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# Measuring Emissions in Vehicle Routing: New Emission Estimation Models Using Supervised Learning

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**Abstract.** In this paper we propose and assess the accuracy of new emission models for vehicle routing. Based on real-world data of instantaneous fuel consumption, time-varying speeds observations, and traffic data related to a large set of shipping operations we propose effective methods to estimate greenhouse gas (GHG) emissions. By carrying out nonlinear regression analysis using supervised learning methods, namely Neural Networks, Support Vector Machines, Conditional Inference Trees, and Gradient Boosting Machines, we develop new emission models that provide more prediction accuracy than classical models. We correctly estimate emissions for time-dependent point-to-point routing under realistic conditions taking into account freight transportation operations during peak hour traffic congestion, stop and go driving patterns, idle vehicle states, and the variation of vehicle loads. Extensive computational experiments under real datasets show the effectiveness of the proposed machine learning emissions models, clearly outperforming the Comprehensive Modal Emissions Model (CMEM) and the Methodology for Estimating air pollutant Emissions from Transport (MEET) in the prediction of hot running traffic emissions according to root mean square error metrics. Based on performance indicators we show that MEET underestimates real-world GHG emissions by 24.94% and CMEM leads to an overestimation of emissions by 13.18% according to observed fuel consumption, while our best machine learning model (Gradient Boosting Machines) exhibited superior estimation accuracy and is off by only 1.70% considering real-world driving conditions. Statistical tests confirm the efficiency of our new models.

**Keywords.** Emissions models, time-dependent routing, traffic congestion, machine learning.

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# 1 Introduction

Freight transportation is known to be an important source of greenhouse gas (GHG) emissions [33]. GHG emissions are proportional to the fuel consumption which in turn, depends on several factors including speed, acceleration, distance, weight of the vehicle, backhauls and roadway slope [10].

Accurate emissions estimation is a valuable information for transportation experts in making effective decisions that improve routing operations. The current literature on GHG emissions for road freight transportation offers different models for estimating emission and fuel consumption, the more well-known being the Comprehensive Modal Emissions Model (CMEM) [2] and the Methodology for Estimating air pollutant Emissions from Transport (MEET) [20]. Over the last few years, CMEM and MEET have been integrated into various routing models, with a focus on environmental impacts in addition to economic implications.

The CMEM is designed for heavy duty vehicles. It computes GHG emissions of route plans considering the traveled distance, vehicle speed, carried load and roadway gradient. Relevant studies on green vehicle routing calculating the amount of GHG emissions following CMEM are those of Bektaş and Laporte [4], Demir et al. [9], and Franceschetti et al. [15] in which the objective is to minimize a function comprising emissions and driver costs. Pathak et al. [28] used CMEM to estimate emissions under real-world driving patterns. Androutsopoulos and Zografos [1] and Huang et al. [22] integrated path selection decision on the vehicle routing problems considering a multigraph representation [17, 31] for the road network that incorporates the set of candidates paths between all pairs of key-destinations. Figliozzi [14], Jabali et al. [23], Qian and Eglese [29], and Ehmke et al. [13] derived emissions from the MEET model, which allows the conversion of speeds into emissions based on fuel consumption rates that have been derived from engine test-bed measurements. MEET considers the impact of load and roadway gradient through error-corrective parameters.

Real-time traffic congestion, the behavior of freight vehicles across road networks, timely fuel consumption data collected by various sensors, and Global Positioning System (GPS) devices are becoming more present in commercial operations [19]. With such rich amount of traffic-related data much attention is now accorded to the computation of emission-minimizing paths on very large road networks based on time-dependent speed observations provided by logistics companies using Intelligent Transportation System (ITS) technology [5]. However, different emission estimation models exist and they are based on very distinct assumptions and yield contrasting results. Making an accurate prediction of

fuel consumption and emissions is an important aspect of a firm's decision-making process as realized emissions and fuel price affects the profitability [11].

Demir et al. [8] elaborated a comparative analysis of several vehicle emission models that have been developed to compute GHG emissions associated with road freight transportation. Emission models vary in their performance according to numerous factors such as speed, acceleration, and vehicle types. Turkensteen [34] evaluated the accuracy of CMEM, indicating that we cannot take for granted that fuel consumption computations assuming fixed speed are accurate in time-dependent routing. The author observed that fixed average speed computations are likely to underestimate emissions. Through sensitivity analysis he showed that much emissions is produced when speed fluctuates and vehicle load increases.

Jaikumar et al. [24] performed a modal analysis of vehicular emissions under real-world driving conditions. They found out that short term events such as acceleration and braking significantly affect emissions. Despite their findings that CMEM underestimates emissions they have only used average speed and acceleration for distances ranging from 1 to 10 *km* based on field data obtained from an on-board diagnostic tool.

It follows from previous studies that approaches based on aggregated speeds can underestimate GHG emissions. Greater estimation accuracy relies on data that reflects real-world operations in road networks. The last decade has seen substantial advances in building prediction models using machine learning methods, which capture complex nonlinear relationships in the systems under study and produce accurate estimations by learning from the available data [6, 26]. There have been a few studies on the application of machine learning methods for establishing practical emission models that can be used in routing problems with both environmental and operational considerations. Inspired by the need of emissions prediction Zeng et al. [36] proposed a new emission model derived from the theory of vehicle dynamics. The parameters of their model were computed with the maximum likelihood estimation (MLE), and its accuracy was validated using GPS data collected for a light duty passenger car through a comparative analysis with the Virginia Tech Microscopic Energy and Emission Model (VT-Micro) [30], Support Vector Machines (SVM) model and Neural Networks (NNET) model. Liu et al. [27] proposed an effective emissions prediction model of a diesel engine using SVM that can be used by diesel engine manufacturers to accurately measure emissions. Due the growing interest of accurate emissions estimations in road freight transportation field, the current study follows previous streams of literature by applying Gradient Boosting Machines (GBM) method in addition to NNET,

SVM and Conditional Inference Trees (CIT) machine learning methods to predict emissions considering relevant variables derived from in-field emissions data considering real-world driving conditions.

From a machine learning point of view a number of opportunities may exist with the availability of time-varying speeds observations, instantaneous fuel consumption, roadway gradient, vehicle load, and stop-and-go traffic data related to vehicle trips of logistics and freight companies across large cities. GPS and on-board real-time emission measurement devices provide real-world observations of emissions of micro scale events under real-world traffic congestion. In this work, we used field data collected across the entire road network of Québec City, which contains up to 50,000 road links. The obtained GPS dataset contains 58,215 instantaneous fuel consumption and speed observations for 1406 deliveries monitored over 97 days between November 2016 and March 2017. In terms of prediction accuracy, families of supervised learning algorithms are shown to be effective in fitting artificial outputs to the real one. Therefore, using supervised learning methods we build nonlinear emission models considering time-varying speeds, vehicle load fluctuations, stop-and-go driving patterns, acceleration, and breaking events. The contributions of this paper are fourfold:

- (i) we propose an effective approach for the computation of GHG emissions in routing considering time-varying speeds;
- (ii) we provide several insights concerning fuel consumption through the analysis of real-world emission data considering shipping operations under a large road network with fluctuating traffic congestion and stop-and-go driving patterns;
- (iii) we develop efficient nonlinear emission models using NNET, SVM, CIT, and GBM supervised learning methods, which are trained by applying the  $k$ -fold cross validation method on real-life GHG emission data acquired by a private-sector retailer from thousands of trips over the course of several months;
- (iv) we demonstrate the effectiveness of the proposed supervised learning models at micro scale events compared to MEET and CMEM that incorrectly predicted emissions under realistic driving conditions.

The remainder of this paper is organized as follows. In the following section we review the literature on emissions models for road freight transportation. Section 3 describes the data collection procedure and provides some initial analysis of the available data. In Section 4 we describe the proposed approach

for modeling GHG emissions using supervised learning methods. In Section 5, we present results of our extensive computational experimentation and sensitivity analysis of several existing and newly introduced emissions models. Conclusions and directions for future research are stated in Section 6.

## 2 Existing emission estimation models

Motivated by the need to account for traffic congestion effects considering variable speeds, this section describes the existing methods to compute emissions in time-dependent networks (multigraphs) using CMEM and MEET. To do so, let  $\mathcal{G}^T = (\mathcal{V}, \mathcal{A}, \mathcal{Z})$  be a multigraph, where  $\mathcal{V}$  is the set of nodes of the road network and  $\mathcal{A}$  is the set of arcs or road segments connecting some pairs of nodes in the network (see Figure 1). Let  $\mathcal{T} = z_0 + \mathcal{H}\delta$  be the length of the planning horizon, where  $\delta > 0$  represents the smallest increment of time over which a change in the speed happens.  $\mathcal{T}$  is divided into a finite number  $\mathcal{H}$  time intervals  $Z_h = [z_0 + \delta(h-1), z_0 + \delta h[$  considering the set  $\mathcal{Z} = \{z_0, z_0 + \delta, \dots, z_0 + \mathcal{H}\delta\}$  of discrete times, with  $h = 1, 2, \dots, \mathcal{H}$ .

Furthermore, let  $\gamma_u(t)$  be a function that provides the arrival time at node  $u$  given a starting time  $t$  at the source. Any path  $p$  from an origin  $o$  to a destination  $d$  follows an ordered sequence of nodes on the road network and is defined by the schedule of traversing it as:

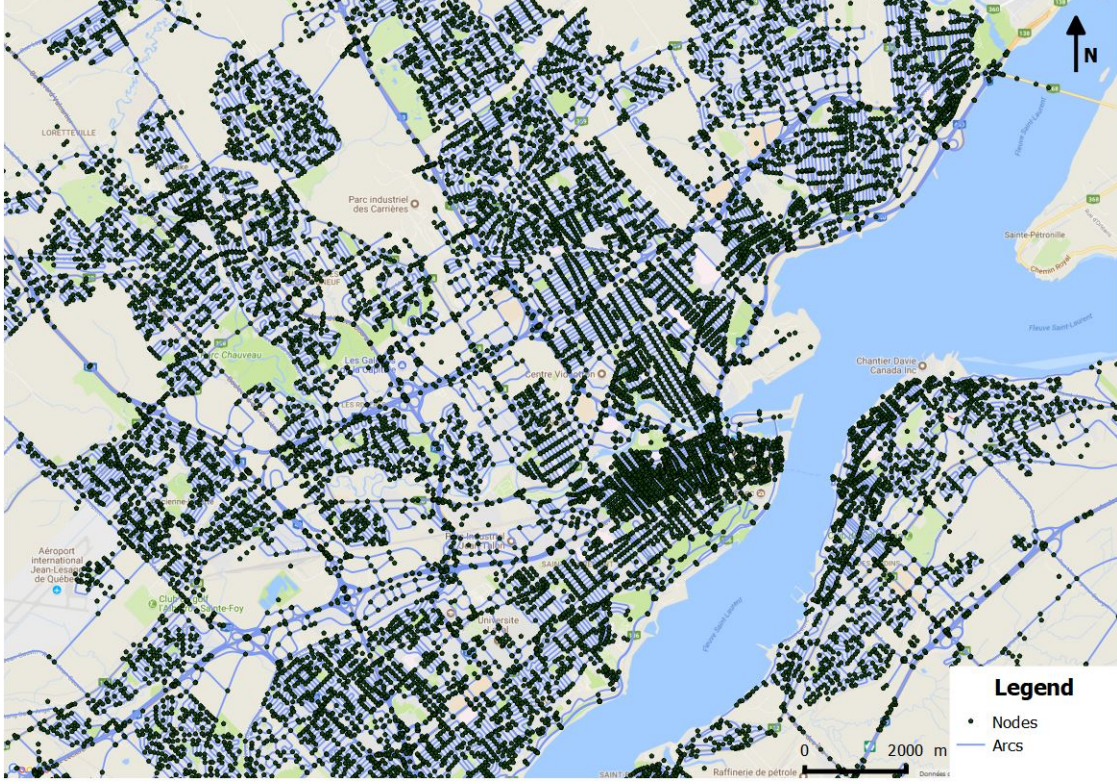
$$p_{od} = (\gamma_o(t), [o = v_0, v_1, \dots, v_{k-1}, v_k = d]) \quad (1)$$

where  $v_k \in \mathcal{V}$  are road nodes, and  $k$  represents the number of nodes of the complete path.

For any road segment  $(u, v) \in \mathcal{A}$  let  $l_{uv}$  denote the distance between nodes  $u$  and  $v$ . Let  $\tau_{uv}(t)$  and  $\mathcal{F}_{uv}(t)$  be the time-dependent travel time and the amount of GHG emissions, respectively, related to traveling across the road segment  $(u, v)$  when the vehicle leaves node  $u$  at time  $t \in \mathcal{T}$ . The travel time function is piecewise linear and satisfies the first-in, first-out (FIFO) rule. With each road segment  $(u, v)$  across a given path is associated a time-dependent travel speed  $s_{uv}(\gamma_u(t))$  at departure time  $t \in Z_h$ .

### 2.1 Time-dependent emission function using CMEM

The CMEM is one of the most used emission models in green vehicle routing. It was designed by Barth and Boriboonsomsin [2] to estimate the amount of emissions generated by a wide variety of vehicles. According to this model, vehicle emissions depend on many environmental and traffic-related



**Figure 1:** Illustration of a portion of the road network in Québec City

parameters, namely load, speed, roadway gradient, among others. Considering vehicle speed  $s$  ( $m/s$ ), total vehicle weight  $\mathcal{M}$  and roadway gradient  $\theta$ , CMEM calculates the instantaneous fuel consumption rate (in liters/second) using the following polynomial function:

$$e_r = \mathcal{E}_0 \left( \mathcal{E}_1 + \left( \frac{(\alpha \mathcal{M} + \beta s^2)s}{\mathcal{E}_2} + \mathcal{P}_{acc} \right) \right), \quad (2)$$

where  $\mathcal{E}_0 = \frac{\zeta}{\omega \psi}$ ,  $\mathcal{E}_1 = k N_e V$ ,  $\mathcal{E}_2 = \frac{1}{\varepsilon 1000 \eta_{tf}}$ ,  $\mathcal{M} = \omega + q$ ,  $\alpha = a + g \sin \theta + g C_r \cos \theta$ , and  $\beta = 0.5 C_d A \rho$  are constant parameters related to the vehicle and its engine such as inertia force, rolling resistance, and other vehicle characteristics.  $\mathcal{P}_{acc}$  is the engine power demand associated with running losses of the engine and additional vehicle accessories such as air conditioning, typically assumed to be zero. All parameter values used are shown in Table 1.

For a given path  $p$  traversed by a vehicle departing from node  $v_i$  at time  $t$ , the corresponding fuel consumption (in liters) can be computed based on equation (3):

**Table 1:** Parameters used by CMEM for the computation of fuel consumption

| Notation    | Description                                          | Typical values |
|-------------|------------------------------------------------------|----------------|
| $w$         | Curb-weight ( $kg$ )                                 | 4500           |
| $q$         | Carried load ( $kg$ )                                | 0-4350         |
| $\zeta$     | Fuel-to-air mass ratio                               | 1              |
| $k$         | Engine friction factor ( $kJ/rev/liter$ )            | 0.25           |
| $N_e$       | Engine speed ( $rev/s$ )                             | 40             |
| $V$         | Engine displacement ( $liter$ )                      | 5.12           |
| $g$         | Gravitational constant ( $m/s^2$ )                   | 9.81           |
| $\rho$      | Air density ( $kg/m^3$ )                             | 1.2041         |
| $C_d$       | Coefficient of aerodynamic drag                      | 0.7            |
| $A$         | Frontal surface area ( $m^2$ )                       | 4.6            |
| $C_r$       | Coefficient of rolling resistance                    | 0.01           |
| $\eta_{tf}$ | Vehicle drive train efficiency                       | 0.4            |
| $\eta$      | Efficiency parameter for diesel engines              | 0.9            |
| $c_f$       | Fuel and GHG emissions cost per liter ( $\$/liter$ ) | 1.05           |
| $c_d$       | Driver wage ( $\$/s$ )                               | 0.0085         |
| $\varpi$    | Heating value of a typical diesel fuel ( $kJ/g$ )    | 44             |
| $\psi$      | Conversion factor ( $g/s$ to $liter/s$ )             | 737            |
| $s^l$       | Lower speed limit ( $m/s$ )                          | 5.555          |
| $s^u$       | Upper speed limit ( $m/s$ )                          | 22.222         |
| $s$         | Average speed at a portion of segment ( $m/s$ )      |                |
| $a$         | Acceleration ( $m/s^3$ )                             | $[-3, 1]$      |
| $\theta$    | Roadway gradient (degree)                            | 0              |

$$\mathcal{F}_{p_{ij}}(t) = \sum_{(u,v) \in p} \mathcal{F}_{uv}^1(t) + \mathcal{F}_{uv}^2(t). \quad (3)$$

The term  $\mathcal{F}^1$  describes the emissions related to the vehicle weight and  $\mathcal{F}^2$  represents the fuel consumption unrelated to the vehicle load:

$$\mathcal{F}_{uv}^1(t) = \tau_{uv}(t) \frac{\alpha \mathcal{M} \mathcal{E}_0}{\mathcal{E}_2} s_{uv}^h = \frac{\alpha \mathcal{M} \mathcal{E}_0}{\mathcal{E}_2} l_{uv}, \quad (4)$$

and

$$\mathcal{F}_{uv}^2(t) = \tau_{uv}(t) \mathcal{E}_0 \left( \mathcal{E}_1 + \frac{\beta}{\mathcal{E}_2} (s_{uv}^h)^3 \right) = \mathcal{E}_0 \mathcal{E}_1 \tau_{uv}(t) + \frac{\beta \mathcal{E}_0}{\mathcal{E}_2} l_{uv} \cdot (s_{uv}^h)^2 \quad (5)$$

## 2.2 Time-dependent emission function using MEET

The MEET emission model was developed by Hickman et al. [20] for estimating vehicle emissions using a variety of polynomial functions of speed and acceleration levels. It computes GHG emissions produced by a vehicle of weights ranging from 3.5 to 32 tons according to travel speed and a wide range of input parameters related to the type of vehicle. Given an unloaded vehicle traveling at speed  $s$  ( $km/h$ ) on a flat surface the MEET calculates the rate of emissions ( $g/km$ ) using the following function:

$$\eta_r = \mathcal{K} + as + bs^2 + cs^3 + d \frac{1}{s} + e \frac{1}{s^2} + f \frac{1}{s^3}. \quad (6)$$

The coefficients  $(\mathcal{K}, a, b, c, d, e, f)$  are defined based on the vehicle type and weights. For example, if we consider the case of a vehicle weighing 3.5-7.5 tons the coefficients for the GHG emissions function for this specific vehicle category are  $(\mathcal{K}, a, b, c, d, e, f) = (110, 0, 0, 0.000375, 8702, 0, 0)$ .

To consider the effect of road gradient for each vehicle category, pollutant and gradient class, MEET proposes the following road gradient correction factor:

$$\eta_g = \mathcal{A}_0 + \mathcal{A}_1 s + \mathcal{A}_2 s^2 + \mathcal{A}_4 s^4 + \mathcal{A}_3 s^3 + \mathcal{A}_5 s^4 + \mathcal{A}_6 s^6. \quad (7)$$

where  $(\mathcal{A}_0 \dots \mathcal{A}_6)$  are coefficients for  $CO_2$  pollutant that vary according to the vehicle category and gradient class. Moreover, to take the effect of the load into account, MEET applies the following load correction factor:

$$\eta_l = \kappa + n\gamma + \rho\gamma^2 + q\gamma^3 + rs + ys^2 + zs^3 + \frac{\varrho}{s}, \quad (8)$$

where  $(\kappa, n, \rho, q, r, y, z, \varrho)$  are coefficients of the load correction function.

Based on MEET the amount of GHG emissions  $\mathcal{E}_{p_{ij}}(t)$  in grams produced by traversing path  $p$  at time  $t$  (with time-varying speeds taken into account) is given by:

$$\mathcal{E}_{p_{ij}}(t) = \sum_{(u,v) \in p} \eta_r(t) \eta_g(t) \eta_l(t) l_{uv}. \quad (9)$$

As GHG emissions are directly proportional to fuel consumption, the amount of fuel consumed can be derived from the amount of emissions according to the study of Coe [7] that set the CO<sub>2</sub> emission from a liter of fuel to 2.66 *kg/liters* (10.1 *kg/gallon*).

### 3 Data collection and analysis of emissions

In collaboration with an important furniture, appliances and electronics retailer from Québec City, on-road fuel consumption data collection was conducted with HINO SERIES 195 heavy-duty vehicles across different time periods of each workday during shipping operations, which covers rush hours times. The vehicles were monitored with a GPS on-board diagnostics and data logging device, which can measure the instantaneous fuel consumption between GPS points. The device incorporates a fuel analyzer sensor, an engine scanning tool, and a communication port for obtaining accurate measurements.

During 97 days between November 2016 and March 2017 up to 58,215 instantaneous speed and fuel consumption observations were collected. Real-time information includes fuel consumption, travel speed, acceleration, deceleration, GPS coordinates and vehicle load. The average travel time between two consecutive measurements is 14.54 seconds.

We now present the characteristics and analysis of real-world, on-road vehicle emissions. The main goal is to quantify and characterize the emissions in a real-world road freight distribution environment regarding relevant input variables. For data validation the daily observed fuel consumption was fitted to fuel invoices showing that the consumption device yields perfect accuracy. Yet, outliers analysis of emission data was done to ensure that there is no time lag between instantaneous emission observations.

Hence, this section describes how data analysis were offset to cleanup any lags in the emission sample that will be used by our machine learning algorithms.

For each observed workday the vehicle travels on average through 14 paths corresponding to shipping trips. Translating journeys into trips involves three main steps:

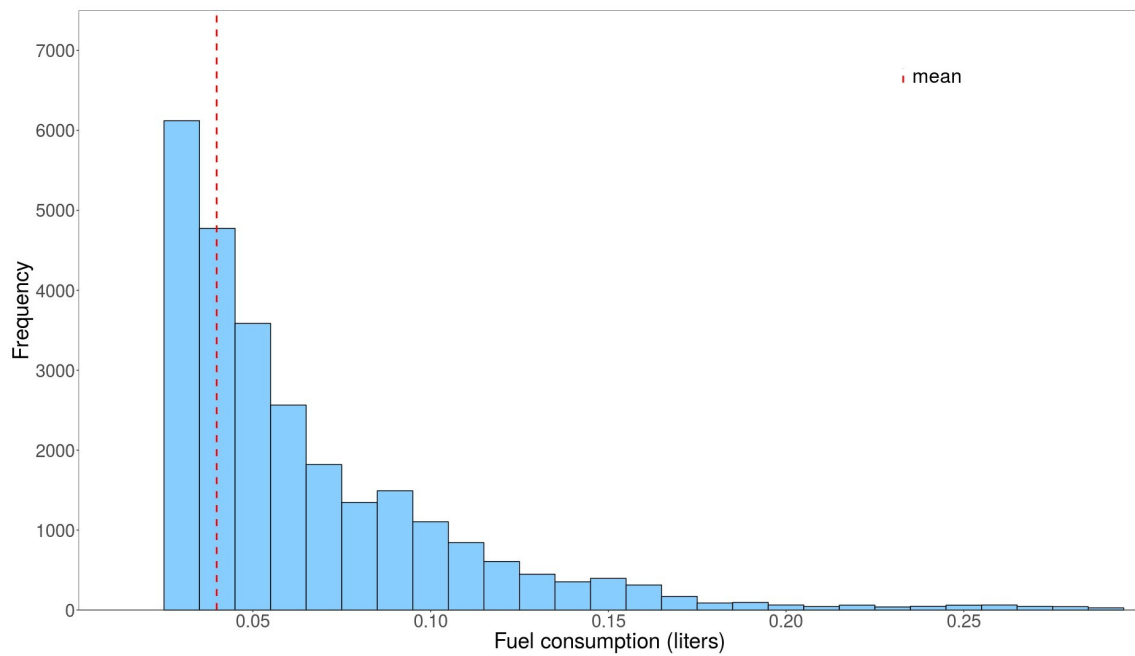
- geomatics and geospatial manipulations by geomatic specialists allow us to match GPS coordinates of each trip to the road links of Québec City. It is therefore essential to combine road segments that form part of a single trip but which have been divided into individual paths according to service time at customers, refueling stops, and/or driver breaks.
- identification of whether a break is a refueling stop or driver break, or service time at a customer where goods are picked up or dropped off, by grouping the observations according to when the vehicle ignition is turned on or off. For the purpose of this study, a trip is defined as a combination of paths traveled across a given workday where the ends are the real location of a pickup or delivery, thus grouping subsequent journeys that include breaks at fuel stations or truck-stops.
- matching the information of GPS points, starting time and idle time with orders details from another database to identify the vehicle load at each GPS point, which is constant throughout the path connecting two customers.

A cleanup process is applied on the prepared data to remove observations corresponding to idle state during breaks or delivery operations. Then, based on the obtained emission sample composed of 46,476 observations we define five explanatory variables: travel speed, acceleration, vehicle load, stop-and-go driving pattern, traveled distance, while the output variable is the amount of fuel consumption produced between two GPS points.

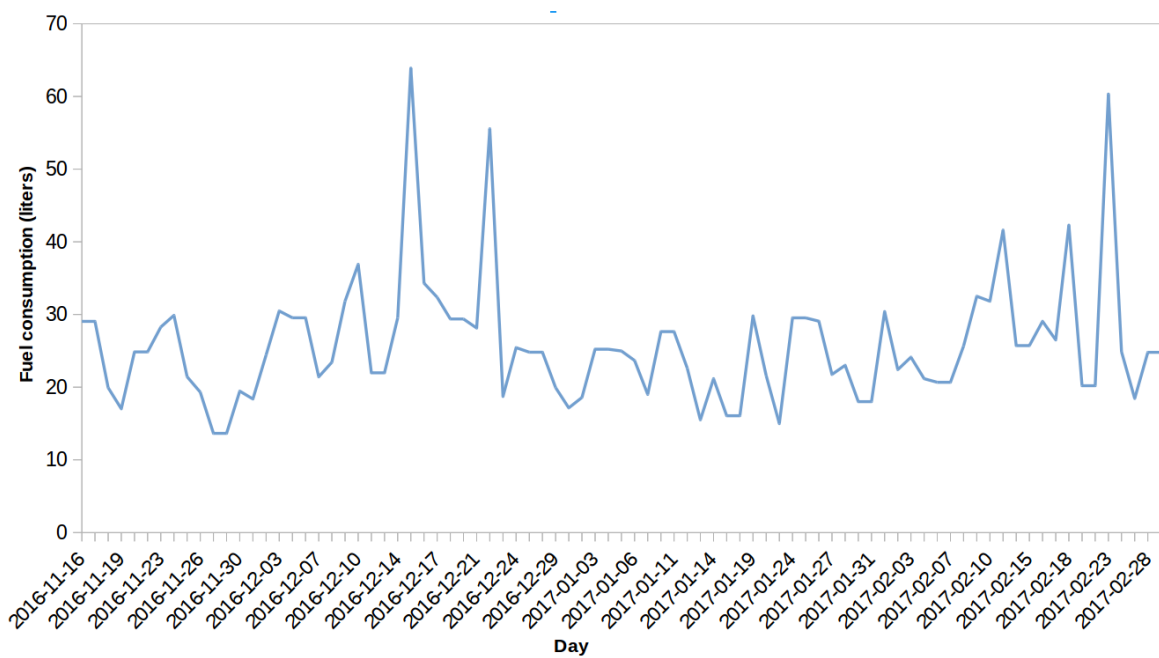
The frequency of link-based fuel consumption observations is displayed in Figure 2. We see that the number of observations is high for low fuel volumes. As shown in Figure 2 the mean of fuel consumption considering all observations is 0.033 liters, respectively.

Figure 3 presents the daily variation of fuel consumption. The different consumption levels between journeys are due to several factors including number of orders, traffic congestion and traveled distance, among others.

A subset of data composed by observations corresponding to steps of 11 seconds is presented in Figure

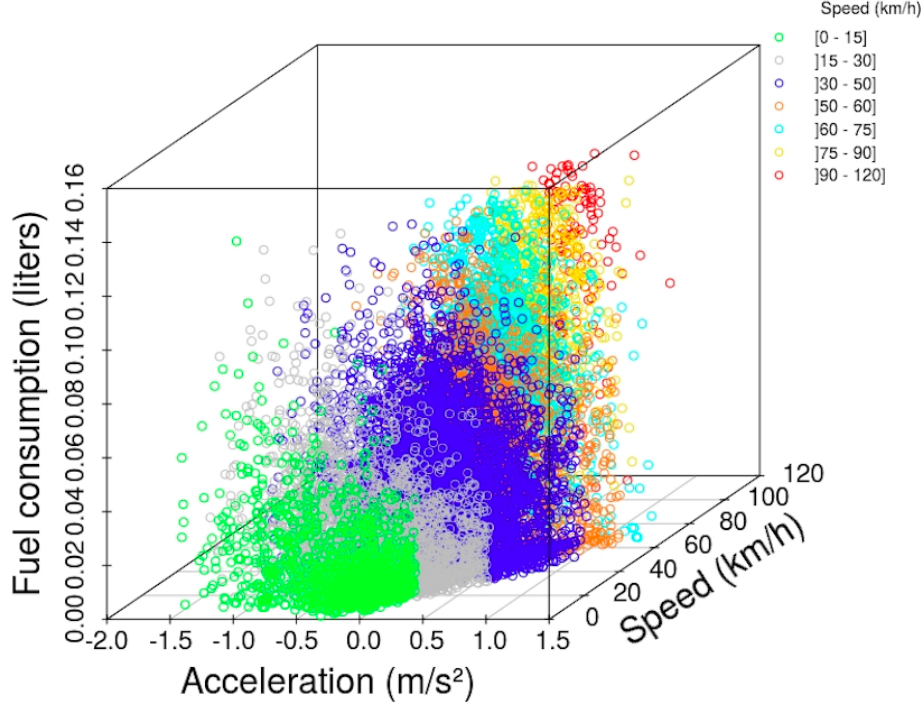


**Figure 2:** Fuel consumption histogram of real-world shipping trips in Québec City



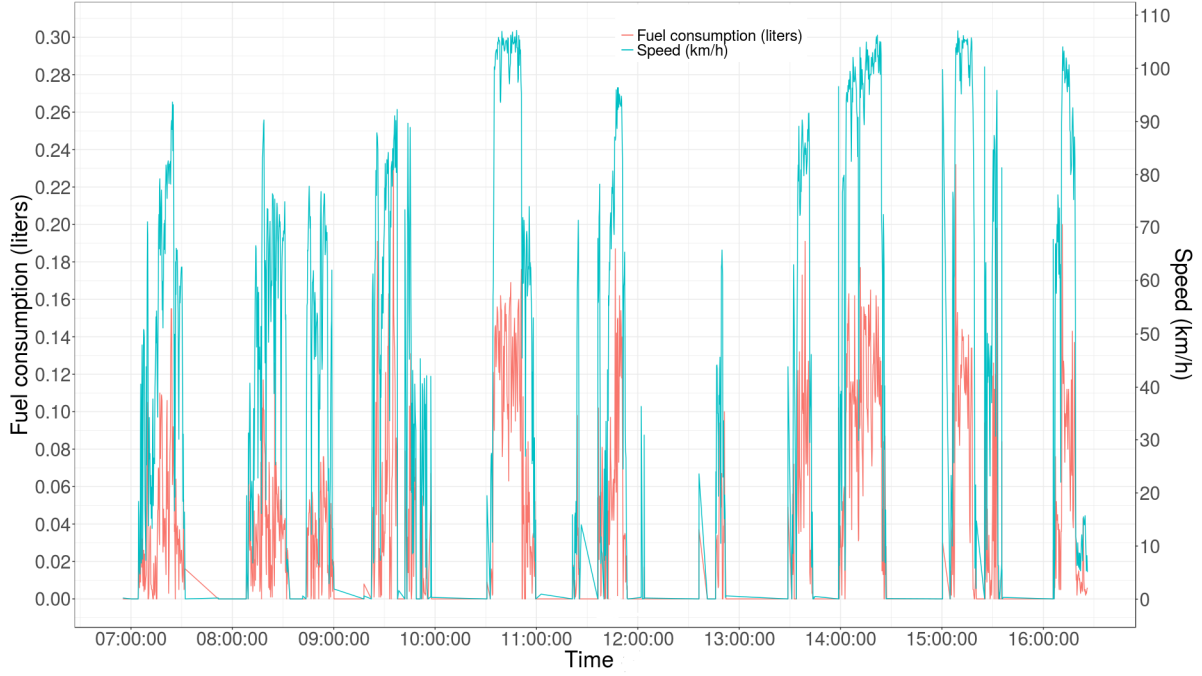
**Figure 3:** Variation of daily fuel consumption of real-world shipping trips in Québec City

4. We see a high level of fuel consumption variability based on speed and acceleration levels. It also illustrates the non-linear behavior of fuel consumption as a function of travel speed and acceleration. When acceleration and speed levels increase, consumption tend to increase. In deceleration, consumption values are generally low.



**Figure 4:** Fuel consumption as a function of instantaneous speed and acceleration for all observations with a travel time of 11 seconds

Figure 5 shows the trade-off between fuel consumption and travel speed over different times of a typical shipping workday. It is remarkable that the fluctuation of fuel consumption is impacted by the speed in the underlying road network. The shape of curves has two distinct phases. In a first stage, we observe that fuel consumption increases with speed. This phase is characterized by a regular form of speed (ascending or descending). The second phase, marked by erratic fluctuations of speed, gives a very accidental relationship between speed and fuel consumption. This situation corresponds to the different phases of acceleration and deceleration. We can see that vehicular consumption during idling and cruising are generally low compared to consumption during acceleration. We also observe that fuel consumption depend on short term events such as rapid acceleration and braking (stop-and-go). The majority of microscopic emission models assume a constant consumption rate when a vehicle is decelerating.



**Figure 5:** Instantaneous variation in fuel consumption and speed during a typical shipping day

To summarize, there is a clear need to perform an effective predictive modeling that takes into account the specificity of fuel consumption/emissions data structures. Therefore, in this study we used model-based machine learning for predicting vehicle emissions.

## 4 Emission modeling with supervised learning methods

This section shows the development of multiple nonlinear emission models using four supervised learning methods: Neural Networks (NNET), Support Vector Machines (SVM), Conditional Inference Trees (CIT) and Gradient Boosting Machines (GBM). Each model-based machine learning uses a set of tuning parameters. These determine the performance profile of each model. To choose the appropriate combination of parameters values while avoiding over-fitting we used grid search method for SVM and CIT and trial-and-error approach for NNET and GBM. For each model we define a set of candidate values for the appropriate tuning parameters according to the relevant literature, sample size and computational resources. We then fit each model with each candidate set using the training dataset on which we apply the  $k$ -fold cross validation method [25] for estimating prediction error. The  $k$ -fold cross validation works by splitting the training dataset into  $k$  roughly equal-sized subsamples or folds. Each supervised learning method performs  $k$  iterations and at each time it excludes one held-out fold

in turn to evaluate their prediction accuracy once the model is estimated using the remaining  $k - 1$  folds. There is no formal rule of defining the value of  $k$ , and we used  $k=10$ . The prediction accuracy of each model is given by the average of  $k$  obtained prediction error measures. For each candidate machine learning model, the optimal settings of tuning parameters is determined according to the obtained performance metrics. Then, we evaluate the performance of their accuracy prediction using a testing dataset (see Section 5).

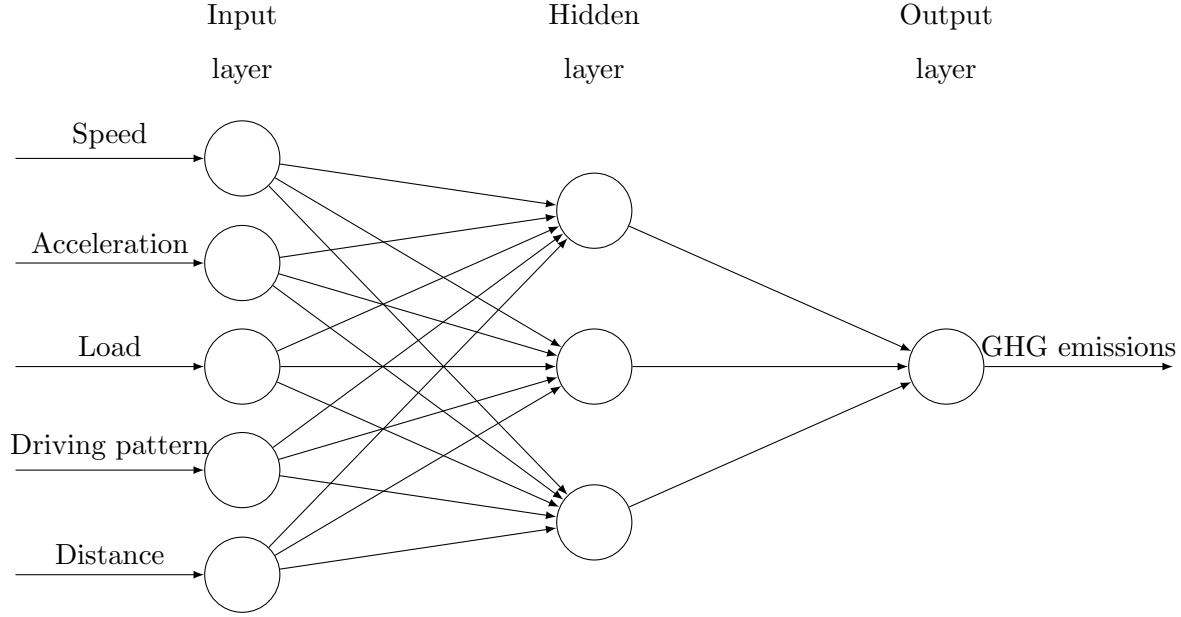
#### 4.1 Neural Networks

NNET learning methods allow the extraction of linear combinations of the inputs to produce a non-linear emission model. NNET is composed of a set of neurons connected together [12]. It uses massive interconnections to fit nonlinear models to multidimensional data [18]. Figure 6 shows a schematic diagram of the proposed NNET used to model GHG emissions. In the network diagram the nodes are the neurons and the arcs are the connections. NNET is a multi-layer network composed of three layers: input layer, hidden layer and output layer. The input layer incorporates five input variables  $x_1, \dots, x_5$  defined based on the chosen parameters affecting emissions, namely speed, acceleration, vehicle load, stop-and-go driving patterns, and distance. The hidden layer incorporates a set of hidden units or unobserved variables used to model the outcome [25]. These hidden units perform intermediate computations using linear combinations of the input variables. The output layer is the combination of obtained hidden units to perform the prediction of emissions.

In this study, several NNET tasks were performed to accurately predict traffic emissions by studying field data. We applied the quasi-Newton back propagation learning algorithm [3]. The linear combinations of the predictors are transformed by a nonlinear activation function (sigmoidal). To reduce over-fitting our NNET algorithm minimizes the following function [25]:

$$\mathcal{G} = \sum_{i=1}^{\mathcal{N}} (y_i - f_i(x))^2 + \eta \left( \sum_{k=1}^{\mathcal{H}} \sum_{j=0}^{\mathcal{P}} \beta_{jk}^2 + \sum_{k=0}^{\mathcal{H}} \gamma_k^2 \right), \quad (10)$$

where  $\mathcal{N}$  is the total number of observations,  $\mathcal{P}$  is the number of predictors,  $\mathcal{H}$  represents the number of hidden units,  $\eta$  is the weight decay, and  $y_i$  is the outcome. The coefficient  $\beta_{jk}$  represents the effect of the  $j$ th predictor on the  $k$ th hidden unit. The function  $f$  defines a linear combination that connects the hidden units to the outcome:



**Figure 6:** Schematic diagram of the NNET emission model

$$f(x) = \gamma_0 + \sum_{k=1}^{\mathcal{H}} \gamma_k h_k, \quad (11)$$

where  $\gamma_k$  are the regression coefficients of hidden layers.

Several combinations of NNET parameter values were investigated by trial-and-error to identify the best learning performance. Four different weight decay  $\eta \in \{15^{-4}, 15^{-3}, 15^{-2}, 15^{-1}\}$  were evaluated along with one hidden layer including between one and 10 hidden units. The convergence to the best NNET model is achieved with a maximum number of iterations equal to 2000. The optimal NNET model used  $\eta = 15^{-3}$  and  $\mathcal{H} = 9$  hidden units.

## 4.2 Support Vector Machines

SVMs is a supervised learning method applied for classification and nonlinear regression [35]. SVM algorithms use a kernel function allowing this model to transform input data to the required form of relationships. There are multiple kinds of kernel functions, such as linear kernel, polynomial, radial basis function, and sigmoid. After several trials, we used a linear kernel function defined as a simple sum of cross products, which have been shown to be effective for the current study.

The SVM regression tries to minimize the following regularized function:

$$\mathcal{W} = \mathcal{C} \sum_{i=1}^{\mathcal{N}} \mathcal{L}(y_i, \mathcal{F}(x_i)) + \sum_{j=1}^{\mathcal{P}} \beta_j^2, \quad (12)$$

where  $x_i$  is the input space-vector,  $\mathcal{L}(\cdot)$  is the loss function,  $\beta$  are coefficients used by the regularization term considering  $\mathcal{P}$  predictors, and constant  $\mathcal{C}$  is the error penalty factor for adjusting the complexity of the model [25].  $\mathcal{F}$  is a prediction equation defined as follows:

$$\mathcal{F}(x) = \sum_{i=1}^{\mathcal{N}} \alpha_i \varphi(x) + \beta_0, \quad (13)$$

where  $\varphi(x)$  is the linear kernel function.

The tuning of regularization parameter  $\mathcal{C}$  through grid search method produced a constant with a value of 1.

### 4.3 Conditional Inference Trees

CIT is a machine learning method that uses unbiased tree-based models for regression and classification [21]. CIT algorithm's estimates regression relationship using a binary recursive partitioning method, which efficiently performs the exhaustive search across the predictors according to split points. A simplified description of this method is provided by the following steps:

1. perform the null hypothesis test of independence between each input variable and the outcome one. The algorithm continues until the hypothesis cannot be rejected;
2. apply a binary split to the selected input variable;
3. recursively repeat steps 1 and 2.

The  $p$ -value statistical test is applied for candidate splits by evaluating the difference between the means of two groups. On our preliminary tests with the training dataset we found that the optimal CIT model is obtained with a value of  $1 - p$  equal to 0.821.

#### 4.4 Gradient Boosting Machines

GBM is gaining a considerable interest in a wide range of data driven applications such as travel time prediction [37] and the modeling of the energy consumption [32]. It is a highly adaptable supervised learning method encompassing both classification and regression in order to find an additive model that minimizes the loss function [16]. GBM iteratively investigates decision trees (basic learner) to reduce the loss function and improve prediction accuracy. The GBM model is defined as follows [16].

Let  $\hat{\mathcal{R}}(x)$  be the regression function that minimizes the expectation of loss function  $\mathcal{S}(y, \mathcal{R})$  over the joint distribution:

$$\hat{\mathcal{R}}(x) = \arg \min_{\mathcal{R}(x)} E_{x,y}[\mathcal{S}(y, \mathcal{R}(x))], \quad (14)$$

where  $\mathcal{R}(x)$  can be formulated as a function with a finite number of parameters  $\beta$  estimated by selecting those values that minimize the loss function  $\mathcal{S}$  using the training sample as shown in equation 15:

$$\hat{\mathcal{R}}(x) = \arg \min_{\beta} \sum_{i=1}^{\mathcal{N}} \mathcal{S}(y_i, \beta). \quad (15)$$

To optimize the GBM model we have performed the tuning of several regularization parameters:

- $d$ : the depth of decision trees that controls the maximum interaction order of the model;
- $I$ : the number of boosting iterations, which also corresponds to the numbers of decision trees;
- $\alpha$ : the learning rate that controls the contribution of each base model or decision trees by shrinking its contribution by a factor between 0 and 1;
- $\delta$ : the subsampling rate or fraction of the training set observations, which is randomly selected to propose the next tree in the expansion.

After the training of the model, the depth of the decision trees  $d$  was selected in the set  $\{2, 5, 7, 9\}$ , the learning rate  $\alpha$  was chosen from 0.01 to 0.5 with a granularity of 0.02. The number of iterations  $I$  was selected within a set spanning from 50 to 250 iterations with a granularity of 50 iterations. The minimum number of observations in trees terminal nodes  $\varphi$  was defined between 5 and 10. The subsampling rate  $\delta$  was fixed to 0.5. The final combination of values used for the GBM model were  $d = 9$ ,  $I = 250$ , and  $\alpha = 0.07$ .

## 5 Numerical experiments

It is not recommended to use the same set of observations for both training and testing. Hence, in this work the assessment of predictive performance has been carried out on an independent sample of field data in order to avoid over-fitting, which is the tendency of the models to fit the training sample too well, at the expense of the predictive accuracy. The preprocessed field dataset composed of 46,476 fuel consumption observations (1406 paths) was split randomly on two subsets using days as the splitting criterion:

- training sample: composed by 80% of days corresponding to 38,004 observations (1263 paths);
- testing sample: composed by 20% of days including 8,472 observations (143 paths).

Each model was trained with the same training dataset with R version 3.4.3 through R-Studio 1.0.153 using a ThinkCenter professional workstation with Intel i7 vPro (8 cores) and 32-gigabyte RAM, running Ubuntu Linux 16.04 LTS x86 operating system. The following R machine learning packages were used to generate nonlinear emission models: nnet, e1071, party, gbm, and caret. The evaluation process was initiated by comparing the models prediction outcomes on in-field observations. More specifically, we assessed the accuracy of studied emissions models considering realistic driving conditions that take into account several factors, such as carried loads, speed, and stop-and-go events. The obtained models were then evaluated on the testing dataset. Their effectiveness was validated by computing and analyzing the following accuracy measures:

- Root Mean Squared Error (RMSE): interpreted as the average distance between the observed values and the model predictions. The RMSE is then computed by taking the square root of the Mean Squared Error (MSE). The smaller the values of RMSE, the closer the predicted values are to the observed ones. The RMSE is computed by squaring the residuals, summing them up and dividing by the number of observations as  $\frac{1}{n} \sum_i^n (y_i - \hat{y}_i)^2$ , where  $y_i$  is the observed value,  $\hat{y}_i$  is the predicted output, and  $n$  is the total number of observations;
- Mean Absolute Error (MAE): is the average magnitude of the errors in a set of predictions. It is computed using the formula  $\frac{1}{n} \sum_i^n |y_i - \hat{y}_i|$ .
- Gap (%): reports how close the corresponding predicted outcome is to the observed value. The percentage gap values are calculated as  $100(y_i - \hat{y}_i)/y_i$ .

## 5.1 Experimental results and analysis

In this section we provide the experimental results and analysis. Table 2 shows the accuracy metrics of CMEM, MEET, NNET, SVM, CIT and GBM predictions. In this table, successive columns give for each emission model the RMSE, the MAE, the Standard Error (Std Error), the mean value, the Gap (%) aggregated across all paths (trips) in the testing dataset, and the computational time (CPU) of training (seconds). Doing so, we estimate the fuel consumption for each road segment, then we aggregate the obtained values for each path. The results obtained for the RMSE metric show that the proposed nonlinear emission models, namely GBM, NNET, CIT and SVM outperform CMEM and MEET and appear to be more accurate in estimating instantaneous vehicle fuel consumption. In fact, we see that the average RMSE ranges from 0.258 to 0.315 for the machine learning models, which are lower than those of the CMEM and MEET models (0.501 and 0.850). More specifically, it can be clearly seen that GBM model exhibited the best estimation accuracy as the fuel consumption predictions are very consistent in trends with in-field observations, with the lowest RMSE of 0.258.

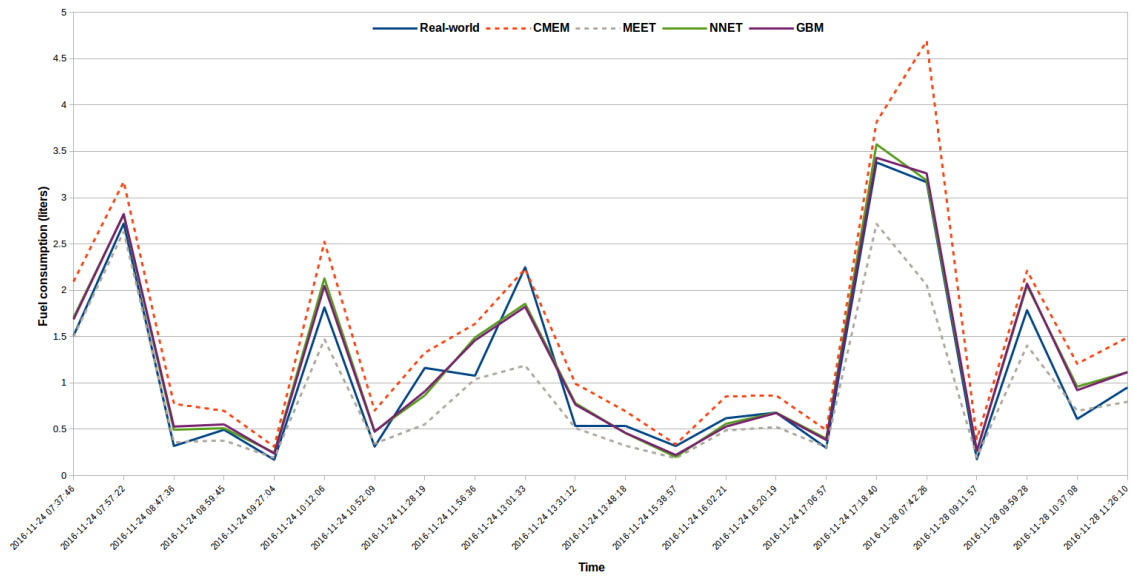
Figure 7 also illustrates that GBM outperforms MEET and CMEM that were found to respectively under- and over-predict fuel consumption. Note however, that GBM algorithm is computationally demanding as it takes over 32354.44 seconds of execution time compared to the case of NNET (5188.85 seconds), SVM (1743.11 seconds) and CIT (404.10 seconds) models.

Regarding the obtained percentage gap values, we observe from Table 2 that the machine learning models give the best prediction results with a gap ranging from -1.930% to 6.173% when compared against MEET underestimating fuel consumption on average by 24.942% and CMEM overestimating fuel consumption by 13.184%. We also see that GBM and CIT yield the lowest underestimation with a gap of -1.709% and -1.453%, respectively.

Additional experiments were performed to study the performance of the developed machine learning models. Figure 8 shows scatter plots that illustrate graphically the prediction accuracy of the studied models superimposed on the field data. On the vertical scale, the observed value of fuel consumption is displayed, whereas the predicted values are presented on the horizontal scale. We observe that NNET, GBM, SVM and CIT models fit similarly as their prediction outcomes are more concentrated and closer to the identity lines represented by red color indicating that the observed and predicted emission values are very close. This implies that the machine learning models yield more effective prediction of fuel consumption than those produced by the classical CMEM and MEET. As expected, machine learning models provide good fitting regarding observed fuel consumption as they are able

**Table 2:** Comparative performance of the proposed machine learning models against MEET and CMEM regarding emission prediction aggregated by paths

| Emission models   | RMSE  | MAE   | Std Error | Mean  | Gap (%) | CPU of training (seconds) |
|-------------------|-------|-------|-----------|-------|---------|---------------------------|
| <b>Real-world</b> | 0     | 0     | 0         | 1.539 | 0       | -                         |
| <b>CMEM</b>       | 0.501 | 0.305 | 0.459     | 1.742 | -13.184 | -                         |
| <b>MEET</b>       | 0.850 | 0.404 | 0.760     | 1.155 | 24.942  | -                         |
| <b>SVM</b>        | 0.315 | 0.170 | 0.301     | 1.444 | 6.173   | 1743.110                  |
| <b>CIT</b>        | 0.264 | 0.151 | 0.263     | 1.561 | -1.453  | 404.100                   |
| <b>NNET</b>       | 0.271 | 0.155 | 0.270     | 1.569 | -1.930  | 5188.850                  |
| <b>GBM</b>        | 0.258 | 0.150 | 0.257     | 1.565 | -1.709  | 32354.440                 |



**Figure 7:** Sample of the estimations produced by CMEM, MEET, NNET and GBM models against real-world fuel consumption.

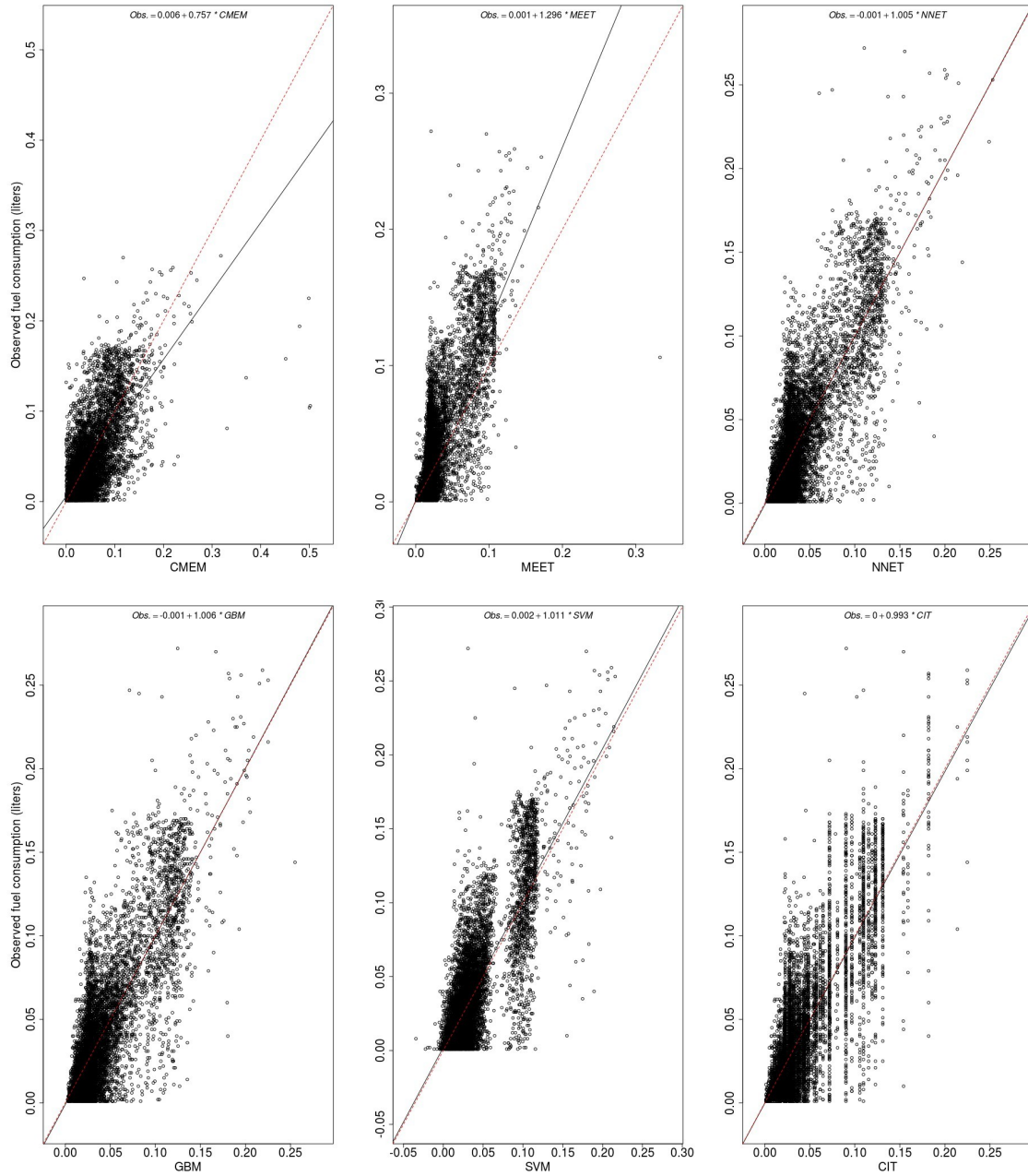
to reflect differences in vehicle emissions that result from traveling on congested areas with frequent stop-and-go events impacting the traffic speed.

Figure 8 also illustrates the difference observed between the identity red line and the black regression line, which shows the variation in prediction between each model results compared to observed data. Notably, this graphical trend was validated by the goodness of fit test. The null hypothesis of this test is performed with a slope=1 and intercept=0. This test leads to the rejection of the null hypothesis with very low  $p$ -value ( $<2.2e-16$ ), lower than the threshold 0.05. Hence, these two models are not preferred candidates for predicting fuel consumption considering estimation at points level. More specifically, the best prediction accuracy belongs to the GBM model yielding the lowest  $p$ -value of 0.314, which is larger than the threshold 0.05. Therefore, the null hypothesis is not rejected which indicates that the prediction outcome of the GBM model is similar to the observed values.

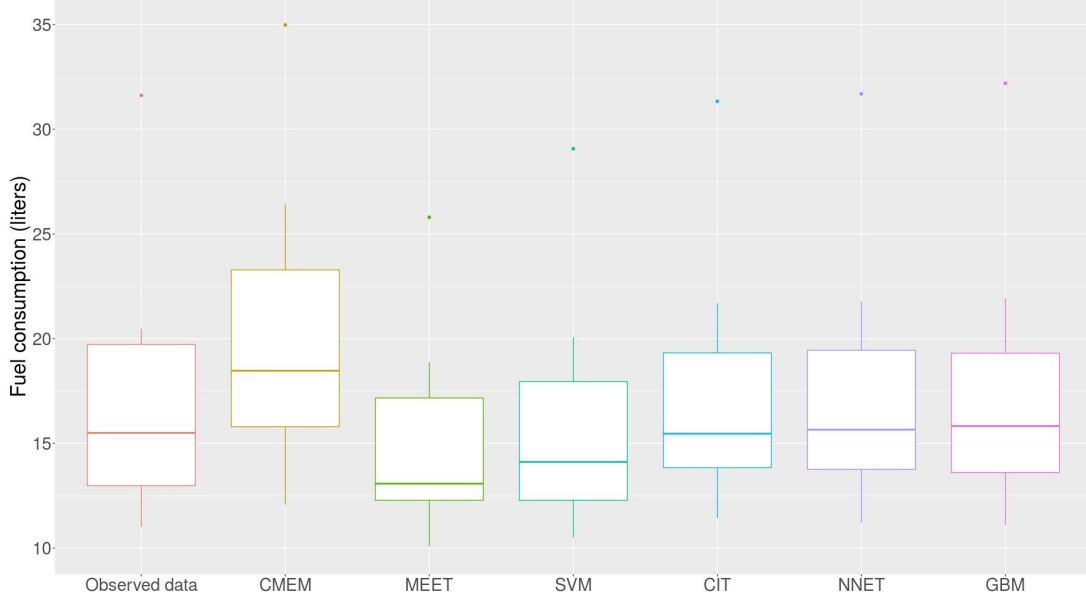
In order to make further analysis on the prediction accuracy of the proposed models the boxplots presented on Figure 9 illustrate numerical outcomes of the studied emission models through their quartiles. Clearly, the median thicknesses of GBM, CIT and NNET models (represented by the lines in the middle of the boxes) seem to be very close to the observed fuel consumption one, exhibiting superior accuracy regarding fuel consumption. When looking at the boxplots of CMEM and MEET, we can see a difference between the medians, indicating that these models tend to incorrectly predict fuel consumption.

To further evaluate the performance of the proposed emission models, a sensitivity analysis is performed to compare their prediction accuracy under multiple criteria: congested (low speeds) and free flow (high speeds) situations, empty and loaded vehicle, stop-and-go driving patterns, and peak and non-peak periods. In Table 3 the performance of emissions estimation of CMEM and MEET is compared against the proposed models with in-field measurements considering each criterion, which includes corresponding mean and gap for the best machine learning model, CMEM, and MEET. Clearly, the degree of estimation varies for all criteria according to real-world driving conditions. We have noticed that the estimation of CMEM and MEET are deteriorated in the case of low speeds with an overestimation of 107.032% and 11.800%, respectively. The result obtained for CMEM is conform with previous literature indicating that potential under prediction is due to its deterministic nature [24]. However, GBM provides a low overestimation of only 3.776%.

For driving pattern criterion, we see that the prediction of CMEM and MEET are affected in the cases of acceleration and deceleration events. As an example, for acceleration observations our experiments



**Figure 8:** Scatter plots of predicted outcomes by CMEM, MEET and machine learning models against observed fuel consumption



**Figure 9:** Boxplots of emissions models prediction performance against observed fuel consumption aggregated by days

indicate that CMEM and MEET emission estimations are inaccurate under fluctuating speeds as they produce a gap of -28.222% and 30.701%, respectively. As expected the GBM model adequately handles acceleration variability when congestion occurs as it has the smallest gap (-1.564%). Regarding loads, GBM gives the lowest gaps (-1.666% for empty vehicles and -1.716% for loaded ones). Interestingly, NNET model shows its performance in peak period cases during the morning between 08h00 and 09h00 providing a gap ranging from 1.107% to 2.783% compared to CMEM and MEET which have a much higher absolute gap between 4.265% and 30.692%.

Based on the results presented in Table 3 it can be argued that GBM and NNET models give the best results and are the most accurate for all aspects, exhibiting a gap just over 3.776%. Further, we can see that the overall performance of both models is very good not only in normal or moderate traffic conditions, but also during traffic congestion. Compared to CMEM and MEET, machine learning models are less sensitive to input variables and maintain superior prediction accuracy.

To summarize, even if emissions estimation is complex and challenging, it is clearly shown that machine learning models enhance emission prediction accuracy by taking into account the interactions among different combinations of input variables. In all experiments presented in this section, we conclude that the proposed machine learning models significantly outperform CMEM and MEET. In fact, machine learning-based emission models, and in particular GBM and NNET models are able to fit complex

nonlinear relationship of vehicle emissions leading to superior emissions prediction accuracy.

## 6 Conclusions and future research

In this paper we have proposed nonlinear emission models using supervised learning methods. The prediction accuracy was compared to the classical MEET and CMEM methods under real-world driving conditions with stop-and-go events, fluctuating speeds and varying road geometry. In our numerical experiments, we have observed that MEET and CMEM incorrectly predicted emissions by 24.942% and  $-13.18\%$ , respectively. Results revealed that the proposed NNET, SVM, CIT and GBM models outperform CMEM and MEET as they improve prediction accuracy in the case of traffic congestion and stop-and-go driving patterns with recurrent acceleration and breaking events. It was also shown that GBM produces the best predictability which is off by only 1.70% according to real-world data. This indicates that we cannot take for granted that existing emission models are sufficiently accurate to be used in green vehicle routing, which requires machine learning models that update them by applying supervised learning methods on collected real-time traffic data and on-road vehicular exhaust emissions.

The results of this work show that using machine learning models and more specifically the GBM and NNET models enhance the prediction accuracy of emissions prediction. A direction of future research is to evolve machine learning emission models by investigating the effects of weather, driver profiles and road-wide factors such as temperature, rain, snow, road maintenance events, etc. Another area of future work will be the integration of machine learning emission models in routing problems and practical road freight transportation applications.

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**Table 3:** Comparative performance statistics of the GBM, NNET, CMEM and MEET models regarding multiple performance indicators

| Criterion               | Aspects                   | NB Obs. | Mean real-world | Best model (RMSE) | Mean BM (%) | Gap BM (%) | CMEM  | Gap CMEM (%) | MEET  | Gap MEET (%) |
|-------------------------|---------------------------|---------|-----------------|-------------------|-------------|------------|-------|--------------|-------|--------------|
| <b>All observations</b> | Testing dataset           | 8472    | 0.041           | GBM               | 0.041       | -1.709     | 0.046 | -13.184      | 0.031 | 24.942       |
|                         | Low speeds (0-15 km/h)    | 1832    | 0.017           | GBM               | 0.017       | -3.776     | 0.034 | -107.032     | 0.018 | -11.800      |
|                         | Moderate speed (~50 km/h) | 175     | 0.034           | GBM               | 0.035       | -2.533     | 0.043 | -28.210      | 0.022 | 34.444       |
|                         | High speed (>75 km/h)     | 1573    | 0.101           | NNET              | 0.101       | 0.529      | 0.090 | 11.252       | 0.074 | 27.160       |
| <b>Load</b>             | Empty vehicle             | 1377    | 0.037           | GBM               | 0.038       | -1.666     | 0.041 | -11.414      | 0.028 | 23.101       |
|                         | Loaded vehicle            | 7095    | 0.041           | GBM               | 0.042       | -1.716     | 0.047 | -13.490      | 0.031 | 25.26        |
| <b>Driving pattern</b>  | Acceleration              | 4703    | 0.044           | GBM               | 0.044       | -1.564     | 0.056 | -28.222      | 0.030 | 30.701       |
|                         | Deceleration              | 3691    | 0.036           | GBM               | 0.037       | -2.081     | 0.033 | 9.002        | 0.031 | 16.255       |
| <b>Period</b>           | 07h30 - 08h00             | 744     | 0.060           | NNET              | 0.060       | 0.867      | 0.062 | -2.671       | 0.044 | 26.650       |
|                         | 08h00 - 08h30             | 776     | 0.050           | NNET              | 0.049       | 1.107      | 0.051 | -4.265       | 0.036 | 26.630       |
|                         | 08h30 - 09h00             | 359     | 0.038           | NNET              | 0.037       | 2.783      | 0.043 | -13.490      | 0.026 | 30.692       |

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