Data-driven Variable Speed Limit Design with Performance Guarantees for Highways

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Abstract—This paper studies the data-driven design of variable speed limits for highways subject to uncertainty, including unknown driver actions as well as vehicle arrivals and departures. With accessibility to sample measurements of the uncertain variables, we aim to find the set of speed limits that prevents traffic congestion and an optimum vehicle throughput with high probability. This results into the formulation of a stochastic optimization problem (P), which is intractable due to the unknown distribution of the uncertainty variables. By developing a distributionally robust optimization framework, we present an equivalent and yet tractable reformulation of (P). Further, we propose an efficient algorithm that provides suboptimal data-driven solutions and guarantees congestion-free conditions with high probability. We employ the resulting control method on a traffic simulator to illustrate the effectiveness of this approach.

I. INTRODUCTION

Transportation networks constitute one of the most critical infrastructure sectors today, with a major impact on the economics, security, public health, and safety of a community. In these networks, the accessibility of routes among large geographical locations is highly dependent on the congestion of the available highways [1]. To mitigate traffic congestion, several control schemes have been proposed in the literature, such as ramp metering control [2]–[5], lane assignment [6], [7], dynamic traffic assignment [8], optimization based control [9], [10], logic-based control [11], extremum seeking control [12], and many other innovative control strategies [13], [14]. More recently, Variable Speed Limit (VSL) has been proposed as an effective congestion control mechanism in transportation [15]–[18]. In particular, the work in [15] studies effects of VSL on highway traffic flows via experiments. A similar insightful view but on general transportation networks is rigorously developed and studied in [16]. In [17], a linear model predictive control of VSL has been proposed as an effective congestion control mechanism in transportation [15]–[18]. In particular, the work in [15] studies effects of VSL on highway traffic flows via experiments. A similar insightful view but on general transportation networks is rigorously developed and studied in [16]. In [17], a linear model predictive control of VSL has been proposed as an effective congestion control mechanism in transportation [15]–[18]. In particular, the work in [15] studies effects of VSL on highway traffic flows via experiments.

Statement of Contributions: This work presents the following contributions: 1) We first extend the CTM to account for random events (due to drivers actions) as well as vehicle arrival and departures. This provides an analytical framework and a stochastic optimization problem formulation for the computation of VSL using the available flow measurements (in Section II). 2) We propose an optimization-based data-driven control approach that extends DRO to account for system dynamics. The resulting approach guarantees congestion elimination with high probability, using only finite flow measurements (in Section III). 3) As the proposed data-driven optimization problem is infinite dimensional and intractable, we propose an equivalent reformulation that reduces the proposed problem into a finite-dimensional optimization problem (in Section III). 4) Yet this problem is non-convex and difficult to solve, so we find an equivalent formulation via a second-order cone relaxation technique. We show that, under mild conditions, the resulting Mixed-Integer Second-Order Cone Problem (MISOCP) is exact, and can be handled by commercial solvers (in Section IV). 5) The resulting MISOCP is still a large-scale problem. We finally propose a computationally efficient algorithm to provide online suboptimal speed limits that ensure congestion elimination and guarantee of highway throughput with high probability (in...
Section V). 6) We numerically demonstrate the performance of the proposed solution techniques and effectiveness of our data-driven approach with performance guarantees, in Section VI.

A preliminary study of this work appeared in [27], however the differences are the following: 1) Our CTM-based model under uncertainty is different (in Section II and III). 2) This work provides equivalent reformulation of the proposed non-convex problem and its exact MISOCP relaxation (in Section IV). 3) This work demonstrates a detailed procedure of the proposed integer-solution search algorithm (in Section V). 4) We study both the effectiveness of the proposed algorithm and distributional robustness of the proposed data driven approach (in Section VI). 5) All the proofs of lemmas, propositions and theorems are provided in Appendix A. 

Notation: See the footnote\(^1\) for basic notations of this work.

\section{Problem Formulation}

In this section, we first introduce a traffic model of one-way highways, and then introduce the set of random inflows and parameters determined by drivers’ actions. Finally, we propose a stochastic optimization problem for designing variable speed limits with performance guarantees.

\subsection{Highway Traffic Model}

Consider a time horizon of length \(Q\), and assume that time is divided into time slots of size \(\delta\). Notice that the time slot duration \(\delta\) needs to be selected carefully in order to obtain accurate discrete-time traffic models (see, e.g., [28], [29]). Let \(T = \{0, 1, \ldots, T\}\) denote the set of time slots, where \(T\) is an integer closest to \(Q/\delta\). We consider a one-way highway of length \(L\), and divide the it into \(n\) segments of equal size \(L/n\). The topology of the highway can be represented by a directed graph \(G = (V, E)\), where \(V = \{0, 1, \ldots, n\}\) and each \(v \in V\) corresponds to the link between two consecutive road segments. Notice that node 0 is a fictitious node representing the inflow into the highway. The edge set is defined as \(E = \{(0, 1), \ldots, (n-1, n)\}\) with each element \(e = (v, v+1) \in E\) corresponding to the road segment between nodes \(v\) and \(v+1\) for all \(v \in \{0, 1, \ldots, n-1\}\). To illustrate this, we refer the reader to Fig. 2. We call node 0 the source node, and node \(n\) the sink node. Further, node \(v \in V \setminus \{0\}\) is called an arrival node if there exists an on-ramp at node \(v\). Similarly, node \(v \in V \setminus \{n\}\) is called a departure node if there exists an off-ramp at node \(v\). Let \(V_A\) and \(V_D\) denote the set of arrival and departure nodes, respectively. By convention, we set node 0 \(\notin V_A\) and node \(n \notin V_D\) for each edge \(e = (v, v+1) \in E\).

1 Let \(\mathbb{R}^{m \times n}\) denote the \(m \times n\)-dimensional real vector space, and let \(1_m\) and \(0_m\) denote the column vectors \((1, \ldots, 1)^T \in \mathbb{R}^m\) and \((0, \ldots, 0)^T \in \mathbb{R}^m\), respectively. For any vector \(x \in \mathbb{R}^m\), let us denote \(x \geq 0_m\) if all the entries are nonnegative. Any letter \(x\) may have appended the following indices and arguments: it may have the subscript \(x_i\) with \(i \in \mathbb{N}\), the argument \(x_i(t)\) with \(t \in \mathbb{N}\), and finally a superscript \(l \in \mathbb{N}\) as in \(x_i(l)\). Given a finite number of elements \(x_i(l) \in \mathbb{R}^e\) where \(e, l, l' \in \mathbb{N}\), we define vectors \(x_i(l') := (x_i(1), x_i(2), \ldots, x_i(l')) \in \mathbb{R}^{e 	imes l'}\), and \(x := (x_1(), x_2(), \ldots)\). Let \(x, y\) and \(x \odot y\) denote the inner and component-wise products of vectors \(x, y \in \mathbb{R}^{e \times l}\), respectively. The component-wise square of vector \(x \in \mathbb{R}^{e \times l}\) is denoted by \(x^2 := x \odot x\). In addition, let \(x \otimes y\) denote the Kronecker product of vectors \(x, y\) with arbitrary dimension. Let \(\|x\|_1\) denote the 1-norm of \(x \in \mathbb{R}^e\), and let \(\|x\|_* := \sup_{\|z\|_1 \leq 1} \langle z, x \rangle\) denote the corresponding dual norm. Notice that \(\|x\|_* = \|x\|_1\).

with starting node \(v\), let \(e'\) denote the on-ramp of edge \(e\) if node \(v \in V_A\) and let \(e''\) denote the off-ramp of edge \(e\) if node \(v + 1 \in V_D\).

A macroscopic model of each road segment can be described by its traffic density, allowable flow rate, and speed limit [1], [19], [28]. Let \(\pi_e, \rho_c,\) and \(\mathcal{T}_e\) denote the maximal free flow speed, the traffic jam density, and the capacity of edge \(e\), respectively. Moreover, \(\rho_c(t)\) denote the traffic density, the allowable flow rate, and the speed limit of edge \(e\) at time slot \(t\), respectively. In this study, we assume that \(u_e(t) = u_e\) is constant over the time horizon \(T\). There is a nonlinear relationship between the allowable flow rate, traffic density, and speed limit of each road segment \(e\). Given a speed limit \(u_e\), the relationship between allowable flow rate \(f_e(t)\) and traffic density \(\rho_e(t)\) can be characterized by the fundamental diagram of edge \(e\). Fundamental diagrams of edge \(e\) for various speed limits are shown in Fig. 1. For more information on fundamental diagrams, we refer the reader to [15], [30].

Our goal is to design speed limits for highways. To achieve this goal, we consider a finite set of speed limits, and then approximate the fundamental diagram of each segment \(e\) with a finite set of piecewise linear functions, as shown in Fig. 1. Let \(\Gamma\) be a finite, feasible set of speed limits for the edges. More precisely, the speed limit of each edge \(e \in E\) must satisfy

\[ u_e \in \Gamma := \{\gamma^{(1)}, \ldots, \gamma^{(m)}\} \]

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The set of real values \(\Gamma\) is determined by the physical structure of the highway as well as its maximal free flow speed and traffic jam density. As mentioned earlier in the footnote, random events, such as accidents, can change these values. Let \(\rho_c'(u_e)\) denote the critical density of edge \(e\) for speed limit \(u_e\).

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The values of parameters \(\pi_e, \rho_c,\) and \(\mathcal{T}_e\) are determined by the physical structure of highways as well as random events, such as accidents and temporary lane closures (see, e.g., [29]).
To compute the traffic density dynamics, let us denote the fraction of the outflow rate that departs the system. Hence, the flow through the off-ramp by \( r_o \) regardless of the flow rates. Using the constraint above and the property \( \tau \) of critical densities, we design speed limits which are robust to the uncertainty \( \Gamma \) and let \( r_o \) be determined by the drivers’ actions. Therefore, \( r_o \) is random, and its value is unknown to the system operator in advance. Each random variable \( r_o \) will have a nonempty support set denoted by \( R_o \subseteq \mathbb{R}_{>0} \) if the ending node of edge \( e \) is a departure node; otherwise, the value of \( r_o \) is zero. Further, let \( f_e(t) \) denote the incoming flow of edge \( e \) at time slot \( t \), and let \( r_o \) denote the fraction of incoming flow through the highway ramp \( e \) at time slot \( t \), respectively. More precisely, the incoming flow to segment \( e \) through the on-ramp \( e' \) is \( f_e(t) := r_o f_e(t) \), where \( r_o \) represents the rate of incoming flow through the highway ramp \( e' \) at time slot \( t \), and \( f_e(t) \) is the traffic density on each edge \( e \) at time slot \( t \). The dynamics of the traffic density on each edge \( e \) can be represented by [19]

\[
\rho_e(t + 1) = \rho_e(t) + h(r_o(t) - f_e(t)), \quad \forall t \in T,
\]

where \( h \) is a random variable and \( \delta \) and \( L \) depend on parameters \( n, \delta \) and \( L \).}

![Fig. 2: Segment of highways and its graph representation. The symbol e indicates a highway segment, and s is its preceding segment.](image)

The traffic density dynamics of each segment \( e \) is equal to the sum of its on-ramp flows and the portion of outgoing flow of its preceding edge that flows into edge \( e \), as shown in Fig. 2. For each edge \( e \in E \) and its preceding edge \( s \in E \), the flow conservation constraint must hold

\[
(1 - r_o(t)) f_e(t) = (1 - r_o(t)) f_s(t), \quad \forall t \in T.
\]

Using the constraint above, the traffic density dynamics at each time slot \( t \in T \setminus \{T\} \) are modeled by

\[
\rho_e(t + 1) = \rho_e(t) + h(1 - r_o(t)) f_s(t) - h f_e(t), \quad \forall e \in E \setminus \{(0, 1)\}.
\]

Recall that \( f_e(t) = u_e \rho_e(t) \) for all \( e \in E \) and \( t \in T \).
out-of-sample performance guarantees within a distributionally robust optimization framework [27]. More precisely, given \( N \) samples of the random variable \( \varpi \), we seek to find a set of speed limits \( u \) with certificate (or objective lower bound) \( J(u) \) such that the out-of-sample performance of \( u \),

\[
\mathbb{E}_\varpi = \frac{1}{N} \sum_{e \in \mathcal{E}, t \in T} \rho_e(t) u_e,
\]

has the following performance guarantee with a desired confidence value \( \beta \in (0, 1) \)

\[
\text{Prob}^N \left( \mathbb{E}_\varpi \left[ \frac{1}{T} \sum_{e \in \mathcal{E}, t \in T} \rho_e(t) u_e \right] \geq J(u) \right) \geq 1 - \beta, \quad (6)
\]

where \( \text{Prob}^N \) denotes the probability of the event \( \mathbb{E}_\varpi = \frac{1}{N} \sum_{e \in \mathcal{E}, t \in T} \rho_e(t) u_e \geq J(u) \), depending on \( u \) and the observed \( N \) outcomes of \( \varpi \). Note that \( \text{Prob}^N \) is defined on the \( N \) product of the sample space of \( \varpi \).

III. PERFORMANCE GUARANTEED SPEED-LIMIT DESIGN

Our goal is to compute a set of speed limits with certain out-of-sample performance guarantees. To achieve this goal, we follow a four-step procedure. First, we reformulate Problem (P) into an equivalent problem (call it Problem (P1)).

Second, we propagate the sample trajectories using the \( N \) measurements of \( \varpi \). Third, we adopt a distributionally robust optimization approach to (P1). The first three steps enable us to obtain a distributionally robust optimization framework for computing speed limits with guarantees equivalent to (6).

Finally, we obtain a tractable problem reformulation.

Step 1: (Equivalent Reformulation of (P)) Traffic densities \( \rho_e(t) \), for all \( e \in \mathcal{E} \) and \( t \in T \setminus \{0\} \), are random since traffic inflows and outflows are random in each segment \( e \). Using this observation, we now consider the variable \( \varpi \) in Problem (P) as a random variable, and derive an equivalent Problem (P1) via a reformulation of the constraints in (P).

Given a speed limit \( u \) that satisfies the constraint (1), let \( \mathbb{P}(u) \) and \( \mathcal{Z}(u) \) denote the probability distribution of variable \( \varpi \) and the support of \( \varpi \), respectively. Recall that in Problem (P), constraints (3) ensure no congestion on the highway. Hence, the given \( u \) should be such that \( \mathcal{Z}(u) \subseteq \{ \rho \in \mathbb{R}^n \mid (3) \} \). Without loss of generality, we consider \( \mathcal{Z}(u) := \{ \rho \in \mathbb{R}^n \mid (3) \} \). To fully characterize random variable \( \varpi \), the distribution of \( \mathbb{P}(u) \) needs to be determined. Using the traffic density dynamics in (5) and flow representation in (4), the probability distribution \( \mathbb{P}(u) \) can be represented as a convolution of the distribution \( \mathcal{P}_\varpi \).

Let \( \mathcal{M}(\mathcal{Z}(u)) \) denote the space of all probability distributions supported on \( \mathcal{Z}(u) \). We now write the objective function of Problem (P) compactly as

\[
H(u; \rho) := \frac{1}{T} \sum_{e \in \mathcal{E}, t \in T} \rho_e(t) u_e,
\]

and reformulate (P) as follows

\[
\text{Problem (P1)} \quad \max_u \quad \mathbb{E}_{\mathbb{P}(u)} \left[ H(u; \rho) \right],
\]

s.t. \( \mathbb{P}(u) \) characterized by (4), (5) and \( \mathcal{P}_\varpi \),

\[
\mathbb{P}(u) \in \mathcal{M}(\mathcal{Z}(u)), \quad (1).
\]

Notice that Problems (P) and (P1) are equivalent. And similarly, we obtain the performance guarantee of (P1) by considering the induced out-of-sample performance on \( \mathbb{P}(u) \), written as \( \mathbb{E}_{\mathbb{P}(u)} \left[ H(u; \rho) \right] \). For all problems derived later, we use the performance guarantees equivalent to (6), as follows

\[
\text{Prob}^N \left( \mathbb{E}_{\mathbb{P}(u)} \left[ H(u; \rho) \right] \geq J(u) \right) \geq 1 - \beta, \quad (7)
\]

Recall that \( \text{Prob}^N \) denotes the probability that the event \( \mathbb{E}_{\mathbb{P}(u)} \left[ H(u; \rho) \right] \geq J(u) \) happens on the \( N \) product of the sample space that defines \( \rho \), the value \( J(u) \) is the certificate to be determined, and \( \beta \in (0, 1) \) is the desired confidence value.

Next, we characterize the probability distribution \( \mathbb{P}(u) \) using the \( N \) sample measurements of \( \varpi \).

Step 2: (Sample Trajectory Propagation) Let \( \mathcal{L} = \{1, \ldots, N\} \) denote the index set for the \( N \) realizations of the random variable \( \varpi \), and let \( \{ \varpi^{(l)} \} \in \ell \subseteq \mathcal{L} \), where \( \varpi^{(l)} := (\omega^{(l)}, \rho^{(l)}(0), r_{in}^{(l)}, r_{out}^{(l)}) \), denote the set of independent and identically distributed (i.i.d.) realizations of \( \varpi \). Given a speed limit \( u \) and measurement \( \varpi^{(l)} \), a unique traffic density trajectory \( \rho^{(l)}(t) \) can be computed by using (4) and (5). Notice that this trajectory is unique since density dynamics (5) is linear (in \( \rho \)) for a given speed limit \( u \) and measurement \( \varpi^{(l)} \). Given these realizations \( \{ \varpi^{(l)} \} \in \ell \subseteq \mathcal{L} \), the sample trajectories \( \{ \rho^{(l)}(t) \} \in \ell \subseteq \mathcal{L} \) of the random traffic flow densities for each edge \( e \in \mathcal{E} \) with its precedent edge \( s \in \mathcal{E} \cup \varnothing \), are given by

\[
\rho_e^{(l)}(t+1) = h \frac{1 - r_{in}^{(l)}(t)}{1 - r_{out}^{(l)}(t)} u_e \rho_e^{(l)}(t) - hu_e \rho_{e+1}^{(l)}(t) + \rho_{e-1}^{(l)}(t), \quad \forall e \in \mathcal{E} \setminus \{0, 1\}, \quad (8)
\]

\[
\rho_{e+1}^{(l)}(t+1) = \rho_{e+1}^{(l)}(t) + h(\omega^{(l)}(t) - u_e \rho_e^{(l)}(t)), \quad e = (0, 1),
\]

for all \( t \in T \setminus \{T\} \) and \( l \in \mathcal{L} \). The following lemma establishes that \( \{ \rho^{(l)}(t) \} \subseteq T \subseteq \mathcal{L} \) are i.i.d. samples from \( \mathbb{P}(u) \).

Lemma III.1 (Independent and identically distributed sample generators of \( \rho \)) Given a speed limit \( u \) and a set of i.i.d. realizations of \( \varpi \), the system dynamics (8) generate i.i.d. sample trajectories \( \{ \rho^{(l)}(t) \} \subseteq T \subseteq \mathcal{L} \) of \( \mathbb{P}(u) \).

We provide the proof in Appendix A, which also contains all the proofs of the later lemmas, propositions and theorems.

Let \( \mathcal{M}_h(\mathcal{Z}(u)) \subseteq \mathcal{M}(\mathcal{Z}(u)) \) denote the space of all light-tailed probability distributions supported on \( \mathcal{Z}(u) \). We make the following assumption on the probability distribution \( \mathbb{P}_\varpi \):

Assumption III.1 (Light-tailed unknown distributions) The distribution \( \mathbb{P}_\varpi \) satisfies \( \mathbb{P}_\varpi \in \mathcal{M}_{h}(\mathcal{Z}(u)) \), i.e., there exists an exponent \( a > 1 \) such that \( b := \mathbb{E}_{\mathbb{P}_\varpi} \left[ \exp \| \varpi \|_a^a \right] < \infty \).

The following lemma shows that the probability distribution of traffic densities is a light-tailed distribution when distribution \( \mathbb{P}_\varpi \) is light-tailed.

Lemma III.2 (Light-tailed distribution of \( \rho \)) If Assumption III.1 holds, then \( \mathbb{P}(u) \in \mathcal{M}_h(\mathcal{Z}(u)) \).

The above Lemmas III.1 and III.2 result in accessible i.i.d. samples of the light-tailed unknown distribution \( \mathbb{P}(u) \), which enable the distributionally robust optimization framework for (P1) in the next step.

3The support \( \mathcal{Z}(u) \) is the smallest closed set such that \( P(\rho \in \mathcal{Z}(u)) = 1 \).

4For any set \( \mathcal{Z} \), we use notion \( M_\varpi(\mathcal{Z}) \) to denote the space of all light-tailed probability distributions supported on \( \mathcal{Z} \).
Step 3: (Performance Guarantee Certificate) Given a speed limit $u$, we design a certificate $J(u)$ that satisfies the performance guarantee condition (7). To achieve this goal, we consider a set of distributions $\mathcal{P}(u)$ that is small, tractable and yet rich enough to contain $\bar{P}(u)$ with high probability. Then by evaluating (P1) under a worst-case distribution of $\mathcal{P}(u)$, we guarantee performance of (P1) in the form of (7).

Consider the Wasserstein ball\(^5\) $B_\epsilon(\bar{P}(u))$ of center $\bar{P}(u) := (1/N) \sum_{i \in \mathcal{I}} \delta_{\rho(i)}$ and radius $\epsilon$. Notice that the center $\bar{P}(u)$ is obtained using the point mass operator $\delta$ under i.i.d. sample trajectories $\{\rho(i)\}_{i \in \mathcal{I}}$ that are distributed according to $\mathcal{P}(u)$, which is a function of the controlled system dynamics (8) and samples of $\varpi$. Then we propose certificates $J(u)$ of (P1) in the following theorem.

**Theorem III.1 (Performance guarantees of (P1))** Assume that Assumption III.1 on light-tailed distributions of $\varpi$ holds. And further, we assume that $N$ i.i.d. samples of $\varpi$, speed limit $u$, and confidence value $\beta$ are given. Then, there exists a Wasserstein radius $\epsilon := \epsilon(\beta)$, depending on the confidence value $\beta$ and Assumption III.1, such that the following set of distributions $\mathcal{P}(u)$ contains $\bar{P}(u)$ as described in (P1) with probability at least $1 - \beta$, i.e.,

$$\operatorname{Prob}^N(\bar{P}(u) \in \mathcal{P}(u)) \geq 1 - \beta,$$

with $\mathcal{P}(u) := B_\epsilon(\bar{P}(u)) \cap M_b(Z(u))$. Further, the following proposed certificate $J(u)$ of (P1) satisfies guarantee (7)

$$J(u) := \inf_{Q \in \mathcal{P}(u)} \mathbb{E}_Q[H(u; \rho)].$$

**Remark III.1 (Effect of Assumption III.1 on $J(u)$)** The certificate $J(u)$ highly depends on the set $\mathcal{P}(u)$ and the Wasserstein radius $\epsilon(\beta)$. In Theorem III.1, the value $\epsilon(\beta)$ is calculated via the parameters $a$ and $b$ in Assumption III.1. As these parameters may not be known, one can determine $\epsilon(\beta)$ in a data driven fashion via (Monte-Carlo type of) simulations. That is, we start by setting $\epsilon(\beta) = 0$ and gradually increase it until the performance guarantees (7) hold with that given $\beta$ for a sufficiently large number of simulation runs.

Theorem III.1 provides each feasible solution $u$ of (P1) with a certificate $J(u)$ that guarantees performance as in (7). This motivates a tractable reformulation of (P1) as follows.

**Step 4: (Tractable Reformulation of (P1))** Our goal is to obtain a speed limit $u$ that maximizes the average flow through the highway as in (P1) while ensuring that the performance guarantee condition (7) is satisfied. Given a set of inflow and outflow samples $\{\varpi(i)\}_{i \in \mathcal{I}}$, a speed limit $u$ that provides the highest $J(u)$ or best objective lower bound, can be computed by solving the following optimization problem

$$\text{(P2)} \quad \sup_{u} \quad J(u).$$

**Problem (P2) consists of $J(u)$, an infinite-dimensional optimization problem that is hard to solve. To obtain a tractable optimization problem, we reformulate Problem (P2) as**

$$\text{(P3)} \quad \max_{u, \rho, \lambda, \mu, \nu, \eta} - \lambda \epsilon(\beta) - \frac{1}{N} \sum_{e \in \mathcal{E}, t \in \mathcal{T}, l \in \mathcal{L}} \int_{e} \rho e \nu e l(t) + \frac{1}{N} \sum_{t \in \mathcal{T}} \left\{ \nu(t), \mu(t) \right\},$$

s.t. $\left[ J + u \circ (\bar{\rho} - \rho^e(\bar{\pi})) \right] \otimes 1_T \circ \eta^l \geq 0_{\mathcal{L}}, \forall l \in \mathcal{L}$,

$$\nu(l) = \mu(l) + 1 \quad u \otimes 1_T, \forall l \in \mathcal{L},$$

$$\left\| \nu(l) \right\|_* \leq \lambda, \forall l \in \mathcal{L},$$

$$\eta^l \geq 0_{\mathcal{L}}, \forall l \in \mathcal{L},$$

where decision variables $(u, \rho, \lambda, \mu, \nu, \eta)$ are concatenated versions of $u_e, \rho_e^l(t), \lambda, \mu_e^l(t), \nu_e^l(t), \eta_e^l(t) \in \mathbb{R}$, for all $l \in \mathcal{L}, t \in \mathcal{T} \setminus \{0\}$, and $e \in \mathcal{E}$. The value $\rho^e(\bar{\pi}) := \int \bar{\rho} / \mathcal{I}$ is the vector of critical densities under the free flow, and $\bar{\pi}$ is the jam density vector.

The following result shows that problems (P2) and (P3) are equivalent for $(u, J)$.

**Theorem III.2 (Tractable reformulation of (P2))** Problem (P2) is equivalent to (P3) in the sense that their optimal objective values coincide and the set of optimizers of (P2) are the projection of that of (P3). Further, for any feasible point $(u, \rho, \lambda, \mu, \nu, \eta)$ of (P3), let $J(u)$ denote the value of its objective function. Then the pair $(u, J(u))$ gives a data-driven solution $u$ with an estimate of its certificate $J(u)$ by $\hat{J}(u)$, such that the performance guarantee (7) holds for $(u, \hat{J}(u))$.

Problem (P3) is inherently difficult to solve due to the discrete decision variables $u$, bi-linear terms $u \otimes 1_T \circ \eta^l$ in the first group of constraints, and the nonlinear sample trajectories $\{\rho^l(i)\}_{i \in \mathcal{I}}$, which motivates our next section.

IV. REFORMULATION AND RELAXATION

Our goal is to compute exact solutions to Problem (P3). To achieve this goal, we do the following: First, we focus on the feasibility set of Problem (P3), and transform its non-convex quadratic terms into a set of mixed-integer linear constraints. We call the new formulation Problem (P4). Second, we propose a second-order cone relaxation for the non-convex quadratic terms in Problem (P4), and a second-order cone relaxation for it. We then present the conditions under which this convex relaxation is exact.

### A. Binary Representation of Speed Limits

Let $\mathcal{O} := \{1, \ldots, m\}$ be the index set of the speed limit set $\Gamma$. For each edge $e \in \mathcal{E}$ and speed limit value $\gamma(i) \in \Gamma$, let us define the binary variable $x_{e,i}$ to be equal to one if $u_e = \gamma(i)$; otherwise $x_{e,i} = 0$. We will then have $u_e = \sum_{i \in \mathcal{O}} \gamma(i) x_{e,i}$ for each edge $e \in \mathcal{E}$. Using this representation, we can reformulate the speed limit constraints (1) as follows.
\[ \gamma^{(1)}(t) \leq \sum_{i \in \mathcal{O}} \gamma^{(i)}(x_{e,i}) \leq \gamma^{(m)}, \forall e \in \mathcal{E}, \]
\[ \sum_{i \in \mathcal{O}} x_{e,i} = 1, \forall e \in \mathcal{E}, \]
\[ x_{e,i} \in \{0, 1\}, \forall e \in \mathcal{E}, i \in \mathcal{O}, \]
and we update the sample trajectories formula (8) for all \( t \in \mathcal{T} \setminus \{T\} \) and \( l \in \mathcal{L} \) as follows
\[ \rho^{(l)}(t + 1) = h \frac{1 - r_{e}^{(0)}(t)}{1 - r_{e}^{(0)}(t)} \sum_{i \in \mathcal{O}} \gamma^{(i)}(x_{e,i}) \rho^{(l)}(t) + \rho^{(l)}(t) \]
\[ - h \sum_{i \in \mathcal{O}} \gamma^{(i)}(x_{e,i}) \rho^{(l)}(t), \forall e \in \mathcal{E} \setminus \{(0,1)\}, \]
\[ \rho^{(l)}(t + 1) = \rho^{(l)}(t) + h \omega^{(t)}(t) - h \sum_{i \in \mathcal{O}} \gamma^{(i)}(x_{e,i}) \rho^{(l)}(t), \quad e = (0,1). \]

In this subsection we are particularly interested in two groups of bi-linear terms: 1) the bi-linear terms \( x_{e,i} \rho^{(l)}(t) \) in the sample trajectories formula (10) and 2) the bi-linear terms \( \sum_{i \in \mathcal{O}} \gamma^{(i)}(x_{e,i}) \eta^{(l)}(t) \) which appear in the first set of constraints (e.g., \( u \otimes 1_{T} \circ \eta^{(l)} \)). Each of these bi-linear terms is comprised of a continuous variable and a binary variable. We represent each of these bi-linear terms with a set of linear constraints using the following linearization technique.

Let us introduce variables \( y_{e,i}^{(l)}(t) \) and \( z_{e,i}^{(l)}(t) \) for all \( e \in \mathcal{E}, i \in \mathcal{O}, t \in \mathcal{T} \setminus \{0\} \) and \( l \in \mathcal{L} \) as follows
\[ y_{e,i}^{(l)}(t) = x_{e,i} \rho^{(l)}(t), \]
\[ z_{e,i}^{(l)}(t) = x_{e,i} \eta^{(l)}(t). \]

We further make the following assumption

**Assumption IV.1 (Bounded dual variable \( \eta \))** There exists a positive constant \( \bar{\eta} \) such that for any optimizers of (P3), the components \( \eta^{(l)}(t) \leq \bar{\eta} \) for all \( e \in \mathcal{E}, t \in \mathcal{T} \setminus \{0\} \) and \( l \in \mathcal{L} \).

We achieve Assumption IV.1 by selecting \( \bar{\eta} \) large enough. This enables the following lemma to represent the non-convex equality constraint in (11) with a set of linear constraints.

**Lemma IV.1 (Linearization technique)** Let us assume that Assumption IV.1 holds. Then for all \( e \in \mathcal{E}, i \in \mathcal{O}, t \in \mathcal{T} \setminus \{0\} \) and \( l \in \mathcal{L} \), the non-convex equality constraint in (11) can be equivalently represented with the following set of linear constraints
\[ 0 \leq z_{e,i}^{(l)}(t) \leq \bar{\eta} x_{e,i}, \]
\[ \eta^{(l)}(t) - \bar{\eta}(1 - x_{e,i}) \leq z_{e,i}^{(l)}(t) \leq \eta^{(l)}(t), \]
\[ 0 \leq y_{e,i}^{(l)}(t) \leq \rho^{(l)}(t), \]
\[ \rho^{(l)}(t) - \bar{\rho}(1 - x_{e,i}) \leq y_{e,i}^{(l)}(t) \leq \bar{\rho} x_{e,i}. \]

In particular, we denote by \( y_{e,i}^{(l)}(0) \) the term \( x_{e,i} \rho^{(l)}(0) \) for each \( e \in \mathcal{E}, i \in \mathcal{O} \) and \( l \in \mathcal{L} \). Then using the new variables \( y_{e,i}^{(l)}(t) \) and \( z_{e,i}^{(l)}(t) \), we can now reformulate the sample trajectories formula (10) as follows
\[ \rho^{(l)}(t + 1) = h \frac{1 - r_{e}^{(0)}(t)}{1 - r_{e}^{(0)}(t)} \sum_{i \in \mathcal{O}} \gamma^{(i)}(y_{e,i}(t)) + \rho^{(l)}(t) \]
\[ - h \sum_{i \in \mathcal{O}} \gamma^{(i)}(z_{e,i}(t)), \forall e \in \mathcal{E} \setminus \{(0,1)\}, \]
\[ \rho^{(l)}(t + 1) = \rho^{(l)}(t) + h \omega^{(t)}(t) - h \sum_{i \in \mathcal{O}} \gamma^{(i)}(y_{e,i}(t)), \quad e = (0,1). \]

Problem (P3) can now be equivalently reformulated as the following optimization problem
\[ \begin{align*}
\max_{x, y, z, \rho, \lambda, \mu, \nu, \eta} & -\lambda e(\hat{\beta}) - \frac{1}{N} \sum_{e \in \mathcal{E}} \sum_{t \in \mathcal{T}} \sum_{l \in \mathcal{L}} \rho^{(l)}(t) \eta^{(l)}(t) + \frac{1}{N} \sum_{e \in \mathcal{E}} \sum_{t \in \mathcal{T}} \sum_{l \in \mathcal{L}} \nu^{(l)}(t) \rho^{(l)}(t), \\
\text{s.t.} & \sum_{i \in \mathcal{O}} \gamma^{(i)}(\bar{\rho} - \rho^{(l)}(t)) \otimes 1_{T} \circ z_{e,i}^{(l)} - \mu^{(l)}, \\
& + \bar{\omega}(\bar{\rho}) \otimes 1_{T} \circ z_{e,i}^{(l)} - \mu^{(l)} \\
& \geq 0, \forall l \in \mathcal{L}, \\
& \nu^{(l)} = \mu^{(l)} + \frac{1}{T} \sum_{i \in \mathcal{O}} \gamma^{(i)}(x_{e,i} \otimes 1_{T}), \forall l \in \mathcal{L}, \\
& \|\nu^{(l)}\|_{*} \leq \lambda, \forall l \in \mathcal{L}, \\
& 0_{n,T} \leq \eta^{(l)} \leq \bar{\eta}, \forall l \in \mathcal{L}, \\
& \text{speed limits (9), dual variable (12),} \\
& \text{sample trajectories (13), (14)).} \end{align*} \]

**Remark IV.1 (Performance guarantee (7) in the setting of Problem (P4))** Let \( \hat{J}(u) \) denote the value of the objective function of (P4) at a computed feasible solution \((x, y, z, \rho, \lambda, \mu, \nu, \eta)\). Then, the resulting speed limits \( u := \sum_{i \in \mathcal{O}} \gamma^{(i)}(x_{e,i}) \) provide a data-driven solution such that \((u, \hat{J}(u))\) satisfies the performance guarantee (7) of (P1). This result exploits the fact that Problem (P4) is equivalent to (P3) and (P3) is equivalent to (P2) as in Theorem III.2.

**B. Second-order Cone Relaxation**

We propose a second-order cone relaxation for the nonconvex quadratic terms \( \{\mu^{(l)} \circ \rho^{(l)}\}_{l \in \mathcal{L}} \) in Problem (P4), and propose a second-order cone relaxation for this problem. To do this, we assume the following:

**Assumption IV.2 (Highway densities are nontrivial)** For all \( e \in \mathcal{E}, t \in \mathcal{T} \) and \( l \in \mathcal{L} \), we assume \( \rho^{(l)}(t) \geq \epsilon(\beta) \), where the parameter \( \epsilon(\beta) \) is the radius of the Wasserstein ball.

**Remark IV.2 (On nontrivial highway densities)** Assumption IV.2 depends on the radius of the Wasserstein ball, which is selected as in Remark III.1. In reality, we could select the value \( \epsilon(\beta) \) to be sufficiently small, even if it potentially sacrifices confidence on performance guarantees. In any case, there are three cases to consider: 1) the density on each segment of highway is just zero, 2) there are zero density values \( \rho^{(l)}(t) \), for some \((e, t, l)\), while the rest of \( \rho^{(l)}(t) \) are upper bounded by a value that is smaller than the maximal-allowable critical density \( \max_{u \in \mathcal{E}} \rho^{(l)}(u) \), and 3) there are some values \( \rho^{(l)}(t) \) that go beyond the maximal-allowable
critical density. In the first case, no congestion would happen and there is no need for VSL control. The second case can be handled by tuning $\delta(\beta)$ to be small enough. In the third case, there is already congestion on some segment of the highway and no feasible VSL would eliminate that congestion.

Assumption IV.2 enables us to explore properties of the optimizers of (P4) as in the following proposition.

**Proposition IV.1 (Optimizers in a cone)** Let $\text{sol}^* := (x^*, y^*, z^*, \lambda^*, \mu^*, \nu^*, \eta^*)$ be any optimizer of Problem (P4). If Assumption IV.2 holds, we have $\nu^* \circ \rho^* \geq 0_{nTN}$.

Proposition IV.1 allows us to explore structure of the bi-linear terms $\{\nu(t) \circ \rho(t)\} \in \mathcal{L}$ via second-order cone constraints. This is achieved by introducing variables $\vartheta_e(t)$ and writing Problem (P4) as follows

$$(P4')$$

$$\max_{s.t.} \frac{1}{N} \sum_{e,t,l} \mathcal{T}_e \mathcal{P}_e \vartheta_e(t) + \frac{1}{N} \sum_{e,t,l} \left( \vartheta_e(t) \right)^2,$$

subject to

$$\vartheta \leq \nu \circ \rho,$$

speed limits (9), sample trajectories $\{(13), (14)\}$,

no congestion $\{(12), (15), (16), (17), (18)\}$.

For each $e \in \mathcal{E}$, $t \in \mathcal{T}$ and $l \in \mathcal{L}$, the constraint (19) can be equivalently written as the following second-order cone:

$$\sqrt{\left( \vartheta_e(t) \right)^2 + \left( \rho_e(t) \right)^2 + 2 \left( \vartheta_e(t) \right)^2} \leq \nu_e(t) + \rho_e(t).$$

Problem (P4) and (P4') are equivalent as the following:

**Lemma IV.2 (Equivalent optimizer sets of (P4) and (P4'))** Problem (P4') is equivalent to (P4) in the sense that their optimal objective values are the same and the set of optimizers of (P4) is the projection of that of (P4'). Further, any feasible solution of (P4') can give us a valid performance guarantee (7) with certificate to be objective function of (P4') evaluated at that feasible solution.

Problem (P4') is still non-convex. To approximate the quadratic terms in the objective, we will first show that variables $\vartheta_e(t)$ are bounded.

**Lemma IV.3 (Bounded variable $\vartheta$)** Assume Assumption IV.1 on bounded $\eta$ holds, then there exist large enough scalar $\overline{\vartheta}$ such that $|\vartheta_e(t)| \leq \overline{\vartheta}$ for all $e \in \mathcal{E}$, $t \in \mathcal{T} \setminus \{0\}$ and $l \in \mathcal{L}$.

Lemma IV.3 enables us to approximate each component of $\vartheta$ by a finite set of points within its range. Let (sufficiently large) $K$ denote the number of points and let us denote the set of these points by $Q := \{\pi_1, \ldots, \pi_K\} \subset \mathbb{R}$. We use the set $Q := \{1, \ldots, K\}$ to index these points. For each edge $e \in \mathcal{E}$, time $t \in \mathcal{T}$ and sample $l \in \mathcal{L}$, we define the binary variable $q_{e,k}(t)$ to be equal to one if $\vartheta_e(t)$ is approximated by $\pi_k$; otherwise $q_{e,k}(t) = 0$. Then for each $e \in \mathcal{E}$, $t \in \mathcal{T}$ and $l \in \mathcal{L}$, we will then represent $\vartheta_e(t)$ by the following constraints

$$\vartheta_e(t) = \sum_{k \in \mathcal{Q}} \pi_k q_{e,k}(t), \quad \sum_{k \in \mathcal{Q}} q_{e,k}(t) = 1, \quad \forall e \in \mathcal{E}, t \in \mathcal{T}, l \in \mathcal{L},$$

Using this representation, we find approximated solutions of (P4') by solving the following

$$(P5)$$

$$\max_{s.t.} \frac{1}{N} \sum_{e,t,l} \mathcal{T}_e \mathcal{P}_e \nu_e(t) + \frac{1}{N} \sum_{e,t,l} \left( \nu_e(t) + \rho_e(t) \right)^2 \leq \nu_e(t) + \rho_e(t),$$

level approximation (21), second-order cone (20),

speed limits (9), sample trajectories $\{(13), (14)\}$,

no congestion $\{(12), (15), (16), (17), (18)\}$.

Problem (P5) is a SOCMIP and can be solved to optimal by commercial solvers, such as GUROBI and MOSEK. Note that for any feasible solution of (P5), it is feasible for (P4') and its objective value is a valid lower bound for that of (P4'). Thus, any feasible solution of (P5) together with its objective value provide performance guarantees (7) via Lemma IV.2. Further, as the number of partition points $K \to \infty$, Problem (P5) is computationally equivalent to Problem (P4'), and therefore the same as Problem (P4).

**V. Computationally Efficient Algorithms**

The solution to Problem (P5) can be hard, especially when the number of partition points $K$ in (P5) is large. Instead of relying on commercial solvers, we propose an alternative solution to compute speed limits. The proposed algorithm that is a decomposition-based method, computes high-quality feasible solutions to (P4) with performance guarantees. Similar algorithms have been proposed in the literature [32], [33]. Such methods allow us to compute sub-optimal solutions to mix-integer nonlinear programs efficiently. The proposed integer-solution search algorithm is shown in Algorithm 1. This algorithm iteratively computes sub-optimal solutions to (P4) until a stopping criteria is met. At each iteration, the algorithm solves an upper-bounding problem to (P4), and then solves a lower-bounding problem to (P4). The upper-bounding Problem (UBP) is obtained through McCormick relaxations of the bi-linear terms $\{\nu(t) \circ \rho(t)\} \in \mathcal{L}$. This upper bounding problem is a mixed-integer linear program and its solution provides us with an upper bound on Problem (P4) and a candidate variable speed limits $\varphi(k)$. We then use the computed speed limit $\varphi(k)$ to construct a set of sample trajectories $\{\varphi(l,k)\} \in \mathcal{L}$ and equivalently reduce Problem (P4) to a linear lower-bounding Problem (LBP) for potential feasible solutions of (P4). If (LBP) is feasible, then the candidate speed limits together with the objective value of (LBP) provide performance guarantee (7) for (P4). Next, we present the upper-bounding and lower-bounding problems in detail.
Algorithm 1 Integer search solution algorithm

1: Initialize \( k = 0 \)
2: \( \text{repeat} \)
3: \( k \leftarrow k + 1 \)
4: Solve Problem \((\text{UBP}_k)\), return \( x^{(k)} \) and UB
5: Generate sample trajectories \( \{\rho^{(k,l)}\}_{l \in L} \)
6: Solve Problem \((\text{LBP}_k)\), return \( \text{obj}_{k} \) and LB
7: \( \text{until} \ UB_a - LB_b \leq \epsilon, \) or \((\text{UBP}_k)\) is infeasible, or
8: \( \text{a satisfactory suboptimal solution is found after certain running time} \ T_{\text{run}} \)
9: \( \text{return} \) data driven solution \( u_{\text{best}} := u^{(q)} \) with certificate \( \tilde{J}(u^{(q)}) \) such that \( q \in \arg\max_{p=1,\ldots,k}\{\text{obj}_{p}\} \)

A. Upper-bounding Problem

Problem \((\text{UBP}_k)\) is constructed in two stages:

\( \text{Stage 1:} \) We use a standard McCormick relaxation to handle the non-convex quadratic terms \( \{v^{(l)}(t)\rho^{(l)}(t)\}_{e \in E, i \in T, l \in L} \) in the objective function of \((\text{P4})\). Notice that the McCormick envelope \([34]\) provides relaxations of bi-linear terms, which is stated in the following remark.

Remark V.1 (McCormick envelope) Consider two variables \( x, y \in \mathbb{R} \) with upper and lower bounds, \( \underline{x} \leq x \leq \overline{x}, \underline{y} \leq y \leq \overline{y} \). The McCormick envelope of the variable \( s := xy \in \mathbb{R} \) is characterized by the following constraints

\[
\begin{align*}
 s & \geq \overline{x}y + xy - \overline{x}y, \quad s \geq \overline{x}y + xy - \underline{x}y, \\
 s & \leq \overline{x}y + xy - \overline{x}y, \quad s \leq \overline{x}y + xy - \underline{x}y.
\end{align*}
\]

To construct a McCormick envelope for \((\text{UBP}_k)\), let us denote \( \nu_e := \nu_e\left( T^{-1} + \overline{x} \overline{y} \right) \) for each edge \( e \in E \).\( \) We have \( 0 \leq \rho^{(l)}(t) \leq \overline{\rho}_c, 0 \leq \rho^{(l)}(t) \leq \overline{\rho}_c \) for all \( e \in E \), \( t \in T \), and \( l \in L \). Therefore, the McCormick envelope of \( s^{(l)}(t) := \nu^{(l)}(t)\rho^{(l)}(t) \) is given by

\[
\begin{align*}
 s^{(l)}(t) & \geq \nu^{(l)}(t)\rho^{(l)}(t) + \nu^{(l)}(t)\overline{\rho}_c - \nu^{(l)}(t)\overline{\rho}_c, \\
 s^{(l)}(t) & \geq \nu^{(l)}(t)\rho^{(l)}(t), \\
 s^{(l)}(t) & \leq \nu^{(l)}(t)\rho^{(l)}(t), \\
 s^{(l)}(t) & \leq \nu^{(l)}(t)\rho^{(l)}(t)\overline{\rho}_c.
\end{align*}
\]

\( \text{Stage 2:} \) We identify appropriate canonical integer cuts to prevent \((\text{UBP}_k)\) from choosing examined candidate variable speed limits \( \{x^{(p)}\}_{p=1}^{k-1} \). Let \( \Omega^{(p)} := \{ (e,i) \in E \times O \mid x^{(p)}_{e,i} = 1 \} \) denote the index set of \( x \) for which the value \( x^{(p)}_{e,i} \) is 1 at the previous iteration \( p \). In addition, let \( c^{(p)} := |\Omega^{(p)}| \) and \( \overline{\Omega}^{(p)} := (E \times O) \setminus \Omega^{(p)} \) denote the cardinality of the set \( \Omega^{(p)} \) and the complement of \( \Omega^{(p)} \), respectively. Therefore, the canonical integer cuts of Problem \((\text{UBP}_k)\) at iteration \( k \) are given by

\[
\begin{align*}
\sum_{(e,i) \in \Omega^{(p)}} x_{e,i} - \sum_{(e,i) \in \overline{\Omega}^{(p)}} x_{e,i} & \leq c^{(p)} - 1, \quad \forall p \in \{1, \ldots, k - 1\}.
\end{align*}
\]

Upper-bounding Problem \((\text{UBP}_k)\) can be formulated as follows

\[
\begin{align*}
\max_{\lambda, \mu, v, \eta} \quad -\lambda \epsilon(\beta) - \frac{1}{N} \sum_{e,t,l} \left( \mathcal{T}_{e} \mathcal{T}_{e} \nu^{(l)}(t) - \nu^{(l)}(t)\rho^{(l)}(t) \right),
\end{align*}
\]

s.t. \( \text{speed limits (9), sample trajectories \{13, 14\}, no congestion \{12, 15, 16, 17, 18\}, McCormick envelope (22), integer cuts (23).} \)

Let UB denote the optimal objective value of \((\text{UBP}_k)\), and let \( x^{(k)} \) denote the integer part of the optimizers of \((\text{UBP}_k)\). Then UB is an upper bound of the original non-convex Problem \((\text{P4})\). We use \( x^{(k)} \) as a candidate speed limit in the lower-bounding problem \((\text{LBP}_k)\).

B. Lower-bounding Problem

Problem \((\text{P4})\) can be equivalently written as

\[
\begin{align*}
\max_{\lambda, \mu, v, \eta} \quad -\lambda \epsilon(\beta) - \frac{1}{N} \sum_{e,t,l} \left( \mathcal{T}_{e} \mathcal{T}_{e} \nu^{(l)}(t) - \nu^{(l)}(t)\rho^{(l)}(t) \right),
\end{align*}
\]

s.t. \( \{z, \lambda, \mu, \nu, \eta \in \Phi(x), (y, \rho) \in \Psi(x), x \in X\} \)

where

\[
\begin{align*}
\Phi(x) := \{ (z, \lambda, \mu, \nu, \eta) \mid \text{no congestion} \},
\Psi(x) := \{ (y, \rho) \mid \text{sample trajectories} \},
X := \{ x \mid \text{speed limits} \}.
\end{align*}
\]

The solution \( x^{(k)} \) to \((\text{UBP}_k)\) at iteration \( k \) provides us with a candidate speed limit \( u^{(k)} := \sum_{i \in O} \gamma^{(i)}(x_{1,i}^{(k)}, \ldots, x_{n_i}^{(k)}) \). For each \( l \in L \) with the given \( u^{(k)} \), the sample trajectory \( \rho^{(l)}(t) \) is uniquely determined by \( (\omega^{(l)}), \rho^{(l)}(0), \gamma^{(i)}(x_{1,i}^{(k)}, \ldots, x_{n_i}^{(k)}) \) using the uniqueness solution of the linear time-invariant systems. Therefore, the element \( (y, \rho) \in \Psi(x^{(k)}) \) is unique. Using the constraints set \( \Psi(x^{(k)}) \), we then construct the unique sample trajectories \( \{\rho^{(l,k)}\}_{l \in L} \). The unique sample trajectories allow us to reduce \((\text{P4})\) to the following lower bounding problem

\[
\begin{align*}
\max_{z, \lambda, \mu, v, \eta} \quad -\lambda \epsilon(\beta) - \frac{1}{N} \sum_{e,t,l} \left( \mathcal{T}_{e} \mathcal{T}_{e} \nu^{(l)}(t) - \nu^{(l)}(t)\rho^{(l,k)}(t) \right),
\end{align*}
\]

s.t. \( \{z, \lambda, \mu, \nu, \eta \in \Phi(x^{(k)})\} \).

Note that \((\text{LBP}_k)\) is a linear program and much easier to solve than the non-convex Problem \((\text{P4})\). Let \( \text{obj}_{k} \) denote the optimal objective value of \((\text{LBP}_k)\). If Problem \((\text{LBP}_k)\) is solved to optimality with a finite \( \text{obj}_{k} \), we will then obtain a feasible solution of \((\text{P4})\) with speed limit \( u^{(k)} := \sum_{i \in O} \gamma^{(i)}(x_{1,i}^{(k)}, \ldots, x_{n_i}^{(k)}) \) and certificate \( J(u^{(k)}) := \text{obj}_{k} \); otherwise, Problem \((\text{LBP}_k)\) is either infeasible or unbounded, i.e., \( \text{obj}_{k} = -\infty \). The lower bound of \((\text{P4})\) can be calculated by \( LB_k = \max_{p=1,\ldots,k}\{\text{obj}_{p}\} \). The stopping criterion of the algorithm can be determined by one of the following criteria

1. \( UB_k - LB_k \leq \epsilon \)
2. \((\text{UBP}_k)\) is infeasible,
3. A satisfactory suboptimal solution is found after certain running time \( T_{\text{run}} \).
In [32], it is shown that such algorithms converge to a global \( \varepsilon \)-optimal solution after finite number of iterations when we use the first and second stopping criteria. The third solution criterion allow us to find a potentially good performance-guaranteed feasible solution within certain running time \( T_{\text{run}} \).

### VI. SIMULATIONS

In this section, we demonstrate in an example how to efficiently find a solution to (P4) that results in a robust data-driven variable-speed limit \( u \) with performance guarantee (7). The analysis of the results are twofold. First, we verify the effectiveness of the proposed integer solution search algorithm by comparing it with the monolith approach that solves an approximation to (P4), Problem (P5). Second, to verify the robustness of the solution and performance guarantees in probability, we compare the resulting distributionally robust data-driven control with the control obtained from the sample-averaged optimization problem. Both controls are applied on a naive highway simulator developed via the standard cell transmission model [19].

#### Simulation setting:
We consider a highway with length \( L = 10 \text{km} \) and we divide it into \( n = 5 \) segments. Let the unit size of each time slot \( \delta = 30 \text{sec} \) and consider \( T = 20 \) time slots for a 10min planning horizon. For each edge \( e \in E \), we assume a traffic jam density of \( \rho_e = 1050 \text{vec}/\text{km}^6 \), a capacity of \( T_e = 3.1 \times 10^8 \text{vec}/\text{h} \) and a maximal speed limit of \( u_e = 140 \text{km}/\text{h} \). Let us consider \( m = 5 \) different candidate speed limits \( \Gamma = \{40 \text{km}/\text{h}, 60 \text{km}/\text{h}, 80 \text{km}/\text{h}, 100 \text{km}/\text{h}, 120 \text{km}/\text{h}\} \). On the \( k \)th edge \( e := (3, 4) \in E \), we assume an accident happens during \( T \) with parameters \( T_e = 2.7 \times 10^3 \text{vec}/\text{h} \). To evaluate the effect of the proposed algorithm, samples of the random variables \( \rho(0), w, r^m \) and \( r^o \) are needed. In real-case studies, samples \( \{\rho(t)(0)\}_{t \in T} \) can be obtained from highway sensors (loop detectors), while samples of the uncertain mainstream flows \( \{w(t)\}_{t \in T} \) and flow fractions \( \{r^m(t)\}_{t \in T} \) can be constructed either from a database of flow data on the highway, or from the current measurements of ramp flows with the assumption that the stochastic process \( \{w(t), r^m(t), r^o(t)\}_{t \in T} \) is trend stationary.

#### Fictitious datasets:
In this simulation example, the index set of accessible samples is given by \( L = \{1, 2, 3\} \). For each \( l \in L \), let us assume that each segment \( e \in E \) initially operates under a free flow condition with an initial density \( \rho_e(0) = 260 \text{vec}/\text{km} \). To ensure sufficient inflows of the system, we let the samples \( \{w_0(t)\}_{t \in L} \) of the mainstream inflow to be chosen from the uniform distribution within interval \([2 \times 10^4, 2.4 \times 10^4] \text{vec}/\text{h}\). For each edge \( e \in E \) and time \( t \in T \), we further assume that samples \( \{r^m_0(t)\}_{t \in L} \) and \( \{r^o_0(t)\}_{t \in L} \) are generated from uniform distributions within interval \([0.5\%], [0.3\%]\), respectively. We also let the confidence value be \( \beta = 0.95 \) and the radius of the Wasserstein Ball \( \epsilon(\beta) = 0.985 \) as calculated in [35].

#### Effectiveness of the algorithm:
To generate feasible solutions that can be carried out for a real time transportation system, we allocate \( T_{\text{run}} = 1\text{min} \) execution time for control design and run algorithms on a machine with two core 1.8GHz CPU and 8G RAM. In this allocated 1 minute, we consider the speed limit design in 2 approaches: 1) we run the proposed Algorithm 1 to solutions of the Problem (P4), and 2) we run optimization solver MOSEK to solutions of the monolith Problem (P5). The partition number \( K = 5 \) is selected for the monolith approach.

We present in Table 1 the comparison of the mentioned two approaches. In 1 minute, the Algorithm 1 executed 19 candidate speed limits where 2 feasible speed limits were found at time 6.7sec and 28.7sec. We verified that \( J(u^{(2)}) = 1.17 \times 10^5 \text{vec}/\text{h} \) is the highest certificate obtained, i.e., \( J(u^{(2)}) \in \arg\max_{p=1,2} \{J(u^{(p)}) \mid u^{(p)} \text{ is feasible}\} \), and the desired speed limits are

\[ u^{(2)} = [120, 100, 80, 80, 100] \text{km}/\text{h}. \]

Compared with the proposed algorithm, the monolith approach returned a feasible solution with the speed limits \( u_{\text{mon}} = [120, 120, 120, 40, 40] \text{km}/\text{h} \) and an approximated throughput \( 3.93 \times 10^4 \text{vec}/\text{h} \). It can be seen that 1) the gap (difference between UB and LB) obtained from the Algorithm 1 is tighter than that obtained from the monolith approach, and 2) the implementable speed limits proposed by the Algorithm 1 results in higher throughput than that achieved by the monolith.

In the following subsection, we use the speed limits \( u^{(2)} \) to verify the guarantees on congestion elimination with high probability.

#### Distributionally robust decisions:
To demonstrate the distributional robustness of our approach, we compare the performance of our speed limits design \( u^{(2)} \) with the performance of the speed limits developed from a sample average optimization problem. In particular, the sample averaged version of (P) (equivalently, (P1)) is the one substitutes the unknown distribution \( \mathbb{P}(u) \) with its empirical distribution \( \hat{\mathbb{P}}(u) \). The resulting tractable formulation of the sample average problem, analogous to (P4), is the following

\[
\begin{align*}
\max_{\mu, \nu, \eta} & \quad -\frac{1}{N} \sum_{c, t, l} J(c) \rho(c, t) + \frac{1}{N} \sum_{c, t, l} \nu(c, t)(u^{(l)}(t)) \\
\text{s. t.} & \quad \sum_{i \in \mathbb{O}} \gamma_i(t) \left( \bar{\eta} - \mu'(\bar{\eta}) \right) \otimes 1_T \otimes z_i(t) - \mu(t) \\
& \quad + \hat{T} \otimes 1_T \otimes \eta(t) \geq 0_{nT}, \forall l \in L, \\
& \quad \nu(t) = \mu(t) + \frac{1}{T} \sum_{i \in \mathbb{O}} \gamma_i(t) x_i \otimes 1_T, \forall l \in L, \\
& \quad 0_{nT} \leq \eta(t) \leq \bar{\eta}, \forall l \in L, \\
& \quad \text{speed limits } (9), \text{ dual variable } (12), \text{ sample trajectories } \{(13), (14)\}.
\end{align*}
\]

---

\( ^a \) Subproblems (UBP_{\text{P4}}) and (LBP_{\text{P4}}) are solved via MOSEK.

\( ^b \) Candidate speed limit.
To verify the performance of \(u^{(2)}\) and \(u^{\text{sav}}\), each trajectory corresponds to a segment \(e \in \{1, 2, \ldots, 5\}\). For simplicity we only label segment (4), which happens to have an accident during the planning horizon. We verified that the density evolution under \(u^{(2)}\) and \(u^{\text{sav}}\) as well as the validation dataset are integrated into a highway simulator with the highway parameter settings described in the Simulation setting paragraph.

Due to space limitations we cannot showcase all sample trajectories for \(10^3\) scenarios, therefore in Fig. 3 we show an average of the sample trajectories, i.e., the function \(\frac{1}{N_{\text{val}}} \sum_{t \in \{1, \ldots, N_{\text{val}}\}} \rho^e(t)\) for each segment \(e\), with speed limits \(u^{(2)}\) and \(u^{\text{sav}}\), and present an arbitrarily chosen scenario 638 in Fig. 4. We select the simulation time horizon to be twice of that the planning horizon’s in order to see the effect of the design clearly. We verified that the density evolution under speed limits \(u^{(2)}\) and, in particular, the density trajectory of accident edge (4), did not exceed the critical density values \(\rho_c^e(80\text{km/h}) = 335\text{vec/km})\) for each sample. Thus the highway \(G\) is kept free of congestion in this planning horizon \(T\) with high probability. However, the same robust behavior can not be guaranteed under speed limits \(u^{\text{sav}}\), as vehicles accumulate significantly on edge (4) for too many samples (contrast to its critical density \(\rho_c^e(60\text{km/h}) = 403\text{vec/km})\), see Fig. 3. We claim the robustness of our design compared to the design from sample average problem, as the latter does not ensure such out-of-sample performance guarantees.

Note that the difference between the previous sample average problem and (P4) is that the former has a Wasserstein Ball radius \(\epsilon(\beta) = 0\) and, thus, unlike (P4), it does not provide a performance guarantee on congestion. We solve the above sample average problem to a suboptimal solution via the Algorithm 1 with the same setting as in solution to \(u^{(2)}\). The resulting speed limit design is the following

\[
u^{\text{sav}} = [60, 60, 80, 60, 60] \text{km/h}.
\]

To verify the performance of \(u^{(2)}\) and \(u^{\text{sav}}\), we generated \(N_{\text{val}} = 10^3\) validation samples of random variables \(\rho(0), u, r^m\) and \(r^\alpha\) that are from the distributions described in the Fictitious datasets paragraph. The speed limit design \(u^{(2)}, u^{\text{sav}}\) as well as the validation dataset are integrated into a highway simulator with the highway parameter settings described in the Simulation setting paragraph.

In this paper, we propose an extension of the cell transmission model that accounts for random inflows, outflows and events along highways. Then, we formulate a data-driven control problem with performance guarantees as a distributional optimization problem. We equivalently reformulate this intractable Problem (P) into a non-convex but tractable Problem (P4), or Mixed Integer Second Order Cone Problem (P5). This is achieved by: 1) extending Distributionally Robust Optimization theory to account for system dynamics; 2) reformulation and relaxation techniques. Finally, we adapt the idea of decomposition and propose an integer-solution search algorithm for efficient solutions of Problem (P4), or commercial solvers for that of Problem (P5). Both approaches provide performance guarantee (6) for Problem (P). Simulations demonstrate the effectiveness of this work.

\section{Conclusions}

In this paper, we propose an extension of the cell transmission model that accounts for random inflows, outflows and events along highways. Then, we formulate a data-driven control problem with performance guarantees as a distributional optimization problem. We equivalently reformulate this intractable Problem (P) into a non-convex but tractable Problem (P4), or Mixed Integer Second Order Cone Problem (P5). This is achieved by: 1) extending Distributionally Robust Optimization theory to account for system dynamics; 2) reformulation and relaxation techniques. Finally, we adapt the idea of decomposition and propose an integer-solution search algorithm for efficient solutions of Problem (P4), or commercial solvers for that of Problem (P5). Both approaches provide performance guarantee (6) for Problem (P). Simulations demonstrate the effectiveness of this work.

\section{Appendix}

\section{Preliminary for Proofs}

A summary of the following theory in Probability and Optimization is used in the proofs.

\textbf{Probability theory:} Let \(\mathcal{M}(Z)\) denote the space of all probability distributions supported on \(Z\). Then for any two distributions \(Q_1, Q_2 \in \mathcal{M}(Z),\) the Wasserstein metric \cite{villani2009optimal} \(d_W : \mathcal{M}(Z) \times \mathcal{M}(Z) \to \mathbb{R}_{\geq 0}\) is defined by

\[
d_W(Q_1, Q_2) := \min_{\Pi} \int_{Z \times Z} \|\xi_1 - \xi_2\|_2 \Pi(d\xi_1, d\xi_2),
\]

where \(\Pi\) is in a set of all distributions on \(Z \times Z\) with marginals \(Q_1\) and \(Q_2\). A closed Wasserstein ball of radius \(\epsilon\) centered at a distribution \(P \in \mathcal{M}(Z)\) is denoted by \(B_{\epsilon}(P) := \{Q \in \mathcal{M}(Z) \mid d_W(P, Q) \leq \epsilon\}\).

\textbf{Optimization theory:} Consider a bounded function \(f : X \to \mathbb{R}\) where \(X \subseteq \mathbb{R}^n\). The function \(f\) is lower semi-continuous on \(X\) if \(f(x) \leq \liminf_{y \to x} f(y)\) for all \(x \in X\). Similarly, the function \(f\) is lower semi-continuous on \(X\) if and only if its sublevel sets \(\{x \in X \mid f(x) \leq \gamma\}\) are closed for each \(\gamma \in \mathbb{R}\). We let \(f^* : X \to \mathbb{R} \cup \{+\infty\}\) denote the convex conjugate
of $f$, which is defined as $f^*(x) := \sup_{y \in X} \{ x, y \} - f(y)$. Further, the infimal convolution of two functions $f$ and $g$ on $X$ is defined as $(f \square g)(x) := \inf_{y \in X} f(x - y) + g(y)$. If $f$ and $g$ are bounded, convex, and lower semi-continuous functions on $X$, we will have $(f + g)^* = (f^* \square g^*)$.

Consider a subset $A \subset X$, and let $\chi_A : X \to \mathbb{R} \cup \{+\infty\}$ denote the characteristic function of $A$, i.e., $\chi_A(x)$ is equal to 0 if and only if $x \in A$ and $+\infty$ otherwise. In addition, let $\sigma_A : X \to \mathbb{R}$ denote the support function of $A$, which is defined as $\sigma_A(x) := \sup_{y \in A} \{ x, y \}$. Notice that $\chi_A$ is lower semi-continuous if and only if $A$ is closed, and that $\sigma_A(x) = [\chi_A]^*(x)$ for all $x \in X$.

**Proof of Lemma III.1**: Continuous functions of i.i.d. random variables generate i.i.d. random variables. Thus, the sample trajectories \{\rho(t)\}_{t \in \mathcal{L}} generated by (8) are i.i.d. realizations of $\mathbb{P}(u)$.

**Proof of Lemma III.2**: The proof consists of two steps. First, we explore the boundedness property of $\rho_e(t)$ w.r.t. $\varpi$, for all $e \in \mathcal{L}$ and $t \in \mathcal{T}$. Second, we claim that there exists an $a > 1$ such that $\mathbb{E}_{\mathbb{P}(u)}[\exp(\|\varpi\|^a)] < \infty$.

**Step 1: (Boundedness of $\rho$)** Consider for each speed limit $u \in \Gamma$ and time $t \in \mathcal{T} \setminus \{0\}$. Let $A(u, t)$ denote the matrix that is consistent with the highway system $\mathcal{G}$, let $B(t)$ denote the column vector that encodes the mainstream flow $\omega$, and write the density $\rho(t)$ in the following compact form

$$\rho(t) = \Phi(t, 0)\rho(0) + \sum_{\tau=0}^{t-1} \Phi(t, \tau + 1)B(\tau),$$

where

$$\Phi(t, \tau) := \begin{cases} I_n, & \text{if } \tau = \tau, \\ A(u, t - 1)A(u, t - 2) \cdots A(u, \tau), & \text{if } \tau > \tau, \end{cases}$$

$$A(u, t) = \begin{bmatrix} m_1 & m_2 & \cdots & m_n \\ n_1(t) & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ n_{t-1}(t) & 0 & \cdots & 0 \end{bmatrix}, \quad B(t) = \begin{bmatrix} h\omega(t) \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

with $m_i := 1 - hu_i$ for $i \in \{1, \ldots, n\}$ and $n_i(t) := \frac{1 - \rho_i(t)}{1 - \rho_i(t)}hu_i$ for $i \in \{1, \ldots, n - 1\}$.

Given each component of $A(u, t)$ is bounded for fixed $u$ and $t$, the induced norm of $A(u, t)$ is also bounded and we denote their universal bound by $A_0$. Then for every $t$ we can bound the infinity norm of $\rho(t)$ as follows

$$\|\rho(t)\|_{\infty} \leq \|\Phi(t, 0)\|_{\infty}\|\rho(0)\|_{\infty} + \sum_{\tau=0}^{t-1} \|\Phi(t, \tau + 1)\|_{\infty}\|\omega(\tau)\|_{\infty},$$

$$\leq A_0\|\rho(0)\|_{\infty} + \sum_{\tau=0}^{t-1} A_0^{t-\tau-1}\|\omega(\tau)\|_{\infty},$$

$$\leq M_1(t) \left( \|\rho(0)\|_{\infty} + \sum_{\tau=0}^{t-1} \|\omega(\tau)\|_{\infty} \right),$$

$$\leq (t + 1)M_1(t)\|\varpi\|_{\infty} \leq (t + 1)M_1(t)\|\varpi\|_{\infty},$$

where $M_1(t) := \max\{A_0^t, h, hA_0^t\}$.

**Step 2: (Light-tailed distribution)** Consider a time $t^* \in \arg\max_{t \in \mathcal{T} \setminus \{0\}} \{\|\rho(t)\|_{\infty}\}$. Then by norm equivalence we have

$$\|\rho\|_{\infty} \leq n\|\rho\|_{\infty} = n \max_{t \in \mathcal{T} \setminus \{0\}} \|\rho(t)\|_{\infty},$$

$$\|\rho(t^*)\|_{\infty} \leq n(t^* + 1)M_1(t^*)\|\varpi\|_{\infty}.$$}

Then for any $a > 1$ with $\mathbb{E}_{\mathbb{P}(u)}[\exp(\|\varpi\|^a)] < \infty$, let $M_2 = \{n(t^* + 1)M_1(t^*)\}^a < \infty$ and we have

$$\mathbb{E}_{\mathbb{P}(u)}[\exp(\|\rho\|^a)] \leq \mathbb{E}_{\mathbb{P}(u)}[\exp(M_2\|\varpi\|^a)],$$

$$= \exp(M_2)^a \mathbb{E}_{\mathbb{P}(u)}[\exp(\|\varpi\|^a)] < \infty.$$}

That is, $\mathbb{P}(u)$ is light tailed.

**Proof of Theorem III.1**: We prove it for a given $u$ in two steps. First, we show the proposed set $\mathcal{P}(u)$ contains the unknown distribution $\mathbb{P}(u)$ with high probability. Then, we show that the proposed certificate $\hat{J}(u)$ provides guarantees as in (7).

**Step 1: (Tractable set containing $\mathbb{P}(u)$)** Under Assumption III.1 and using $N$ i.i.d. samples of $\varpi$, we obtain i.i.d. samples \{\rho(t)\}_{t \in \mathcal{L}} of $\mathbb{P}(u)$ via Lemma III.1. Then with the distribution

$$\hat{\mathbb{P}}(u) := \frac{1}{N} \sum_{t \in \mathcal{L}} \hat{\rho}(t),$$

we quantify the relation between $\hat{\mathbb{P}}(u)$ and $\mathbb{P}(u)$ via Lemma III.2 and the following theorem:

**Theorem A.1 (Measure concentration [37, Theorem 2])** If $\mathbb{P}(u) \in \mathcal{M}_b(\mathcal{Z}(u))$, then

$$\mathbb{P}^N \{d_{\mathcal{W}}(\mathbb{P}(u), \hat{\mathbb{P}}(u)) > \epsilon\} < \begin{cases} c_1 e^{-c_2 N \max(2, \ell)}, & \text{if } \ell \leq 1, \\ c_1 e^{-c_2 N a}, & \text{if } \ell > 1, \end{cases}$$

for all $N \geq 1$, $\ell \neq 2$, and $\epsilon > 0$, where the parameter $\ell$ is the dimension of $\rho$, and parameters $c_1$, $c_2$ are positive constants that only depend on $\ell$, $a$ and $b$ as in Assumption III.1. □

Let us select $\epsilon := \varepsilon(\beta)$ to be the following

$$\varepsilon(\beta) := \begin{cases} \left( \frac{\log(c_1 \beta^{-1})}{c_2 N} \right)^{1/\max(2, \ell)}, & \text{if } N \geq \frac{\log(c_1 \beta^{-1})}{c_2}, \\ \left( \frac{\log(c_1 \beta^{-1})}{c_2 N} \right)^{1/a}, & \text{if } N < \frac{\log(c_1 \beta^{-1})}{c_2}, \end{cases}$$

then Theorem A.1 leads to

$$\mathbb{P}^N \{d_{\mathcal{W}}(\mathbb{P}(u), \hat{\mathbb{P}}(u)) > \varepsilon(\beta)\} < \beta,$$

or, equivalently,

$$\mathbb{P}^N \{d_{\mathcal{W}}(\mathbb{P}(u), \hat{\mathbb{P}}(u)) \leq \varepsilon(\beta)\} \geq 1 - \beta.$$

From the definition of the Wasserstein ball $\mathcal{B}_{\varepsilon(\beta)}(\hat{\mathbb{P}}(u))$ and the fact that $\mathbb{P}(u) \in \mathcal{M}_b(\mathcal{Z}(u))$, we have

$$\mathbb{P}^N \{\mathbb{P}(u) \in \mathcal{B}_{\varepsilon(\beta)}(\hat{\mathbb{P}}(u))\} \geq 1 - \beta,$$

$$\mathbb{P}^N \{\mathbb{P}(u) \in \mathcal{M}_b(\mathcal{Z}(u))\} = 1,$$

which results in

$$\mathbb{P}^N \{\mathbb{P}(u) \in \mathcal{P}(u)\} \geq 1 - \beta.$$
with 
\[ \mathcal{P}(u) := \mathbb{B}_{\epsilon(\beta)}(\hat{\mathbb{P}}(u)) \cap \mathcal{M}_h(\mathcal{Z}(u)). \]

**Step 2: (Certificate of (P1))** From the previous reasoning, for a given \( u \) we have \( \mathbb{P}(u) \in \mathcal{P}(u) \) with probability at least \( 1 - \beta \). Then, with the probability at least \( 1 - \beta \) the objective value of (P1) satisfies the following

\[ \mathbb{E}_{\mathbb{P}(u)}[H(u; \rho)] \geq \inf_{Q \in \mathcal{P}(u)} \mathbb{E}_Q[H(u; \rho)]. \]

Let \( J(u) \) be

\[ J(u) := \inf_{Q \in \mathcal{P}(u)} \mathbb{E}_Q[H(u; \rho)], \]

which results in

\[ \text{Prob}^N(\mathbb{E}_{\mathbb{P}(u)}[H(u; \rho)]) \geq J(u) \geq 1 - \beta. \]

Then the proposed certificate \( J(u) \) of (P1) satisfies guarantee (7), which completes the proof. ■

**Proof of Theorem III.2:** We achieve it by three steps. First, we show that Problem (P2) can be equivalently reduced to a finite-dimensional problem. Then we equivalently reformulate the resulting problem into a maximization problem. Finally, we show the performance guarantees of (P3).

**Step 1: (Finite-dimensional reduction of (P2))** We express \( J(u) \) as follows

\[ J(u) = \begin{cases} \inf_Q & \int_{\mathcal{Z}(u)} H(u; \rho) Q(dp), \\ \text{s.t.} & Q \in \mathcal{M}_h(\mathcal{Z}(u)), d_{TV}(Q, \hat{\mathbb{P}}(u)) \leq \epsilon(\beta), \\ & \int_{\mathcal{Z}(u)} H(u; \rho) Q(dp), \\ & \text{s.t.} \int_{\mathcal{Z}(u) \times \mathcal{Z}(u)} ||\rho - \rho^\prime||_{\Pi}(dp, d\rho^\prime) \leq \epsilon(\beta), \end{cases} \]

\[ \Pi \] is a distribution of \( \rho \) and \( \rho^\prime \) with marginals \( Q \) and \( \hat{\mathbb{P}}(u) \in \mathcal{M}_h(\mathcal{Z}(u)), \]

\[ = \begin{cases} \inf_{Q, l \in \mathcal{L}} & \frac{1}{N} \sum_{i \in \mathcal{L}} \int_{\mathcal{Z}(u)} H(u; \rho) Q^{(i)}(dp), \\ \text{s.t.} & Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u)), \forall l \in \mathcal{L}, \\ & \text{as} \quad (8), \end{cases} \]

where the first equality applies the definition of the expectation operation; the second equality uses the definition of Wasserstein metric; the third equality exploits the fact that the joint distribution \( \Pi \) can be characterized by the marginal distribution \( \hat{\mathbb{P}}(u) \) of \( \rho^\prime \) and the conditional distributions \( Q^{(i)} \) of \( \rho \) given \( \rho^\prime = \rho_{\rho^\prime}^{(i)}, l \in \mathcal{L} \), written as

\[ \Pi := \frac{1}{N} \sum_{l \in \mathcal{L}} \delta_{\rho_{\rho^\prime}^{(i)}} \otimes Q^{(i)}, \]

with \( N \) the number of samples.

**Step 2:** [Lemma 3.4], the order of the inf-sup operator in the resulting representation of \( J(u) \) can be switched, resulting in the following expression

\[ J(u) = \left\{ \begin{array}{ll} \sup_{\lambda \geq 0} \inf_{Q^{(i)}, l \in \mathcal{L}} & -\lambda \epsilon(\beta) \\ & + \frac{1}{N} \sum_{l \in \mathcal{L}} \int_{\mathcal{Z}(u)} \left( \lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho) \right) Q^{(i)}(dp), \\ \text{s.t.} & (8), Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u)), \forall l \in \mathcal{L}, \end{array} \right. \]

Move the inf operator into the sum operator, we have

\[ J(u) = \left\{ \begin{array}{ll} \sup_{\lambda \geq 0} & -\lambda \epsilon(\beta) \\ & + \frac{1}{N} \sum_{l \in \mathcal{L}} \left\{ \inf_{Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u))} \mathbb{E}_{Q^{(i)}}[\lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho)] \right\}, \\ \text{s.t.} & (8). \end{array} \right. \]

For each \( l \in \mathcal{L} \), we claim that

\[ \inf_{Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u))} \mathbb{E}_{Q^{(i)}}[\lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho)] \\ = \inf_{\rho^\prime \in \mathcal{Z}(u)} \left( \lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho) \right). \]

The above claim can be clarified as the following

(a) Let \( p^* \) denote the value of the second term. Then, for any \( \rho \in \mathcal{Z}(u) \), we have

\[ p^* \leq \lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho), \]

implying

\[ p^* \leq \mathbb{E}_{Q^{(i)}}[\lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho)], \]

holds for any probability distribution \( Q^{(i)} \in \mathcal{M}(\mathcal{Z}(u)) \), so does for \( Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u)) \). Therefore, we have

\[ p^* \leq \inf_{Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u))} \mathbb{E}_{Q^{(i)}}[\lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho)]. \]

(b) Next, we claim that the set \( \mathcal{M}_h(\mathcal{Z}(u)) \) contains all the Dirac distributions supported on \( \mathcal{Z}(u) \). Then, for any \( \rho^\prime \in \mathcal{Z}(u) \), we have

\[ \delta_{\rho^\prime} \in \mathcal{M}_h(\mathcal{Z}(u)), \]

resulting in

\[ \inf_{Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u))} \mathbb{E}_{Q^{(i)}} \left[ \lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho) \right] \leq \lambda ||\rho^\prime - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho^\prime), \forall \rho^\prime \in \mathcal{Z}(u), \]

which implies

\[ \inf_{Q^{(i)} \in \mathcal{M}_h(\mathcal{Z}(u))} \mathbb{E}_{Q^{(i)}} \left[ \lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho) \right] \leq p^*. \]

Therefore, we equivalently write \( J(u) \) as

\[ J(u) = \sup_{u, \lambda \geq 0} -\lambda \epsilon(\beta) + \frac{1}{N} \sum_{l \in \mathcal{L}} \inf_{\rho^\prime \in \mathcal{Z}(u)} \left( \lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho) \right), \]

s.t. (1), (8).

Finally, we write Problem (P2) as follows

\[ (P2') \]

\[ \sup_{u, \lambda \geq 0} -\lambda \epsilon(\beta) + \frac{1}{N} \sum_{l \in \mathcal{L}} \inf_{\rho^\prime \in \mathcal{Z}(u)} \left( \lambda ||\rho - \rho_{\rho^\prime}^{(i)}|| + H(u; \rho) \right), \]

s.t. (1), (8).
Step 2: (Equivalent reformulation of \((P2')\)) Using the definition of the dual norm and moving its sup operator we can write Problem \((P2')\) as
\[
\sup_{u,\lambda \geq 0} -\lambda \epsilon(\beta) + \frac{1}{N} \sum_{l \in L} \inf_{\rho \in \mathcal{Z}(u)} \sup_{\rho \in \mathcal{Z}(u)} \left( \langle \nu(l), \rho - \rho(l) \rangle + H(u; \rho) \right),
\]
s.t. \((1), (8)\).

Given \(\lambda \geq 0\), the sets \(\{\nu(l) \in \mathbb{R}^{nT} \mid \|\nu(l)\|_* \leq \lambda\}\) are compact for all \(l \in L\). We then apply the minmax theorem between inf and the second sup operators. This results in the switch of the operators, and finally using the definition of conjugate functions. The function \(h^l(u)\) results in the following form
\[
h^l(u) := \inf_{\rho \in \mathcal{Z}(u)} \left( \langle \nu(l), \rho \rangle + H(u; \rho) \right), \forall l \in L.
\]

For each \(l \in L\), we rewrite \(h^l(u)\) firstly taking a minus sign out of the inf operator, then exploiting the equivalent representation of sup operation, and finally using the definition of conjugate functions. The function \(h^l(u)\) results in the following relation
\[
h^l(u) = -\sup_{\rho \in \mathcal{Z}(u)} \left( \langle -\nu(l), \rho \rangle - H(u; \rho) \right),
\]
\[
= -\sup_{\rho} \left( \langle -\nu(l), \rho \rangle - H(u; \rho) - \chi_{\mathcal{Z}(u)}(\rho) \right),
\]
\[
= - [H(u; \cdot) + \chi_{\mathcal{Z}(u)}(\cdot)]^* (-\nu(l)).
\]

Further, we apply the inf-convolution operation and push the minus sign back into the inf operator, for each \(h^l(u)\), \(l \in L\). The representation of \(h^l(u)\) results in the following relation
\[
h^l(u) = -\inf_{\mu} \left( [H(u; \cdot)]^* (-\mu(l) - \nu(l)) + \chi_{\mathcal{Z}(u)}(\cdot)^* (\mu(l)) \right),
\]
\[
= \sup_{\mu} \left( -[H(u; \cdot)]^* (-\mu(l) - \nu(l)) - \chi_{\mathcal{Z}(u)}(\cdot)^* (\mu(l)) \right).
\]

By substituting \(-\nu(l)\) by \(\nu(l)\), the resulting optimization problem has the following form
\[
\sup_{u,\lambda,\mu,\nu} -\lambda \epsilon(\beta) - \frac{1}{N} \sum_{l \in L} \left( [H(u; \cdot)]^* (-\mu(l) + \nu(l)) + \chi_{\mathcal{Z}(u)}(\cdot)^* (\mu(l)) - \langle \nu(l), \rho(l) \rangle \right),
\]
s.t. \((1), (8)\), \(\lambda \geq 0\),
\[
\|\nu(l)\|_* \leq \lambda, \forall l \in L.
\]

Given \(u\), the strong duality of linear programs is applicable for the conjugate of the function \(H(u; \cdot)\) and the support function \(\sigma_{\mathcal{Z}(u)}(\mu(l))\). Using the strong duality and the definition of the support function, we compute
\[
[H(u; \cdot)]^* (\mu(l) - \nu(l)) := \begin{cases} 0, & \nu(l) = \mu(l) + \frac{1}{N} u \otimes 1_T, \forall l \in L, \\
\infty, & \text{o.w.,}
\end{cases}
\]

and
\[
\chi_{\mathcal{Z}(u)}(\cdot)^* (\mu(l)) = \sigma_{\mathcal{Z}(u)}(\mu(l)) = \begin{cases} \sup_{\xi} \langle \mu(l), \xi \rangle, & \text{s.t.} \ 0 \leq \xi(v) \leq \rho^*(\xi(u)), \forall v \in \mathcal{E}, \\
\inf_{\eta} \sum_{v \in \mathcal{E}, t \in T, l \in L} \tilde{J}_e \sigma_{\mathcal{E}_l}(\eta(l)), & \text{s.t.} \ \tilde{J} + u \circ (\tilde{\beta} - \rho^*(\tilde{\eta}(l))) \otimes 1_T \circ \eta(l) \\
\eta(l) \geq 0_{nT}, \forall l \in L.
\end{cases}
\]

We substitute these parts for that in the objective function, take a minus sign out of the above inf operator, and obtain
\[
\sup_{u,\rho,\lambda,\mu,\nu,\eta} -\lambda \epsilon(\beta) - \frac{1}{N} \sum_{e \in \mathcal{E}, l \in T, l \in L} \tilde{J}_e \sigma_{\mathcal{E}_l}(\eta(l)),
\]
s.t. \(\tilde{J} + u \circ (\tilde{\beta} - \rho^*(\tilde{\eta}(l))) \otimes 1_T \circ \eta(l) \geq 0_{nT}, \forall l \in L,
\]
\[
\nu(l) = \mu(l) + \frac{1}{N} u \otimes 1_T, \forall l \in L,
\]
\[
\|\nu(l)\|_* \leq \lambda, \forall l \in L,
\]
\[
\hat{J}(u) \leq J(u), \forall l \in L,
\]
\[
\hat{J}(u) \geq 0_{nT}, \forall l \in L,
\]
\[
(1), (8).
\]

Given that all the reformulations in this step hold with equalities, we therefore claim that the above problem is equivalent to \((P2)\). Finally, we claim that the sup operation is indeed achievable, due to the fact that 1) the variable \(u\) is in a finite set \(\Gamma\) and 2), for any \(u \in \Gamma\) that is feasible to the above problem, the above problem with that fixed \(u\) satisfies the Slater’s condition, which implies that the above problem is achievable. We therefore claim \((P2)\) is equivalent to \((P3)\).

Step 3: (Performance guarantees of \((P3)\)) Given any feasible point \((u, \rho, \lambda, \mu, \nu, \eta)\) of \((P3)\), we denote its objective value by \(J(u)\). The value \(J(u)\) is a lower bound of \((P3)\) and therefore a lower bound for \((P2)\), i.e., \(J(u) \leq J(u)\). Thus \(J(u)\) is an estimate of the certificate for the performance guarantee \((7)\). Therefore, \((u, J(u))\) is a data-driven solution and certificate pair for \((P1)\).

Proof of Lemma IV.1: The proof follows by the application of the following proposition on each bilinear term in \((11)\):

Proposition A.1 (Equivalent reformulation of bi-linear terms [39, Section 2]) Let \(Y \subset \mathbb{R}\) be a compact set. Given a binary variable \(x \in \mathbb{R}\) and a linear function \(g(y)\) in a continuous
variable $y \in \mathcal{Y}$, $z$ equals the quadratic function $xzg(y)$ if and only if
\[
qx \leq z \leq \bar{q}x, \\
g(y) - q \cdot (1 - x) \leq z \leq g(y) - q \cdot (1 - x),
\]
where $q = \min_{y \in \mathcal{Y}} \{g(y)\}$ and $\bar{q} = \max_{y \in \mathcal{Y}} \{g(y)\}$. □

**Remark A.1 (Regularization technique)** In a later program, we add the following extra constraints to speed up the internal computation of solvers
\[
\sum_{i \in O} z_{e,i}^{(l)}(t) = \eta_{e}^{(l)}(t), \\
\forall e \in \mathcal{E}, t \in \mathcal{T} \setminus \{0\}, l \in \mathcal{L}, \\
\sum_{i \in O} y_{e,i}^{(l)}(t) = \rho_{e}^{(l)}(t), \\
\forall e \in \mathcal{E}, t \in \mathcal{T} \setminus \{0\}, l \in \mathcal{L}.
\]
These are adapted from the binary representation (9) and the definition of $y_{e,i}^{(l)}(t)$ and $z_{e,i}^{(l)}(t)$.

**Proof of Proposition IV.1:** Knowing that $\rho^* \geq 0_{\mathcal{E} \times \mathcal{T} \times \mathcal{N}}$ by constraints (13), we only need to show $\nu^* \geq 0_{\mathcal{E} \times \mathcal{T} \times \mathcal{N}}$. To prove this, let us assume there exists an optimizer $\text{sol}^*$ such that, for at least one $e \in \mathcal{E}, \tau \in \mathcal{T}$ and $l \in \mathcal{L}$, it holds $\nu_e^{\text{sol}^*}(\tau) < 0$. Then, using constraint (16), we claim $\mu_e^{\text{sol}^*}(\tau) < 0$. Next, we show the contradiction to an optimizer by constructing a feasible solution that gives us higher objective value than that resulted from $\text{sol}^*$. To achieve this, we perturb variables $\lambda^*, \mu_e^{\text{sol}^*}(\tau)$ and $\nu_e^{\text{sol}^*}(\tau)$, and leave other components the same as that in $\text{sol}^*$. With such perturbation, only constraints (15), (16), and (17) are varied.

Let $\text{sol} := (x^*, y^*, z^*, \rho^*, \bar{\lambda}, \bar{\mu}, \bar{\nu}, \eta^*)$ denote the feasible solution we are to construct. We denote by $h^* := \sum_{e \in O} \gamma_{e}^{(l)}(\bar{p} - \rho_e^{\text{sol}}(\pi)) \otimes 1 \circ z_{e}^{(l)}(\bar{p}) + \bar{f} \otimes 1_{\mathcal{T}} \circ \eta_{e}^{(l)}(\pi)$ the unperturbed part in constraint (15) and construct $\bar{\nu}$ as follows
\[
\bar{\nu}_e^{(l)}(t) = \begin{cases} 
\mu_e^{\text{sol}^*}(\tau), & \text{if } (e, t, l) \neq (e, \tau, l), \\
\min\{\rho_e^{\text{sol}^*}(\tau), -\mu_e^{\text{sol}^*}(\tau)\}, & \text{o.w.}
\end{cases}
\]

The above construction ensures the feasibility of constraints (15) and furthermore, because $h_e^{\text{sol}^*}(\tau) \geq 0$ and $\mu_e^{\text{sol}^*}(\tau) < 0$, we claim $\bar{\nu}_e^{(l)}(\tau) \geq 0$. Then let us denote by $g^* := \frac{1}{\mathcal{T}} \sum_{e \in O} \gamma_{e}^{(l)}(x_{e}^{*} \otimes 1_{\mathcal{T}})$ the unperturbed part of constraints (16) and construct variable $\bar{\mu}$ as follows
\[
\bar{\mu}_e^{(l)}(t) = \begin{cases} 
\mu_e^{(l)}(t), & \text{if } (e, t, l) \neq (e, \tau, l), \\
\mu_e^{\text{sol}^*}(\tau) + g_{\tau}^*(\tau), & \text{o.w.}
\end{cases}
\]

Again, we have $\bar{\nu}_e^{(l)}(\tau) \geq 0$. Then by letting $\tilde{\lambda} := \max\{\lambda^*, \bar{\nu}_e^{(l)}(\tau)\}$, constraints (17) are satisfied. In this way, a feasible solution sol is constructed.

Next, we evaluate the difference of the objective values of (P4) resulting from sol and sol* in the following
\[
\text{objective(sol)} - \text{objective(sol*)} = \left( -\tilde{\lambda} + \lambda^* \right) \epsilon(\beta) + \left( \tilde{\nu}_e^{(l)}(\tau) - \nu_e^{\text{sol}^*}(\tau) \right) \rho_e^{\text{sol}^*}(\tau), \\
\geq \left( -\tilde{\lambda} + \lambda^* + \tilde{\nu}_e^{(l)}(\tau) - \nu_e^{\text{sol}^*}(\tau) \right) \epsilon(\beta), \\
= \min\{\lambda^* - \tilde{\nu}_e^{(l)}(\tau), \lambda^* + \tilde{\nu}_e^{(l)}(\tau) \} \epsilon(\beta) - \nu_e^{\text{sol}^*}(\tau) \epsilon(\beta), \\
> 0,
\]
where the first equality cancels out unperturbed terms; the second inequality applies Assumption IV.2 and the fact that $\tilde{\nu}_e^{(l)}(\tau) \geq 0$ and $\nu_e^{\text{sol}^*}(\tau) < 0$; the third equality applies construction of $\tilde{\lambda}$; and the last inequality is achieved by summing the nonnegative first term and the strict positive second term.

By the above computation, we constructed a feasible solution sol with a higher objective value than that of sol*, contradicting the assumption that sol* is an optimizer. ■

**Proof of Lemma IV.2:** Let us denote by ($P4^\nu$) the Problem (P4) with an extra set of constraints $\nu \geq 0_{\mathcal{E} \times \mathcal{T} \times \mathcal{N}}$. We prove the lemma in two steps.

**Step 1:** (Equivalence of optimizers sets) First, we use Proposition IV.1 to claim that the set of optimizers of (P4) is the same as that of ($P4^\nu$). Second, we claim that for any optimizer of ($P4^\nu$), all the constraints in (19) are active. This means that the set of optimizers of ($P4^\nu$) are the same as the projection of that of (P4). Therefore, the optimizers set of (P4) and ($P4^\nu$) are equivalent.

**Step 2:** (Performance guarantees) First, any feasible solution of ($P4^\nu$) correspond to a feasible solution of (P4). This holds because any feasible solution of ($P4^\nu$) satisfies all the constraints of (P4). Next, the objective value of ($P4^\nu$) gives a lower bounds of that of (P4). This can be verified using constraints (19). Finally, the performance guarantees (7) of feasible solution of ($P4^\nu$) can be derived from that of (P4) as in Remark IV.1.

**Proof of Lemma IV.3:** We construct $\bar{\mu}$ by showing boundedness of $\nu \circ \rho$. It’s known for each $e \in \mathcal{E}, t \in \mathcal{T}$ and $l \in \mathcal{L}$, the density $\rho_e^{(l)}(t)$ is nonnegative and bounded above by $\max_{e \in \mathcal{E}} \{\bar{\pi}_e\}$. Then we only need to find the upper bound of $\nu_e^{(l)}(t)$. By Assumption IV.1, the variable $\eta_e^{(l)}(t)$ is bounded. Then computations via constraints (15) and (16) result in upper bound of $\nu_e^{(l)}(t)$ as the following
\[
\nu_e^{(l)}(t) \leq \max_{e \in \mathcal{E}} \left\{ \left( f_e + u_e (\bar{\pi}_e - \rho_e^{(l)}(\bar{\pi}_e)) \right) \eta + \frac{1}{\mathcal{T}} u_e \right\}, \\
= \max_{e \in \mathcal{E}} \left\{ \bar{\pi}_e \rho_e \eta + \frac{1}{\mathcal{T}} u_e \right\}.
\]

By letting $\bar{u} = \sqrt{\max_{e \in \mathcal{E}} \left\{ \bar{\pi}_e \rho_e^2 \eta + \frac{1}{\mathcal{T}} u_e \right\}}$, we complete the proof. ■
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