NeuralMOVES: Extracting and Learning Surrogates for Diverse Vehicle Emission Models

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1 INTRODUCTION

The transportation sector is a pivotal contributor to global greenhouse gas (GHG) emissions, accounting for 28.5% of the U.S.'s total CO_2 emissions and consuming 37% of its energy (EPA, 2023). As the largest source of GHG emissions in the U.S., it represents both a significant challenge and a substantial opportunity for climate change mitigation. Innovations such as electrification, automation, and intelligent infrastructure are revolutionizing this sector, offering paths to significant emissions reductions (Sciarretta *et al.*, 2020, International Energy Agency, 2023, McKinsey Center for Future Mobility , 2023). However, the real-world impacts and effectiveness of these innovations hinges critically on the availability of accurate and adequate emission models to design and motivate the deployment of these technologies.

The emission model space is vast (Mądziel, 2023), but the Motor Vehicle Emission Simulation (MOVES) (USEPA, 2022) serves as the official and state-of-the-science emission modeling framework in the US; provided, enforced and maintained by the Environmental Protection Agency (EPA). Despite its technical certification and established use, MOVES' processing and software is designed for specific governmental uses (i.e. State Implementation Plans and Conformity Analyses) and its use beyond trained practitioners poses important challenges, including a steep learning curve, high computing time, extensive inputs, and multiple technical complexities. Moreover, MOVES follows a macroscopic modeling framework, and it is unsuitable for numerous microscopic approaches.

These challenges and limitations are particularly important in the field of Intelligent Transportation Systems (ITS). In this field, emerging technologies are studied that involve analyzing, controlling and optimizing vehicular dynamics, like eco-driving (Mintsis *et al.*, 2020), stop-and-go wave mitigation (Wu *et al.*, 2019), Lagrangian control (Vinitsky *et al.*, 2018), variable speed limit optimization (Zegeye *et al.*, 2010), among others. For these approaches, the emission models are essential not only for post-hoc emission quantification but also in the optimization process and problem formulation itself, as they aid in the development of objective functions. In contrast to the macroscopic modeling framework of MOVES, which computes emissions from an entire trajectory under a highly aggregated scenario, these applications require a microscopic emission model able to compute, in real-time, emissions from a single action taken at each time step for a specific vehicle and environment.

Motivated by bridging MOVES' emission modeling with applications that require faster, programmatic and microscopic processing, MOVES variants have been developed. On the one hand, MOVES-Matrix (Liu *et al.*, 2016) pre-calculates over 90 billion emission rates from MOVES using high-performance computing cluster, and provides an expansive (in the order of hundreds of Gb) matrix of the results. As a lookup table, MOVES-Matrix can output MOVES emissions calculations significantly faster than MOVES, while maintaining MOVES' comprehensive set of scenario parameters (i.e. vehicles types, ages, fuel types, regions, road grade, etc.). This model is particularly suitable for existing users of MOVES that want to speed up their processing, as it requires MOVES expertise and the same input format and resolution.

On the other hand, MOVEStar (Wang *et al.*, 2020), takes a bottom-up approach and replicates MOVES' processing framework in a reduced and streamlined fashion. This variant serves as an accessible, lightweight and microscopic version of MOVES, but without an accuracy measure and for a reduced subset of scenario parameters, including 2 vehicles types and a fixed and unique region, temperature, humidity, fuel, and road grade. While these variants are a significant step in making MOVES accessible and suitable for more users and applications, a significant portion of ITS approaches still need a an emission model with the right combination of features.

In response, this paper presents NeuralMOVES, a new generation of MOVES surrogate as an effort go get microscopic models that are diverse enough (i.e. with comprehensive set of scenario parameters) to capture real-world conditions, accurate enough to serve as a valid MOVES substitute, and lightweight enough to run in real time and be accessible for all types of users and use cases.

The main differentiators of NeuralMOVES are the use reverse engineering to extract instantaneous emission from MOVES, and surrogate learning to perform function approximation of the instantaneous emission space as a Neural Network. As MOVES-Matrix, we pre-extract an extensive and diverse dataset from MOVES, but we design inputs to get instantaneous emission an get a microscopic model. Then, we apply Machine Learning techniques to capture Gigabytes of data in just a short list of Neural Net weight paramters. We perform an exhaustive validation to compare the surrogate models against MOVES to validate their accuracy and robustness.

The implications of our work are twofold: our models simplify GHG emission evaluation in transportation-related analyses by providing a faster, programmatic alternative to MOVES and enable control and optimization approaches by offering microscopic and environment feature-rich models compared to alternative models.

2 METHODOLOGY

This study introduces a novel suite of surrogate CO_2 emission models developed through the reverse engineering of MOVES and the application of surrogate learning techniques. Our methodology encompasses three primary phases: data collection through reverse engineering, surrogate model development, and validation.

Data Collection: We devised a reverse-engineering approach to MOVES, generating a comprehensive dataset by extracting instantaneous emissions data. This was achieved by designing custom trajectory inputs into MOVES to isolate emissions attributable to specific vehicular actions.

Model Development: We then constructed surrogate models using machine learning techniques to fit the instantaneous emissions data. including neural networks and decision trees. These models were designed to capture the complex relationships between vehicle dynamics and environmental conditions, thereby enabling precise emission predictions at a microscopic level.

Validation: The surrogate models were validated against MOVES using a set of diverse driving trajectories. This process involved comparing the emissions computed by our models

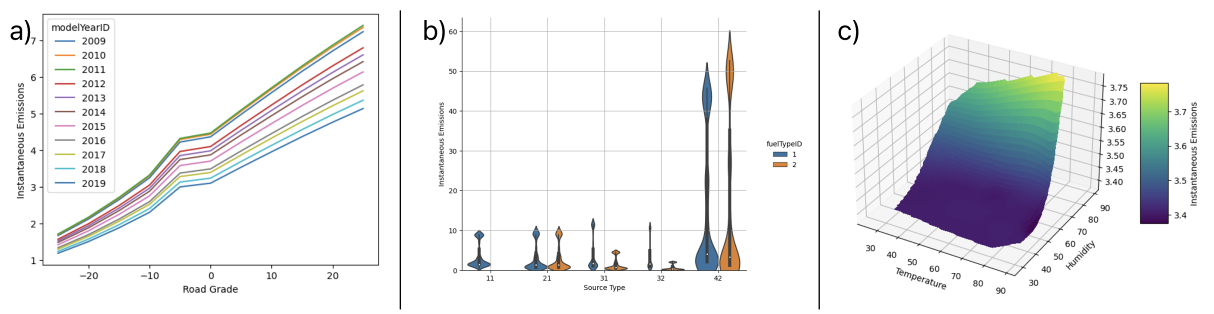

Figure 1 – *Variations of raw instantaneous emissions extracted by reverse-engineering MOVES across a) Vehicle Age and Road Grade; b) Type of Vehicle (Source Type) and Fuel Type; and c) Temperature and Humidity. Results highlight the significant impact on parameters that reduce-order emission model tend to ignore. Road grade, in particular, shows a variability of around 500% across different road grades. On the other hand, temperature and humidity shows a modes 10% variability in emissions, suggesting that emissions estimations can be extended across different regions with small correction factors.*

with those obtained from MOVES across various vehicle types and environmental conditions. The validation helped in refining the models and confirming their accuracy and reliability.

Through this methodology, we developed a robust toolset capable of providing rapid and accurate emissions assessments, facilitating enhanced decision-making in transportation planning and environmental policy.

3 RESULTS

The key results from the study are as follows:

Instantaneous Emission Dataset: Through reverse engineering moves, extensive instantaneous emission data were extracted. The study successfully generated a dataset with over 121 million data points mapping various vehicle and environmental parameters to instantaneous emissions. This data is the backbone and ground truth used, and the surrogate models are function approximations to replicate and interpolate the data.

Diversity Importance: Figure 1 shows the relationship between emissions and factors such as vehicle age, type, road grade, temperature, and humidity. The analysis revealed that the diversity of emission model is paramount, as parameters that are not usually considered in reduced-order models affect emissions greatly. Newer vehicles tend to emit less, and road grade significantly affects emissions, with some grades leading to emissions four times higher than others. Weather conditions also influenced emissions, although the maximum variation observed was about 10%.

Surrogate Model Accuracy: The surrogate models achieved a mean absolute percentage error (MAPE) of 6.013% when compared to MOVES across all scenarios. Figure 2 shows a detailed breakdown of error distributions across different model dimensions.

Model Architecture: As shown in Table 1. Various machine learning models were explored, with neural networks showing the best performance. The optimal neural network architecture consisted of three layers with a hyperbolic tangent activation function and a hidden dimension of 64.

Trajectory Validation: As the final step of our validation analysis, we conducted a detailed examination of individual trajectories to gain insights into specific driving cycle properties that may influence the surrogate models' performance. Figure 3 shows the performance of the models when applied to different trajectory types.

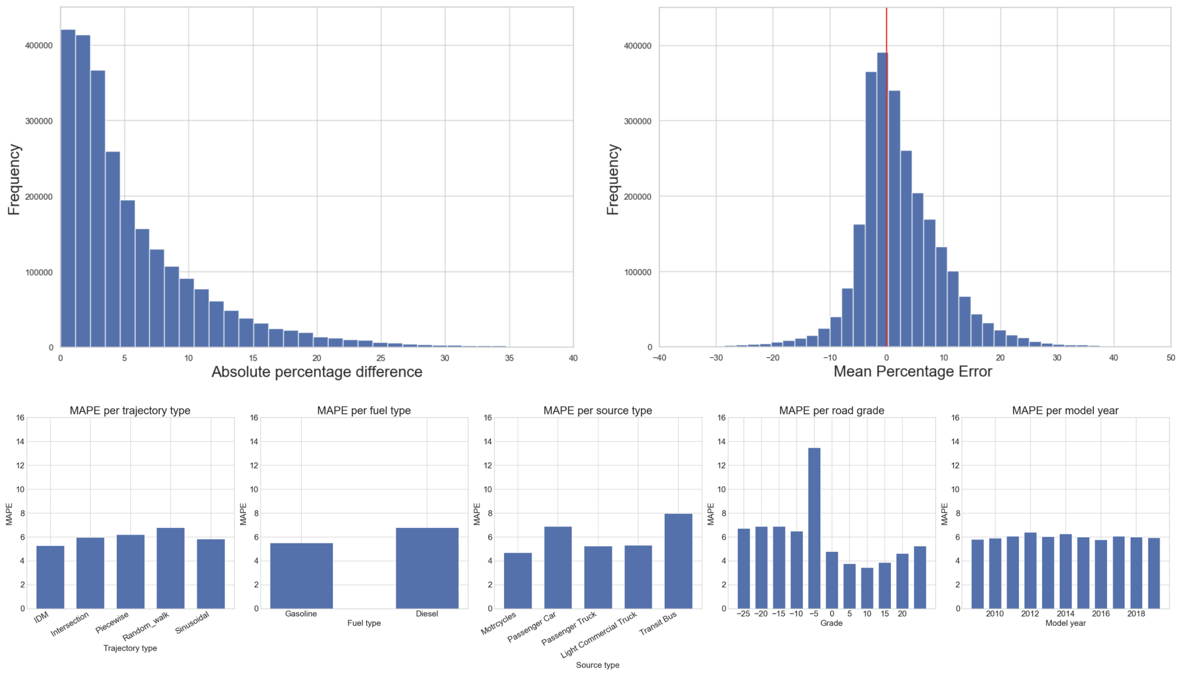

Figure 2 – *Distribution of Mean Absolute Percentage Error (MAPE) across over 2 million tests, evaluating the performance of surrogate models against the MOVES standard for representative trajectories and diverse environments. The MAPE, averaging 6.013%, illustrates the deviation between the surrogate models' emissions estimates and those calculated by MOVES. The error distribution, centered around zero, indicates a high precision and consistent accuracy of the surrogate models in estimating emissions across diverse scenarios and trajectories. This figure highlights the models' robustness and reliability as substitutes for MOVES, suitable for both micro and macro-scale environmental analysis.*

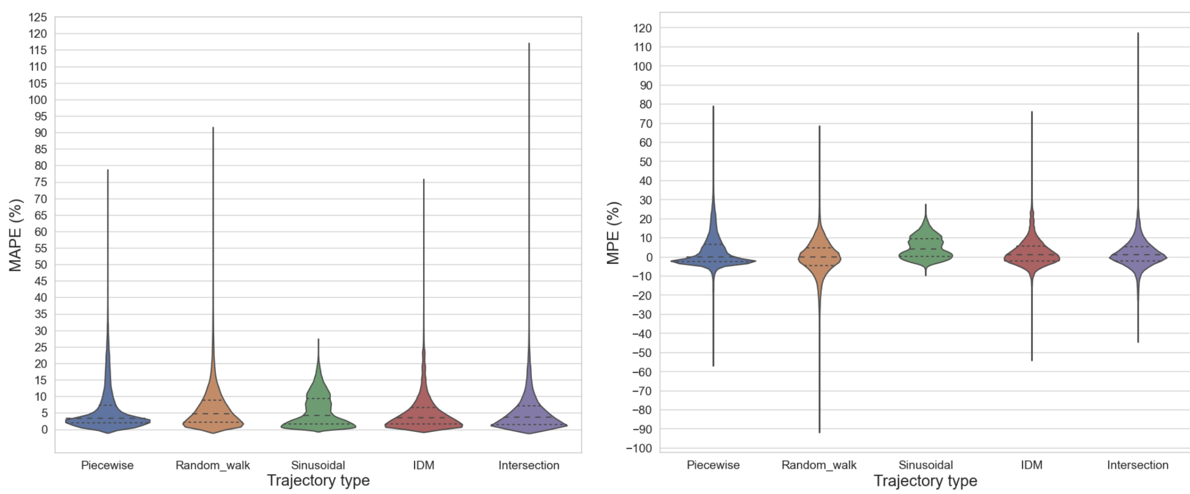

Figure 3 – *Distribution of Mean Absolute Percentage Error (MAPE) and Mean Percentage Error (MPE) for various trajectory types evaluated across all surrogate models, environments, and validation runs. The MAPE values are closely clustered around 6% for all trajectory types, with median values consistently below 5%, indicating a uniform error distribution irrespective of trajectory behavior. This uniformity across different driving behaviors such as IDM, Intersection, Piecewise, Random Walk, and Sinusoidal trajectories, which range from 5.77% to 6.877% in MAPE, underscores the models' consistent performance in diverse scenarios.*

Table 1 – *Surrogate model architectures and ablations with end-to-end error statistics.*

Model type	Architecture	Training	MAPE (%)	MPE (%)	MdPE (%)	StdPE
Polynomial	3rd order		31.04	8.9	5.22	50.16
Decision Tree	Depth 50		6.17	5.37	3.78	**7.75**
NN	2 layers, dim 5	11 epochs	149.73	124.43	65.64	165.17
NN	3 layers, dim 64	11 epochs	11.54	10.91	8.63	11.56
NN	2 layers, dim 5	300 epochs	7.85	6.04	4.81	9.44
NN	2 layers, dim 5 0.97 scaling	300 epochs	**6.01**	**2.46**	**1.22**	8.90

4 DISCUSSION

With a 6% mean absolute percentage end- to-end error, the surrogate models effectively capture the essence of MOVES and can serve as reliable substitutes for a wide range of applications. The lightweight and user-friendly nature of the surrogate models empowers transportation professionals and stakeholders, enabling them to reliably conduct microscopic and macroscopic (like control-based approaches and eco-driving) analyses with ease and efficiency. This level of precision signifies a substantial advancement in the field, providing a more accessible and computationally efficient alternative to the industry-standard emission model. Moreover the surrogate models' ability to accurately capture the diverse emission profiles across a wide spectrum of vehicle types, fuels, ages, road grades, and weather conditions, with over 22,000 unique profiles, enables more realistic modeling and marks a significant improvement over existing reduced-order models. **Future Directions and Considerations** include the integration of these models into traffic simulation tools and the replication of this methodology to get models for other pollutants.

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