

**Proof:** As \([f^*, f_{dmy}^T]^T\) solves the VI model (19), according to Wang et al (2019b), the revised travel costs of all routes with positive flows are equal for both HDVs and CAVs. Note that the flows for all dummy routes are positive (i.e, \(f_{dmy,z}^w > 0, \forall z, w\)) and the revised travel costs for these dummy routes are 0. Then the revised travel costs of all real routes with positive flows are 0. This indicates that the route flow pattern \(f^*\) satisfies the CNL-ED condition and the UE-ED condition in Eq. (5) and Eq. (14) simultaneously. Thereby, it solves the VI problem (15). This completes the proof.

Proposition 3 indicates that at the equilibrium state \([f^*, f_{dmy}^T]^T\) of VI problem (21), the traffic demand for an arbitrary vehicle class \(z\) and OD pair \(w\) in the real network is \(q_z^w = \sum_{k \in R_z^w} f_{k,z}^w = D(S_z^w (f^*))\). This implies that the flow on the dummy route between OD pair \(w\) for vehicle class \(z\) is \(\tilde{q}_z^w = D(S_z^w (f^*))\). Thereby, the main idea to solve the MTA-ED problem using a solution algorithm for fixed demand-based MTA problem (21) is to add a dummy route between each OD pair in the real network to hold the surplus OD demand for both HDVs and CAVs so that the equilibrium flows on the real routes for the VI problem (21) and the VI problem (15) are the same.

### 2.2.2 Solution algorithm for the VI problem (21)

This section presents the detailed steps to implement the RSRS-MSRA algorithm to solve the VI problem (21), which helps to obtain the equilibrium route flow solution for the VI problem (15) based on Proposition 3. Let \(\tilde{f}\) be the vector of the flow of all routes in the augmented network, \(\tilde{f} = [f^*, f_{dmy}^T]^T\), and \(\tilde{f}_n\) be the value of \(\tilde{f}\) at iteration \(n\). At iteration \(n + 1\), the flows of all routes in the augmented network
are updated using the following models
\[
\mathbf{f}_{n+1} = \mathbf{f}_n + \beta_n \Phi(\mathbf{f}_n) = \left[ \mathbf{f}_{n,H} \right] + \beta_n \left[ \Phi_H(\mathbf{f}_n) \right] \tag{22a}
\]
where \( \Phi_H(\mathbf{f}_n) = (\phi_{k,H}^w(\mathbf{f}_n), \forall k \in R_H^w, w \in W_H) \) and \( \Phi_A(\mathbf{f}_n) = (\phi_{k,A}^w(\mathbf{f}_n), \forall k \in R_A^w, w \in W_A) \) are updated by:
\[
\phi_{k,H}^w(\mathbf{f}_n) = \sum_{g \in R_H^w} \left[ f_{g,H}^w(n) \left( C_{g,H}^w(\mathbf{f}_n) - C_{k,H}^w(\mathbf{f}_n) \right)_+ - f_{k,H}^w(n) \left( C_{k,H}^w(\mathbf{f}_n) - C_{g,H}^w(\mathbf{f}_n) \right)_+ \right] \tag{22b}
\]
\[
\phi_{k,A}^w(\mathbf{f}_n) = \sum_{g \in R_A^w} \left[ f_{g,A}^w(n) \left( C_{g,A}^w(\mathbf{f}_n) - C_{k,A}^w(\mathbf{f}_n) \right)_+ - f_{k,A}^w(n) \left( C_{k,A}^w(\mathbf{f}_n) - C_{g,A}^w(\mathbf{f}_n) \right)_+ \right] \tag{22c}
\]
The step \( \beta_n \) is computed as
\[
\beta_n = \frac{1}{h_n \chi_n} \tag{22d}
\]
\[
h_n = \max \left( h_{i,z}^w(n) \mid h_{i,z}^w(n) = \sum_{g \in R_Y}(C_{g,z}^w(\mathbf{f}_n) - C_{i,z}^w(\mathbf{f}_n))_+, \forall i \in R_z^w, \forall w \in W_z, \forall z \in Z \right) \tag{22e}
\]
\[
\chi_n = \begin{cases} 
\geq 2; & \text{if } n = 1 \\
\chi_{n-1} + Y_1; & \text{if } \| \Phi(\mathbf{f}_n) \| \geq \| \Phi(\mathbf{f}_{n-1}) \| \text{ and } n \geq 2 \\
\chi_{n-1} + Y_2; & \text{if } \| \Phi(\mathbf{f}_n) \| < \| \Phi(\mathbf{f}_{n-1}) \| \text{ and } n \geq 2 
\end{cases} \tag{22f}
\]
where \( h_{i,z}^w(n) \) is the flow of route \( i \) for vehicle class \( z \) between OD pair \( w \) at iteration \( n \). \( (x)_+ = x \) if \( x > 0 \), otherwise, \( x = 0 \); \( \beta_n \) is the step size. It decides how far the current route flow goes along the descent direction \( \Phi_H(\mathbf{f}_n) \). The term \( 1/h_n \) ensures that the total flow swapped from an arbitrary route to other routes is not larger than the flow on this route. \( Y_1 \) and \( Y_2 \) are predetermined parameters.

The full steps to solve the VI problem (21) can be summarized as follows

**Step 1**: Let \( n = 0 \). Set a sufficiently large demand for each OD pair for both CAVs and HDVs. Assign the OD demand to all real and dummy routes between corresponding OD pairs. Denote the resulted route flow as \( \mathbf{f}_0 \).

**Step 2**: Compute the OD demand in the real network based on all real route flows, i.e., \( \mathbf{q}_n = \left[ \Lambda^H \right] \mathbf{f}_n \).

Then compute the vector of inverse of all demand functions \( \mathbf{D}^{-1}(\mathbf{q}_n) \), the vector of all revised route travel costs \( \mathbf{G}_n \) and the vector of all generalized route travel costs \( \mathbf{G}_n \) in the augmented network sequentially.

**Step 3**: Update the route flows according to Eq. (22a).

**Step 4**: Let \( n = n + 1 \). If \( \mathbf{f}_n \) satisfies the convergence criteria, then stop. Otherwise, go to step 2.

It should be noted that in each iteration, the RSRS-MSRA algorithm only computes the route flows. The OD demand is updated based on the route flows. To measure the solution quality, the convergence criteria (denoted as \( \varepsilon_1 \)) is formulated as:
\[
\varepsilon_1 = \frac{\mathbf{f}_n \cdot \mathbf{G}_n}{\mathbf{f}_n \cdot \mathbf{G}_n} \tag{23}
\]

Eq. (23) shows that if \( \mathbf{f}_n \) computed by the RSRS-MSRA algorithm is closer to the equilibrium route flow solution, then \( \varepsilon_1 \) is closer to 0.

It should be noted that in the case when multiple solutions of the MTA-ED problem (17) exist (i.e.,
the RSRS-MSRA algorithm only give a local equilibrium solution $x^*$, which depends on the initial route flow pattern $\bar{f}_0$, i.e., if the initial route flow pattern $\bar{f}_0$ locates in a local convex hall containing the locally optimal solution $x^*$, the RSRS-MSRA algorithm will converge to an equilibrium route flow $f^*$ which results in $x^*$. This indicates that if the RSRS-MSRA algorithm is applied with more number of initial points in the feasible set, more number of the local equilibrium solution $x^*$ will be found. This character will be useful to find the optimal toll rates in Section 3.3 when multiple solutions of the MTA-ED problem (17) exist.

3. Optimal toll design problems

This study considers the second-best pricing problem where only a subset of links in the network can be tolled to maximize the design objectives. The tolls are only set for HDVs. The CAVs are toll-free on any roads in the network. The main motivation for this toll strategy is to reduce the proportion of the HDVs on the toll roads to increase the link capacity so that the traffic congestion can be mitigated. To better demonstrate the usefulness of this toll strategy, we consider three optimal toll problems, i.e., the maximum total revenue problem, the maximum customer surplus problem, and the maximum total demand problem. The three network design problems seek to find the optimal toll rates for the AVT links to maximize the total tolls, the customer surplus, and the total trips in the network, respectively. The maximum total revenue problem is designed for the interest of the private-sector stakeholders while the rest two problems are designed from the interest of the public-sector stakeholders.

Let $\Gamma_T$ be the set of AVT links in the network. Denote $\tau_a, a \in \Gamma_T$ as the toll rate for HDVs on AVT link $a$, and $\tau = [\tau_a, \forall a \in \Gamma_T]$ be the vector of toll rates for all AVT links in the network. Denote $F_{TR}, F_{CS}$ and $F_{TD}$ as the total revenue, customer surplus, and total demand in the network, formulated as

$$F_{TR}(x(\tau), \tau) = \sum_{a \in \Gamma_T} v_{a,H} \cdot \tau_a \quad (24a)$$

$$F_{CS}(x(\tau), \tau) = \sum_{z \in Z} \sum_{w \in W_z} \int_0^{q_{w}^z} D_z^{-1,w}(s) ds - \sum_{a \in I_T} (v_{a,H} \cdot t_{a,H}) - \sum_{a \in I_A} (v_{a,A} \cdot t_{a,A}) \quad (24b)$$

$$F_{TD}(x(\tau), \tau) = \sum_{w \in W_H} q_{H}^w + \sum_{w \in W_A} q_{A}^w \quad (24c)$$

As mentioned before, we cannot analytically show that the MTA-ED problem (17) has a unique solution. However, numerical applications in different networks using the RSRS-MSRA algorithm with a large set of different initial points found that they always converge to the same optimal point. This indicates that the solution of the HDV route flows, the CAV link flows, and the OD demand of the CAVs at the MTA-ED equilibrium state can be unique. This phenomenon occurs perhaps because the link travel cost functions for both CAVs and HDVs used in this study only differ in fixed terms and are monotonic increasing in CAV and HDVs flows. Nevertheless, as we cannot guarantee the solution $x^*$ is unique in all cases, we will formulate two categories of optimal toll design problems based on whether the solution of the MTA-ED problem (17) is found to be unique or not. The optimal toll design problems with a unique solution of the MTA-ED problem (17) are the basis to formulate and solve the optimal toll design problems with multiple solutions to the MTA-ED problem (17).
3.1 Optimal toll design problems when the MTA-ED problem (17) has a unique solution

When the solution of the MTA-ED problem (17) is unique, the three optimal toll design problems are formulated as the following bi-level programming problems. The upper-level programming problem is

\[
\begin{align*}
\min_{\tau} & \quad -F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau}) \\
\text{s.t.} & \quad v_{a,H}^{*}(\mathbf{\tau}^H) + v_{a,A}^{*}(\mathbf{\tau}) - Q_{a}^{*}(v_{a,H}^{*}, v_{a,A}^{*}, \mathbf{\tau}) \leq 0, \; \forall a \in \Gamma_{T} \\
\tau_a & \leq \tau_{\max}, \; \forall a \in \Gamma_{T} \\
\tau_a & \geq 0, \; \forall a \in \Gamma_{T}
\end{align*}
\] (25a)

(25b)

(25c)

(25d)

where \(\mathbf{x}^*(\mathbf{\tau})\) is the equilibrium flow solution of the lower-level MTA-ED problem (17).

In Eq. (25), \(F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\) denotes the objective function for the three optimal toll design problems, i.e., \(F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau}) = F_{TR}(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\) for the maximum total revenue problem, \(F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau}) = F_{CS}(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\) for the maximum customer surplus problem and \(F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau}) = F_{TD}(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\) for the maximum total demand problem. \(v_{a,H}^{*}(\mathbf{\tau})\) and \(v_{a,A}^{*}(\mathbf{\tau})\) are equilibrium flows on link \(a\) under toll strategy \(\mathbf{\tau}\) for HDVs and CAVs, respectively. \(Q_{a}^{*}(v_{a,H}^{*}, v_{a,A}^{*}, \mathbf{\tau})\) is the capacity of the AVT link \(a\) at the equilibrium state under toll strategy \(\mathbf{\tau}\).

The inequality constraints (25b)-(25d) are the same for the three optimal toll design problems. Inequality (25b) ensures that the sum of HDV flow and CAV flow on each ATV link is less than the link capacity to avoid traffic congestion. Inequalities (25c) and (25d) present the upper and lower bounds of the toll rates charged on each AVT link, respectively. They show that all toll rates are nonnegative and are no larger than \(\tau_{\max}, \tau_{\max} > 0\). For simplicity, we denote \(\Omega_{\tau}\) as the set of all \(\mathbf{\tau}\) which satisfying the inequality constraints (25b)-(25d) simultaneously.

3.2 Optimal toll design problems when the MTA-ED problem (17) has multiple solutions

When multiple solutions are found for the MTA-ED problem (17), to assure a minimum level of network performance after deploying the AVT links, we will develop robust optimization problems to find the optimal toll rates for the AVT links to increase the network performance (value of a performance indicator in Eq. (24)) in the worst-case. Let \(\Omega_{x,\tau}\) be the set of equilibrium solutions of the lower-level MTA-ED problem (17) with toll strategy \(\mathbf{\tau}\). Then, the local solution of the MTA-ED problem (17) with toll strategy \(\mathbf{\tau}\) which minimizes the value of the performance indicator can be found by solving the problem \(\min_{\mathbf{x}^*(\mathbf{\tau})} F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\), where \(F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\) represents the value of a performance indicator in Eq. (24) at a local solution \(\mathbf{x}^*(\mathbf{\tau})\). The system performance in the worst-case under toll strategy \(\mathbf{\tau}\) (i.e., at a local solution where the value of the performance indicator is minimum among others) can be written as \(\min_{\mathbf{x}^*(\mathbf{\tau})} F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\). The three optimal toll design problems are formulated as the following robust optimization problems.

\[
\begin{align*}
\max_{\tau \in \Omega_{\tau}} \min_{\mathbf{x}^*(\mathbf{\tau})} F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})
\end{align*}
\] (26a)

where \(\mathbf{x}^*(\mathbf{\tau})\) and the set \(\Omega_{x,\tau}\) in problem (26a) are obtained by solving the lower-level MTA-ED problem (17). Similarly, in (26a), the performance indicator \(F(\mathbf{x}^*(\mathbf{\tau}), \mathbf{\tau})\) is different for the three optimal toll design problems.

The problem (26a) seeks to find the optimal solution \(\mathbf{\tau}^*\) to maximize the system performance in the
worst-case (i.e., the value of \( \min_{\mathbf{x}^*(\tau) \in \Omega_{x^*}} F(\mathbf{x}^*(\tau), \tau) \)). Let \( \Phi(\tau) = \min_{\mathbf{x}^*(\tau) \in \Omega_{x^*}} F(\mathbf{x}^*(\tau), \tau) \). Note that the solution of \( \tau \) to the problem \( \max_{\tau \in \Omega_{x^*}} \Phi(\tau) \) and the problem \( \min_{\tau \in \Omega_{x^*}} - \Phi(\tau) \) are the same, we can solve the following robust optimization problem to obtain the solution of \( \tau \) to the problem (26a).

\[
\min_{\tau \in \Omega_{x^*}} - \Phi(\tau) = \min_{\tau \in \Omega_{x^*}} - \min_{\mathbf{x}^*(\tau) \in \Omega_{x^*}} F(\mathbf{x}^*(\tau), \tau)
\]  

(26b)

A solution algorithm for the problem (26b) will be developed in the next section to find the optimal toll strategy on AVT links to maximize the system performance in the worst-case so that a minimum level of system performance (e.g., total revenue, customer surplus, total demand) can be guaranteed.

3.3 Method to solve the problem (26b) using the solution algorithm for the problem (25)

Suppose the MTA-ED problem (17) has a unique solution. Let \( \mathbf{x}^*(\tau) \) be the vector-valued function that characterizes the equilibrium flow solution of the MTA-ED problem (17) when \( \tau \) changes. Thereby, \( \mathbf{x}^*(\tau) \) maps \( \tau \) into a unique vector (i.e., the unique equilibrium solution of the MTA-ED problem (17)). Then, problem (25) can be written equivalently as \( \min_{\tau \in \Omega_{x^*}} - F(\mathbf{x}^*(\tau), \tau) \). We will discuss the method to solve this problem in Section 4. In the following, we will show how to solve the problem (26b) by leveraging the solution algorithm for the problem (25).

Suppose the MTA-ED problem (17) has multiple solutions; as the solutions of the MTA-ED problem (17) are locally unique (see Section 2.1.4), the number of these solutions must be finite. Let \( \mathbf{x}_i^*(\tau), \mathbf{x}_2^*(\tau), \ldots, \mathbf{x}_N^*(\tau) \) be the locally optimal solutions for the MTA-ED problem (17) with toll strategy \( \tau \), where \( N \) is the total number of locally optimal solutions \( (N = |\Omega_{x^*}|) \). As \( \mathbf{x}_i^*(\tau), \forall i = 1, 2, \ldots, N \) is unique for given \( \tau \), and the cost functions \( \left[ C_{h i}, t_{h i}^*, (-D_{A}^{-1})^T \right] \) in the MTA-ED problem (17) are continuous in \( \tau \); \( \mathbf{x}_1^*(\tau), \mathbf{x}_2^*(\tau), \ldots, \mathbf{x}_N^*(\tau) \) change continuously in \( \tau \). We will denote \( \mathbf{x}_i^*(\tau), \forall i = 1, 2, \ldots, N \) as a vector-valued function which maps \( \tau \) into a unique locally optimal solution of the MTA-ED problem (17). Thereby, problem (26b) can be written equivalently as

\[
\min_{\tau \in \Omega_{x^*}} - \Phi(\tau) = \min_{\tau \in \Omega_{x^*}} - \left[ \min_{\mathbf{x}_i^*(\tau)} \left( F(\mathbf{x}_1^*(\tau), \tau), F(\mathbf{x}_2^*(\tau), \tau), \ldots, F(\mathbf{x}_N^*(\tau), \tau) \right) \right]
\]  

(27)

The following Proposition discusses the solutions for the problem (27).

**Proposition 4:** If \( \mathbf{x}^* \) is a locally optimal solution for the problem (26b), then it must be a locally optimal solution for at least one of the problems \( \min_{\tau \in \Omega_{x^*}} - F(\mathbf{x}_i^*(\tau), \tau), i = 1, 2, \ldots, N \).

**Proof:** Without loss of generality, let \( \Phi(\mathbf{x}^*) = \min \left( F(\mathbf{x}_1^*(\mathbf{x}^*), \mathbf{x}^*), F(\mathbf{x}_2^*(\mathbf{x}^*), \mathbf{x}^*), \ldots, F(\mathbf{x}_N^*(\mathbf{x}^*), \mathbf{x}^*) \right) = F(\mathbf{x}_j^*(\mathbf{x}^*), \mathbf{x}^*) \), where \( j \) is an integer between 1 and \( N \). As the performance indicator \( F(\cdot) \) is a continuous function of \( \mathbf{x} \) and \( \mathbf{x}_j^*(\mathbf{x}^*) \), \( i = 1, 2, \ldots, N \) are isolated points, there exists a sufficiently small area (ball) centered at \( \mathbf{x}^* \) (denoted as \( B_1(\mathbf{x}^*) \)) such that \( \Phi(\mathbf{x}) = F(\mathbf{x}_j^*(\mathbf{x}), \mathbf{x}), \mathbf{x} \in B_1(\mathbf{x}^*) \cap \Omega_{x^*} \). Similarly, as \( \mathbf{x}^* \) is a locally optimal solution for problem (26b), there exists another sufficiently small area (ball) centered at \( \mathbf{x}^* \) (denoted as \( B_2(\mathbf{x}^*) \)) such that \( \min_{\mathbf{x} \in B_2(\mathbf{x}^*) \cap \Omega_{x^*}} - \Phi(\mathbf{x}) = - \Phi(\mathbf{x}^*) \). Therefore,

\[
- \Phi(\mathbf{x}^*) = \min_{\mathbf{x} \in B_1(\mathbf{x}^*) \cap \Omega_{x^*}} - \Phi(\mathbf{x}) = \min_{\mathbf{x} \in B_1(\mathbf{x}^*) \cap \Omega_{x^*}} - F(\mathbf{x}_j^*(\mathbf{x}), \mathbf{x}) = - F(\mathbf{x}_j^*(\mathbf{x}^*), \mathbf{x}^*)
\]  

(28)
Eq. (28) indicates that $\boldsymbol{\tau}^*$ is also a locally optimal solution of the problem $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_j^*(\tau), \tau)$. This completes the proof of Proposition 4.

Note that the problem $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_j^*(\tau), \tau)$ is very similar to the problem (25) as the locally optimal solution $\mathbf{x}_j^*(\tau)$ is unique. It can be solved using the same algorithm as used for problem (25) which will be discussed in Section 4. According to Proposition 4, the optimal solution $\boldsymbol{\tau}^*$ to the problem (26b) can be found as follows

**Step 1:** Obtain an arbitrary vector of toll rates $\boldsymbol{\tau}^0$ in $\Omega_{\tau}$ and set it as the starting point. Generate a large set of initial route flows and use the RSRS-MSRA algorithm to solve the fixed demand-based MTA problem (21) for each of these initial route flows at $\boldsymbol{\tau}^0$. Let $\mathbf{x}_1^*(\boldsymbol{\tau}^0), \mathbf{x}_2^*(\boldsymbol{\tau}^0), \ldots, \mathbf{x}_N^*(\boldsymbol{\tau}^0)$ be the isolated local equilibrium solution found by the RSRS-MSRA algorithm.

**Step 2:** Solve the problems $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_i^*(\tau), \tau), i = 1, 2, \ldots, N$ using the method introduced in Section 4. Let $\tau_i^1, \tau_i^2, \ldots, \tau_i^N$ be the locally optimal solution to these problems, respectively. According to Proposition 4, the optimal solution $\boldsymbol{\tau}^*$ to the problem (26b) must be one of the $\tau_i^j, i = 1, 2, \ldots, N$. Step 3 will be used to find the exact $\tau_i^j$ which solves problem (26b).

**Step 3:** Compute $F(\mathbf{x}_i^*(\tau_i^j), \tau_i^j), \forall i = 1, 2, \ldots N, \forall j = 1, 2, \ldots N$. Find a $i^*$ between 1 and $N$ such that $\min_{i^*} F(\mathbf{x}_i^*(\tau_i^{j^*}), \tau_i^{j^*}), j = 1, 2, \ldots, N = F(\mathbf{x}_{i^*}^*(\tau_{i^*}^{j^*}), \tau_{i^*}^{j^*})$, then $\tau_{i^*}^{j^*}$ solves problem (26b), i.e., $\boldsymbol{\tau}^* = \tau_{i^*}^{j^*}$.

In the first step, if only one solution is found by using the RSRS-MSRA algorithm, then problem (25) will be used instead to obtain the optimal toll rates for the AVT links. If multiple solutions are obtained, then steps 2 and 3 will be applied to solve the problem (26b).

It should be noted that similar to other bi-level programming problems, both problem (25) and problem (26b) are intrinsically non-convex. Therefore, we only seek to find a locally optimal solution $\boldsymbol{\tau}^*$ for the two problems, the solution for which depends on the presumed initial toll rates $\boldsymbol{\tau}^0$.

The remaining question for solving the problem (26b) is how to obtain the optimal solution for the problem $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_i^*(\tau), \tau)$ in Step 2. In the next section, we will discuss the solution algorithm for the problem $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_i^*(\tau), \tau)$ (i.e., problem (25)) where the solution of the lower-level MTA-ED problem (17) is unique. This algorithm can also be used to solve $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_i^*(\tau), \tau)$. To do this, we only need to

1. find an initial feasible flow $\mathbf{f}^0$ by which the RSRS-MSRA algorithm will converge to the initial locally optimal point $\mathbf{x}_i^*(\mathbf{f}^0)$, and
2. in each iteration $n$, set the initial route flow in the RSRS-MSRA solution algorithm sufficiently close to the equilibrium solution $\mathbf{x}_i^*(\mathbf{f}^n)$. We will discuss why the solution algorithm for the problem $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_i^*(\tau), \tau)$ can also be used to solve $\min_{\tau \in \Omega_{\tau}} - F(\mathbf{x}_i^*(\tau), \tau), \forall i$ at the end of Section 4.1.

For simplicity, in the next section, we will introduce the solution algorithm for the problem (25) in which the solution of the MTA-ED problem (17) is assumed to be unique. Further, we note that the solution to the MTA-ED problem (17) is found to be unique for different networks analyzed in the numerical section.
4. Solution algorithm for optimal toll design problem (25) when the MTA-ED problem (17) has a unique solution

In literature, many solution algorithms have been proposed to solve the second-best pricing problem in which the embedded equilibrium traffic assignment model has a unique solution (e.g., UE, SUE, etc.), including the sensitivity analysis-based algorithm (Friesz, 1990), the non-smooth approach (Chiou, 2006), the marginal function-based approach (Yang et al., 2004), etc. A review of the algorithms can be found in Wang et al. (2010). While these algorithms can effectively solve the corresponding optimal toll design problems, some of them are heuristic that may not be convergent for some initial points (Friesz, 1990), and other algorithms are only locally convergent (Yang et al., 2004) or require strong assumption for convergence (e.g., the objective function is convex, Chiou, 2006).

This section revises the norm-relaxed method of feasible direction (NRMFD) proposed by Cawood and Kostreva (1994) to solve the three optimal toll design problems (25) when the MTA-ED problem (17) has a unique solution. Compared with other existing algorithms in the literature, the revised NRMFD has two advantages: First, it can converge for non-convex optimization problems; Second, it is globally convergent (Chen and Kostreva, 2000) if the MTA-ED problem (17) has a unique solution, i.e., it converges to a locally optimal solution from an arbitrary initial point in the feasible set. The revised NRMFD can generate a sequence of points in the feasible set (i.e., points that satisfy the inequality constraints) to decrease the objective function. In the following, we will discuss the details for solving problem (25) using the revised NRMFD.

4.1 The revised NRMFD solution algorithm

As mentioned before, the bi-level optimal toll design problem (25) can be reformulated as a single-level nonlinear programming problem \( \min_{\tau \in \Omega_T} -F(x^*(\tau), \tau) \). Let \( \tau^n \) be the vector of toll rates obtained at iteration \( n \). Cawood- Kostreva's NRMFD solves the following quartic optimization problem to find a descent direction \( d = [d_a, \forall a \in \Gamma_T] \) for the problem (25) at \( \tau^n \).

\[
\begin{align*}
\min \quad & \vartheta \in \mathbb{R}^m, \quad d \in \mathbb{R}^m \quad \text{subject to} \\
& \frac{\partial}{\partial \vartheta} \frac{\partial}{\partial d} \left( \frac{\partial}{\partial d} \right)^T \cdot H \cdot \frac{\partial}{\partial d} d \leq \vartheta \quad \text{(29a)} \\
& -\nabla_\tau F(x^*(\tau^n), \tau^n) \cdot d^n \leq \vartheta \quad \text{(29b)} \\
& \sum_{x \in Z} v_{a,x}^*(\tau^n) - Q_a^*(v_{a,H}, v_{a,A}, \tau^n) + \left( \sum_{x \in Z} \nabla_\tau v_{a,x}^*(\tau^n) - \nabla_\tau Q_a^*(v_{a,H}, v_{a,A}, \tau^n) \right) d^n \leq \vartheta, \forall a \in \Gamma_T \quad \text{(29c)} \\
& \tau^n - \tau_{max} + d^n \leq \vartheta, \forall a \in \Gamma_T \quad \text{(29d)} \\
& -\tau^n - d^n \leq \vartheta, \forall a \in \Gamma_T \quad \text{(29e)}
\end{align*}
\]

where \( H \) is a symmetric positive definite matrix; \( \vartheta \) is a positive parameter; \( \nabla_\tau F(x^*(\tau^n), \tau^n) \) is the vector of derivatives of the objective function with respect to link toll variables at the equilibrium state \( x^*(\tau^n) \); \( \nabla_\tau v_{a,x}^*(\tau^n) \) is the gradient of the flow of vehicle class \( z \) on link \( a \) with respect to \( \tau \) at the equilibrium state \( x^*(\tau^n) \); \( \nabla_\tau Q_a^*(v_{a,H}, v_{a,A}, \tau^n) \) is the gradient of the capacity of link \( a \) with respect to \( \tau \) at the equilibrium state \( x^*(\tau^n) \);

Inequality (29b) ensures that the first-order change of the objective function is less than \( \vartheta \); The left-hand side of inequalities (29c)-(29e) linearize the nonlinear anonymous functions in inequalities (25b)-(25d), respectively, assuming the toll rates are changed by \( d^n \) from \( \tau^n \). The inequalities (29c)-(29e)
ensure the first-order approximation of the functions in inequalities (25b)-(25d) is less than $\theta$ after the link tolls are changed by $d^n$ from $\tau^n$.

Inequalities (29b)-(29e) linearizes the nonlinear programming problem (25) at the equilibrium state $x^*(\tau^n)$. It can be found that if $[d^n,\theta]$ satisfies the inequalities (29b)-(29e) and $\theta < 0$, then $d^n$ is a descent direction of the objective function (25a) at the point $\tau^n$. Further, it also guarantees that the inequalities (25b)-(25d) are held if $\tau^n$ goes along the direction $d^n$ for a sufficiently small step (i.e., $\tau^n + r \cdot d^n$, $r$ is a small positive value). Thereby, the first term in the objective function seeks to minimize the value of $\theta$. Further, as the gap between the linearized system (29b-29e) and the original nonlinear system (25) increases with respect to the difference between the new toll vectors and $\tau^n$, the second term in the objective function (29a) seeks to minimize the $H$-norm of the direction $d^n$.

After obtaining a feasible descent direction $d^n$, Cawood and Kostreva (1999) solves a one-dimension optimal problem to find the optimal step size $r$ to minimize the function $-F(x^*(\tau^n + r \cdot d^n), \tau^n + r \cdot d^n)$, where $\tau^n + r \cdot d^n \in \Omega_\tau$. However, as the function $F(x^*(\tau^n + r \cdot d^n), \tau^n + r \cdot d^n)$ is anonymous whose value can only be computed by solving the MTA-ED problem (17), finding the exact optimal step size $r$ to decrease the objective function is very computationally expensive. Therefore, this study proposes a method to approximate the optimal step size. The main idea is to proportionally expand or shrink a randomly generated initial step size $r_0$ until the objective function cannot be reduced or one of the inequalities in problem (25) cannot be held at the new point. The details of the method will be shown later in this section.

To implement the revised NRMFD, the starting point $\tau^0$ should be feasible, i.e., $\tau^0 \in \Omega_\tau$. As the link flows of HDVs decrease monotonically with respect to link toll rate and the link capacity increases monotonically with respect to link toll rate, the feasible initial $\tau^0$ can be found by setting the toll rate on each AVT link sufficiently large (should be less than $\tau_{max}$). The full steps to solve the optimal toll problem (25) using the revised NRMFD are as follows.

**Step 1**: Find an initial feasible point $\tau^0$ by setting the toll rate on each AVT link large enough within their bound. Let $f^0$ be the initial route flow for the RSRS-MSRA algorithm. Let $n = 0$.

**Step 2**: Solve the MTA-ED problem using the RSRS-MSRA algorithm with toll strategy $\tau^n$ and initial flow $f^0$. Let $f^*(\tau^n)$ be the computed equilibrium route flow solution, and $x^*(\tau^n)$ be the corresponding solution of HDV route flows, CAV link flows, and CAV OD demand. Compute the gradients $\nabla_z F(x^*(\tau^n), \tau^n)$, $\nabla_z Q^*_a(v^*_{a,H}, v^*_{a,A}, \tau^n)$, and $\nabla_z v_{a,z}(\tau^n)$, $\forall a \in I_\tau, z \in Z$. Input these gradients into problem (29).

**Step 3**: At the equilibrium state $f^*(\tau^n)$ (or equivalent, $x^*(\tau^n)$), solve the quadric optimization problem (29) to find the feasible descent direction $d^n$. If $\theta > 0$, then output $\tau^n$ and stop the iteration. Otherwise, go to step 4.

**Step 4**: Approximate the optimal step size $r$ as follows.

**Step 4.1**: Let $l = 0$. Randomly generate a small initial step size $r_l$. Let $F_{Ev} = -F(x^*(\tau^n), \tau^n)$. Compute the MTA-ED problem to obtain the equilibrium flows and the value of the objective function (25a) with toll strategy being $\tau^n + r_l \cdot d^n$ and initial route flows being $f^*(\tau^n)$. Let $f^*(\tau^n + r_{l+1} \cdot d^n)$ be the corresponding equilibrium route flow solution.

**Step 4.2**: If $\tau^n + r_l \cdot d^n \in \Omega_\tau$ and $-F(x^*(\tau^n + r_l \cdot d^n), \tau^n + r_l \cdot d^n) < F_{Ev}$, then let $F_{Ev} =
\[-F(x^*(\tau^n + r_l \cdot d^n), \tau^n + r_l \cdot d^n), \quad r_{l+1} = \omega \cdot r_{l}, \quad v_l = \omega, \] where \( \omega \in (1,2) \) and \( v_l \) is an indicator. Otherwise, \( r_{l+1} = \frac{1}{\omega} \cdot r_0, \quad v_l = \frac{1}{\omega}. \)

**Step 4.3:** If \( l \geq 2, \) \( v_{l+1} = \frac{1}{\omega} \) and \( v_l = \omega, \) then let \( \tau^{n+1} = \tau^n + r_l \cdot d^n, \) go to step 5. If \( l \geq 2, \) \( v_{l+1} = v_l = \omega, \) then let \( \tau^{n+1} = \tau^n + r_{l+1} \cdot d^n, \) go to step 5. Else, go to step 4.4.

**Step 4.4:** Compute the MTA-ED problem to obtain the equilibrium flows and the value of the objective function (25a) with toll strategy being \( \tau^n + r_{l+1} \cdot d^n \) and initial route flow being \( f^*(\tau^n + r_{l+1} \cdot d^n). \) Let \( l = l + 1. \) Go to step 4.2.

**Stop 5:** If \( |F(x^*(\tau^{n+1}), \tau^{n+1}) - F(x^*(\tau^n), \tau^n)|/F(x^*(\tau^n), \tau^n) < \varepsilon_2, \) then stop iteration, output \( \tau^{n+1}. \)

Otherwise, let \( n = n + 1, \) go to step 3.

In **Step 5**, \( \varepsilon_2 \) is a predetermined threshold for convergence. If the change of the objective function is less than \( \varepsilon_2, \) the algorithm stops. In **Step 4.2**, if \( r_1 \) increases from \( r_0, \) it implies that the initial step size \( r_0 \) is too small. We will keep increasing the step size until the objective function cannot be reduced or the new point becomes infeasible. Similarly, if \( r_1 \) decreases from \( r_0, \) it implies that the initial step size \( r_0 \) is too large. We will keep reducing the step size until the new point is feasible and value of the objective function at the new point is less than \(-F(x^*(\tau^n), \tau^n). \) In theory, \( \omega \) can be an arbitrary value in \((1,2). \)

In this study, we set it as the golden ratio, i.e., \( \omega = 1.618. \)

Cawood and Kostreva (1994) showed that the above solution algorithm is globally convergent when the optimal step \( r \) is found at each iteration. However, in the revised NRMFD, the optimal step \( r \) is approximated other than computed exactly. Nevertheless, our algorithm is still globally convergent. The following Theorem will be used to show that the proposed algorithm is globally convergent.

**Theorem 1** (Chen and Kostreva, 1999): Suppose \( d^n \) is the optimal solution to problem (29); if \( \tau^n \) is not an optimal solution to problem (25), then \( d^n \) is a feasible descent direction for problem (25) at \( \tau^n. \)

**Proposition 5:** The revised NRMFD is globally convergent when the lower level MTA-ED problem (17) has a unique solution.

**Proof:** Without loss of generality, we will take the maximum total revenue problem as an example. Let \( \tau^0 \) be a vector of initial feasible toll pricing, and \( \tau^0, \tau^1, \tau^2, \cdots \) be a sequence of \( \tau s \) found in each iteration by the revised NRMFD. Note that the objective of the maximum revenue problem (i.e., \(-F_T(x^*(\tau), \tau)\) is bounded for \( \tau \in \Omega. \) As \( x^*(\tau) \) is unique, \(-F_T(x^*(\tau), \tau) \) is unique. Further, according to Theorem 1, \(-F_T(x^*(\tau^{n+1}), \tau^{n+1}) < -F_T(x^*(\tau^n), \tau^n) \); then, the sequence \( \tau^0, \tau^1, \tau^2, \cdots \) must converge (Rudin, 1964). Let \( \tau^* \) be the point where the sequence converges to. We will prove that \( \tau^* \) is an optimal solution to the maximum total revenue problem by contradiction. Suppose \( \tau^* \) is not an optimal point of the maximum revenue problem. According to Theorem 1, a new feasible descent direction \( d \) can be found by solving the problem (29) at \( \tau^* \) and a step \( r \) can be found by the revised NRMFD such that the constraints (25b)-(25d) hold at the new point \( \tau^* + rd \), and \(-F_T(x^*(\tau^* + rd), \tau^* + rd) < -F_T(x^*(\tau^*), \tau^*). \) This indicates that the sequence \( \tau^0, \tau^1, \tau^2, \cdots \) does not converge to \( \tau^*, \) which contradicts with the presumed condition. Thereby, \( \tau^* \) must be an optimal solution to the maximum total revenue problem. Proposition 5 is proved.

It should be noted that the NRMFD converges linearly to the optimal solution, where the parameter \( \sigma \) and the matrix \( H \) significantly impact the convergence rate (Korycki and Kostreva, 1996a). Korycki
and Kostreva (1996b) found that the maximum convergence speed of the NRMFD is usually achieved when \( H \) is set as an identity matrix and \( \sigma \) is set between 0.5 and 2. In our numerical example, we found that the convergence speed of the proposed algorithm is faster for various networks when \( \sigma \) is set between 0.5 and 10, and \( H \) is set as an identity matrix.

It is important to note that when the MTA-ED problem (17) has multiple solutions, the revised NRMFD is used to solve the problem \( \min_{\tau \in \Omega_{\tau}} F(x^*_i(\tau), \tau) \), where \( x^*_i(\tau) \) is a locally optimal solution of the MTA-ED problem (17) with toll strategy \( \tau \), and \( x^*_i(\tau^0) \) is determined by the initial flow pattern \( f^0 \). Note that \( x^*_i(\tau) \) is unique. Thereby, the NRMFD is convergent when applied to solve the problem \( \min_{\tau \in \Omega_{\tau}} F(x^*_i(\tau), \tau) \). The main problem for the application of the NRMFD is to compute the locally optimal solution \( x^*_i(\tau) \) for an arbitrary toll strategy \( \tau \). Note that in Step 4.1 and Step 4.4 in the revised NRMFD, we set the initial route flow pattern as \( f^*(\tau^0 + r_i \cdot d^0) \) for the RSRS-MSRA algorithm, which is sufficiently close to the equilibrium route flow solution with toll strategy \( \tau^0 + r_{i+1} \cdot d^0 \) that results in the locally optimal solution \( x^*_i(\tau^0 + r_{i+1} \cdot d^0) \) (because \( r_{i+1} \) is very close to \( r_i \)). Thereby, the RSRS-MSRA algorithm will converge to the unique local solution (i.e., \( x^*_i(\tau^0 + r_{i+1} \cdot d^0) \)) at each iteration \( l \) as it searches the solution in a very small local area around \( x^*_i(\tau^0 + r_{i+1} \cdot d^0) \). This indicates that the NRMFD can be leveraged to solve the problem (26b).

If the MTA-ED problem (17) has a unique solution, the initial route flow pattern for the RSRS-MSRA algorithm in Step 4.1 and Step 4.4 in the revised NRMFD can be set as an arbitrary point in the feasible set \( \Omega_f \).

### 4.2 Sensitivity analysis of the VI problem (15)

This section presents the analytical method for sensitivity analysis of the MTA-ED problem (15). It aids in obtaining the derivatives of the objective function, equilibrium link flows and link capacity with respect to \( \tau \) at Step 2 of the revised NRMFD algorithm. Note that the application of this method only requires that the solution of the MTA-ED problem (17) is locally unique. Thereby, it can also be leveraged by the proposed revised NRMFD to obtain a solution for problem (26b) when the MTA-ED problem (17) has multiple solutions. For simplicity, We will omit the notation \( \tau \) when describing the equilibrium flows, i.e., \( f^* \) means \( f^*(\tau) \).

Without loss of generality, suppose the \( f^* = [f^*_H, f^*_A] \) is the equilibrium route flow solution under toll strategy \( \tau \). The KKT conditions for the VI problem (15b) can be summarized as

\[
C_H(f^*) - \pi^*_H - \Lambda_H^T \mu_H^* = 0 \\
C_A(f^*) - \pi^*_A - \Lambda_A^T \mu_A^* = 0 \\
\begin{bmatrix}
\Lambda_H & \Lambda_A
\end{bmatrix}
\begin{bmatrix}
f_H^* \\
f_A^*
\end{bmatrix} - \begin{bmatrix}
q_{H}^* \\
q_{A}^*
\end{bmatrix} = 0
\]

\[
\pi^*_H f^*_H = 0 \\
\pi^*_A f^*_A = 0 \\
f_A^* \geq 0; f_H^* \geq 0 \\
\pi^*_H \geq 0; \pi^*_A \geq 0
\]

where \( \pi^*_H \) and \( \mu^*_A \) are the vectors of Lagrange multipliers associated with the inequality and equality constraints for vehicle class \( z \), respectively in the set \( \Omega_f \). \( q^*_H \) and \( q^*_A \) are vectors of equilibrium demand of all OD pairs for HDVs and CAVs, respectively.
Define the equilibrated routes as these routes whose revised travel cost is 0 at equilibrated state. Let \( \tilde{f}_H \) and \( \tilde{f}_A \) be the flows of the equilibrated routes for both HDVs and CAVs, respectively. As flows of non-equilibrated routes are strictly 0 for small perturbations of link toll rates \( \tau \), the non-equilibrated routes can be excluded for sensitivity analysis. Thereby, Eq. (30) can be simplified as

\[
\begin{align*}
\tilde{c}_H(\tilde{f}^*) - \tilde{\pi}^*_H - \bar{\lambda}_H^* \bar{\mu}_H^* &= 0 \\
\tilde{c}_A(\tilde{f}^*) - \tilde{\pi}^*_A - \bar{\lambda}_A^* \bar{\mu}_A^* &= 0 \\
\begin{bmatrix} \bar{\lambda}_H & \bar{\lambda}_A \end{bmatrix} \begin{bmatrix} \tilde{f}_H^* \\ \tilde{f}_A^* \end{bmatrix} - \begin{bmatrix} q_H^* \\ q_A^* \end{bmatrix} &= 0 \\
\tilde{\pi}^*_H \tilde{f}_H^* &= 0 \\
\tilde{\pi}^*_A \tilde{f}_A^* &= 0 \\
\tilde{f}_A^* &\geq 0; \tilde{f}_H^* > 0 \\
\tilde{\pi}^*_H &\geq 0; \tilde{\pi}^*_A \geq 0
\end{align*}
\]

where \( ^* \) denotes the corresponding variables associated with the equilibrated routes for either CAVs or HVDs.

Note that the route flow solution for CAVs at the equilibrium state is non-unique. To derive the analytical method for sensitivity analysis of the MTA-ED problem, the following method proposed by Yang and Bell (2007) will be used to obtain a route flow pattern for CAVs with desired uniqueness. Let \( \bar{\lambda}_A \) and \( \bar{\lambda}_A \) be the link-path and OD-path matrices for equilibrated routes of CAVs at the equilibrium state. Denote \( \begin{bmatrix} \bar{\lambda}_A \\ \bar{\lambda}_A \end{bmatrix} \) as a full column matrix constituted by column vectors in \( \begin{bmatrix} \bar{\lambda}_A \\ \bar{\lambda}_A \end{bmatrix} \) that has the same rank as \( \begin{bmatrix} \bar{\lambda}_A \\ \bar{\lambda}_A \end{bmatrix} \). Let \( \tilde{f}_A \) be the flows of routes with link-path and OD-path matrix \( \begin{bmatrix} \bar{\lambda}_A \\ \bar{\lambda}_A \end{bmatrix} \), and \( \tilde{f}_A \) be the flows of other equilibrium routes for CAVs. Assume an equilibrium route flow solution exists for CAVs such that the flow of all equilibrated routes is positive at the unperturbed state. Let \( \tilde{f}_A^* = \begin{bmatrix} \tilde{f}_A^* \\ \tilde{f}_A^* \end{bmatrix} (\tilde{f}_A^* > 0; \tilde{f}_A^* > 0) \) be such a route flow solution for CAVs. When link toll rates change for a small value from the unperturbed state, only \( \tilde{f}_A \) can change, the route flow \( \tilde{f}_A \) remains fixed. As \( \begin{bmatrix} \bar{\lambda}_A \\ \bar{\lambda}_A \end{bmatrix} \) is a full column matrix, this route flow variation method helps to generate a unique route flow solution for CAVs when link toll rates vary.

The following assumption will be useful to derive the analytical model for sensitivity analysis of VI problem (15b).

**Assumption 2.** The equilibrium route flow solution \( f^* \) for the VI problem (15b) is non-degenerate.

Assumption 2 is not strong as the possibility for \( f^* \) being degenerate is almost 0 (Wang et al., 2019b). Note that \( \tilde{f}_H^*, \tilde{f}_A^* > 0, \tilde{\pi}^*_H = 0 \) and \( \tilde{\pi}^*_A = 0 \). Under assumption 3, \( \tilde{\pi}^*_H \) and \( \tilde{\pi}^*_A \) will remain 0 for small perturbation of \( \tau \). Thereby, Eq. (31) can be simplified as

\[
\begin{align*}
\bar{g}_H(f^*) - D_H^{-1}(q_H^*) - \bar{\lambda}_H^* \bar{\mu}_H^* &= 0 \\
\bar{g}_A(f^*) - D_A^{-1}(q_A^*) - \bar{\lambda}_A^* \bar{\mu}_A^* &= 0 \\
\begin{bmatrix} \bar{\lambda}_H & \bar{\lambda}_A \end{bmatrix} \begin{bmatrix} \tilde{f}_H^* \\ \tilde{f}_A^* \end{bmatrix} - \begin{bmatrix} q_H^* \\ q_A^* \end{bmatrix} &= 0
\end{align*}
\]
where $D^{-1}_H(q^*_H)$ and $D^{-1}_A(q^*_A)$ are vectors of the inverse of all demand functions for HDVs and CAVs at equilibrium state, respectively.

According to Eq. (5) and Eq. (14), at equilibrium state, the revised route travel costs for all equilibrated routes are 0. Thereby, $\tilde{G}_H(f^*, 0) - D^{-1}_H(q^*_H) \equiv 0$ and $\tilde{G}_A(f^*, 0) - D^{-1}_H(q^*_H) \equiv 0$, which indicate that $\tilde{\pi}_H^* = 0$ and $\tilde{\pi}_A^* = 0$. Eq. (32a) and Eq. (32b) can be simplified as

$$\tilde{G}_H(f^*) - D^{-1}_H(q^*_H) = 0$$  \hspace{1cm} (33a)
$$\tilde{G}_A(f^*) - D^{-1}_A(q^*_A) = 0$$  \hspace{1cm} (33b)

Let

$$\varphi_{H,H}^w(f^*, 0) = \frac{1}{\mu} c_{k,H}^w - \frac{1}{\theta} H_{k,H}^w + \frac{1}{\theta} \ln(f_{k,H}^w)$$  \hspace{1cm} (34)

Denote $\tilde{\varphi}_H(f^*, 0)$ as the vector of $\varphi$ for all equilibrated routes for HDVs. Submit Eq. (3) and Eq. (32) into Eq. (33b), we have

$$\tilde{\varphi}_H(f^*, 0) - \frac{1}{\theta} \tilde{\Lambda}_H \cdot \ln(q_{H}^*) - D^{-1}_H(q^*_H) = 0$$  \hspace{1cm} (35)

Note that $\nabla \tilde{\Phi}_A^* \equiv 0$. Differentiate both side of Eq. (35), Eq. (33b) and Eq. (32c) with respect to $\tau$, we have

$$\nabla \tilde{\Phi}_H(f^*) + \nabla f_{l_H} \tilde{\Phi}_H(f^*) \nabla \tilde{\Phi}_H - \nabla \tilde{\Phi}_H \cdot \nabla \varphi_{H} = 0$$  \hspace{1cm} (36a)
$$\nabla \tilde{G}_A(f^*) + \nabla f_{l_A} \tilde{G}_A(f^*) \nabla \tilde{G}_A - \nabla \varphi_{A} = 0$$  \hspace{1cm} (36b)
$$\left[ \tilde{\Lambda}_H \right] \left[ \nabla \tilde{\Phi}_H \right] - \left[ \nabla \tilde{\Phi}_A \right] = 0$$  \hspace{1cm} (36c)

where

$$\nabla \tilde{\Phi}_H = \left( \frac{1}{\theta} \tilde{\Lambda}_H \cdot \text{diag} \left( \frac{1}{\varphi_{H}} \right) + \tilde{\Lambda}_H \cdot \nabla q_{H} D^{-1}_H(q^*_H) \right)$$  \hspace{1cm} (36d)

Submitting Eq. (36c) into Eq. (36a) and Eq. (36b), yields

$$\nabla \tilde{\Phi}_H(f^*) + \nabla f_{l_H} \tilde{\Phi}_H(f^*) \nabla \tilde{\Phi}_H - \nabla \tilde{\Phi}_H \cdot \nabla \varphi_{H} = 0$$  \hspace{1cm} (37a)
$$\nabla \tilde{G}_A(f^*) + \nabla f_{l_A} \tilde{G}_A(f^*) \nabla \tilde{G}_A - \nabla \varphi_{A} = 0$$  \hspace{1cm} (37b)

According to Eq. (37), the derivatives of $\tilde{f}_H^*$ and $\tilde{f}_A^*$ with respect to $\tau$ can be formulated as

$$\left[ \nabla \tilde{f}_H^* \right] = - \left[ \nabla f_{l_H} \tilde{\Phi}_H(f^*, 0) - \nabla \tilde{\Phi}_H(f^*, 0) \right]^{-1} \left[ \nabla \tilde{\Phi}_H(f^*, 0) \right]$$  \hspace{1cm} (38)

In Eq. (38)

$$\nabla f_{l_H} \tilde{\Phi}_H(f^*) = \frac{1}{u} \tilde{\Delta}_H^* \cdot \nabla q_{H} \tilde{\Phi}_H \cdot \tilde{\Delta}_H - \frac{(1 - u)}{u} \rho^* \tilde{\Delta}_H^* \cdot \nabla q_{H} \tilde{\Phi}_H \cdot \tilde{\Delta}_H + \frac{1}{\theta} \text{diag} \left( \frac{1}{\tilde{f}_H^*} \right)$$  \hspace{1cm} (39a)
$$\nabla f_{l_A} \tilde{\Phi}_H(f^*) = \frac{1}{u} \tilde{\Delta}_H^* \cdot \nabla q_{A} \tilde{\Phi}_H \cdot \tilde{\Delta}_A - \frac{(1 - u)}{u} \rho^* \tilde{\Delta}_H^* \cdot \nabla q_{A} \tilde{\Phi}_H \cdot \tilde{\Delta}_A$$  \hspace{1cm} (39b)
$$\nabla f_{l_H} \tilde{G}_A(f^*) = \tilde{\Delta}_H^* \cdot \nabla q_{H} \tilde{G}_A \cdot \tilde{\Delta}_H$$  \hspace{1cm} (39c)
$$\nabla f_{l_A} \tilde{G}_A(f^*) = \tilde{\Delta}_A^* \cdot \nabla q_{A} \tilde{G}_A \cdot \tilde{\Delta}_A$$  \hspace{1cm} (39d)
$$\nabla \tilde{\Phi}_H(f^*) = \frac{1}{u} \tilde{\Delta}_H^* \cdot \nabla \tilde{\Phi}_H - \frac{(1 - u)}{u} \rho^* \tilde{\Delta}_H^* \cdot \nabla \tilde{\Phi}_H$$  \hspace{1cm} (39e)
$$\nabla \tilde{G}_A(f^*) = \tilde{\Delta}_A^* \cdot \nabla \tilde{G}_A$$  \hspace{1cm} (39f)

where $\tilde{\nu}_z$ is the vector of flows of all links used by vehicles in class $z$ (i.e., links with the non-zero flow)
at equilibrium state and $\tilde{z}$ is the vector of corresponding equilibrium link travel costs. $\rho^* = [\rho^w_{k,l}, \forall k, l \in R^w_H, w \in W]$, and

$$
\rho^w_{k,l} = \frac{\sum_{m \in R^w_{l,u}} (\alpha^w_{m,k})^{\frac{1}{a}} \left( \sum_{l \in R^w_{u,l}} (\alpha^w_{m,l}) \exp \left(-\theta c^w_{l,u} \right) \right)^{\frac{1}{a}}} {\sum_{m \in R^w_{l,u}} (\alpha^w_{m,k})^{\frac{1}{a}} (\alpha^w_{m,l}) \exp \left(-\theta c^w_{l,u} \right)} \left[ \alpha^w_{m,l} \exp \left(-\theta c^w_{l,u} \right) \right]^{\frac{1}{a} - 2} \left( \sum_{l \in R^w_{u,l}} (\alpha^w_{m,l}) \exp \left(-\theta c^w_{l,u} \right) \right)^{\frac{1}{a} - 1} \left( \alpha^w_{m,l} \right)^{\frac{1}{a}} \exp \left(-\theta c^w_{l,u} \right)
$$

(40g)

According to Eq. (38),

$$
\nabla \tilde{z}^*_H = \Delta_H \cdot \nabla \tilde{f}^*_H
$$

(40a)

$$
\nabla \tilde{z}^*_A = \Lambda_A \cdot \nabla \tilde{f}^*_A
$$

(40b)

$$
\nabla \tilde{q}^*_H = \Lambda_H \nabla \tilde{f}^*_H
$$

(40c)

$$
\nabla \tilde{q}^*_A = \Lambda_A \nabla \tilde{f}^*_A
$$

(40d)

Let $\tau_a$ be a variable in $\tau$, the derivatives of the link capacity, total revenue, total customer surplus and total demand with respect to $\tau_a$ can be formulated, respectively, as

$$
\nabla \tau_a Q^*_b = \nabla v_{a,b} Q_b \cdot \nabla \tau_a v_{a,b}^* + \nabla v_{a,b} Q_b \cdot \nabla \tau_a v_{a,b}^*
$$

(41a)

$$
\nabla \tau_a F_{TR} = \sum_{a \in T} \left( \nabla \tau_a v_{a,b}^* \cdot \tau_a + v_{a,b}^* \right)
$$

(41b)

$$
\nabla \tau_a F_{TCS} = \sum_{z \in Z} \nabla \tau_a q^w \cdot v_{z}^T \cdot D^{-1}_z(q^z) - \sum_{z \in Z} \nabla \tau_a z^T \cdot \tilde{z}^T \cdot D^{-1}_z(q^z) - \sum_{z \in Z} \nabla \tau_a q^w \cdot \tilde{v}^T \cdot D^{-1}_z(q^z) + \tilde{v}^T \cdot \nabla \tau_a \tilde{f}^*_H
$$

(41c)

$$
\nabla \tau_a F_{TD} = \sum_{w \in W_H} \nabla \tau_a q^w + \sum_{w \in W_A} \nabla \tau_a q^w
$$

(41d)

where $Q^*_b$ is the equilibrium capacity of an arbitrary AVT link $b, b \in T$ in the network.

5. Numerical example

5.1 Effectiveness of the solution algorithm for the MTA-ED problem

5.1.1 A small numerical example

![Figure 3. A small network](image)

Table 1. Inputs for the small network in Figure 1

<table>
<thead>
<tr>
<th>Links</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Free flow travel time ($l_a$)</td>
<td>4</td>
<td>7</td>
<td>1</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>Toll rate ($\tau_a$)</td>
<td>0.5</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Capacity of HDVs ($Q_{a,H}$)</td>
<td>30</td>
<td>40</td>
<td>10</td>
<td>30</td>
<td>30</td>
</tr>
</tbody>
</table>
In this section, a small network shown in Figure 3 will be used to demonstrate the details for implementing the solution algorithm for the fixed demand-based MTA problem (21). It helps to obtain the equilibrium route flow solution for the MTA-ED problem (15). The small network contains one OD pair (from node O to node D), five links, and three routes, i.e., route 1: links 1-4, route 2: links 2-5, and route 3: links 1-3-5. Suppose only link 1 is the AVT link and the toll rate on link 1 is 0.5 dollars, i.e., all HDVs need to pay 0.5 dollars to access link 1. Suppose one dollar equals 0.5 units of travel time. The dispersion parameter and the nesting degree are \( \theta = 0.5 \) and \( u = 0.5 \), respectively. The OD demand for both HDVs and CAVs is formulated as

\[
D_H^w(S_H^w) = q_{H,0}^w \cdot \exp \left( -b_H \frac{S_H^w}{S_{H,0}} \right) = 40 \cdot \exp \left( -0.2 \frac{S_H^w}{5.63} \right) \tag{42a}
\]

\[
D_A^w(S_A^w) = q_{A,0}^w \cdot \exp \left( -b_A \frac{S_A^w}{S_{A,0}} \right) = 40 \cdot \exp \left( -0.2 \frac{S_A^w}{9} \right) \tag{42b}
\]

where \( b, z \in Z \) are coefficients. \( S_{z,0}^w, z \in Z \) is the expected perceived travel cost for vehicle class \( z \) between OD pair \( w \) under free flow scenario. \( q_{H,0}^w \) and \( q_{A,0}^w \) denotes the maximum number of trips by HDVs and CAVs between OD pair \( w \), respectively. For simplicity, we call \( q_{H,0}^w + q_{A,0}^w \) the maximum demand for OD pair \( w \) and \( q_{A,0}^w/(q_{H,0}^w + q_{A,0}^w) \) the market penetration rate of CAVs. As only one OD pair exists in this small network, the superscript ‘w’ will be omitted thereafter. The inputs of the small network can be found in Table 1.

As discussed in Section 3, to enable the application of the RSRS-MSRA solution algorithm, a dummy route will be added to connect the origin and the destination directly. The dummy route can be used by both CAVs and HDVs. Note that the expected perceived travel cost \( S_{z}^w, z \in Z \) is larger than 0 for this network. Therefore, \( D_H(S_H) < D_H(0) = 40 \) and \( D_A(S_A) < D_A(0) = 40 \). According to Proposition 2, the fixed OD demand is set as 40 for both HDVs and CAVs in the augmented network. At the initial step, the fixed OD demand is assigned uniformly to all the routes between the OD pair (include the dummy route). Therefore, we have

\[
f_{1,H}(1) = 10; f_{2,H}(1) = 10; f_{3,H}(1) = 10; f_{dmy,H}(1) = 10
\]

\[
f_{1,A}(1) = 10; f_{2,A}(1) = 10; f_{3,A}(1) = 10; f_{dmy,A}(1) = 10
\]

The traffic demand of HDVs and CAVs for the actual network can be computed by summing the flow on the three real routes between, which are \( q_H = 30 \) and \( q_A = 30 \), respectively. The inverse of the demand functions for HDVs and CAVs are computed as \( D_H^{-1}(q_H) = 8.098 \) and \( D_A^{-1}(q_A) = 12.946 \), respectively. The generalized travel costs of the three real routes for HDVs and CAVs are

\[
G_{1,H}(1) = 9.459; G_{2,H}(1) = 7.872; G_{3,H}(1) = 20.046
\]

\[
G_{1,A}(1) = 11.156; G_{2,A}(1) = 10.096; G_{3,A}(1) = 19.594
\]

The revised travel costs of the three real routes for HDVs and CAVs are computed as \( C_{i,z} = G_{i,z}(1) - D_{i,z}^{-1}(q_A), i = 1,2,3; z \in Z \), respectively. Thereby,

\[
C_{1,H}(1) = 1.362; C_{2,H}(1) = -0.226; C_{3,H}(1) = 11.949
\]

\[
C_{1,A}(1) = -1.789; C_{2,A}(1) = -2.877; C_{3,A}(1) = 6.648
\]

Note also that for the dummy route, \( C_{dmy,H} \equiv C_{dmy,A} \equiv 0 \). According to Eq. (22),

<table>
<thead>
<tr>
<th>Capacity of CAVs (( Q_{A,A} ))</th>
<th>60</th>
<th>80</th>
<th>20</th>
<th>60</th>
<th>60</th>
</tr>
</thead>
</table>

26
Let $\chi = 4$, we have

$$\beta_1 = \frac{1}{h_1} = \frac{1}{\frac{1}{4} \max \{h_{lx}(1) \mid h_{lx}(1) = \sum_{j \in \mathbb{R}_x} (C_{jlx}(\tilde{f}_1) - C_{ilx}(\tilde{f}_1))_+ \}, i \in \mathbb{R}_x; \forall z \in \mathbb{Z}}$$

$$= \frac{1}{4 \cdot 34.71} = 0.0072$$

Thereby,

$$\tilde{f}_{2,h} = [f_{1,h}(2) \ f_{2,h}(2) \ f_{3,h}(2) \ f_{dmy,h}(2)]$$

$$= \tilde{f}_{1,h} + \beta_1 \Phi(\tilde{f}_{n,h})$$

$$= [11.100 \ 12.015 \ 5.000 \ 11.885]$$

$$\tilde{f}_{2,a} = [f_{1,a}(2) \ f_{2,a}(2) \ f_{3,a}(2) \ f_{dmy,a}(2)]$$

$$= \tilde{f}_{1,a} + \beta_1 \Phi(\tilde{f}_{n,a})$$

$$= [11.317 \ 11.943 \ 6.595 \ 10.285]$$

Repeat the above steps, the equilibrium route flow solutions for both HDVs and CAVs on the augmented network can be obtained by the RSRS-MSRA solution algorithm.

\[\Phi_{1,h}(\tilde{f}_1) = \sum_{g \in \mathbb{R}_h} \left[ f_{g,h}(1) \left( C_{g,h}(\tilde{f}_1) - C_{1,h}(\tilde{f}_1) \right)_+ - f_{1,h}(n) \left( C_{1,h}(\tilde{f}_1) - C_{g,h}(\tilde{f}_1) \right)_+ \right] \]

$$= 10 \times \{-1.588 + 10.587 - 1.362\}$$

$$= 76.38$$

$\Phi_{2,h}(\tilde{f}_1) = 139.87; \Phi_{3,h}(\tilde{f}_1) = -347.10; \Phi_{4,h}(\tilde{f}_1) = 130.85,$

$\Phi_{1,a}(\tilde{f}_1) = 91.399; \Phi_{2,a}(\tilde{f}_1) = 134.88; \Phi_{3,a}(\tilde{f}_1) = -246.10; \Phi_{4,a}(\tilde{f}_1) = 19.82,$

Figure 4. Convergence performance of the RSRS-MSRA algorithm for the VI problem (21)
Figure 4 shows the evolution of the value of the convergence criteria. As can be seen, the value of convergence criteria is lower than $1 \times 10^{-8}$ after 180 iterations. Further, Figure 5 demonstrates that the route flows for both CAVs and HDVs computed by the RSRS-MSRA solution algorithm are very close to the equilibrium state after only 40 iterations. These results indicate the RSRS-MSRA solution algorithm can solve the MTA-ED model very effectively and efficiently.

Based on Figure 5, the equilibrium demand for HDVs and CAVs can be obtained by summing the corresponding flows on routes 1, 2, and 3, which are 29.605 and 31.979, respectively. It can verify that the elastic demand functions (37a) and (37b) will give the same results by submitting the expected perceived travel cost for HDVs and CAVs at the equilibrium state into the two functions, respectively.

### 5.1.2 Application to three larger networks

To further illustrate the convergence performance of the RSRS-MSRA algorithm, the Nguyen-Dupuis, the Sioux Falls, and the Anaheim network are used. The Nguyen-Dupuis network is a small network with four OD pairs, 19 links, and 25 routes. The Sioux Falls network consists of 24 nodes, 76 links, and 552 O-D pairs. The Anaheim network is a mid-size network containing 416 nodes, 914 links, and 1406 OD pairs. The link penalty approach proposed by De La Barra et al. (1993) is used to find the routes that are likely to be used by travelers. To reduce the impacts of the chosen route set on the equilibrium solution, the number of routes for each OD pair (i.e., $K$) is set as 15. Thereby, 7920 and 21038 routes are found in total by the link penalty approach for the Sioux Falls and Anaheim networks, respectively.
Figure 6. Convergence performance of the RSRS-MSRA algorithm for the three larger networks

Figure 6 shows the evolution of the value of the convergence criteria. It demonstrates that the values of convergence criteria decrease monotonically for all testing networks. However, the RSRS-MSRA solution algorithm converges slower if more number of routes is involved. Nevertheless, it can find a route flow solution with a value of convergence criteria lower than $1 \times 10^{-4}$ within 2000 iterations for all networks.

5.2 Sensitivity analysis of the MTA-ED problem

Sensitivity analysis of the MTA-ED problem is one critical step to solve the three optimal toll design problems. This section demonstrates the details to perform the sensitivity analysis method to obtain the derivatives of equilibrium link flows, link capacity, and the three objective functions in Eq. (24) with respect to link toll rates, which are used in the revised RNMFD. For simplicity, the small numerical example in section 5.1 is also used. Based on Figure 5, the equilibrium flow solution of the three real routes for HDVs and CAVs are

$$f^*_H = [10.747 \ 12.832 \ 6.026]; f^*_A = [13.767 \ 18.2112 \ 0]$$

Note that HDVs use all three routes while the CAVs only use routes 1 and 2 at the equilibrium state. Further, the link-path and OD-path vectors of route 1 and route 2 are independent. Thereby

$$\tilde{f}^*_H = [10.747 \ 12.832 \ 6.026]; \tilde{f}^*_A = \tilde{f}^*_A = [13.767 \ 18.211]$$

and

$$\bar{\Delta}_H = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \ 0 & 1 & 0 & 0 & 1 \ 1 & 0 & 1 & 0 & 1 \end{bmatrix}^T; \bar{\Delta}_A = \begin{bmatrix} 1 & 0 \ 0 & 1 \ 1 & 0 \ 0 & 1 \end{bmatrix}; \bar{A}_H = [1 \ 1 \ 1]; \bar{A}_A = [1 \ 1]$$

Submit the equilibrium route flow solutions into Eq. (40), we have

$$\nabla_{f_H} \Psi_H (f^*_H, 0) - \tilde{\Psi}_H = \begin{bmatrix} 1.277 & 0.869 & 0.982 \\ 0.876 & 1.208 & 0.977 \\ 1.013 & 1.010 & 1.674 \end{bmatrix}$$
Suppose only the toll on link 1 changes, then
\[
\nabla_{\bar{f}_1} \tilde{\varphi}_H(f^*, 0) = \begin{bmatrix}
0.104 & -0.007 \\
-0.004 & 0.085 \\
0.0651 & 0.063
\end{bmatrix}
\]
\[
\nabla_{\bar{f}_1} \tilde{\varphi}_A(f^*, 0) = \begin{bmatrix}
0.198 & 0 & 0.131 \\
0 & 0.166 & 0.108
\end{bmatrix}
\]
\[
\nabla_{\bar{f}_1} \tilde{\varphi}_A(f^*, 0) - \tilde{\lambda}_A^T \nabla_{\bar{q}_A} D_H^{-1}(\bar{q}_A) \tilde{\lambda}_A = \begin{bmatrix}
1.506 & 1.407 \\
1.407 & 1.490
\end{bmatrix}
\]

Suppose the toll on link 1 changed, then
\[
\nabla_{\bar{f}_1} \tilde{\varphi}_H(f^*, 0) = \frac{1}{u} \tilde{\lambda}_H^T \cdot \nabla_{\bar{f}_1} \bar{f}_H - \frac{(1 - u)}{u} \rho^* \tilde{\lambda}_H^T \cdot \nabla_{\bar{f}_1} \bar{f}_H = [0.5 \quad -0.028 \quad 0.560]^T
\]
\[
\nabla_{\bar{f}_1} \tilde{\varphi}_A(f^*, 0) = \tilde{\lambda}_A^T \cdot \nabla_{\bar{f}_1} \bar{f}_A = [0 \quad 0]^T
\]

Submit the above results into Eq. (38), we have
\[
\begin{bmatrix}
\nabla_{\bar{f}_1} \bar{f}_H^* \\
\nabla_{\bar{f}_1} \bar{f}_A^*
\end{bmatrix} = [-1.458 \quad 1.704 \quad -0.484 \quad 3.212 \quad -3.188]^T
\]

Thereby,
\[
\nabla_{\bar{f}_1} \hat{\varphi}_H = \tilde{\lambda}_H \nabla_{\bar{f}_1} \bar{f}_H = [-1.942 \quad 1.704 \quad -0.484 \quad -1.458 \quad 1.22]^T
\]
\[
\nabla_{\bar{f}_1} \hat{\varphi}_A = \tilde{\lambda}_A \nabla_{\bar{f}_1} \bar{f}_A = [3.212 \quad -3.187 \quad 3.212 \quad -3.187]
\]
\[
\nabla_{\bar{f}_1} Q^* = [2.160 \quad -2.989 \quad 0 \quad 2.634 \quad -1.579]^T
\]
\[
\nabla_{\bar{f}_1} F_{TT} = 15.802; \nabla_{\bar{f}_1} F_{CS} = -4.425; \nabla_{\bar{f}_1} F_{TD} = -0.214
\]

where \(Q^*\) is the vector of all link capacity at equilibrium state. Suppose the toll on link 1 changed from 0.5 to 1, using first-order approximation approach, we have
\[
\hat{\varphi}_H(1) = [15.802 \quad 13.684 \quad 5.784 \quad 10.018 \quad 19.468]^T
\]
\[
\hat{\varphi}_A(1) = [15.373 \quad 16.618 \quad 15.373 \quad 16.618]
\]
\[
Q^*(1) = [39.810 \quad 55.108 \quad 10 \quad 43.030 \quad 38.979]^T
\]
\[
\hat{F}_{TT}(1) = 16.287; \hat{F}_{CS}(1) = 2214.59; \hat{F}_{TD}(1) = 61.477
\]

where \(\hat{\varphi}_H(1), \hat{\varphi}_A(1), Q^*(1), \hat{F}_{TT}(1), \hat{F}_{CS}(1)\) and \(\hat{F}_{TD}(1)\) are link flows for HDVs, link flows for CAVs, link capacity, total revenue, customer surplus and total demand estimated at \(\tau_1 = 1\). The computed values using RSRS-MSRA solution algorithm are
\[
\varphi_H(1) = [15.803 \quad 13.687 \quad 5.778 \quad 10.026 \quad 19.463]^T
\]
\[
\varphi_A(1) = [15.368 \quad 16.623 \quad 15.368 \quad 16.623]
\]
\[
Q^*(1) = [39.815 \quad 55.113 \quad 10 \quad 43.016 \quad 38.977]^T
\]
\[
F_{TR}(1) = 15.803; F_{CS}(1) = 2214.78; F_{TD}(1) = 61.480
\]

As can be seen, the estimated values are all very close to the computed ones. This indicates that the first-order approximation approach can provide good estimation of the equilibrium flow solution and network performance when link tolls are changed for small values.

5.3 Optimal toll designs problems

5.3.1 Convergence performance of the revised NRMFD

To show the convergence performance of the revised NRMFD, suppose the tolls are set to charge
HDVs on links 4 and 5 in the Nguyen-Dupuis network and on links 29 and 48 in Sioux Falls network, respectively, to reduce traffic congestion on these links. To determine if the MTA-ED problem (17) has a unique solution, 500 different initial points and 6000 different initial points are generated for the RSRS-MSRA solution algorithm to compute the equilibrium flows for the Nguyen-Dupuis network and the Sioux Falls network, respectively. Note that the RSRS-MSRA solution algorithm with each of these initial points converges to the same equilibrium flow $\mathbf{x}^*$. Thereby, the MTA-ED problem (17) may have a unique solution and problem (25) will be used to find the optimal toll rates for the AVT links to improve the network performance. It should be noted that the volume/capacity (V/C) is over 1.1 on these links at the equilibrium state when no tolls are set.

For Nguyen-Dupuis network, the initial point for the revised NRMFD is $[\tau^0_4, \tau^0_5] = [10, 6.5]$ for all the three optimal toll design problems. For Sioux Falls network, the initial point for solving the maximum total revenue problem, the maximum customer problem and the maximum total demand problem are set as $[\tau^0_{29}, \tau^0_{48}] = [10, 20]$, $[\tau^0_{29}, \tau^0_{48}] = [10, 20]$ and $[\tau^0_{29}, \tau^0_{48}] = [10, 14.5]$, respectively. Let $H = I_2$, set $\sigma$ as 10 and 1 for the Nguyen-Dupuis and the Sioux Falls network, respectively. $I_2$ is the 2-dimension identity matrix.

(a)  \hspace{1cm} (b)  
(c)  \hspace{1cm} (d)
Figure 7. Contour of the objective functions and solution trajectories (blue lines) for different optimal toll design problems in different networks; (a) Maximum total revenue problem for Nguyen-Dupuis network; (b) Maximum total revenue problem for Sioux Falls network; (c) Maximum customer surplus problem for Nguyen-Dupuis network; (d) Maximum customer surplus problem for Sioux Falls network; (e) Maximum total demand problem for Nguyen-Dupuis network; (f) Maximum total demand problem for Sioux Falls network.

Figure 7 shows the contour of the objective functions and solution trajectories of the revised NRMFD for different optimal toll design problems. It demonstrates that revised NRMFD only takes a few iterations to find the optimal solution of all toll design problems in both networks. Thereby, this algorithm can solve the optimal toll problem very efficiently. It should be noted that in Figure (7d)-(7e), the total flow of HDVs and CAVs on one AVT link equals the link capacity at the optimal toll state, which prevents further improvement of the objective function.

5.3.2 Three optimal toll design problems with more number of AVT links

In this section, three numerical examples will be demonstrated to find the optimal toll rates for the AVT links to improve the three performance indicators, respectively. By applying the RSRS-MSRA solution algorithm with a large set of initial points, the solution of the MTA-ED problem (17) in all numerical examples are also found to be unique. Thereby, the optimal toll design problem (25) will be used in the three numerical examples shown as follows.

5.3.2.1 Maximum revenue problem

Suppose the private-sector stakeholder plans to charge the HDVs on the 8 links shown in red in the Sioux Falls network (see Figure 8) to reduce traffic congestion while maximizing the total revenue. The V/C on most of these links at equilibrium state without tolls are over 1.15 (except links 30 and 51). The elastic demand functions for both HDVs and CAVs are shown in Eq. (42). The maximum total demand for each OD pair can be found in Leblanc (1973). The market penetration rate of the CAVs is assumed to be 50%.
Figure 8. AVT links (marked in red) on the Sioux Falls network

Table 2. Solution trajectory of the NRMFD for maximum total revenue problem

<table>
<thead>
<tr>
<th>Iterations</th>
<th>$\tau_{29}$</th>
<th>$\tau_{30}$</th>
<th>$\tau_{48}$</th>
<th>$\tau_{49}$</th>
<th>$\tau_{51}$</th>
<th>$\tau_{52}$</th>
<th>$\tau_{53}$</th>
<th>$\tau_{58}$</th>
<th>Total revenue</th>
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<td>1</td>
<td>35</td>
<td>35</td>
<td>35</td>
<td>35</td>
<td>35</td>
<td>35</td>
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<td>35</td>
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<tr>
<td>3</td>
<td>32.26</td>
<td>32.26</td>
<td>32.26</td>
<td>32.26</td>
<td>32.26</td>
<td>32.26</td>
<td>17.06</td>
<td>32.41</td>
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<tr>
<td>4</td>
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<td>32.39</td>
<td>32.39</td>
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<td>32.39</td>
<td>18.02</td>
<td>31.41</td>
<td>73656.78</td>
</tr>
<tr>
<td>6</td>
<td>31.8</td>
<td>29.31</td>
<td>31.8</td>
<td>31.8</td>
<td>31.8</td>
<td>31.8</td>
<td>18.46</td>
<td>31.28</td>
<td>74776.1</td>
</tr>
<tr>
<td>7</td>
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<td>31.18</td>
<td>31.18</td>
<td>31.18</td>
<td>31.18</td>
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<td>30.66</td>
<td>75461.45</td>
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<td>9</td>
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<td>31.5</td>
<td>30.02</td>
<td>18.12</td>
<td>30.98</td>
<td>76035.12</td>
</tr>
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<td>30.1</td>
<td>30.56</td>
<td>30.41</td>
<td>30.5</td>
<td>30.74</td>
<td>18.29</td>
<td>31.11</td>
<td>76132.00</td>
</tr>
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<td>29.92</td>
<td>37.31</td>
<td>29.06</td>
<td>32.19</td>
<td>31.53</td>
<td>17.94</td>
<td>20.02</td>
<td>77480.31</td>
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<tr>
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<td>29.92</td>
<td>35.69</td>
<td>29.06</td>
<td>32.19</td>
<td>31.53</td>
<td>17.94</td>
<td>20.02</td>
<td>77880.59</td>
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<td>13</td>
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<td>30.22</td>
<td>34.07</td>
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<td>32.3</td>
<td>18.03</td>
<td>19.84</td>
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<td>30.36</td>
<td>33.45</td>
<td>30.11</td>
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<td>32.57</td>
<td>18.07</td>
<td>19.82</td>
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</tr>
<tr>
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<td>29.84</td>
<td>33.29</td>
<td>34.34</td>
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<td>36.72</td>
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<td>17.31</td>
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</tr>
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<td>16</td>
<td>30.52</td>
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<td>34.13</td>
<td>31.65</td>
<td>36.42</td>
<td>17.46</td>
<td>17.18</td>
<td>78362.02</td>
</tr>
</tbody>
</table>

Suppose all the initial toll rates for the 8 links are set as 35. Table 2 shows the toll rates on the 8 AVT links and corresponding total revenue computed by the revised NEMFD at each iteration. As can be seen, it only takes 16 iterations for this algorithm to converge. The computational time is 2258.4 seconds. At the optimal state, the total revenue collected by charging the HDVs on the 8 links is 78362.02.
Figure 9. Comparison of link flows with no toll and these with optimal toll (a) Comparison of link flows of HDVs, (b) Comparison of link flows of CAVs

Figure 9 compares the equilibrium link flows of HDVs and CAVs with no tolls and these with the optimal tolls shown in Table 2. As can be seen, after the optimal toll rates are deployed on these links, the HDV flows are reduced dramatically while the CAV flows are increased significantly. Thereby, setting tolls for HDVs of AVT links can significantly increase the proportion of CAV flows in the mixed traffic, which dramatically increases the link capacity (see Figure 10). Figure 11 shows that the link travel time is reduced by over 40% while the total link flows are reduced by less than 30% for most of the 8 links. Further, it can be found that the percentage reduction of total link flows on AVT links 29 and 48 are negative, implying that the total flows on the two links are increased after the optimal toll is deployed. Nevertheless, the link travel times on the two AVT links are still reduced significantly due to enhanced
link capacity. These results indicate that charging HDVs can effectively reduce traffic congestion in a local area.

![Figure 10. Capacity of the 8 AVT links at equilibrium state before and after the setting of the optimal tolls](image)

**Figure 10.** Capacity of the 8 AVT links at equilibrium state before and after the setting of the optimal tolls

![Figure 11. Effects of link tolls on link travel time and total link flows](image)

**Figure 11.** Effects of link tolls on link travel time and total link flows

### 5.3.2.2 Maximum customer surplus problem

Suppose the market penetration rate of CAVs is 50% and the public-sector stakeholder plans to set tolls for HDVs on links 7, 9, 10, 11, 13, and 19 in the Nguyen-Dupuis network (see Figure 12) to
maximize the customer surplus. Table 3 shows that the revised NRMFD only takes 8 iterations to find the optimal toll solution. The computational time is 43.2 seconds. At the optimum state, the customer surplus is 226538.4, larger than it is at the equilibrium state with no tolls, which is 225953.15. Thereby, under mixed traffic environments, trips by HVDs may significantly reduce the total customer surplus as they reduce the effects of CAVs on link capacity, which increases the travel costs of both HDVs and CAVs. The introduction of AVT links can not only reduce traffic congestion is a local area, but may also improve the global network performance compared to it is with no AVT links, which is hard to be seen in the context of pure HDV flows (Glazer and Niskanen, 2000).

![Nguyen-Dupuis network](image)

**Figure 12.** Nguyen-Dupuis network

<table>
<thead>
<tr>
<th>Iterations</th>
<th>$\tau_7$</th>
<th>$\tau_9$</th>
<th>$\tau_{10}$</th>
<th>$\tau_{11}$</th>
<th>$\tau_{13}$</th>
<th>$\tau_{19}$</th>
<th>Customer surplus</th>
</tr>
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<td>1</td>
<td>5</td>
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<td>5</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>223983.0</td>
</tr>
<tr>
<td>2</td>
<td>4.97</td>
<td>4.97</td>
<td>4.97</td>
<td>1.9</td>
<td>1.9</td>
<td>4.97</td>
<td>225598.9</td>
</tr>
<tr>
<td>3</td>
<td>8.23</td>
<td>8.23</td>
<td>8.23</td>
<td>1.21</td>
<td>5.51</td>
<td>8.57</td>
<td>225943.5</td>
</tr>
<tr>
<td>4</td>
<td>8.28</td>
<td>8.28</td>
<td>8.28</td>
<td>0.34</td>
<td>5.56</td>
<td>8.62</td>
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</tr>
<tr>
<td>5</td>
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</tr>
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</tr>
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<td>0</td>
<td>5.6</td>
<td>8.67</td>
<td>226538.4</td>
</tr>
</tbody>
</table>

5.3.2.2 **Maximum total demand problem**

Suppose the market penetration rate of CAVs is 70% and the public-sector stakeholder plans to set tolls on links 2, 5, 7, 9, 10, 11, 16, and 18 in the Nguyen-Dupuis network to maximize the total demand. Table 4 shows that the revised NRMFD only takes 4 iterations to find the optimal toll solution. The computational time is 18.6 seconds. Note that the total demand at the equilibrium state with no tolls is 1520.955. The optimal results shown in Table 4 indicate that charging the HDVs on the 8 AVT links can
increase the total demand. To look into this phenomenon, Figure 13 shows the change of demand for HDVs and CAVs between each OD pair after the optimal tolls are set on the 8 AVT links. It demonstrates that controlling the accessing of HDVs on the AVT links can significantly increase the demand of CAVs for most OD pairs with no dramatic negative impacts on the OD demand of HDVs. This is because a reduction of HDV flow on the AVT links will significantly reduce the travel time of both HDVs and CAVs, which attracts more number of CAV-based trips and partly compensate for the reduction in level of service for HDVs due to tolls on AVT links. These results further demonstrate the necessity to constraint the use of HDVs in certain areas under mixed traffic environments. The proposed HDV-based toll strategy helps the decision-makers to find the optimal toll rates for HDVs to maximize the designed network performance.

### Table 4. Solution trajectory of the revised NRMFD for the maximum total demand problem

<table>
<thead>
<tr>
<th>Iterations</th>
<th>$\tau_2$</th>
<th>$\tau_5$</th>
<th>$\tau_7$</th>
<th>$\tau_9$</th>
<th>$\tau_{10}$</th>
<th>$\tau_{11}$</th>
<th>$\tau_{16}$</th>
<th>$\tau_{18}$</th>
<th>Total demand</th>
</tr>
</thead>
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<td>4</td>
<td>7</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1538.92</td>
</tr>
<tr>
<td>2</td>
<td>3.97</td>
<td>7</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0.27</td>
<td>1.99</td>
<td>1539.73</td>
</tr>
<tr>
<td>3</td>
<td>3.83</td>
<td>6.88</td>
<td>1.88</td>
<td>1.88</td>
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</tr>
<tr>
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<td>1.88</td>
<td>0</td>
<td>1.85</td>
<td>1540.39</td>
</tr>
</tbody>
</table>

### Figure 13. Comparison of OD demand for both HDVs and CAVs before and after setting the optimal toll rates on the AVT links

6. **Concluding comments**

The AVT links can effectively control the proportion of HDVs in mixed traffic environments by charging HDVs with a certain amount of tolls. It is a useful strategy for traffic operators to reduce traffic congestion and encourage the adoption of CAVs in the transition period. This study seeks to find the optimal toll rates for HDVs in AVT links to maximize the network performance. To do this, an MTA-ED problem is proposed to better estimate the impacts of link tolls on equilibrium network flows. The MTA-ED problem characterizes the HDV and CAV travelers’ route choice behavior using the CNL-ED model and UE-ED model, respectively. The two models capture the effects of HDV and CAV travelers’
knowledge level of traffic conditions on their route choices. Further, it also models the changes in OD demand induced by tolls charged for HDVs. Thereby, the proposed model enhances behavior realism. To solve the MTA-ED problem, an equivalent fixed demand-based MTA model is formulated. It enables the application of the route-swapping-based solution algorithm proposed by Wang et al. (2019). Further, based on the needs of both private-sector and public-sector stakeholders, two categories of the optimal toll design problems are formulated according to whether the MTA-ED problem has a unique solution or not. These optimal toll design problems help to find the optimal toll rate on each AVT link to maximize the designed performance indicator in the worst case. These problems are solved by a revised NRMFD constructed upon the analytical model for sensitivity analysis of the MTA-ED problem. This algorithm is globally convergent even if the optimal design problems are non-convex.

The numerical application finds that the revised NRMFD can effectively solve the three optimal toll design problems. It converges very fast for different networks. Further, under mixed traffic environments, HDV-based trips have dramatic negative effects on link capacity. It can significantly increase the link travel time, which may deteriorate the system performances including the customers’ surplus and total demand (i.e., they are not maximum when no tolls are introduced to control HDV flows). This phenomenon shows the necessity to control the access of HDVs on some links. The proposed method in this study helps to find the optimal toll rates on AVT links to control the HDV flows to maximize the network performance.

The current work can be extended in a few directions.

First, while we cannot analytically prove that the proposed MTA-ED problem (17) has a unique solution, numerical analysis suggests that its solution is unique. A future research direction is to analyze the conditions under which the solution of the MTA-ED problem (17) is unique. Further, we will explore whether a case exists for which the MTA-ED problem (17) has multiple solutions, and apply problem (26b) to determine the optimal toll rates for AVT links to improve the network performance in the worst case.

Second, the embedded link capacity model in the BPR function significantly impacts its link travel time prediction performance. In this study, the link capacity model considers the impacts of two critical factors, i.e., the heterogeneous reaction time of HDVs and CAVs, and the market penetration rate of CAVs. Other factors such as CAV platoon size, the order of CAVs and HDVs in the flow, and the number of lanes may also impact the link travel time. Hence, a future research direction is to develop and calibrate a new link travel time function for mixed traffic flows to holistically consider the impacts of these factors.

Third, when CAV technology is not mature (≤ level 3 automation), the drivers may need to take over driving frequently. To better characterize the network flow in this context, we will study the analytical relations between the travelers' driving mode choice and the potential impact factors (such as road conditions, traffic environments, human factors, etc.). We will divide the travelers and the roads into multiple classes based on the likelihood of using autonomous driving mode. A new multiclass traffic assignment model will be formulated to improve the prediction performance of network flows in a mixed traffic environment under level 3 (or less) automation.

Fourth, the revised NRMFD only converges linearly to the optimal point as it is built upon the linearized system of the upper-level nonlinear programming problem (25) (Cawood and Kostreva, 1994). New solution algorithms will be designed for the optimal toll design problems to enable superlinear convergence to the optimal point.
Acknowledgments

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