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A freight origin-destination synthesis model with mode choice

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ABSTRACT

This paper develops a novel procedure to conduct a Freight Origin-Destination Synthesis (FODS) that jointly estimates the trip distribution, mode choice, and the empty trips by truck and rail that provide the best match to the observed freight traffic counts. Four models are integrated: (1) a gravity model for trip distribution, (2) a binary logit model for mode choice, (3) a Noortman and Van Es' model for truck, and (4) a Noortman and Van Es' model for rail empty trips. The estimation process entails an iterative minimization of a nonconvex objective function, the summation of squared errors of the estimated truck and rail traffic counts with respect to the five model parameters. Of the two methods tested to address the nonconvexity, an interior point method with a set of random starting points (Multi-Start algorithm) outperformed the Ordinary Least Squared (OLS) inference technique. The potential of this methodology is examined using a hypothetical example of developing a nationwide freight demand model for Bangladesh. This research improves the existing FODS techniques that use readily available secondary data such as traffic counts and link costs, allowing transportation planners to evaluate policy outcomes without needing expensive freight data collection. This paper presents the results, model validation, limitations, and future scope for improvements.

1. Introduction

A country's freight system is a major pillar of its economy. For instance, over 45% of commercial establishments in the US are directly dependent on the freight system for their operations (Holguín-Veras et al., 2018a,b). An efficient freight system is also vital to improving trade and the quality of life of a society. However, the freight transportation sector is also one of the major contributors to such negative externalities as energy consumption, emissions, congestion, and noise, with the potential for those externalities to grow rapidly in the coming decades (International Energy Agency, 2016). A sustainable freight system is essential to tackling global climate change, as transportation is the third-largest contributor to global energy consumption, of which freight trucks represent more than half the share (International Energy Agency, 2016). Freight transportation planning endeavors to help the public sector in evaluating policy outcomes designed to minimize these negative impacts, and promote the sustainable use of natural resources, without hindering economic growth. The primary goal of this research is to provide freight policymakers with the necessary methodologies to estimate freight demand and mode choice more efficiently, cost-effectively, and within data limitations.

In the US, the available modes of freight transportation are truck, rail, inland waterways, pipelines, and air. Among these, the predominant modes are truck and rail, with shares of 41%, and 27% in ton-miles, 72% and 9% in tons, and 73% and 1.4% in value,

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respectively (Bureau of Transportation Statistics, 2020). Similarly, trucks dominate freight transport in other parts of the world. For instance, trucks contributed to more than 75% of freight mode share in ton-kilometers in Europe in 2019 (Eurostat, 2020), 71% in India in 2020 (NITI Aayog et al., 2021), and around 80% in Bangladesh (Gota and Anthapur, 2016). The exception is Australia, which has a higher rail share (about 49%) in ton-kilometers, mainly dominated by mining activity. Iron ore and coal constitute 80% of total rail cargo by ton-kilometers in Australia. In recent years, several countries, e.g., the US, India, Bangladesh, and Australia, have witnessed a steady rise in the truck volumes (BITRE, 2014; Gota and Anthapur, 2016; NITI Aayog et al., 2021). These studies showed that rail dominates in the transportation of low-valued bulk cargo for longer distances, whereas truck is an irreplaceable option for medium-haul intercity (urban) freight and last-mile deliveries.

Nevertheless, there is a huge difference in the externalities caused by these two modes. Compared to truck, rail is nearly four times as fuel-efficient and emits less emissions per ton-mile transported (Association of American Railroads, 2014). Kruse (2012) estimated that the distance transported by truck and rail for a ton of cargo per gallon of fuel is 155 and 413 miles, respectively. Trucks contributed to over 16% of total energy consumption and greenhouse gas emissions in the US in 2016, and in the past decade, the truck share in total petroleum consumption has been increasing at an alarming rate of 1.7% a year (Davis and Boundy, 2019). Also, trucks contribute to higher freight-related fatalities, over 88% in the US in 2017 (Sprung, 2017). Therefore, promoting sustainable freight mode shifts plays an important part in regional (intercity) or national-level freight planning.

One of the key challenges in freight transportation planning, specifically in freight mode choice modeling, is the lack of available data, as collecting a survey at the national level is extremely expensive and time-consuming (Russo et al., 2009; Nuzzolo et al., 2013; Tavasszy and Friedrich, 2019). In addition, the existing freight data are either confidential or privately owned in most cases. As a result, the literature on freight mode choice rarely uses national-level datasets, with notable exceptions: Abate et al. (2019) and Holguín-Veras et al. (2021), which used the confidential versions of Commodity Flow Survey (CFS) micro-data for Sweden and the US, respectively. Moreover, the existing modeling techniques to estimate freight mode choice either focus on urban freight, typically specific types of trucks, or require large amounts of input data to estimate mode choice, including costs, travel times, shipment size, origin, destination, and commodity type (Holguín-Veras, 2002; Leachman, 2008; Reis, 2014; Roman et al., 2017; Zhang and Lee Lam, 2018). Thus, there is an urgent need to develop efficient modeling techniques to evaluate freight mode choices that work well within the constraints of time, money, and the availability of data.

One of the major contributions of this research is to incorporate mode choice in the Freight Origin-Destination Synthesis (FODS) methods, which aim to estimate freight demand using readily available secondary data such as partial trip distribution, traffic counts, link costs, payloads, zonal productions, and attractions. In addition to mode choice, this paper jointly estimates the empty trip models for different transportation modes (e.g., truck and rail). Empty trips are a vital component of freight traffic, with an estimated share varying between 30 and 50% for truck (Holguín-Veras and Thorson, 2003a,b) and between 33 and 46% for an average freight railcar (Cambridge Systematics Inc., 2007). In summary, this research makes an important contribution to the FODS literature by developing and calibrating an integrated freight demand model that jointly estimates a gravity model for distribution, a binary logit model for mode choice (between truck and rail), and Noortman and Van Es' model for empty trips. The methodology is tested using a hypothetical example of estimating a nationwide freight demand model for Bangladesh. These procedures provide better predictions for the outcomes of policies designed to improve sustainability and social welfare.

The remainder of this paper is organized as follows. Section 2 presents a thorough literature review on the existing FODS models and freight mode choice. Section 3 explains the methodology, model selection, model formulations, and proof for the nonconvexity of the objective function. Section 4 presents the solution procedure. Section 5 illustrates the model application on a hypothetical case of developing a nationwide freight model for Bangladesh. Section 6 summarizes with concluding remarks, limitations, and the scope for future research.

2. Literature review

This section is divided into two parts. The first part reviews the literature on Freight Demand Synthesis (FDS) methods, followed by discussions of the literature on freight mode choice models.

2.1. Freight demand synthesis

The early research on demand synthesis started in passenger transportation (Robillard, 1975; Willumsen, 1978; Fisk and Boyce, 1983), which was later adopted and improved to analyze the case of freight transportation. FDS models could be divided into two categories: (1) Freight Origin-Destination Synthesis (FODS) and (2) Freight Tour Synthesis (FTS) models (Ortúzar and Willumsen, 2011). FODS deals with estimating the freight flows between the Origin and Destination zones (OD-Table) from secondary data, typically either by weight of cargo or trips by a single mode, mostly truck. In contrast, FTS deals with estimating freight tours, mostly relevant in urban scenarios, where a single truck starts the trip from a warehouse, then delivers to multiple locations and ultimately returns to the same warehouse it started from (Sánchez-Díaz et al., 2015; Gonzalez-Calderon and Holguín-Veras, 2019; Comi et al., 2021; Holguín-Veras et al., 2021). Recent developments in freight tour synthesis approaches include estimating tours from a logit-based probabilistic model using the automated delivery vehicle monitoring data (Comi et al., 2021) and a novel multi-class, multi-commodity synthesis approach (Holguín-Veras et al., 2021).

Table 1 shows a summary of the FODS and FTS literature. As shown in the table, studies on FODS or FTS are very limited compared to studies of passenger transport. The literature on FODS could be divided into two categories, structured and unstructured. The studies in the structured category use trip distribution models with a closed functional form, e.g., gravity model (Tamin and Willumsen, 1989; Tamin and Willumsen, 1992; Holguín-Veras and Patil, 2007; Holguín-Veras and Patil, 2008; Levine et al., 2009). In contrast, the publications in the unstructured group do not consider any functional form for the trip distribution, e.g., genetic algorithm or entropy maximization (Gédéon et al., 1993; List and Turnquist, 1994; Nozick et al., 1996; Crainic et al., 2001; Rios et al., 2002; Al-Battaineh and Kaysi, 2005; Ma et al., 2012). One of the earliest studies of FODS, Tamin and Willumsen (1989), belongs to the structured category; it examined various combinations of distribution, assignment models, and solution techniques and concluded that the gravity model with All-or-Nothing (AON) traffic assignment provided a better fit while estimated using optimization techniques. Tamin and Willumsen (1992) found that estimating FODS by commodity, i.e., considering a separate distribution model for various commodities, improves the model performance by decreasing the Root Mean Squared Error (RMSE) for traffic counts by 15%. There are a few studies in the structured category that consider different freight modes; for instance, Tavasszy et al. (1994) estimated a multi-modal OD-Table for international goods movement using the base OD-Table instead of traffic counts, assuming the choice of the OD is multinomially distributed. Another such study is Levine et al. (2009), which considered truck and rail modes in obtaining the container flows to 84 zones in the US. The input data are the partial OD-Table and the Waybill sample for rail flows and a gravity model to represent the trip distribution.

A major contribution to the FODS literature was carried out by Holguín-Veras and Patil (2007), which incorporated empty trips, using Noortman and Van Es' model (Noortman and Van Es, 1978) and a gravity model for the distribution. Two objective functions were considered based on the availability of traffic count data on empty trips. Holguín-Veras and Patil (2008) concluded that incorporating empty trips improves the FODS model's performance, and adding a multi-commodity gravity model further improved the accuracy compared to the single commodity model. The research conducted in this paper is inspired by the modeling approach followed in Holguín-Veras and Patil (2007).

Among the studies in the unstructured group, Gédéon et al. (1993) developed a bi-level multimodal optimization model to estimate an OD-Table, which is solved using a steepest-descent algorithm. List and Turnquist (1994) estimated the OD-Table by minimizing the weighted sum of deviations between the estimated and observed OD-Table, productions, and attractions for three truck types (vans, medium, and large) during three different time intervals (morning peak, midday, and evening peak). Similar to List and Turnquist (1994), Nozick et al. (1996) obtained the freight distribution by value between the United States and Mexico for multiple commodities. Crainic et al. (2001) extended the approach by Gédéon et al. (1993) to estimate a multimodal and multi-commodity freight OD-Table from observed trip distribution, transfers, and link flows. Rios et al. (2002) evaluated various input data on an entropy maximization approach and proved that the quality of the traffic counts is the most significant input affecting the FODS performance, with a small deviation of 10% in the traffic counts capable of increasing the RMSE threefold. Al-Battaineh and Kaysi (2005) estimated a truck OD-Table using a genetic algorithm with the link flows, trip productions, and attractions. The major limitation of Al-Battaineh and Kaysi (2005) is its huge run-time. Ma et al. (2012) used a Bayesian networks approach to estimate FODS using the previously available OD-Table and traffic counts from the loop detectors, assuming the trips are normally distributed. A base OD-Table is a mandatory input for this method, which may not always be available. Recently, Teye and Hensher (2021) developed a new entropy maximization model to facilitate the optimal utilization of available datasets to estimate freight trip distribution by commodity and vehicle type in Australia.

As shown in Table 1, a few studies on FODS considered multiple modes or vehicle types either in the trip distribution or in the optimization model. However, there is no study estimating a mode choice model. The freight mode choice literature is presented next.

2.2. Freight mode choice

The studies on freight mode choice predominantly use random utility models estimated from surveys (stated or revealed preference). A few studies adopt optimization techniques (McGinnis et al., 1981; Casavant et al., 1993; Blauwens et al., 2006; Leachman, 2008; Stewart et al., 2008; Zhang and Lee Lam, 2018), mostly based on the inventory theory approach proposed by Baumol and Vinod (1970). Other methods applied in analyzing freight mode choice include artificial neural network (Abdelwahab and Sayed, 1999), elimination by aspects (Young et al., 1982), hierarchical integration approach (Norojono and Young, 2003), experimental economics (Holguín-Veras et al., 2011), agent-based modeling (Reis, 2014), and latent class modeling (Kim et al., 2017; Roman et al., 2017).

Multinomial logit (MNL) is the most widely used random utility model to study freight mode choice except Winston (1981), who used a probit model. Freight mode choice could be classified into three types in terms of the way the shipment size is considered (Holguín-Veras et al., 2011; Tavasszy and De Jong, 2013). The choice of freight mode is intertwined with the choice of shipment size. The first type of model assumes that shipment size is independent of the mode choice (McFadden et al., 1986; Nam, 1997; Brooks et al.,

Table 1
Summary of FODS and FTS Literature.

FODS/FTS Studies		Model Adopted: Trip Distribution – Furness/ Fratar-II	Opportunities (OP)	Gravity model (GR)	Gravity Opportunity (GO)	Genetic Algorithm (GA)	Entropy maximization	Bayesian	Optimizaton models
Structured	Tamin and Willumsen (1989)	✓	✓	✓	✓				
	Tamin and Willumsen (1992)	✓	✓	✓	✓				
	Tavasszy et al. (1994)			✓					
	Holguín-Veras and Patil (2007)			✓					
	Holguín-Veras and Patil (2008)			✓					
	Levine et al. (2009)			✓					
Unstructured	Gédéon et al. (1993)								✓
	List and Turnquist (1994)								✓
	Nozick et al. (1996)								✓
	Crainic et al. (2001)								✓
	Rios et al. (2002)						✓		
	Al-Battaineh and Kaysi (2005)					✓			
	Ma et al. (2012)							✓	
	Teye and Hensher (2021)					✓		✓	
Tours	Wang and Holguín-Veras (2008)						✓		
	González-Calderón (2014)						✓		
	Sánchez-Díaz et al. (2015)						✓		
	Gonzalez-Calderon and Holguín-Veras, (2019)						✓		
	Comi et al (2021)							✓	
	Holguín-Veras et al. (2021)						✓		
Current Research				✓					

2012; Comi and Polimeni, 2020). The second type of model assumes a one-way interaction, whereby the shipment size influences the mode choice (Jiang et al., 1999; Norojono and Young, 2003). The majority belongs to the third type of model, which assumes that shipment size and mode choice are interdependent; hence, a discrete-continuous model is applied (Abdelwahab and Sargious, 1991; Holguín-Veras, 2002; Pourabdollahi et al., 2013; Abate and de Jong, 2014; Arencibia et al., 2015; Larrañaga et al., 2017; Stinson et al., 2017; Abate et al., 2019; Keya et al., 2019; Holguín-Veras et al., 2021).

Table 2 summarizes the methodologies used in various studies on freight mode choice. In summary, the table concludes that the discrete choice models, especially the MNL model, is best suited to study freight mode choice. The MNL model is adopted in estimating the freight mode choice modeling in several countries, including Sweden, Italy, and Norway, to name a few (de Jong et al., 2004). Also, Comi and Polimeni (2020) proved that the MNL model provides better results at aggregated level mode choice in estimating the potential benefits of various short sea shipping scenarios. Similarly, in the case of chain behavior in freight mode choice that involves a joint decision of multiple modes, the nested logit model is found to provide a better fit (Jensen et al., 2019). The mode choice model parameters are typically estimated using statistical techniques (maximum likelihood estimation, MLE) based on either revealed (RP) or stated preference (SP) datasets. However, a simultaneous estimation of shipment size and mode is required, as the researchers found that the mode choice is dependent on the shipment size, and the choice of shipment size also depends on the mode choice (Holguín-Veras et al., 2021).

As shown in Tables 1 and 2, no previous research in FDS has combined FODS, mode choice modeling, and empty trip models in the estimation of freight demand. Also, no study has inferred the mode choice model parameters from the secondary data using either optimization or synthesis approaches instead of the MLE on SP or RP datasets. This research addresses these gaps by improving the existing FODS techniques by estimating a binary logit model for the mode choice between truck and rail along with the empty trip

Model Adopted				Attributes Considered							
Routing											
All or Nothing (AON)	User Equilibrium (UE)	System optimum (SO)	Stochastic UE	O-D table/ model	Tour flows	Commodity type	Vehicle type/class	Multiple modes	Empty trips	Dynamic flows	Mode choice model
✓			✓	✓							
✓				✓		✓					
✓				✓				✓			
✓				✓					✓		
✓				✓		✓			✓		
		✓						✓			
		✓		✓				✓			
			✓	✓			✓			✓	
			✓	✓		✓					
		✓		✓		✓		✓			
✓				✓							
✓				✓		✓					
✓				✓							
✓				✓		✓	✓				
					✓						
	✓				✓		✓				
					✓					✓	
					✓						
✓					✓	✓					
					✓		✓				
✓				✓					✓		✓

Table 2
Summary of Freight Mode Choice Literature.

No.	Methodology	Literature (Selected)
1	Discrete/Continuous Choice Models (Random Utiltiy Theory)	McGinnis et al. (1981); Winston (1981); Gray (1982); McFadden et al. (1986); Abdelwahab and Sargious (1991); Nam (1997); Abdelwahab (1998); Holguín-Veras (2002); Norojono and Young (2003); Brooks et al (2012); Pourabdollahi et al. (2013); Abate and Jong (2014); de Jong et al (2004); Arencibia et al. (2015); Kim et al. (2017); Larrañaga et al. (2017); Roman et al. (2017); Stinson et al. (2017); Abate et al. (2019); Keya et al. (2019); Jensen et al (2019); Comi and Polimeni (2020); Holguín-Veras et al. (2021)
2	Optimization (inventory theory)	Baumol and Vinod (1970); McGinnis et al. (1981); Gray (1982); Hall (1985); Leachman (2008); Zhang and Lee Lam (2018)
3	Elimination by Aspects	Young et al. (1982)
4	Artificial Neural Network	Abdelwahab and Sayed (1999)
5	Simulation	Reis (2014)
6	Game Theory	Holguín-Veras et al. (2011)

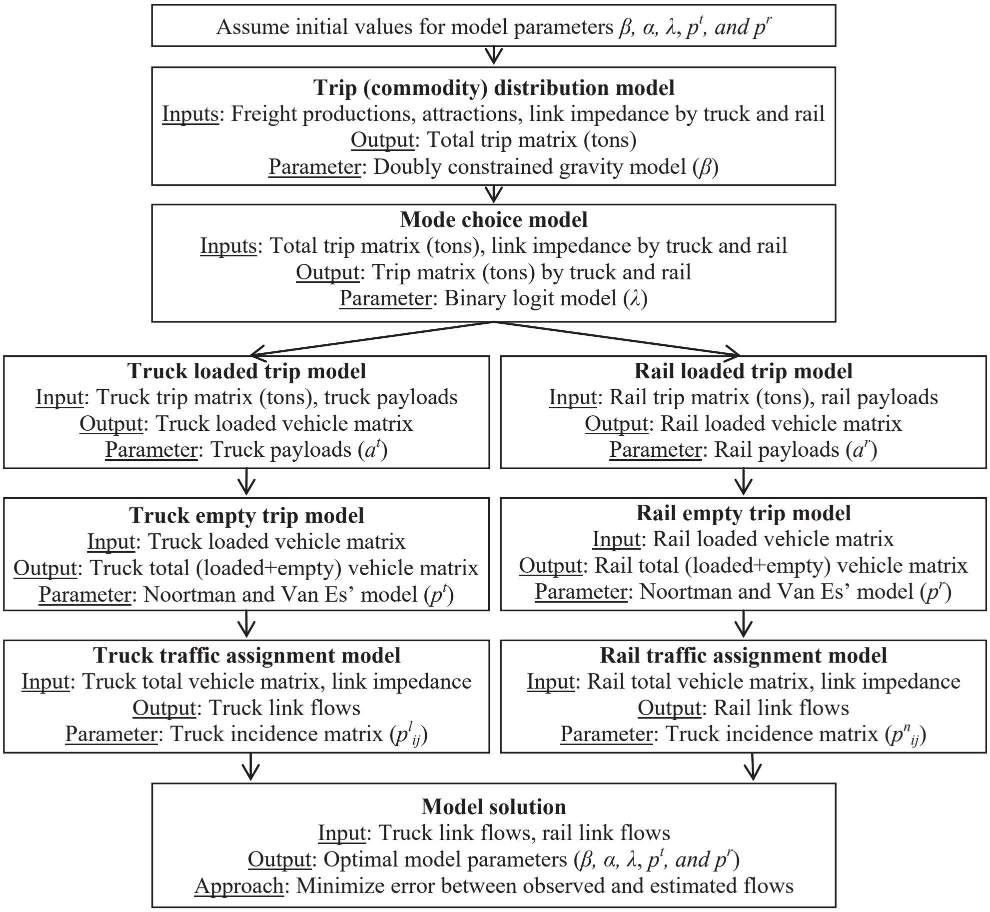

Fig. 1. FODS-MC Model Overview.

models. A solution procedure is proposed to estimate the model parameters based on the zonal productions, attractions, and the observed traffic count data for both truck and rail. The subsequent sections provide a detailed explanation of the methodology, model formulation, and solution procedure.

3. Methodology

A schematic of the Freight Origin-Destination Synthesis with Mode Choice (FODS-MC) model—inputs, outputs, and model parameters—is shown in Fig. 1. The FODS-MC model aims to estimate the freight flows, vehicle freight trips (including the empty trips) by truck and rail between the Origins and the Destinations (OD). The required input data are freight productions and attractions, payloads, network data for truck and rail, and link traffic counts for truck and rail. The FODS-MC model estimates the parameters for four interdependent models based on the observed traffic counts of truck and rail. These models are: (1) trip distribution model, which estimates the flow of cargo between an OD; (2) mode choice model, which splits the total cargo into cargo by truck and rail; (3) loaded trip model, which converts the cargo flows to truck and rail vehicle flows based on payloads; and (4) empty trip models for truck and rail, which estimate the empty vehicle flows between an OD. The total (loaded and empty) estimated vehicle trips are then assigned to the truck and rail networks to compare with the observed traffic counts. Additional details for these models are provided next.

3.1. Trip distribution model

A doubly constrained Gravity Model (GM) is used to represent the commodity flows (weights or volumes) between origins and destinations. The basic formulation of GM used is shown in Equation (1). The GM is selected as it provides an easy and effective way to estimate the freight flows between the ODs and incorporates spatial interactions such as zonal productions, attractions, and impedances. The GM is simply a pragmatic assumption to minimize the problems associated with model calibration, as, unlike the freight flows, the vehicle flows often display chaining behavior (Holguín-Veras and Thorson, 2000; Holguín-Veras and Patil, 2005). Tamin and Willumsen (1989) concluded that the GM provided better results than other commodity flow distribution models, including Furness, opportunities, and gravity opportunity models. Also, the GM, with an exponential impedance function presented in Equation (1), best captures the distribution as it could be derived from the entropy maximization method with a linear constraint on the total cost, which is widely used in modeling freight and passenger trips (Wilson, 1970; Fisk, 1988; Kawakami et al., 1992; Rios et al., 2002; Ortúzar and Willumsen, 2011; Kumar et al., 2016; de Grange et al., 2017).

$$m_{ij} = A_i B_j O_i D_j e^{-\beta c_{ij}} \tag{1}$$

where,

m_{ij} = Weight of cargo transported from zones i to zone j, including all modes
A_i, B_j = Balancing factors for freight productions and attractions respectively
O_i = Total weight of cargo originating at zone i (includes all modes)
D_j = Total weight of cargo destined at zone j (includes all modes)
$e^{-\beta c_{ij}}$ = Impedance (deterrence) function (negative exponential)
c_{ij} = Average impedance of trip from zone i to zone j
β = GM parameter to be estimated ($\geqslant 0$)

Since the impedance function includes a negative sign for β, the parameter (β) obtained from the optimization procedure must be non-negative, as the number of trips has to decrease with an increase in the impedance (c_{ij}). Since m_{ij} is the total cargo including all modes, the c_{ij} should consider the impedance of both truck and rail. Thus, it is necessary to formulate a methodology to estimate the average impedance (c_{ij}) and the modal split simultaneously, as c_{ij} depends on the mode choice model.

3.2. Mode choice model

The freight mode or vehicle choice is widely modeled using the Random Utility Theory (RUT), which is based on the hypothesis that the users are rational individuals who try to maximize the perceived utility from the choice (Domencich and McFadden, 1975). The utility function has two components. The first component is the systematic (observed) component (V_k), which could be measured as a function of attributes either relevant to the choice or the user. The second component is the error component (ε_k) introduced by the factors that lead to observational randomness. Hence, for a choice set '*N*' with two alternatives (*k and l*), the probability of choosing the choice k over l is given in Equation (2).

$$Pr(k) = Pr(V_k - V_l \geqslant \varepsilon_k - \varepsilon_l) \tag{2}$$

where, the systematic (observed) components (V_k and V_l) are expressed as a linear function of vector of '*N*' independent variables (X)

$$V_k = \sum_{n=1}^{N} \beta_n X_{nk} \tag{3}$$

Assuming the extreme value Type 1 (Gumbel) distribution for the error components leads to the Multinomial Logit (MNL) model for the probability of choosing a choice '*k*' from the choice set '*M*' as shown in Equation (4).

$$Pr(k) = \frac{e^{V_k}}{\sum_{m=1}^{M} e^{V_m}} \tag{4}$$

The MNL model is used for mode choice at either the disaggregate (shipment) or aggregate (market) level (Modenese-Vieira, 1992). The disaggregate models seek to explain the decision making of the shipper/carrier in transporting a specific shipment, whereas the aggregate models estimate the mode share combined at various levels of geography, region (OD), commodity, or industry sector as a function of aggregate independent variables such as average travel times, costs, distances, etc. The MNL models are typically calibrated using maximum likelihood estimations techniques. However, in the special scenario of a Binary Logit (BL) model with the number of choices (modes) of just two, the market share models could also be calibrated using logistic or Ordinary Least Square (OLS) regression estimation.

In this research, for numerical purposes, the estimation of market shares (q_{ij}) of truck and rail between an OD using a binary logit model is considered, with the utility function dependent only on the impedance of the trip between an OD (c_{ij}). The truck and rail are mutually exclusive and collectively exhaustive modes. The assumption of the logit model is reasonable since it is widely used in the freight mode choice literature, as shown in Table 2. There is a need to consider a constant term in addition to the travel impedance because the mode choice may depend on other unobserved factors. The mode choice models estimating the market shares are shown in Equations (5) and (6):

$$q^t_{ij} = \frac{e^{\alpha - \lambda c^t_{ij}}}{e^{\alpha - \lambda c^t_{ij}} + e^{-\lambda c^r_{ij}}} \tag{5}$$

$$q^r_{ij} = 1 - q^t_{ij} = \frac{e^{\lambda c^r_{ij}}}{e^{\alpha - \lambda c^t_{ij}} + e^{-\lambda c^r_{ij}}} \tag{6}$$

where,

$q^t{}_{ij}$ = Market share of selecting truck from zone i to zone j
$q^r{}_{ij}$ = Market share of selecting rail from zone i to zone j
$c^t{}_{ij}$ = Impedance of trip from zone i to zone j by truck
$c^r{}_{ij}$ = Impedance of trip from zone i to zone j by rail
α = Constant term of mode choice model to be estimated
λ = Impedance intercept of mode choice model to be estimated (≥ 0)

Where, the trip impedance ($c^t{}_{ij}$ and $c^r{}_{ij}$), in its most general form, could be expressed as generalized cost as a function of relevant cost elements such as rates (r_{ij}), distances (d_{ij}), travel times (t_{ij}), transfer times (tr_{ij}), reliability (rl_{ij}), shipment size (s_{ij}), and shipment value (v_{ij}) as shown in Equation (7). Also, Holguín-Veras et al. (2021) concluded that the generalized cost as a function of travel time, value, and cost produced better discrete choice models to capture the shippers' freight mode choice. In the numerical example in Section 5, the travel times (t_{ij}) between origin 'i' and destination 'j' for different modes are considered as impedances.

$$c^k_{ij} = f\left(r^k_{ij}, d^k_{ij}, t^k_{ij}, tr^k_{ij}, rl^k_{ij}, s^k_{ij}, v^k_{ij}\right) \forall k \in truck(t) \ or \ rail(r) \tag{7}$$

The average impedance c_{ij} can be calculated from the market shares in Equations (5) and (6), as shown in Equation (8).

$$c_{ij} = q^t_{ij} c^t_{ij} + q^r_{ij} c^r_{ij} \tag{8}$$

The weight of cargo transported by truck and rail between zones i and j is obtained by multiplying the respective market shares in Equation (5) and (6) with total cargo obtained in Equation (1).

$$m^t_{ij} = q^t_{ij} m_{ij} \tag{9}$$

$$m^r_{ij} = q^r_{ij} m_{ij} \tag{10}$$

3.3. Vehicle flow estimation model

The commodity flows by the truck and rail obtained from Equations (8) and (9) have to be converted to the respective vehicle trips to assign them to the corresponding network. This conversion is not straightforward, especially for the trucks, as they have a wide range of capacities in both weights and volumes. Also, the vehicle flows would include the empty trips, where the truck or railcars run vacant. The empty trips are inevitable due to the asymmetry in the distribution of commodity flows, where some zones have more inclination toward either supply (origins) or demand (destinations). The vehicles need to go back to the supply zones mostly empty to transport goods back to demand zones. Hence, this research considers both loaded and empty trips separately, as explained below.

3.3.1. Loaded trip model

The loaded trips (x_{ij}) by truck and rail are obtained by dividing the commodity distribution (m_{ij}) with the average payload, as given in Equation (11).

$$x^k_{ij} = \frac{m^k_{ij}}{a^k_{ij}} \tag{11}$$

As shown in Equation (11), the payload is a function of origin and destination pair (ij) to account for the specificity of the trip between an OD. For example, a trip between an OD could belong to transporting iron ore to the steel plant, which would obviously have higher payloads than usual. The vehicle flows from the above equation estimate the number of vehicles with respect to the average payload of a typical truck and railcar and do not consider various types of vehicles in each mode.

3.3.2. Empty trip model

Empty trip modeling differs from that of loaded trips, as the former is a result of imbalances in the commodity flows between the ODs. For instance, a truck that makes a loaded trip in one direction (*zone i to zone j*) makes an empty return trip (*zone j to zone i*) if there is no sufficient cargo from *zone j to i*. Therefore, the number of empty trips between two zones depends on two factors. The first factor is the number of loaded vehicles traveling in one direction, and the second is the availability of sufficient cargo flow in the opposite direction to fill the truck for the return trip. Hence, the proper technique to include empty vehicle trips is to use complementary models that estimate the empty trips as a function of either the loaded trips or including the higher order trip chain behavior (Noortman and Van Es, 1978; Hautzinger, 1984; Holguín-Veras and Thorson, 2003a,b; Moeckel and Donnelly, 2016; Hvolby et al., 2019; Gonzalez-Calderon et al., 2021).

This research used the basic version of the Noortman and Van Es' model, which is widely used in the freight literature to estimate empty trips. This model estimates the empty trips (y_{ij}) between *zones i and j* as a fraction of loaded trips between *zones j and i* (Noortman and van Es, 1978), as given in Equation (12). The basic formulation of Noortman and Van Es' is adopted to reduce the computational complexity, which assumes the order of trip chain being zero, i.e., the empty trips depend only on the primary trip between the OD. Hence, the empty parameter (p^k) in Equation (12) depends on the vehicle flow between the OD.

$$y_{ij}^{k} = p^{k}x_{ji}^{k} \tag{12}$$

The total vehicle trips (z_{ij}) is obtained by adding the loaded and the empty trips

$$z_{ij}^{k} = x_{ij}^{k} + p^{k}x_{ji}^{k} \tag{13}$$

where

k = Truck (t) or rail (r)
a^{t}_{ij}, a^{r}_{ij} = Average payloads from zone i to zone j by truck and rail, respectively.
p^{t}, p^{r} = Empty trip parameters (between 0 and 1) by truck and rail, respectively.

The estimated total (loaded and empty) number of vehicle trips by different modes does not incorporate the freight tours (common in an urban scenario) and intrazonal trips. The scope of this research is limited to estimating the freight demand at a regional or national level. However, for relatively smaller zones, these aggregate OD matrices, complemented with additional data on trip chain behavior, could assist in investigating the possibilities of regional freight tours (Comi et al., 2021).

3.4. Estimated link flows

The total vehicle flows between the zones need to be assigned to the respective truck and rail networks for two major reasons: 1) to be able to compare with the observed link traffic counts, which constitute the basis of the FODS-MC model and 2) to assess the impacts of freight vehicle traffic on the transportation infrastructure. Traffic assignment models allocate these OD flows to the respective network either by considering congestion effects such as User Equilibrium (UE), System Optimal (SO), Stochastic User Equilibrium (SUE), or without considering the congestion effects, such as All-or-Nothing (AON) (Sheffi, 1985). In this research, the total vehicle trips (z_{ij}) obtained from Equation (13) is assigned to truck and rail networks using the AON assignment. The AON assignment assumes that trips between zones i and j take the shortest path that minimizes the total impedance. In the unlikely event of multiple shortest paths at the nation-level network, the assignment takes one of the shortest paths randomly. Previous studies found that AON provides better estimates for FODS than SUE (Tamin and Willumsen, 1989). The AON assignment also reduces the computational time while not compromising the quality of parameter estimation. Estimated link flows by truck (v_l^{est}) and rail (v_n^{est}) are shown in Equations (14) and (15). In the case of multimodal transport, the estimated link flows comprise all the modes used by the cargo, including rail-truck chain behavior.

$$v_l^{est} = \sum_{i,j} p_{ij}^{l} z_{ij}^{t} \ \forall l \in L \tag{14}$$

$$v_n^{est} = \sum_{i,j} p_{ij}^{n} z_{ij}^{r} \ \forall n \in N \tag{15}$$

where,

$p_{ij}^{l} \in \{0,1\}$ = Equal to one if the link 'l' falls in the shortest path between zone i and zone j by truck.
$p_{ij}^{n} \in \{0,1\}$ = Equal to one if the link 'n' falls in the shortest path between zone i and zone j by rail.
L = Set of links in truck network and
N = Set of links in rail network

3.5. Objective function

The FODS-MC model seeks to maximize the agreement between the observed and the estimated traffic counts (link flows) for truck and rail. This is because compared to zonal productions (O_i) and attractions (D_j), the traffic count data (v^{obs}) are either readily available or could be easily obtained from the traffic sensors or toll plazas. Hence, the objective function (F_v) in Equation (16) is the summation of squared errors between the observed and the estimated link flows. The objective function considers only the total traffic counts since they are the most widely available. If the traffic counts are available in greater detail, such as by type of vehicle (truck and railcar), empty and loaded trips, Equation (16) should be expanded to minimize the errors between estimated and observed counts at the finest levels of detail possible.

$$F_v = \sum_{l} \left(v_l^{est} - v_l^{obs}\right)^2 + \sum_{n} \left(v_n^{est} - v_n^{obs}\right)^2 \tag{16}$$

where,

v_l^{obs} = Observed truck link flows
v_n^{obs} = Observed rail link flows

Substituting the observed link flows (v_l^{ob} *and* v_n^{obs}) from Equations (14) and (15) in Equation (16)

$$F_v = \sum_l (\{\sum_{i,j} p_{ij}^l z_{ij}^t\} - v_l^{obs})^2 + \sum_n (\{\sum_{i,j} p_{ij}^n z_{ij}^r\} - v_n^{obs})^2 \quad (17)$$

Substituting total vehicle trips (z_{ij}) from Equation (13) in Equation (17)

$$F_v = \sum_l (\{\sum_{i,j} p_{ij}^l (x_{ij}^t + p^t x_{ji}^t)\} - v_l^{obs})^2 + \sum_n (\{\sum_{i,j} p_{ij}^n (x_{ij}^r + p^r x_{ji}^r)\} - v_n^{obs})^2 \quad (18)$$

The function F_v, in Equation (18), could be written as the sum of truck (F_{vt}) and rail (F_{vr}) error components as shown in Equation (19).

$$F_v = F_{vt} + F_{vr}$$

where,

$$F_{vt} = \sum_l (\{\sum_{i,j} p_{ij}^l (x_{ij}^t + p^t x_{ji}^t)\} - v_l^{obs})^2 and F_{vr} = \sum_n (\{\sum_{i,j} p_{ij}^n (x_{ij}^r + p^r x_{ji}^r)\} - v_n^{obs})^2 \quad (19)$$

Substituting the loaded vehicle trips (x_{ij}) from Equation (11) in Equation (19) followed by expanding the truck and rail cargo flows (m^k_{ij}) as a function of market share (q^k_{ij}) and total cargo flows (m_{ij}) as given in Equations (8) and (9), Equations (20) and (21) can be obtained. These Equations allow for a convex optimization of objective function (F_v) as a function of market shares (q_{ij}), see Section 4.1.

$$F_{vt} = \sum_l (\{\sum_{i,j} p_{ij}^l (\frac{q_{ij}^t m_{ij}}{a_{ij}^t} + p^t \frac{q_{ji}^t m_{ji}}{a_{ji}^t})\} - v_l^{obs})^2 \quad (20)$$

similarly,

$$F_{vr} = \sum_n (\{\sum_{i,j} p_{ij}^n (\frac{q_{ij}^r m_{ij}}{a_{ij}^r} + p^r \frac{q_{ji}^r m_{ji}}{a_{ji}^r})\} - v_n^{obs})^2 \quad (21)$$

3.6. FODS-MC model formulation

The FODS-MC model could be expressed as an optimization program, as shown below. The objective function minimizes Equation (16), which is the summation of squared errors between observed and estimated link flows for truck and rail. The constraints in Equations (22) to (24) correspond to the doubly constrained GM, for which the average impedances are computed from the constraint in Equation (27). Equations (23) and (24) ensure that the sum of rows and columns in the trip distribution matrix add up to given zonal productions (O_i) and attractions (D_j). The constraints in Equations (25) and (26) represent the binary logit model for the mode choice; Equations (28) and (29) convert the commodity flows to vehicle flows using the payloads; Equations (30) and (31) provide the total (loaded + empty) vehicle trips using the Noortman and van Es' empty trip model, and Equations (32) and (33) estimate the links flows for truck and rail assuming AON assignment. Equation (34) is the upper bound constraint on the empty trip model parameters for truck and rail.

Parameters (Decision variables):

Gravity model (β), mode choice model (α, λ), truck empty trip (p^t), and rail empty trip model (p^r)

Input data:

Freight productions (O_i), and attractions (D_j) by weight of cargo
Truck and rail network link impedances (c^t_{ij} and c^r_{ij}), assignment matrix (p^l_{ij} and p^n_{ij})
Observed traffic counts by truck (v_l^{obs}) and rail (v_n^{obs})
Average payload by truck (a^t_{ij}) and rail (a^r_{ij})

Objective function:

$\underset{\alpha,\beta,\lambda,p^t,p^r}{Min} F_v = \sum_l (v_l^{est} - v_l^{obs})^2 + \sum_n (v_n^{est} - v_n^{obs})^2$(Sum squared errors of estimated traffic counts)

Constraints (subject to):

$$m_{ij} = A_i B_j O_i D_j e^{-\beta c_{ij}} \ \forall ij \quad \text{(Gravity model)} \quad (22)$$

$$A_i = \frac{1}{\sum_j B_j D_j e^{-\beta c_{ij}}} \forall ij \quad \text{(Balancing factor for productions)} \quad (23)$$

$$B_j = \frac{1}{\sum_i A_i O_i e^{-\beta c_{ij}}} \forall ij \quad \text{(Balancing factor for attractions)} \tag{24}$$

$$q^t_{ij} = \frac{e^{\alpha - \lambda c^t_{ij}}}{e^{\alpha - \lambda c^t_{ij}} + e^{-\lambda c^r_{ij}}} \forall ij \quad \text{(Market share of truck)} \tag{25}$$

$$q^r_{ij} = (1 - q^t_{ij}) \ \forall ij \quad \text{(Market share of rail)} \tag{26}$$

$$c_{ij} = q^t_{ij} c^t_{ij} + q^r_{ij} c^r_{ij} \ \forall ij \quad \text{(Average impedance for gravity model)} \tag{27}$$

$$x^t_{ij} = \frac{q^t_{ij} m_{ij}}{a^t_{ij}} \ \forall ij \quad \text{(Truck loaded trips)} \tag{28}$$

$$x^r_{ij} = \frac{q^r_{ij} m_{ij}}{a^r_{ij}} \ \forall ij \quad \text{(Rail loaded trips)} \tag{29}$$

$$z^t_{ij} = x^t_{ij} + p^t x^t_{ji} \ \forall ij \quad \text{(Truck total trips)} \tag{30}$$

$$z^r_{ij} = x^r_{ij} + p^r x^r_{ji} \ \forall ij \quad \text{(Rail total trips)} \tag{31}$$

$$v^{est}_l = \sum_{i,j} p^l_{ij} z^t_{ij} \ \forall L \quad \text{(Estimated truck link flows)} \tag{32}$$

$$v^{est}_n = \sum_{i,j} p^n_{ij} z^r_{ij} \ \forall N \quad \text{(Estimated rail link flows)} \tag{33}$$

$$p^t, p^r \leqslant 1 \quad \text{(Upper bound for empty trip parameters)} \tag{34}$$

$$\beta, \lambda, p^t, p^r \geqslant 0 \quad \text{(Non − negativity constraints)} \tag{35}$$

The mathematical proof for the nonconvexity of the objective function F_v is provided in Appendix A.

4. Solution procedure

This section is divided into two subsections. Section 4.1 presents the solution process followed in estimating the FODS-MC model parameters. Section 4.2 demonstrates the performance of two nonconvex solution methods (i. Multi-Start and ii. Convex + OLS) and provides the proof for selecting the Multi-Start method as the best alternative. The solution process is explained below.

4.1. FODS-MC model solution process

The model outlined in Section 3 requires an iterative process to estimate the parameters due to various computational challenges. Firstly, the objective function is nonconvex. Secondly, the average impedance in the gravity model (c_{ij}) is a function of mode choice parameters α, λ. Hence, there is an interdependency between the mode choice and trip distribution. Considering these challenges, the model calibration procedure is divided into five iterative steps.

Fig. 2 shows the solution process for the estimation of the FODS-MC model parameters (β, α, λ, p^t and p^r), which minimizes the objective function explained in Equation (16). The iteration process begins ($N = 0$) by assigning the initial values for the model parameters. A reasonable assumption for the initial values of β, α, p^t, and p^r could be obtained from the existing data and literature. More specifically, β in the GM is approximately equal to the inverse of the total average impedance of the trip distribution (Ortúzar and Willumsen, 2011). Similarly, as demonstrated by Holguín-Veras and Thorson (2003a,b), solid starting values of the parameters of the empty trip models, p^t and p^r, can be obtained from estimates of the percentage of total empty trips in the area (see Equation (36)). These values could also be used to further validate the parameter estimates obtained from the FODS-MC model.

$$P^k_e = \frac{p^k}{1 + p^k} \tag{36}$$

where, k = truck (t) or rail (r)

Step 1: Compute the average impedance (c_{ij}) matrix from the impedances by truck ($c^t{}_{ij}$), rail ($c^r{}_{ij}$), and the mode choice model parameter obtained in each iteration (λ_N), as shown in Equations (5)-(7).

Step 2: Compute the commodity distribution (m_{ij}) by applying the doubly constrained GM in Equation (1) using the freight productions (O_i), and attractions (D_j), impedance (c_{ij}) obtained in the previous step, and the GM parameter in each iteration (β_N). The balancing factors (A_i and B_j) are estimated using the standard computation procedures for the doubly constrained GM.

Step 3: Minimize F_v with respect to the GM parameter (β_{N+1}) by assuming α_N, λ_N, $p^t{}_N$, and $p^r{}_N$ from the previous step. The balancing

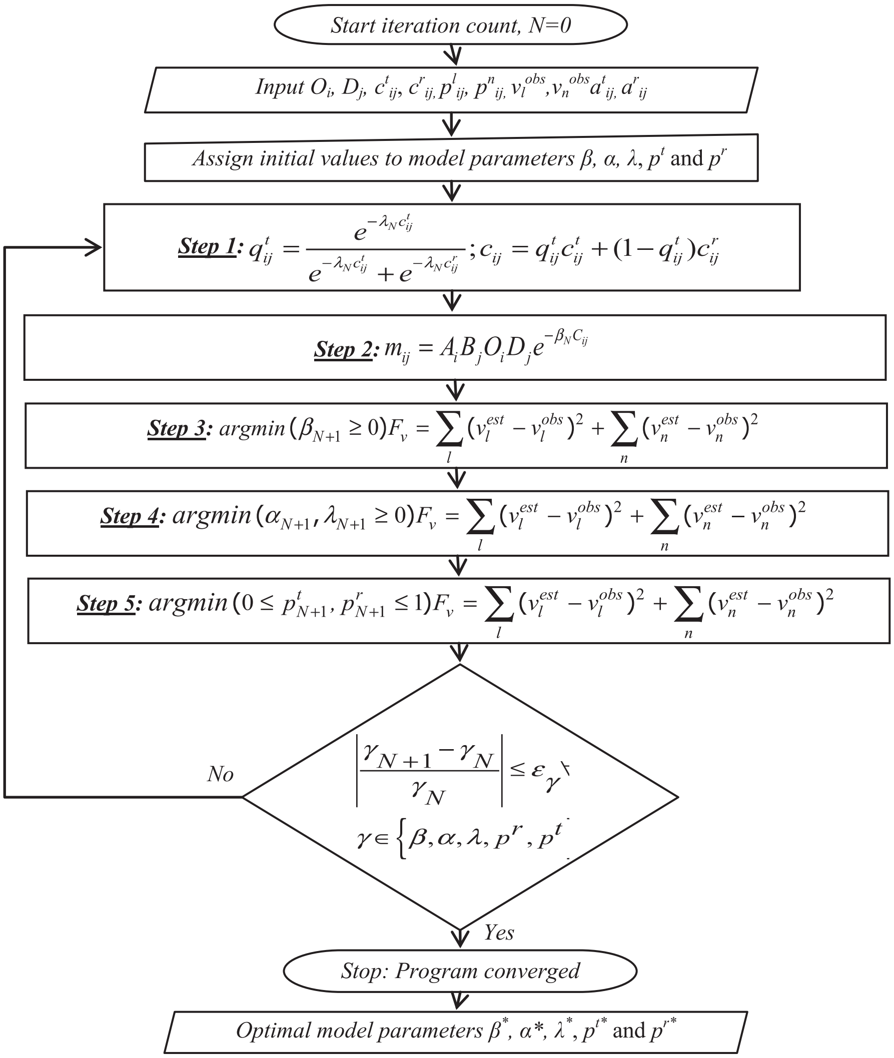

Fig. 2. FODS-MC Model Solution Process.

factors (A_i, B_j) are assumed to be independent of β, which does not affect the optimum solution as the tolerance for convergence (ε) is relatively small to change A_i and B_j.

Step 4: Minimize F_v with respect to the mode choice model parameters (α_{N+1}, λ_{N+1}) by assuming β_{N+1}, $p^t{}_N$, and $p^r{}_N$ from the previous steps. Two methods (Multi-Start and Convex + OLS) were tested to address the nonconvexity of F_v, which are explained in Section 4.1. The average impedance c_{ij} is assumed to be independent of the mode choice model parameters α and λ. However, this assumption does not affect the optimum solution since the stopping criteria (ε) is relatively small.

Step 5: Minimize F_v with respect to the empty trip model parameters ($p^t{}_{N+1}$ and $p^r{}_{N+1}$) by assuming β_{N+1}, α_{N+1}, λ_{N+1} from the previous steps. This step includes a constraint to ensure that $p^t{}_N$ and $p^r{}_N$ are less than or equal to one.

The calibration procedure ends when the relative change in each of β_{N+1}, α_{N+1}, λ_{N+1}, $p^t{}_{N+1}$, and $p^r{}_{N+1}$ compared to the values from the previous iteration is less than or equal to the stopping criteria (ε). If not, steps 1–5 are repeated until the stopping criteria are met.

4.2. Nonconvex solution methods

This research tested two methods to address the nonconvexity of F_v in estimating mode choice model parameters (α, λ) in step 4 of the model solution process outlined in Fig. 2. The first method (Multi-Start algorithm) finds the local optimal solutions for a set of randomly generated starting points. The second method (Convex + OLS) infers the best fit λ for the optimal market shares (q_{ij}) for truck and rail using Ordinary Least Squares (OLS) regression. As neither method guarantee the global optimal, it is necessary to determine which method provides the solution closest to the optimal solution. The subsequent sections provide a brief description of these methods, followed by a test case to select the best method.

1. Multi-Start Algorithm with Interior Point Method (Multi-Start)

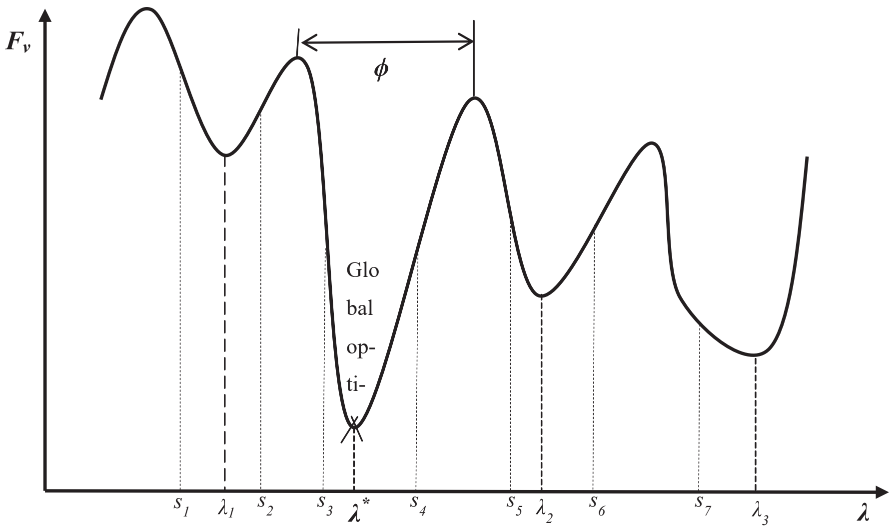

Fig. 3. Multi-Start Method.

In the interior point method in the Multi-Start algorithm, the main problem (see Equation (37)) is solved using a set of barrier sub-problems (see Equation (38)), as shown below, where μ is the barrier parameter that converges to zero and η_i (≥ 0) is the slack of each constraint *i*.

Main problem:

$$Min\, f(x),\ \text{S.t. } g(x) \leqslant 0 \tag{37}$$

Barrier sub-problem:

$$Min\, f(x) - \mu \sum_i Ln(\eta_i),\ \text{S.t. } g(x) + \eta = 0 \tag{38}$$

The Interior Conjugate Gradient (ICG) method is used to obtain the local optimal solution for the nonconvex objective function *f(x)*. ICG is similar to the Newton method, where the step length is calculated by minimizing a sequential quadratic program of the Lagrangian function. Trust region strategies in the ICG algorithm permit the direct use of second derivative information to solve the Karush-Kuhn-Tucker (KKT) conditions. For the nonconvex objective function, the local optimal does not coincide with the global optimal. For example, the parameter values λ_1, λ_2, λ_3 in Fig. 3 provide the local optimal for the objective (F_v) while λ^* gives the global optimal.

The Multi-Start method estimates the local optimal for a set of randomly generated starting points (S_1, S_2... S_7), among which starting points S_3 and S_4 lead to the global optimal. Unless a starting point falls in the optimal region ϕ, the global optimal solution is not guaranteed. The greater the number of randomly generated starting points, the greater the chance that at least one of the starting points will fall in the region ϕ. Although the Multi-Start method does not ensure global optimality, the solution obtained from this method could be much closer to the global optimal. For a detailed explanation of the algorithm, please refer to (Byrd et al., 1999; Byrd et al., 2006; Waltz et al., 2006).

2. Convex Programming with OLS Regression (Convex + OLS)

In this method, the mode choice model parameter (λ) is estimated in two steps. The first step is solving a quadratic program shown below (see Equations (39) and (40)), which obtains the optimal mode choice market shares for truck (q^t_{ij}) and rail (q^r_{ij}) since the objective function F_v as a function of market shares is convex. The constraints ensure that the market shares that add up to one also lie between zero and one.

Minimize:

$$F_v = \sum_l (\{\sum_{i,j} p^l_{ij} (\frac{q^t_{ij} m_{ij}}{a^t_{ij}} + p^t \frac{q^t_{ji} m_{ji}}{a^t_{ji}})\} - v^{obs}_l)^2 + \sum_n (\{\sum_{i,j} p^n_{ij} (\frac{q^r_{ij} m_{ij}}{a^r_{ij}} + p^r \frac{q^r_{ji} m_{ji}}{a^r_{ji}})\} - v^{obs}_n)^2 \tag{39}$$

Subject to:

$$0 \leqslant q^t_{ij}, q^r_{ij} \leqslant 1 \ and\ q^t_{ij} + q^r_{ij} = 1 \tag{40}$$

The second step estimates the best fit λ for the optimal market shares from the previous step, using the Ordinary Least Squares (OLS) regression method, which minimizes the sum squared errors shown below. This method is based on the procedure developed by Berkson (Berkson, 1944) to estimate the binary logit model by aggregating the individual observations into subgroups. This method is adopted in the transportation mode choice methodology by Ben-Akiva and Lerman (1985).

$$\underset{\alpha,\lambda}{Min}\sum_{ij}(Y-\lambda X)^2 \tag{41}$$

where: $Y = ln\left(\left(1/q_{ij}^{t}\right)-1\right)$ and $X = c_{ij}^{t} - c_{ij}^{r}$

The expressions shown above for Y and X are obtained from Equation (5) after taking natural logarithms and solving for Y and X. The λ estimated from the OLS may or may not provide a good fit to the market shares. Also, the quadratic program in the first step could have multiple optimal solutions, which would lead to multiple values for λ in the second step. Thus obtained, the λ minimizes the error in the estimated market shares, which does not guarantee the optimal value in minimizing the error in estimated traffic counts in F_v. The performance of both methods discussed above is evaluated using a test case; see Appendix B. Appendix B proves that the Multi-Start method gives better and more reliable parameter estimates compared to that of the Covex + OLS method. The methodology and the model solution techniques discussed in the previous sections are applied on a quasi-real-life case study of estimating a nation-wide freight demand model for Bangladesh, as explained in the subsequent section.

5. Numerical example: Bangladesh fods-MC model

This numerical example assesses the performance of the methodology developed in this paper to infer the FODS-MC model parameters in a quasi-real-life test case. The case used in this section is inspired by a national freight demand model developed for Bangladesh (Herrera et al., 2019; Holguín-Veras et al., 2019; Holguín-Veras et al., 2020a,b), funded by the World Bank (WB). As part of this WB study, a team from Rensselaer Polytechnic Institute (RPI) estimated the freight trip distribution and empty trip models for truck using the methodology developed by Holguín-Veras and Patil (2007) and Holguín-Veras and Patil (2008). The numerical example varies from a real-life case study, as some parameters such as the rail traffic counts (${v_n}^{obs}$), rail link travel times, and payloads were not available. An approximate value of the rail link flows was estimated from the demand data, which was then incorporated in the FODS-MC model estimation along with a few scenarios of truck payloads and rail travel times. The entire process of model estimation and assignment (AON) for this numerical example is carried out using the KNITRO solver version 10.3 from Artleys, interfacing with MATLAB R2019b (Artelys, 2017), on a computer with 64 GB memory and a 3.5 GHz processor.

This section is organized as follows: Section 5.1 presents an overview of the economy and freight system in Bangladesh; Section 5.2 explains the process to obtain the secondary data that serve as the input to the FODS-MC model, and Section 5.3 presents the FODS-MC model results for various scenarios of truck payload, and rail speeds.

5.1. Overview

Bangladesh (BGD), with a population of 158 million, is the tenth densest country in the world and is divided into eight divisions and 64 districts. The districts were used as the Transportation Analysis Zones (TAZs) for this study. The capital city is Dhaka, and major cities include Chittagong, Khulna, and Rajshahi (Bangladesh National Portal, 2017). The economy of BGD is growing at a rate of 6–8% a year, driven by the growth of small establishments (68% with less than three employees). Agriculture provides employment to more than 50% of the population, followed by manufacturing and other sectors. Textiles and garments are the major exports. More than 90% of the imports and exports occur through the port at Chittagong. Fig. 4 shows the districts and the transportation network in BGD.

The transportation infrastructure in BGD includes 27,000 km of roads, 2,900 km of rail lines, and 6,000 km of navigable rivers. Three major rivers (Brahmaputra, Padma, and Meghna) divide the country into three parts, which makes the lack of proper bridges an important hurdle in transporting cargo between these parts. Freight mode share in ton-km is 80% for road, 16% for inland waterways, and 4% for rail (Smith and Guillossou, 2009). The road network is congested, with heavily overloaded trucks. Due to lack of geographic coverage, and the deteriorating quality of freight rail service with low average speeds between 10 and 12.5 kmph, the rail mode share decreased from 28% to 4% in the past 30 years (Bangladesh Railway, 2014). The existing freight models developed for the WB estimate the total truck vehicle trips (including the empty trips) between the TAZs (districts) using the FODS techniques developed by Holguín-Veras and Patil (2008). Due to the high economic growth, population density, and the multi-purpose road-rail bridge (Padma) that is being constructed, BGD needs a solid freight modeling framework to assist the public sector in developing policies that will promote sustainable freight transportation. This research assists in estimating modal split by adding a mode choice model and empty trips for rail to the existing freight models for BGD.

5.2. Data preparation

One of the first steps to implementing a FODS-MC model is the preparation of input data parameters (despite being secondary data), i.e., freight productions (O_i), attractions (D_j), link impedances (c_{ij}), traffic counts (v^{obs}), and payloads (a_{ij}), as explained in Section 3.6. The sections below provide a brief description of the process of obtaining these input parameters, along with the associated assumptions and limitations. All the datasets explained below belong to the year 2013. For a detailed explanation of the freight survey, data collection, sampling plan, industry sectors, geographic coverage, freight generation models, estimation procedures, and the estimation of road link travel times using the GPS data, please refer to Herrera et al. (2019) and Holguín-Veras et al., (2018a,b).

Transportation analysis zones (TAZs)

The 64 districts, which cover the entire country (refer to Fig. 4A), were chosen as the Transportation Analysis Zones (TAZs), based on their homogeneity with respect to freight activity, their being part of existing administrative boundaries, and their size being

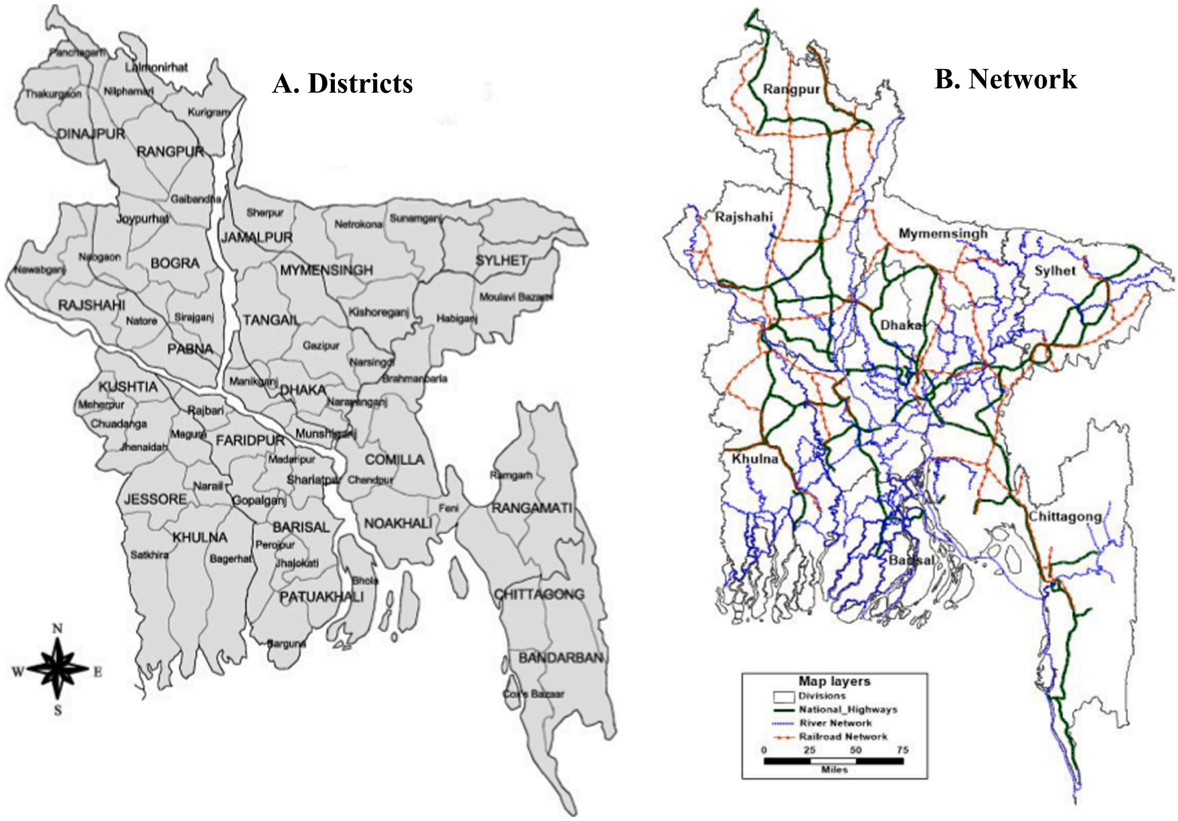

Fig. 4. BGD Districts (TAZs) and Transportation Network.

compatible for choosing a proper centroid (Ortúzar and Willumsen, 2011). However, a TAZ in the northeast of BGD (Khurigram) was removed due to a lack of economic census data to estimate the freight productions (O_i) and attractions (D_j), which reduces the total number of TAZs considered to 63. Since the FODS-MC model aims to estimate a nationwide regional freight demand model, no external zone (outside BGD) is considered. Therefore, the trip distribution would estimate the trips between the 63 districts inside BGD.

Freight Generation

The freight productions (O_i) and attractions (D_j) in tons per day were estimated from a national-level freight survey conducted by Holguín-Veras et al. (2019). The survey collected freight generation data from around 4000 establishments spread across the country. This survey is complemented with econometric modeling (i.e., multiple linear regression models) techniques that estimated the freight productions and attractions as a function of industry sector (by two-digit Bangladesh Standard Industry Classification, BSIC) and the number of full-time equivalent employees in the establishment. These models were applied to the census data (agriculture and economic) to estimate the freight generation by industry sector in each TAZ, i.e., 63 districts in BGD. A few assumptions are made to ensure that the O_i and D_j include only the regional or intercity freight generation. For instance, establishments with less than three employees are ignored in the estimation of O_i and D_j, as these firms mainly deal with the freight that is locally produced and consumed. Firms with more than a thousand employees are also neglected, assuming that they mainly focus on international cargo. For further details on the estimation of O_i and D_j, please refer to Holguín-Veras et al. (2019).

Link Impedances

The travel time in hours for each link in the road (c^t_{ij}) and rail (c^r_{ij}) network is considered as the link impedances. Due to lack of data, other factors influencing the impedance, e.g., transfers, reliability, shipment size, shipment value (as explained in Section 3.2), were not included. The GPS data were collected for about 15% of the links in the country, mainly comprising of free-flow travel times. For the links with no travel time data available, an approximate value of travel times was randomly assigned assuming a uniform distribution for space mean speeds of the other links (with GPS data available) in the given TAZ. These space mean speeds are converted into the link travel times based on the link distances estimated from the GIS layer. For more information on truck link travel times, please refer to Holguín-Veras et al. (2019). Since the data on travel times for rail links were also unavailable, they were calculated for each link assuming a uniform speed of 10 or 12 kmph (Bangladesh Railway, 2014). The FODS-MC models are estimated for both cases of rail average speeds. These link travel times, along with the mode choice model, are required to obtain the impedance matrix (c_{ij}) in the GM in Section 3.1. Also, they are required to estimate the AON assignment matrix for truck (p^t_{ij}) and rail (p^r_{ij}) flows, as explained in Section 3.4. Due to lack of data, the time taken for loading (at origin TAZ) and unloading (at the destination TAZ) and transfers were neglected in both c_{ij} and p_{ij}, for both truck and rail links.

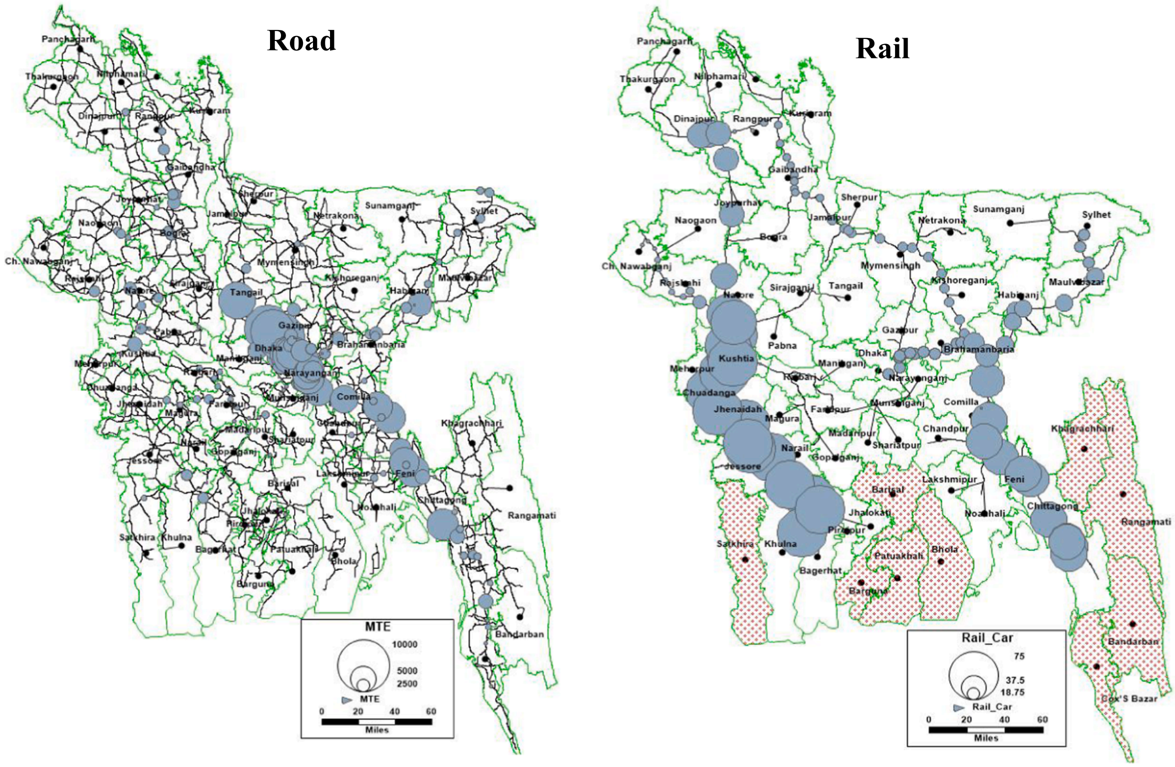

Fig. 5. BGD Observed Truck and Rail Link Flows (Holguín-Veras et al., 2020a,b).

Observed Link Flows

Fig. 5 shows the truck and rail network with traffic counts. The truck flows are concentrated between the major districts of Dhaka and Chittagong, while the major rail flows are occurring along the east and west corridors. The road network is fully connected between any two TAZs, whereas the rail network is not fully connected, as nine districts in the south (Bandarban, Barguna, Barisal, Bhola, Cox's Bazar, Khagrachhari, Patuakhali, Rangamati, and Satkhira; highlighted in Fig. 5) are not connected by the rail. The rail link impedances (c_{ij}) either from or to these districts were assumed to be infinite.

Truck traffic counts (v_l^{obs}) were available for 1,520 out of 4,848 links. Since the traffic counts comprise various types of trucks carrying local and international cargo, it is necessary to separate the regional or intercity traffic. Using the customs data, followed by distribution and traffic assignment techniques, the imports/exports flows are removed from the traffic counts. Utility vehicles (two- or three-wheelers) are neglected from the traffic counts since these vehicles mainly contribute to local freight trips. The truck types in the traffic counts are largely classified into three categories: 1) small (two-axle, four-tire), 2) medium (two-axle, six-tire), and 3) large (four or more axles). Truck flows are in Medium Truck Equivalent (MTE), and rail flows are in number of rail wagons/railcars. Different types of trucks in the traffic counts are converted into MTE, based on their respective average payloads, as given in Equation (42) below. On average, the small and large trucks are found to carry one-third and twice the load carried by the medium trucks, respectively. The payload data are obtained from one of the biggest truck manufacturers in BGD (Tata Motors Bangladesh, 2018) and corrected for overloading based on surveys conducted by the local partner. For more detail, please refer to Holguín-Veras et al. (2020a, b).

$$MTE = \frac{1}{3}(Small\ trucks) + (Medium\ trucks) + 2(Large\ trucks) \tag{42}$$

The observed traffic count (v_n^{obs}) data are not available for rail. However, the average annual OD flows in tons of cargo and number of wagons transported by rail between the terminals were provided by the World Bank. These OD flows, complemented with payload data of the wagons/railcar, were assigned to the rail network, which resulted in the estimated traffic counts for 304 out of 478 links. These estimated rail traffic counts were inputted as the observed rail traffic counts (v_n^{obs}) in the model estimation. Since the OD flows are partial, the aggregate share of empty trips in the OD flows cannot be used to validate the empty trip parameter estimates from the FODS-MC model results. It is assumed that rail flows comprise just one type of railcar; they do not contain any local cargo, and they contribute to just 2% of the international freight flows. Also, the trip from the origin zonal centroid to the nearest rail terminal (first leg) and the trip from the destination rail terminal to the zonal centroid (last leg) is carried out by truck.

Payloads

The payloads (a^t_{ij}) for various types of trucks observed in the traffic count data are not available. Hence, assumptions on payloads

Table 3
FODS-MC Model Results: Parameter Estimation.

Scenario	Avg. rail speed (kmph)	Truck payload (tons)	Rail payload (tons)	Gravity model (β)	Mode choice (λ)	Truck empty trip (p^t)	Rail empty trip (p^r)	Run-time (h:mm:ss)	Toleranace (ε)
1	10	15	50	0.443	0.171	0.488	0.313	02:23:14	0.5%
2		20	50	0.248	0.170	0.483	0.498	02:09:02	1.0%
3	12	15	50	0.422	0.215	0.481	0.285	03:01:52	0.5%
4		20	50	0.238	0.219	0.480	0.501	01:41:39	1.0%

were made based on the design loads of different truck models available from one of the major truck manufacturers in BGD (Tata Motors Bangladesh, 2018). As per Tata Motors Bangladesh (2018), the design payloads of medium trucks vary from 11.61 tons (truck model "16 Tonners") to 23.2 tons (truck model "31 Tonner Rigid"). Also, a medium truck typically has a designed volume of around 45 cubic meters (7.2 m length X 2.5 m width X 2.5 m height). Assuming the truck is fully loaded with highly dense cargo, the payload should vary between 15 and 20 tons. Also, Herrera et al. (2019) found that reshaping of the chassis and overloading of trucks are prevalent in BGD. To account for the lack of data on payloads and overloading, the FODS-MC model is estimated for two cases of payloads for a medium-size truck: 15 and 20 tons. For rail, the average payload of the wagon/railcar is available from the data provided by the WB. The average payload of a rail wagon is around 49.45 tons. Hence, the FODS-MC models are estimated by considering the average payload of a railcar (all railcars are uniform) as 50 tons.

Because of the data constraints explained above, the FODS-MC models are estimated for four scenarios, two cases of rail speeds (10 and 12 kmph), and two cases of truck payloads (15 and 20 tons). The next section presents the FODS-MC model results and analysis for all four scenarios. It is important to verify that the basic assumptions of the logit model are fulfilled in this numerical example. Firstly, the dependent variable, the mode choice of truck or rail between an OD, is strictly a binary (discrete) outcome. Also, the choices of mode between the OD pairs are independent of each other, and the sample size (63 OD pairs) is sufficiently large for just one independent (explanatory) variable. Another vital aspect is that there should not be any multicollinearity among the independent variables. In this numerical example, we considered only one explanatory variable (travel times as impedance). Since the distances and travel times are correlated, only one of them, preferably the better variable to include, is the travel times.

5.3. Results and analysis

The FODS-MC methodology discussed in Section 3 and the estimation procedure with the Multi-Start method explained in Section 4 were applied to the BGD case. Table 3 shows the FODS-MC model results for four scenarios of average rail speeds and truck payloads, the rail mode share, run-time, and the stopping criteria (ε), considered equal for all four model parameters β, λ, p^t, and p^r, as explained in Fig. 2. The run-time varies from 1.5 to 3 h. The gravity (β) and the mode choice (λ) model parameters have the unit of inverse of travel impedance (per hour), while empty trip parameters (p^t, and p^r) are dimensionless.

The performance of the FODS-MC model is assessed based on the values estimated for the model parameters (β, λ, p^t, and p^r) and their consistency across various scenarios. The estimated β from the FODS-MC model is in the range of 0.24–0.44 per hour, indicating that the average travel time of all the trips by rail and truck in BGD is between 2.3 and 4.2 h, which is in line with the findings from Holguín-Veras et al. (2018a,b). For example, β decreased from 0.44 to 0.25 between Scenario 1 and 2. The mode choice parameter λ indicates the marginal effect of the utility of choosing the truck or rail with respect to the impedance (travel time). λ has not changed significantly with increases in the truck payloads, i.e., between Scenarios 1 and 2 ($\sim$0.17), Scenarios 3 and 4 ($\sim$0.22). λ increased with increase in the average rail speed. The truck empty trip parameter (p^t) is nearly constant in all four scenarios, which makes sense because the parameter of the empty trip model depends on the symmetry of the commodity flow matrix (Holguín-Veras and Thorson, 2003a,b). The rail empty trip parameter (p^r) increased with an increase in the truck payload (e.g., between Scenarios 1 and 2). However, for a given truck payload, p^r showed negligible change with an increase in rail speeds (e.g., between Scenarios 1 and 3). The empty trip share for truck estimated using Equation (36) is about 32% ($p^t \sim 0.48$), which is similar to findings from the literature (González-Calderón et al., 2012). p^r varies from 0.28 to 0.50, corresponding to 22–33% of the rail trips being empty.

The performance of the FODS-MC is further investigated by comparing the observed traffic counts with the estimated values from the model. Table 4 shows the results from the OLS regression between the observed and estimated link flows, with the intercept being zero.

All coefficients of truck and rail flows are close to one (0.98 or 0.99) and significant at 1% level (t-stat greater than 2.58). The estimated truck flows have better explanatory power, with R^2 close to 0.5. The low R^2 (0.15–0.16) for estimated rail flows could be attributed to three major data-related issues: 1) unavailability of actual rail link flows; 2) the available rail OD flows are approximate values; and 3) the existence of more variance in the rail payloads, as this research considered a uniform railcar with a payload of 50 tons. Based on the results shown in Tables 3 and 4, the authors believe that Scenario 3 is the best scenario among the four scenarios. Also, a truck payload of 15 tons and a rail speed of 12 kmph is closer to the findings from the previous studies (Bangladesh Railway, 2014). Hence, the model estimated from Scenario 3 is used to illustrate some sample applications of the FODS-MC model and the traffic count sampling plan, as explained in the subsequent sections.

Table 4
FODS-MC Model Results: Observed vs. Estimated Link Flows.

Scenario	Avg. rail speed (kmph)	Truck payload (tons)	Rail payload (tons)	Actual vs. estimated flows: Truck Coeff	Truck t-stat	Truck R^2	Truck RMSE	Rail Coeff	Rail t-stat	Rail R^2	Rail RMSE	Tolerance (ε)
1	10	15	50	0.98	21.59	0.48	#####	0.98	7.41	0.15	49.04	0.5%
2		20	50	0.99	21.77	0.48	#####	0.99	7.34	0.15	49.12	1.0%
3	12	15	50	0.98	21.50	0.47	#####	0.98	7.60	0.16	48.85	0.5%
4		20	50	0.99	21.76	0.48	#####	0.99	7.54	0.16	48.91	1.0%

Table 5
FODS-MC Model Results: Rail Mode Shares.

Rail Share								
Scenario	Avg. rail speed (kmph)	Truck payload (tons)	Rail payload (tons)	tons	Tons		Ton-hours	
					Loaded Trips	Empty Capacity*	Loaded Trips	Empty Capacity*
1	10	15	50	10.39%	10.39%	6.91%	19.55%	13.47%
2		20	50	7.78%	7.78%	8.00%	13.76%	14.12%
3	12	15	50	10.93%	10.93%	6.79%	17.63%	11.27%
4		20	50	8.05%	8.05%	8.37%	12.08%	12.55%

Note: * Assuming the empty truck or railcar is loaded with their respective payloads.

5.4. Policy implications

The FODS-MC model has a huge potential in evaluating various freight policy implications to help the transportation planners (at regional or national level) achieve sustainable freight goals. A few examples are presented below based on the numerical example in Section 6.3 on BGD. For the model to produce better results, it is important to have the actual link travel times, payloads, and traffic counts (rail) for both truck and rail. Due to the above-mentioned reasons, this section is limited to presenting examples on how the FODS-MC could be used, but not to derive or compare the results with other studies (Smith and Guillossou, 2009).

Promoting Sustainable Mode Split

The FODS-MC model could assist in evaluating the effect of policy interventions targeted to promote the use of sustainable freight mode choice. For instance, Table 5 shows the rail mode shares by tons and ton-hours transported for all four scenarios. The mode choice model parameter (λ) alone does not solely reflect the total mode share of truck or rail. The aggregate mode share (in tons or ton-hours) of truck or rail depends on all model parameters (β, λ, p^t, and p^r) and the respective impedance matrices. The share in tons and ton-hours is divided into loaded trips and empty capacity. The share of loaded trips estimates the actual tons and ton-hours transported, whereas the share of empty capacity is estimated assuming the empty vehicles (trucks or railcars) are loaded to their respective payloads.

In the case of the BGD example presented, a policy supporting the increase in the weight limit of the trucks is not beneficial to increase the rail mode share. An increased payload as per Table 5, would result in a shift of freight traffic from rail to truck contributing to the higher energy consumption, emissions, and traffic congestion. Table 10 shows that the rail mode share decreases significantly with an increase in the truck payload in both tons and ton-hours. However, the share of rail empty trips decreases with an increase in truck payload. The ton-hours cannot be compared between different rail speeds, as the share is affected by the decrease in the travel times. The higher share of rail in ton-hours compared to tons may be attributed to the low rail speeds compared to truck. Though not comparable, the values in Table 5 are not far from the actual mode share (4% for rail in ton-km) provided by Smith and Guillossou (2009), which includes other modes in addition to truck and rail.

Evaluation of Infrastructure Investments

The FODS-MC model is useful in estimating the impacts of infrastructure investments such as establishing a new rail terminal at a TAZ, constructing a new rail line, bridges, mining, or manufacturing units, to name a few. An example of such could be found in Holguín-Veras et al. (2020a,b), where a single mode (truck) demand synthesis approach is used to evaluate the benefits associated with the construction of the Padma multipurpose bridge and improving the efficiency of ferry operations at multiple locations. The FODS-MC model is capable of similar analysis at a higher level, including the impact on different freight modes. For instance, Table 6 presents the Vehicle Hours Traveled (VHT) per day by loaded and empty trips for all four scenarios.

As shown in Table 6, an increase in the rail speeds (for a given truck payload) from 10 to 12 kmph reduces the VHT for both truck and rail. Hence, in case of a new rail line or renovating the existing rail infrastructure to support higher speeds, the model could estimate the total vehicle hours saved in both modes. For example, comparing Scenarios 1 and 3, the truck VHT per day decreases by 519 (189,435 VHT per year) and rail VHT reduces by 1,158 (422,670 VHT per year). Assuming a railcar is nearly three times the value of truck (based on the payloads), the total VHT savings between Scenarios 1 and 3 is about 1.5 million medium-truck VHT a year. Also,

Table 6
FODS-MC Model Results: Vehicle Hours Traveled per Day.

Scenario	Avg. rail speed (kmph)	Truck pay-load (tons)	Rail pay-load (tons)	Truck VHT				Rail VHT			
				Loaded	Empty	Total	% Empty	Loaded	Empty	Total	% Empty
1	10	15	50	88,567	43,247	1,31,814	32.81%	6,456	2,019	8,475	23.82%
2		20	50	86,119	41,638	1,27,757	32.59%	5,498	2,739	8,237	33.26%
3	12	15	50	88,659	42,636	1,31,295	32.47%	5,692	1,624	7,316	22.20%
4		20	50	86,191	41,340	1,27,531	32.42%	4,738	2,372	7,110	33.37%

increasing the truck payload from 15 to 20 tons brings considerable savings to VHT, about 1.7 million medium-truck VHT a year between Scenarios 1 and 2. This shows that policies targeted at increasing truck sizes, and road/bridge capacities to accommodate them, may improve the quality of the freight system in BGD, assuming the rail traffic counts used in this example were real.

Optimal Data Collection for Freight Planning

In addition to the policy assessment in promoting sustainable freight modes, the FODS-MC model helps in data gaps in the freight demand modeling. Since the collection process requires a significant amount of time and money, it is important to maximize the benefits associated with investments made in freight data collection. The FODS-MC procedure provides guidelines for vital issues pertaining to the freight data collection plan, such as what data to collect? (e.g., travel times, traffic counts, freight generation, freight trip generation), where to collect from? (e.g., which links the traffic counts data should be collected from to maximize the return for investments), and what should the sample size be? (e.g., collect traffic counts from 10% of the randomly selected links in national highways). The modeling procedures of such presented in this paper support a thorough experimental design for freight surveys which are crucial for countries or regions where freight data are scarce.

The numerical example explained above shows the ability of the FODS-MC methodology developed in this research to provide a reasonably good model to estimate regional freight demand (including mode choice and empty trips) and to evaluate various policy outcomes with the use of limited input data that are easier and relatively inexpensive to obtain. One of the major inputs for the above model is traffic counts from truck (v_l^{obs}) and rail (v_n^{obs}), which could be obtained from tolls, cargo invoices, and loop detectors. The next section analyzes the influence of the traffic count sample on the FODS-MC model, followed by recommendations for a traffic count data collection plan to maximize the model performance.

6. Concluding remarks

The Freight Origin-Destination Synthesis with Mode Choice (FODS-MC) model developed in this paper infers the commodity and vehicle (both loaded and empty) flows by mode between origins and destinations using secondary data in the form of traffic counts and estimates of freight generation. This feat is accomplished by the integration of multiple sub-models—commodity distribution, vehicle trip estimation (loaded and empty), and traffic assignment for both truck and rail—that represent the various freight demand processes. In doing so, the methodology described in the paper is the first reported in the literature that conducts Freight Origin-Destination Synthesis (FODS) jointly with the estimation of a freight mode choice model. A solution technique is developed to estimate the FODS-MC model, which has been tested using a quasi-real-life numerical example of developing a nationwide freight demand model for Bangladesh (BGD). The FODS methods, like the one discussed in this paper, bypass the need for expensive and time-consuming freight data collection efforts by using secondary data such as traffic counts, link costs, distances, travel times, payloads, zonal productions, and attractions as major inputs. FODS-MC models provide transportation planners and policymakers with an efficient, fast, and inexpensive way to analyze freight policy outcomes.

The FODS-MC model incorporates a doubly constrained GM with a negative exponential impedance function for the trip distribution, a binary logit model for mode choice, and the Noortman and Van Es' model for truck and rail empty trips. The solution procedure involves an iterative estimation of four model parameters—gravity model (β), mode choice model (λ), empty trip model for truck (p^t) and empty trip model for rail (p^r)—that maximizes the agreement between the estimated and observed truck and rail link flows (traffic counts). The estimated link flows are based on the All-or-Nothing (AON) assignment, which assumes that trips take the shortest path in terms of generalized cost between a given Origin-Destination (OD) pair. The model assumes an AON assignment, as the regional networks are typically simple with a limited number of paths between any given OD pair. The inclusion of the mode choice model makes the estimation of the FODS-MC model more complex, as the impedance function in the GM is dependent on the mode choice model. Also, the objective function with respect to the mode choice parameters ($F_v(\alpha,\lambda)$), minimizing the summation of squared errors between the estimated and observed traffic counts, is found to be nonconvex.

Two nonconvex solution methods (Multi-Start method and Convex + OLS) were examined in estimating the optimal λ^* (assuming $\alpha = 0$), as close as possible to the global optimal using a test network. The Multi-Start method, an interior point method with random starting points, outperformed the Convex + OLS method in estimating a reliable, faster, and better optimal solution for λ. The Multi-Start method estimates the local optimal for a set of randomly generated starting points. The higher the number of starting points, the higher the chances of achieving the global optimal. The Convex + OLS technique has two steps. The first step estimates the optimal market shares using a quadratic program. The second step finds the parameter that best fits the market shares using an Ordinary Least Squared (OLS) regression. Compared to the Multi-Start method, the Convex + OLS method had difficulties in converging when the stopping criteria for the parameter estimation was less than 5%. In addition, the Root Mean Square Errors (RMSE) between the estimated and “true” parameters and traffic counts are higher for the Convex + OLS method. The Multi-Start method also showed better consistency in the parameter estimation, with higher stopping criteria leading to an increase in the RMSEs and faster run-times. When the stopping criteria for empty trip model parameters (p^t and p^r) is increased from 4% to 5%, the run-time of the Multi-Start method drops from 282 to 45 s, and RMSE for truck and rail flows increase by 16% and 25% respectively. Hence, the Multi-Start method was chosen for the FODS-MC model estimation.

The FODS-MC model was applied in estimating a hypothetical nationwide freight demand model for BGD. The FODS-MC model parameters were estimated for four scenarios of different truck payloads and rail speeds. The model results were validated based on the consistency in the parameter estimation, findings from past studies, and their ability to estimate actual traffic counts. The estimated β is between 0.24 and 0.44, corresponding to 2.3–4.2 h of average travel times, which is found to be reasonable for BGD (Holguín-Veras et al., 2020a,b). The average travel time increases (β decreases) with an increase in the truck payload. The mode choice parameter (λ) is found to be more sensitive to rail speeds compared to truck payloads. The truck empty trip share is nearly constant, 32% ($p^t \sim 0.48$), which is close to the values estimated by Holguín-Veras and Thorson (2003a,b) for all scenarios of payloads and rail speeds.

Notwithstanding its significance, the FODS-MC model has limitations. A key limitation, especially at the national level, is the binary nature of the mode choice model. For example, in BGD, three modes (truck, rail, and inland waterways) are found to play a major role in regional freight transportation, while the current research is limited to just two modes. Besides the logit model, other choice models, e.g., a piece-wise linear form, should be tried to circumvent the issues associated with the nonconvexity of the objective function. In case of the availability of actual payload data, a weighted objective function would be appropriate, as railcars transport more cargo than trucks. The objective function could also be divided into loaded and empty flows if the traffic count data have that information. The incorporation of various industry sectors or commodity types would enhance the model’s performance considerably, as the trip distribution and mode choice were found to be highly dependent on the commodity type. Advanced modeling forms to estimate empty trips that depend on the OD pair could also be incorporated to enhance the current model’s performance. In the case of dense networks or the presence of multiple shortest paths, User Equilibrium (UE) or stochastic UE assignment models could replace the AON assignment used in this paper. Nevertheless, the current research enhances the FODS techniques and provides freight planners with a better, reliable, and faster way to analyze policies and infrastructure investments.

CRediT authorship contribution statement

Lokesh Kalahasthi: Conceptualization, Methodology, Software, Writing – original draft, Writing – review & editing. **José Holguín-Veras:** Conceptualization, Formal analysis, Writing – review & editing, Project administration, Funding acquisition, Supervision. **Wilfredo F. Yushimito:** Software, Formal analysis, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Proof for nonconvexity of F_V

This section provides a mathematical proof showing that the objective function F_v is nonconvex with respect to the mode choice parameters α, and λ (assuming c_{ij} is independent of α, and λ). To prove the nonconvexity, it is necessary to prove that the Hessian shown in Equation (43) is not positive semidefinite.

$$Hessian = \begin{bmatrix} \frac{\partial^2 F_v}{\partial \alpha^2} & \frac{\partial^2 F_v}{\partial \alpha \lambda} \\ \frac{\partial^2 F_v}{\partial \lambda \alpha} & \frac{\partial^2 F_v}{\partial \lambda^2} \end{bmatrix} \tag{43}$$

The differential of F_v with respect to either α or λ is symmetric, as both (α and λ) are exponential part of the logit model as explained in Equations (5) and (6). Also, it could be observed from Equation (43) that the Hessian is symmetric, as the first derivative of F_v is also differentiable. Hence, this section simplifies the proof by assuming $\alpha = 0$ and showing that one of the diagonals of Hessian ($\partial^2 F_v/\partial\lambda^2$) is negative. To show that a two-by-two symmetric matrix is positive semidefinite, it is sufficient to prove that one of the diagonals is negative.

The Hessian of F_v is the sum of Hessians of truck (F_{vt}) and rail (F_{vr}) components of the objective function as shown in the Equation (44).

$$\frac{\partial^2 F_v}{\partial \lambda^2} = \frac{\partial^2 F_{vt}}{\partial \lambda^2} + \frac{\partial^2 F_{vr}}{\partial \lambda^2} \tag{44}$$

Hessian of the truck component of the objective function (F_{vt})

Let the difference between the estimated and the observed link flows for given link 'l' in the road network L is U_l, defined as shown in Equation (45):

$$U_l = \left\{ \sum_{i,j} p_{ij}^l \left(\frac{q_{ij}^t m_{ij}}{a_{ij}^t} + p^t \frac{q_{ji}^t m_{ji}}{a_{ji}^t} \right) \right\} - v_l^{obs} and F_{vt} = \sum_l U_l^2 \tag{45}$$

Differentiating with respect to λ,

$$\frac{\partial F_{vt}}{\partial \lambda} = 2 \sum_l (U_l \frac{\partial U_l}{\partial \lambda}) \tag{46}$$

$$\frac{\partial^2 F_{vt}}{\partial \lambda^2} = 2 \sum_l \{ \left(\frac{\partial U_l}{\partial \lambda} \right)^2 + U_l \frac{\partial^2 U_l}{\partial \lambda^2} \} \tag{47}$$

Equation (45) could be solved by using the chain rule, a sequential substitution of Equations (48) to (53) into Equation (47)

$$let\, E_{ij} = e^{\lambda \left(c_{ij}^t - c_{ij}^r \right)} \forall ij \, then\, q_{ij}^t = \frac{1}{1 + E_{ij}} \forall ij \tag{48}$$

$$\frac{\partial E_{ij}}{\partial \lambda} = (c_{ij}^t - c_{ij}^r) E_{ij} \forall ij \, and \, \frac{\partial^2 E_{ij}}{\partial \lambda^2} = (c_{ij}^t - c_{ij}^r)^2 E_{ij} \forall ij \tag{49}$$

$$\frac{\partial q_{ij}^t}{\partial \lambda} = \frac{-1}{(1 + E_{ij})^2} \frac{\partial E_{ij}}{\partial \lambda} = - \left(q_{ij}^t \right)^2 \frac{\partial E_{ij}}{\partial \lambda} \forall ij \tag{50}$$

$$\frac{\partial^2 q_{ij}^t}{\partial \lambda^2} = (q_{ij}^t)^2 \{ 2 q_{ij}^t \left(\frac{\partial E_{ij}}{\partial \lambda} \right)^2 - \frac{\partial^2 E_{ij}}{\partial \lambda^2} \} \forall ij \tag{51}$$

$$\frac{\partial U_l}{\partial \lambda} = \sum_{i,j} p_{ij}^l (\frac{m_{ij}}{a_{ij}^t} \frac{\partial q_{ij}^t}{\partial \lambda} + \frac{p^t m_{ji}}{a_{ji}^t} \frac{\partial q_{ji}^t}{\partial \lambda}) \forall l \tag{52}$$

$$\frac{\partial^2 U_l}{\partial \lambda^2} = \sum_{i,j} p_{ij}^l (\frac{m_{ij}}{a_{ij}^t} \frac{\partial^2 q_{ij}^t}{\partial \lambda^2} + \frac{p^t m_{ji}}{a_{ji}^t} \frac{\partial^2 q_{ji}^t}{\partial \lambda^2}) \forall l \tag{53}$$

Similarly, the Hessian of rail component F_{vr} could be obtained by defining the difference between the estimated and observed link flows for given link 'n' in the rail network N (V_n), as shown in Equation (54):

$$V_n = \{ \sum_{i,j} p_{ij}^n (\frac{q_{ij}^r m_{ij}}{a_{ij}^r} + p^r \frac{q_{ji}^r m_{ji}}{a_{ji}^r}) \} - v_n^{obs} \forall n \tag{54}$$

Hessian of the rail component of the objective function (F_{vr})

$$\frac{\partial^2 F_{vr}}{\partial \lambda^2} = 2 \sum_n \{ \left(\frac{\partial V_n}{\partial \lambda} \right)^2 + V_n \frac{\partial^2 V_n}{\partial \lambda^2} \} \tag{55}$$

Equation (54) could be solved by using the chain rule from a sequential substitution of Equations (56) to (61) into Equation (55) Let

$$F_{ij} = e^{\lambda \left(c_{ij}^r - c_{ij}^t \right)} \forall ij \, then\, q_{ij}^r = \frac{1}{1 + F_{ij}} \forall ij \tag{56}$$

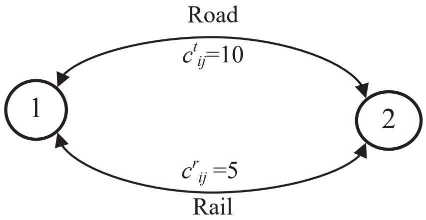

Fig. 6. Nonconvexity of F_v: Sample network.

Table 7
Nonconvexity of F_v: Sample Network Parameters.

OD/Link	Payload (tons)				Observed link flows				OD impedance				Trips (tons)	
	Truck (a^t)		Rail (a^r)		Truck (v_l^{obs})		Rail (v_m^{obs})		Truck (c^t)		Rail (c^r)		m_{ij}	
	1	2	1	2	1	2	1	2	1	2	1	2	1	2
1	1	1	3	3	0	100	0	20	Inf	10	Inf	5	0	200
2	1	1	3	3	100	0	20	0	10	Inf	5	Inf	200	0
Empty trip parameters: $p^t = 0.35$, $p^r = 0.45$														

Note: Inf = Infinite.

$$\frac{\partial F_{ij}}{\partial \lambda} = (c^r_{ij} - c^t_{ij})F_{ij}\forall ij \text{ and } \frac{\partial^2 F_{ij}}{\partial \lambda^2} = (c^r_{ij} - c^t_{ij})^2 F_{ij}\forall ij \tag{57}$$

$$\frac{\partial q^r_{ij}}{\partial \lambda} = -(q^r_{ij})^2 \frac{\partial F_{ij}}{\partial \lambda}\forall ij \tag{58}$$

$$\frac{\partial^2 q^r_{ij}}{\partial \lambda^2} = (q^r_{ij})^2 \{2q^r_{ij}\left(\frac{\partial F_{ij}}{\partial \lambda}\right)^2 - \frac{\partial^2 F_{ij}}{\partial \lambda^2}\}\forall ij \tag{59}$$

$$\frac{\partial V_n}{\partial \lambda} = \sum_{i,j} p^n_{ij}\left(\frac{m_{ij}}{a^r_{ij}}\frac{\partial q^r_{ij}}{\partial \lambda} + \frac{p^r m_{ji}}{a^r_{ji}}\frac{\partial q^r_{ji}}{\partial \lambda}\right)\forall n \tag{60}$$

$$\frac{\partial^2 V_n}{\partial \lambda^2} = \sum_{i,j} p^n_{ij}\left(\frac{m_{ij}}{a^r_{ij}}\frac{\partial^2 q^r_{ij}}{\partial \lambda^2} + \frac{p^r m_{ji}}{a^r_{ji}}\frac{\partial^2 q^r_{ji}}{\partial \lambda^2}\right)\forall n \tag{61}$$

The Hessian shown in Equation (43) could be estimated sequentially using Equations (44)–(61). However, it is not straightforward to prove that the objective function (F_v) is nonconvex because the Hessian is positive for some values of λ, i.e., the function F_v is not globally convex. But for some values of λ, the function becomes nonconvex, which prevents the model from achieving global optimal. Hence, the nonconvexity should be proved using a small test case network (see Fig. 6) where it is necessary and sufficient to show that the Hessian becomes negative definite for some value of λ for the test case example.

Therefore, to prove the nonconvexity, a network with two nodes and four links is considered (see Fig. 6). The nonconvexity of the objective function (F_v) could be proved by showing that the Hessian is negative for desirable values of λ ($\geq$0) for this network with two zones (nodes 1 and 2) connected by a two-way truck and rail link each, as shown in Fig. 6.

The parameters such as payloads, observed link flows, impedances, and distribution matrix are shown in Table 7. Internal flows are ignored in the trip distribution matrix, i.e., m_{11} and m_{22} both equal to zero. The link cost is assumed to be the same in both directions, i.e., $c_{12} = c_{21}$ for both rail and truck. The payload of truck and railcar is 1 and 3 tons, respectively. The observed traffic in both directions is 100 trucks and 20 railcars. The empty trip parameter for truck (p^t) is 0.35 and (p^r) 0.45 for rail.

Table 8 shows estimation of the Hessian of F_v following the process described in Equations (44)–(61), for two cases. For $\lambda = 0.3$ (case 1), the Hessian of F_v is negative (-898.84), which shows that the objective function F_v is concave. For $\lambda = 0.2$ (case 2), the Hessian of F_v is positive (206,242.28), which shows that the objective function F_v is convex. Since the Hessian is negative for some values of λ, the function F_v is not globally convex. Hence, this proves that F_v as a function of λ (assuming c_{ij} is independent of α, and λ) is nonconvex. Therefore, the Hessian in Equation (43) is not positive semidefinite, and F_v is nonconvex.

Table 8
Nonconvexity of F_v: Results.

Case 1: λ=0.3

Hessian of truck flows F_{vt}

OD/Link	E		q^t		$dE/d\lambda$		$d^2E/d\lambda^2$		$dq^t/d\lambda$		$d^2q^t/d\lambda^2$		U_l		$dU_l/d\lambda$		$d^2U_l/d\lambda^2$			β	*0.1*
	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2		λ	0.3
1	1.0	4.5	0.5	0.2	0.0	22.4	0.0	112.0	0.0	−0.7	0.0	2.4	0	−51	0	−201	0	639		p^t	0.35
2	4.5	1.0	0.2	0.5	22.4	0.0	112.0	0.0	−0.7	0.0	2.4	0.0	−51	0	−201	0	639	0		p^r	0.45

32372.04

Hessian of rail flows F_{vr}

OD/Link	F		q^r		$dF/d\lambda$		$d^2F/d\lambda^2$		$dq^r/d\lambda$		$d^2q^r/d\lambda^2$		V_n		$dV_n/d\lambda$		$d^2V_n/d\lambda^2$			β	*0.1*
	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2		λ	0.3
1	1.0	0.2	0.5	0.8	0.0	−1.1	0.0	5.6	0.0	0.7	0.0	−2.4	0	59	0	72	0	−229		p^t	0.35
2	0.2	1.0	0.8	0.5	−1.1	0.0	5.6	0.0	0.7	0.0	−2.4	0.0	59	0	72	0	−229	0		p^r	0.45

−33270.88

Hessian of F_v

Case 2: $\lambda = 0.2$

Hessian of truck flows F_{vt}

OD/Link	E		q^t		$dE/d\lambda$		$d^2E/d\lambda^2$		$dq^t/d\lambda$		$d^2q^t/d\lambda^2$		U_l		$dU_l/d\lambda$		$d^2U_l/d\lambda^2$			β	*0.1*
	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2		λ	0.2
1	1.0	2.7	0.5	0.3	0.0	13.6	0.0	68.0	0.0	−1.0	0.0	2.3	0	−27	0	−265	0	613		p^t	0.35
2	2.7	1.0	0.3	0.5	13.6	0.0	68.0	0.0	−1.0	0.0	2.3	0.0	−27	0	−265	0	613	0		p^r	0.45

214622.31

Hessian of rail flows F_{vr}

OD/Link	F	q^r	$dF/d\lambda$	$d^2F/d\lambda^2$	$dq^r/d\lambda$	$d^2q^r/d\lambda^2$	V_n	$dV_n/d\lambda$	$d^2V_n/d\lambda^2$		β	*0.1*	OD/Link	F	q^r	$dF/d\lambda$	$d^2F/d\lambda^2$	$dq^r/d\lambda$	$d^2q^r/d\lambda^2$	V_n	$dV_n/d\lambda$
	1	2	1	2	1	2	1	2	1	2	1	2		1	2	1	2	1	2	1	2
1	1.0	0.4	0.5	0.7	0.0	−1.8	0.0	9.2	0.0	1.0	0.0	−2.3	0	51	0	95	0	−220		p^t	0.35
2	0.4	1.0	0.7	0.5	−1.8	0.0	9.2	0.0	1.0	0.0	−2.3	0.0	51	0	95	0	−220	0		p^r	0.45

−8380.03

Hessian of F_v **206242.28**

Appendix B. Evaluation of nonconvex solution methods

By design, the test cases are simplified versions of what may be expected in real-life conditions. To reduce the number of influencing factors, a simplified mode choice model without a constant term (α) is assumed without the loss of generality. This section focuses on assessing the performance of the FODS-MC model and the nonconvex optimization methods (Multi-Start and Convex + OLS) using a small test case. More specifically the tests assess how well these alternative procedures retrieve the known "true" FODS-MC model parameters (β, λ, p^t, *and* p^r) for a hypothetical network with five nodes and 14 links each for truck and rail (see Fig. 7). The figure also shows the link flows for both truck and rail. Both methods are implemented on Knitro solver version 10.3 from Artleys, interfacing with MATLAB R2018b (Artelys, 2017), on a computer with 64 GB memory and an Intel Xeon E3-1240 v5 3.5 GHz processor.

The nodes in Fig. 7 represent the centroids of a zone. The zonal productions (O_i) and attractions (D_j) in multiples of 10 tons per day are shown in Table 9, where the sum of productions is equal to the sum of attractions for all five zones.

Table 10 shows the link impedances from which the impedance matrix for the gravity model (c_{ij}), and the shortest path matrix (p_{ij}) for the AON assignment model for truck and rail, are estimated. The payloads for truck (a^t_{ij}) and rail (a^r_{ij}) are assumed as 10 tons and 30 tons, respectively. The link flows for all 14 links of truck (v_l) and rail (v_n) shown in Table 10 are estimated from Equations (1) to (14), assuming the "true" FODS-MC model parameters as $\beta = 0.1$, $\lambda = 0.2$, $p^t = 0.4$, *and* $p^r = 0.6$.

The FODS-MC model is calibrated by Multi-Start and Convex + OLS methods, using the link flows shown in Table 10 as the observed flows (v_l^{obs} and v_n^{obs}) in the objective function F_v given in Equation (15). Table 11 shows the results obtained for seven different scenarios of stopping criteria (ε) for convergence in the parameter estimation explained in Fig. 2, along with the respective

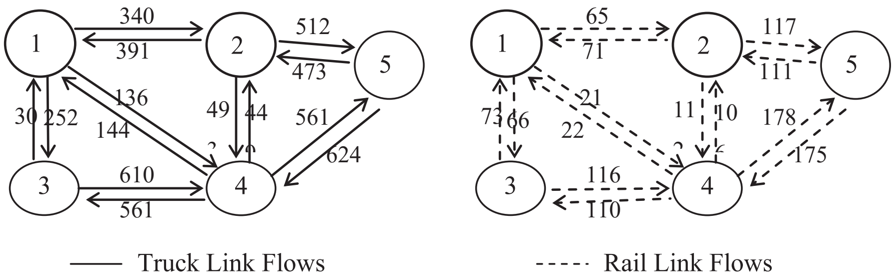

Fig. 7. Test Case: Truck and Rail Network Flows.

Table 9
Test Case: Freight Generation.

Zone	Cargo Flow (10 tons/day)	
	Production (O_i)	Attraction (D_j)
1	720	999
2	1,395	1,035
3	1,080	828
4	1,296	1,458
5	1,269	1,440
Total	**5,760**	**5,760**

Table 10
Test Case: Impedance and Observed Flows.

Link Truck/Rail	Origin node	Destination node	Impedance		Obs. Flows (per day)	
			Truck	Rail	Truck (v_l)	Rail (v_n)
1	1	2	10	13	340	65
2	1	3	7	9.1	252	66
3	1	4	15	19.5	136	21
4	2	1	10	13	391	71
5	2	4	6	7.8	493	112
6	2	5	6	7.8	512	117
7	3	1	7	9.1	301	73
8	3	4	9	11.7	610	116
9	4	1	15	19.5	144	22
10	4	2	6	7.8	449	106
11	4	3	9	11.7	561	110
12	4	5	3	3.9	650	178
13	5	2	6	7.8	473	111
14	5	4	3	3.9	624	175

Table 11
Test case: FODS-MC Results by Multi-Start and Convex + OLS Methods.

Scenario	Parameters	Stopping Criteria			Gravity model (β)	Mode choice (λ)	Truck empty trip (p^t)	Rail empty trip (p^r)	RMSE		Run time (s)
		Gravity model (ε_β)	Mode choice (ε_λ)	Empty trip ($\varepsilon_{pt}/\varepsilon_{pr}$)					Truck flows	Rail flows	
Test Case	True Values	NA			0.10	0.20	0.40	0.60	0.00	0.00	
1	Convex + OLS	1%	5%	2%	Did not converge						
	Multi-Start			2%	0.08	0.20	0.38	0.58	27.20	19.18	335.95
2	Convex + OLS	1%	5%	3%	Did not converge						
	Multi-Start	1%	5%	3%	0.07	0.20	0.35	0.61	28.12	21.34	287.97
3	Convex + OLS	1%	5%	4%	Did not converge						
	Multi-Start	1%	5%	4%	0.07	0.21	0.34	0.61	29.72	21.91	282.78
4	Convex + OLS	5%	5%	5%	2.62	2.72	0.20	0.90	62.81	33.65	162.94
	Multi-Start	5%	5%	5%	0.14	0.31	0.33	0.83	34.54	27.82	45.81
5	Convex + OLS	7%	7%	7%	2.72	2.67	0.20	0.90	60.68	32.18	164.85
	Multi-Start	7%	7%	7%	0.14	0.31	0.33	0.83	34.54	27.82	46.02
6	Convex + OLS	10%	10%	10%	0.14	0.46	0.21	0.90	37.92	29.03	50.69
	Multi-Start	10%	10%	10%	0.14	0.31	0.33	0.83	34.54	27.82	43.50
7	Convex + OLS	20%	20%	20%	0.21	1.58	0.20	0.90	42.82	31.39	47.27
	Multi-Start	20%	20%	20%	0.14	0.31	0.33	0.83	34.54	27.82	46.32

Note: Run-time shown is in seconds (s).

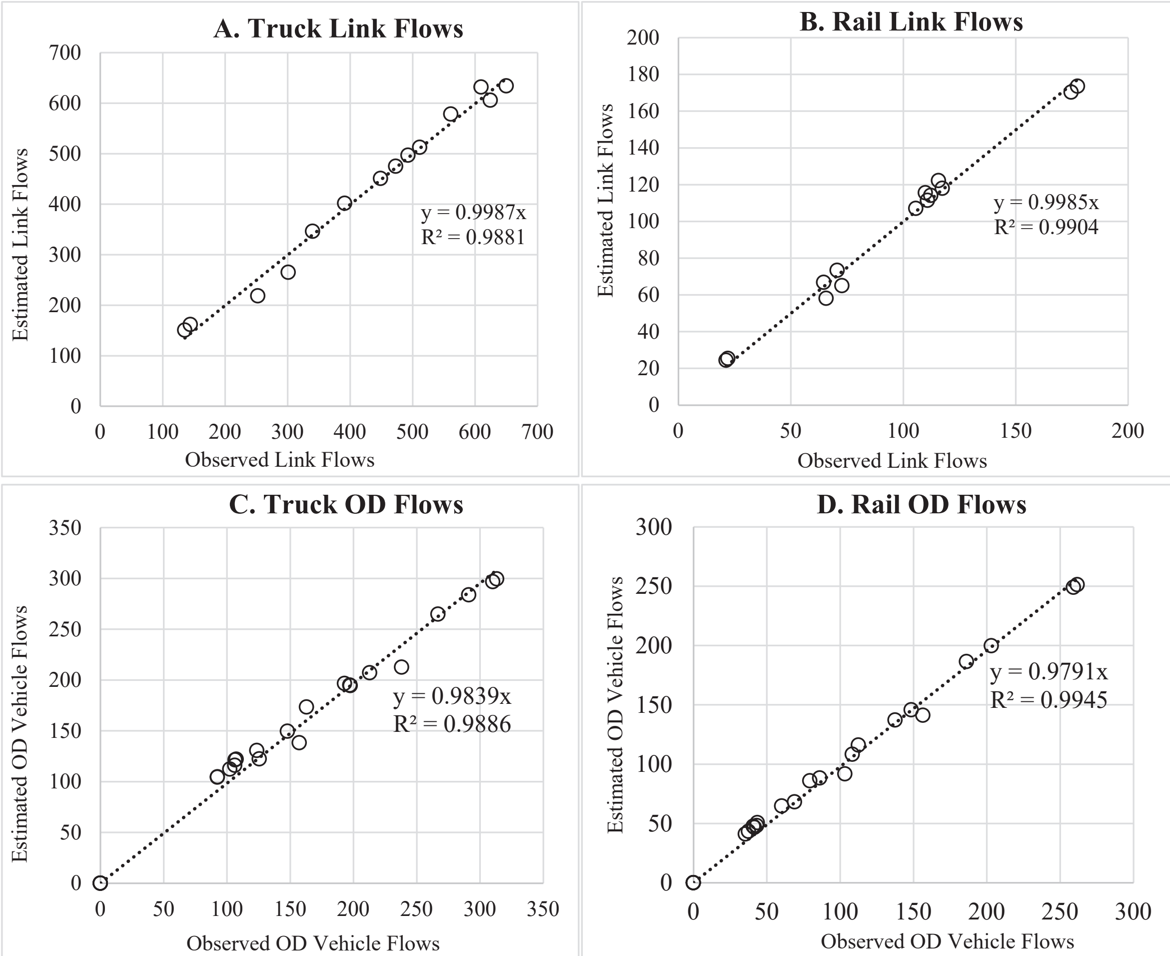

Fig. 8. Observed vs. Estimated Flows (Scenario 1, Multi-Start Method in Table 11).

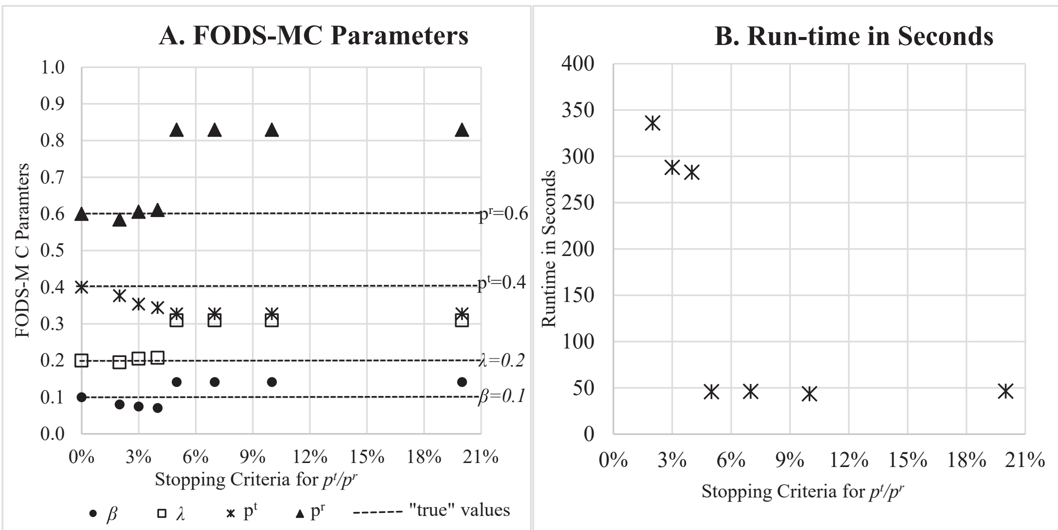

Fig. 9. Multi-Start Method Performance and Run-time (Scenario 1, Multi-Start Method in Table 11).

run-time in seconds. The same stopping criteria are selected for the convergence of truck (ε_{pt}) and rail (ε_{pr}) empty trip parameters. The number of random starting points in the Multi-Start algorithm is fixed to 15. The performance of each method is assessed based on four different criteria: (1) agreement between the "true" and the estimated parameters, (2) reliability of the stopping criteria (ε), (3) run-time (s), and (4) consistency in the accuracy of parameter estimation. An efficient solution process must be able to retrieve the parameters as close as possible to the "true" values, with stopping criteria reliable to achieve the converge of the iterations and in the minimum run-time.

Table 11 also shows the Root Mean Squared Errors (RMSE) between the estimated and "true" values of truck and rail traffic counts. Overall, the Multi-Start method provides the estimates closest to the "true" parameter values, though it converges at lower stopping criteria in Scenarios 1 to 3. With respect to the run-time, the Multi-Start method is much faster compared to that of the Convex + OLS method. The Multi-Start method with the best solution (Scenario 1) required nearly six minutes to converge. The run-time of the Multi-Start method does not decrease monotonously with increases in the stopping criteria, as the convergence depends on the probability of the randomly generated starting points falling in the optimal region. In the case of Convex + OLS, the run-time consistently decreases with increases in the stopping criteria. The Multi-Start method performs better with respect to consistency in the parameter estimation as well. The quality of parameter results from the Multi-Start method improves with decrease in the stopping criteria, while that of the Convex + OLS method is inconsistent. For example, Scenario 6 in the Convex + OLS method produced better estimates than Scenario 4 and Scenario 5. In addition, the performance of the Multi-Start method in the most stringent scenario (1) is shown in Fig. 8 below. It is important to compare the estimated link flows (Fig. 8A and 8B) and OD Table (Fig. 8C and 8D) with that of observed values, as the trip distribution is more sensitive to the FODS-MC model parameter values. In the test case, the observed OD Table is available, whereas the link flows are the only inputs available to validate the model in the real-life scenario. In Fig. 8, the slope (intercept) of the linear regression and R^2 are close to one for both OD Table and the link flows, showing a better goodness of fit. Hence, the Multi-Start method is found to be efficient, faster, and more reliable in estimating the mode choice parameter (λ).

Fig. 9 shows the effects of the stopping criteria for empty trip model parameters on the quality of parameter estimates (Fig. 9A) and the run-time (Fig. 9B) for the Multi-Start method in Scenario 1. As expected, the estimation error (difference between the estimated and the "true" values) for the parameters are increasing with increase in the stopping criteria. Also, the run-time surges drastically from 45 s to 280 s when the stopping criteria change from 4% to 5%. However, compared to the reduction in the estimation errors from stopping criteria 5% to 4% (by 38% for p^r, see Fig. 9A), the increase in the run-time is reasonable (see Fig. 9B). The run-time depends on the stopping criteria of the parameter estimation (ε), number of links for which the observed flows (v^{obs}) are available, and the number of random starting points used in the Multi-Start method and the size of the network. An appropriate stopping criterion for each parameter is required to estimate the FODS-MC model in an appropriate duration without compromising the quality of the results. In all cases, the Multi-Start method should be complemented with a process to validate the FODS-MC parameters estimated from this model. In case the estimated FODS-MC parameters do not pass the validation, the program should be re-run, adding new constraints to eliminate the previous optimal solutions.

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