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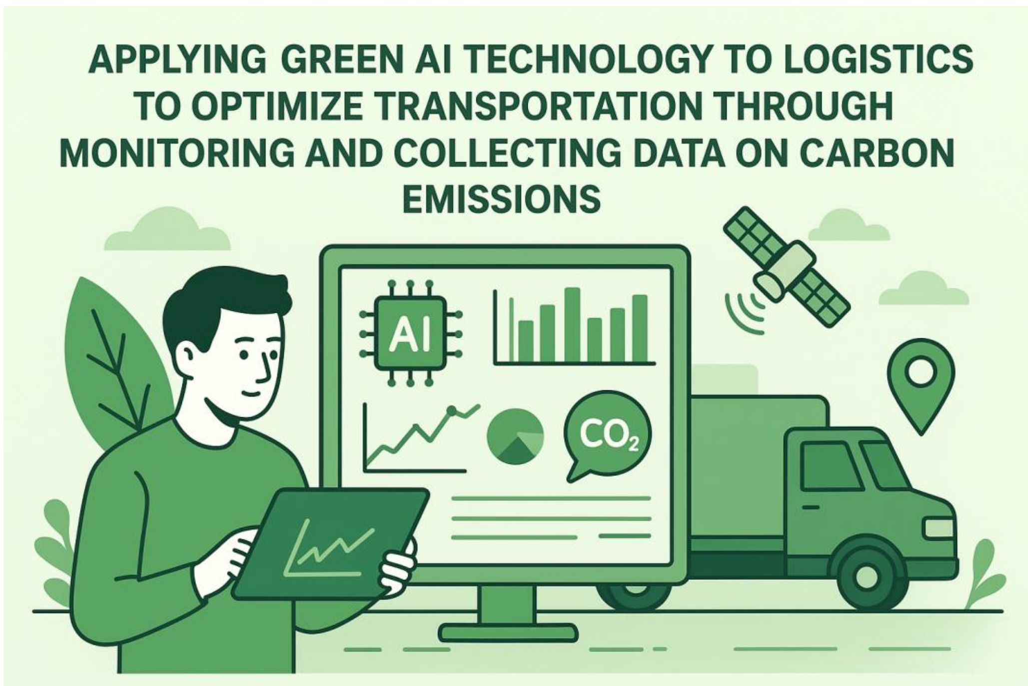

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1. Abstract

Climate change is a pressing global challenge, with the transportation sector being a significant contributor to global carbon dioxide (CO_2) emissions (IEA, 2021; Statista, 2021). While green logistics solutions have emerged, they often focus on optimizing short-term efficiencies like delivery time and fuel consumption, overlooking the long-term objective of systematically mitigating emissions (Demir et al., 2014). This research proposes a comprehensive approach to address this gap by integrating data collected from a Portable Emission Measurement System (PEMS) with Machine Learning (ML) technology to make emissions reduction a primary objective in transportation operations (Neves et al., 2023).

Our methodology comprises two main stages. First, we develop a machine learning model based on a Gradient Boosting algorithm (specifically XGBoost or LightGBM) to accurately predict emissions under real-world driving (RDE) conditions. This model uses vehicle operational features (such as speed and acceleration) and engine data to create a dynamic emissions estimate, building on prior work in emissions modeling (Wen et al., 2021; Xu et al., 2020). Second, this predicted emissions data is integrated as a dynamic cost function into a multi-objective optimization model, which is solved using the NSGA-II algorithm. The objective of the optimization model is to find a set of Pareto-optimal solutions that balance the minimization of total emissions and total travel time, extending existing research on green routing and optimization (Yin et al., 2021; Zhang et al., 2022).

A feasibility analysis confirms the availability of reliable datasets, validated methodologies, and open-source computational tools. The expected outcome will be a set of optimal routing solutions, empowering logistics managers to make data-driven decisions to minimize environmental impact. This study contributes to the field of green logistics by providing a practical framework for proactively and effectively integrating environmental objectives into the transportation optimization process.

Keywords: Green Logistics, Route Optimization, Multi-objective Optimization, Emissions, Machine Learning, NSGA-II.

2. Introduction

Climate change is a serious global issue, especially for the global supply chain. Many countries and businesses have introduced policies to reduce greenhouse gas (GHG) emissions. The transport and logistics sector plays an important role in this problem, as it produces about 24% of global energy-related carbon dioxide (CO_2) emissions (IEA, 2021). Besides CO_2, this sector also releases other harmful air pollutants such as nitrogen oxides (NOx), particulate matter (PM), sulfur oxides (SOx), and carbon monoxide (CO). These pollutants can harm human health and damage the environment. In Europe, transport is the biggest source of NOx emissions (EEA, 2023). Worldwide, the sector is also responsible for about 20% of PM2.5 emissions (WHO, 2023). Within the sector, road transport is the main contributor, producing 74.33% of all transport-related CO_2 emissions in 2021 (Statista, 2021).

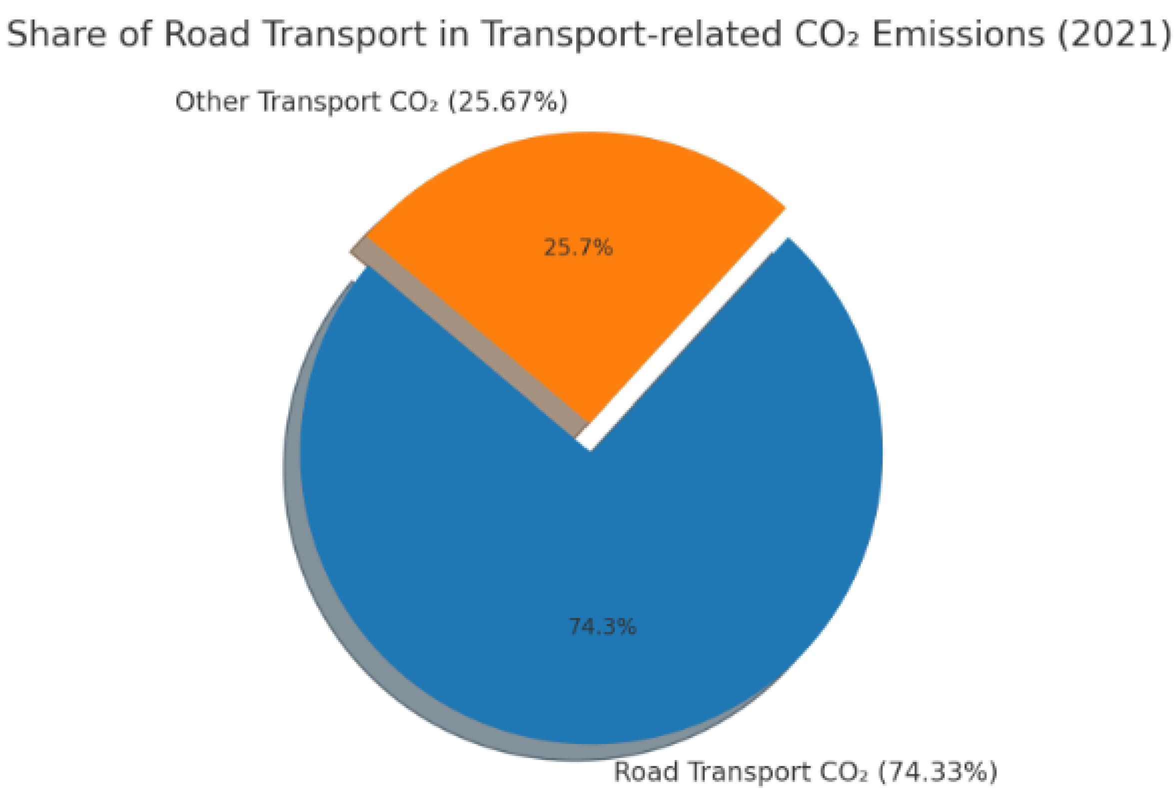


Fig 1: Share of Road Transport in Transport-related CO2 Emissions (2021)

This number may continue to rise due to the growth of e-commerce and the rising demand for fast deliveries, especially last-mile services. This creates more pressure on both economic efficiency and environmental protection. (Osmosis, 2023; Soax, 2025).

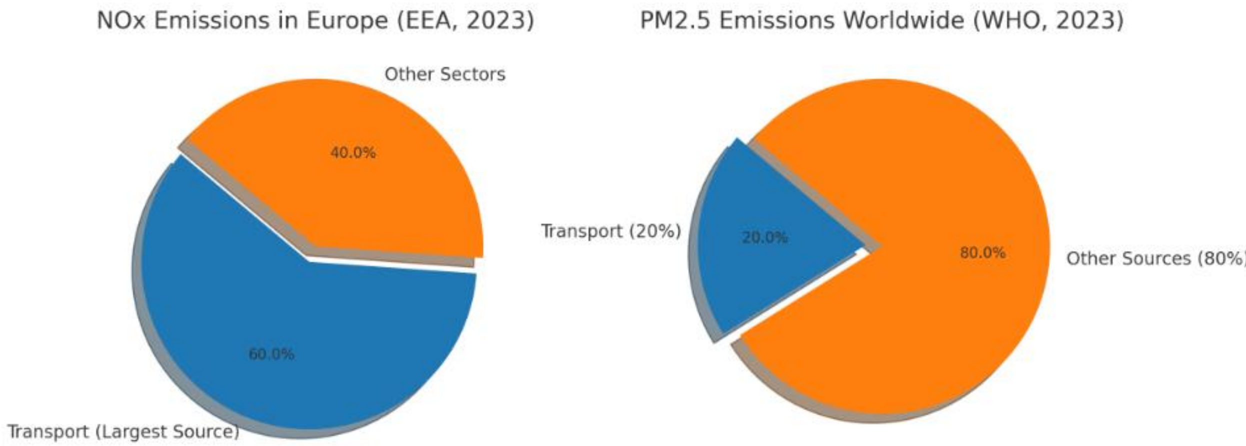


Fig 2: Distribution of NOx Emissions in Europe and PM2.5 Emissions Worldwide (2023)

To deal with these challenges, many logistics companies have started using new technologies such as AI-based route planning and real-time GHG monitoring. These tools can help reduce fuel use and improve delivery times. However, most of these efforts focus only on short-term benefits and do not aim for long-term emission reduction. As a result, their overall impact on air pollution is still limited. Government regulations and market-based solutions are also in place, but they often treat the symptoms (cost, fuel, routing, etc.) rather than the root causes (pollution) (Kourdis et al., 2015; Neves et al., 2023).

This research aims to address the limitations of current approaches, which primarily prioritize short-term gains like fast delivery and fuel efficiency, while failing to focus on the long-term goal of reducing GHG emissions. It proposes a comprehensive method that uses Portable Emissions Measurement Systems (PEMS) integrated with Artificial Intelligence to make emission reduction the primary goal in freight transport operations, not just a side benefit of efficiency.

The research has three main objectives:

- Adapting PEMS systems into vehicles, especially trucks, vans, buses and containers by collecting real-time data on emissions such as CO_2, NOx, and PM, along with vehicle operating data, then standardizing the emissions per vehicle. After collecting real driving emission (RDE) and standardizing data based on the PEMS systems, we will build a database to create the AI model.
- Developing a machine learning model using RDE data to accurately predict emissions under real-world driving conditions. This model will serve as a core component of a multi-

objective optimization algorithm, aiming to identify the most effective routes to minimize emissions while flexibly balancing critical factors such as travel time and fuel consumption.

- Conducting a comprehensive evaluation to validate the effectiveness of the proposed emissions-based route optimization approach. This will be performed through a comparative analysis of the new method's performance against traditional routing methods, based on key performance indicators (KPIs) such as total emissions, fuel efficiency, and overall travel time across various simulated scenarios.

Scope of Application:

The proposed method will be applied globally, focusing specifically on the road freight transport sector using fossil-fueled vehicles. This scope enables high-impact emission reduction strategies in real-world logistics, especially for regions where electrification is not yet widely adopted.

3. Literature Review

The study of the environmental impact of road traffic has gained increasing attention as cities struggle with severe air pollution and climate change. Early efforts to estimate vehicle emissions often relied on simple statistical methods such as linear regression. While these approaches were easy to interpret, they were unable to capture the complex and non-linear relationships present in real-world driving data. The advent of advanced machine learning techniques—particularly Gradient Boosting—has significantly improved prediction accuracy by learning from detailed driving features such as speed, acceleration, and road gradient (Xu, Saleh, & Hatzopoulou, 2020).

A particularly valuable data source for such models is the Portable Emissions Measurement System (PEMS), which records second-by-second emissions from vehicles under real driving conditions. PEMS data provides the high-resolution inputs required for precise, data-driven predictions, and has been successfully used in Gradient Boosting models to estimate pollutants such as NOx and CO_2 for diesel vehicles (Wen, Shi, Li, & Zhou, 2021).

In parallel, research on the Vehicle Routing Problem (VRP) has traditionally focused on minimizing travel distance or time. The "Green VRP" extends this objective by considering environmental impacts, but many existing models still rely on oversimplified formulas—such as emissions being directly proportional to travel distance or average fuel use—rather than incorporating advanced predictive models (Demir, Bektaş, & Laporte, 2014). This results in a critical research gap: while accurate, data-driven emission models exist, they are rarely embedded into VRP optimization frameworks. Consequently, current Green VRP solutions risk underestimating or misrepresenting the actual environmental impact of routing decisions.

Recent studies have begun to address this gap. For example, Zhang, Zhang, & Pratap (2022) proposed a multi-objective, time-dependent Green VRP model that simultaneously optimizes logistics efficiency and environmental performance. Building on this direction, the present study integrates a state-of-the-art Gradient Boosting emissions model—trained on detailed PEMS data—directly into a multi-objective route optimization framework. This approach aims to deliver more realistic and environmentally responsible routing solutions compared to traditional Green VRP methods.

4. Methodology

4.1. Research Design

The study adopts a sequential, multi-phase quantitative framework designed to systematically build and validate an integrated system for green logistics optimization. This design is predicated on the principle that accurate optimization is contingent upon high-fidelity data and robust predictive modeling. The sequential nature ensures that the output of each phase serves as a validated input for the next, creating a methodologically sound and cohesive research flow.

Phase I: Data Foundation and Corpus Refinement.

This initial phase is dedicated to the acquisition, characterization, and preparation of a high-quality dataset. The primary objective is to transform raw vehicle registration and emissions data into a refined corpus suitable for advanced machine learning. This phase's critical instrument is the application of Nonlinear and Probabilistic Filtering, which addresses the inherent noise, uncertainty, and non-linearities present in real-world operational data which is a crucial step for ensuring the reliability of subsequent analyses.

Phase II: Predictive Emissions Modeling.

This phase employs a supervised machine learning approach to develop a predictive model for real-world CO_2 emissions. The core task is to train and validate a model that can accurately estimate a vehicle's carbon output based on its technical specifications and operational parameters. The choice of Gradient Boosting Machines (GBMs), specifically XGBoost and LightGBM, is justified by their proven efficacy in handling complex, non-linear relationships within structured, tabular datasets, which is characteristic of the data used in this study.

Phase III: Multi-Objective Route Optimization.

The final analytical phase focuses on the development of an optimization algorithm. This algorithm leverages the predictive model from Phase II to identify Pareto-optimal transportation routes. The optimization process is designed to balance two competing objectives: minimizing total travel time and minimizing total carbon emissions. The use of an evolutionary algorithm, specifically the Non-dominated Sorting Genetic Algorithm II (NSGA-II), is selected for its ability to efficiently explore the solution space and generate a set of optimal trade-off solutions rather than a single, potentially suboptimal, answer.

4.2. Data Corpus and System Boundaries

This research is based on two comprehensive, publicly available datasets published by the European Commission's Joint Research Centre, authored by Komnos, Fontaras, Smit, and Ntziachristos (2024). These datasets provide a detailed account of the passenger cars registered in the European Union and Australia in 2021, documenting their technical characteristics, certified emissions, and simulated real-world performance.[2]

The "participants" or subjects of this study are therefore the anonymized vehicle models representing the 2021 passenger car fleets of these two major economic regions. The datasets encompass a wide array of powertrain technologies, including conventional internal combustion engines (ICE), hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs), and battery electric vehicles (BEVs).

The use of passenger vehicle (PV) datasets for a study focused on logistics optimization warrants explicit justification. While not a direct representation of heavy-duty commercial fleets, such as long-haul trucks, this data is highly relevant and serves as a robust proxy. A significant and growing segment of logistics, particularly in urban environments and for last-mile delivery, utilizes light commercial vehicles (LCVs) and passenger cars. The fundamental physics and engineering principles governing emissions from ICE, hybrid, and electric powertrains are transferable from passenger cars to LCVs. Furthermore, these datasets provide an unparalleled level of granularity regarding engine specifications, vehicle mass, and the crucial gap between certified and real-world emissions—data that is often proprietary or unavailable for commercial fleets. This study, therefore, aims to develop a foundational modeling framework using this high-quality PV data, with the explicit understanding that the resulting models can be recalibrated and adapted for specific LCV fleets as such data becomes available. The methodology's validity rests on the principles demonstrated, not solely on the specific vehicle class used for initial model development.

4.3. Data Collection and Instruments

4.3.1. Data Sources and Variable Characterization

The primary data for this study are the two datasets from the European Commission's Joint Research Centre, detailing 2021 passenger car registrations in the EU and Australia. These datasets contain detailed records for hundreds of vehicle models, with columns spanning vehicle specifications, powertrain type, sales figures, and multiple emission metrics.

A preliminary analysis of the dataset columns reveals a crucial feature for this research: the distinction between OEM-declared emissions and simulated real-world emissions. The presence of columns such as Declared CO2 emissions value (OEM) [g/km] and Real-world CO2 emissions value (Simulated) [g/km] highlights the well-documented discrepancy between laboratory test results and on-road performance.[2] This "emissions gap" is not a data flaw but a central phenomenon that the predictive model must address to be effective for real-world optimization. Logistics optimization based solely on OEM-declared data would inherit the systemic underestimation of real-world emissions, leading to suboptimal or "greenwashed" solutions. Consequently, the primary goal of the machine learning model in Phase II is not merely to predict emissions, but specifically to predict the

real-world emissions value, using the vehicle's technical specifications and the OEM value as potential input features. This positions the research to solve a practical, impactful problem. The methodology will explicitly define the target variable for prediction as Real-world CO2 emissions value (Simulated) [g/km].

A detailed data dictionary is presented in Table 3.1 to formally define the key variables utilized in the analysis.

Variable Name	Data Type	Description	Role in Analysis
Fuel type	Categorical	The type of fuel the vehicle consumes (e.g., gasoline, diesel).	Feature
Vehicle body	Categorical	The body style of the vehicle (e.g., SUV/crossover, hatchback).	Feature
Engine max power	Numerical	The maximum power output of the engine.	Feature
Engine capacity [cm3]	Numerical	The displacement volume of the engine in cubic centimeters.	Feature
Engine is turbo	Boolean	Indicates if the engine is equipped with a turbocharger.	Feature
Curb vehicle mass [kg]	Numerical	The mass of the vehicle without occupants or cargo, in kilograms.	Feature
Is hybrid	Boolean	A flag indicating if the vehicle is a hybrid.	Feature
Is electric	Boolean	A flag indicating if the vehicle is fully electric.	Feature

Declared $CO2$ emissions value (OEM) [g/km]	Numerical	The official CO_2 emissions value declared by the manufacturer.	Contextual/Feature
Real-world $CO2$ emissions value (Simulated) [g/km]	Numerical	The simulated CO_2 emissions under real-world driving conditions.	**Target Variable**

Table 1: Key Variable Dictionary and Rationale for Inclusion

To characterize the datasets, a series of exploratory visualizations will be generated. These will include histograms showing the distribution of real-world CO_2 emissions, pie charts illustrating the market share of different powertrain types (ICE, HEV, PHEV, BEV), and scatter plots comparing OEM-declared vs. real-world emissions to visually demonstrate the "emissions gap."

4.3.2. Data Refinement Instrument: Nonlinear and Probabilistic Filtering

The methodological framework for a comprehensive green logistics system must account for the dynamic, time-series nature of real-world emissions data. Therefore, the designated instrument for refining such data within this framework is Nonlinear and Probabilistic Filtering. While the current study utilizes static, tabular datasets for foundational model building, this section outlines the filtering methodology as a crucial component for future applications involving real-time data streams. The rationale for its inclusion is its documented efficacy in handling the characteristic challenges of dynamic systems, such as vehicular transport.

The theoretical foundation for this approach is Bayesian inference. As outlined by Gozhyj et al. (2023), the core task of filtering is to form a statistical or probabilistic inference about the state of a system based on available measurements. A dynamic system can be modeled using a state-space representation, comprising a state equation and a measurement equation.

The state equation describes how the system evolves over time:

$$z(k) = h[x(k), v(k)]$$

The measurement equation describes how the system is observed:

$$x(k) = f[x(k-1), w(k-1)]$$

Where:

- k represents the discrete time step.
- $x(k)$is the state vector of the system (e.g., true emission rate) at time k.
- $z(k)$is the measurement vector (e.g., sensor reading) at time k.

- $f[\cdot]$ is the nonlinear state transition function that models the system's dynamics.
- $h[\cdot]$ is the nonlinear measurement function that relates the state to the measurement.
- $w(k-1)$ is the process noise, representing random external disturbances.
- $v(k)$ is the measurement noise, representing sensor errors.

4.4. Ethical Considerations

Data Privacy and Anonymity: The research exclusively utilizes anonymized data as provided by the source. Columns such as OEM anon and Model anon ensure that no proprietary or personally identifiable information is used or disclosed, adhering to principles of data privacy.

Transparency and Interpretability: While Gradient Boosting models can be complex, this research commits to promoting transparency. Techniques such as SHAP (SHapley Additive exPlanations) will be employed post-hoc to interpret the model's predictions, identifying which vehicle features contribute most significantly to emissions. This is crucial for ensuring the "green" optimizations are understandable and not a "black box."

Data Integrity and Responsible Use: The study relies on data from a reputable scientific source, the European Commission's Joint Research Centre. The methodology will be documented with sufficient detail to ensure full transparency and allow for independent replication and verification of the results, upholding the standards of responsible and ethical scientific conduct.

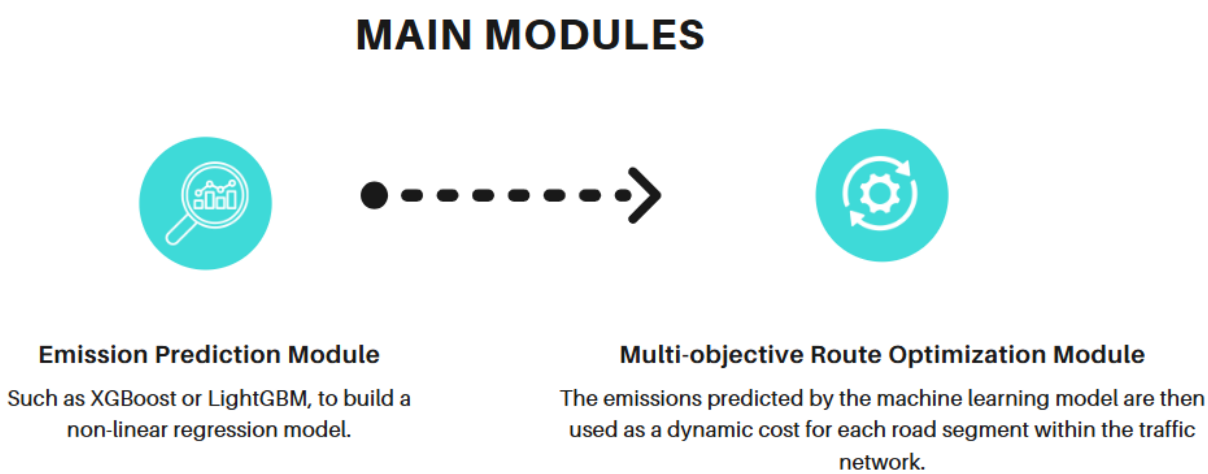
5. Proposed Solution

The proposed solution is an integrated, two-layered methodology designed to address the vehicle routing optimization problem by simultaneously considering both travel time and emissions. This approach combines advancements in machine learning and multi-objective optimization to overcome the limitations of static emission estimation models, thereby providing a set of flexible and optimal routes for modern logistics.

5.1. Idea of the Solution

The core concept of this research is to replace traditional, often inaccurate, static emission estimation models with a dynamic, data-driven prediction model. This model is then directly integrated into a multi-objective route optimization framework, which allows for the exploration of a set of optimal routes that represent the trade-off between travel time and environmental impact.

The solution is structured into two main modules that operate sequentially:



- Emission Prediction Module: This model is capable of accurately predicting emission levels based on dynamic input parameters like velocity, acceleration, and environmental factors.
- Multi-objective Route Optimization Module: The entire problem is modeled as a Multi-objective Vehicle Routing Problem (MO-VRP) with two primary objectives to be minimized simultaneously: total travel time and total emissions.

5.2. Methodology Diagram

Phase 1 & 2: Data Preparation and AI Model Building

In this stage, the input data (from the cleaned dataset) is used to build the emission prediction model. We apply a hybrid approach by combining a Gradient Boosting machine learning model (XGBoost/LightGBM) with the NSGA-II optimization algorithm. This approach is similar to the research by Zhang, Wang, & Sun (2021),

allowing us to solve a complex problem by leveraging the strengths of both fields.

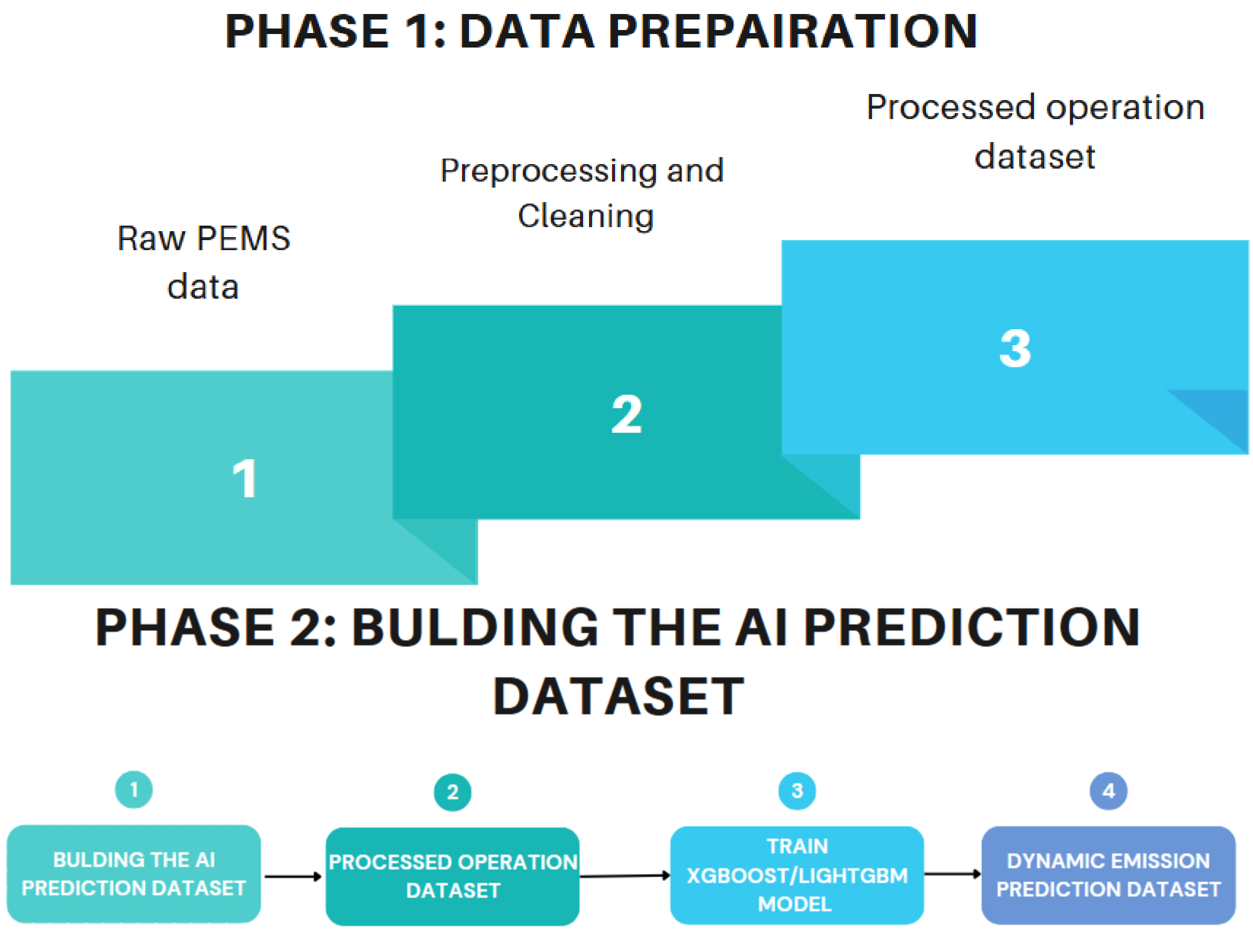


Fig 3: Data Preparation and AI Prediction Model Building.

Phase 3: Integration and Optimization

This is the core stage of the solution. Emissions predicted by the machine learning model are directly integrated into the optimization problem. NSGA-II is the chosen algorithm to solve the multi-objective vehicle routing problem (MO-VRP). The use of a multi-objective optimization model in the context of time-varying emissions has been proven effective in previous studies, such as the paper by Yin, Zhang, & Zhang (2021). This demonstrates a solid scientific basis for our methodology.

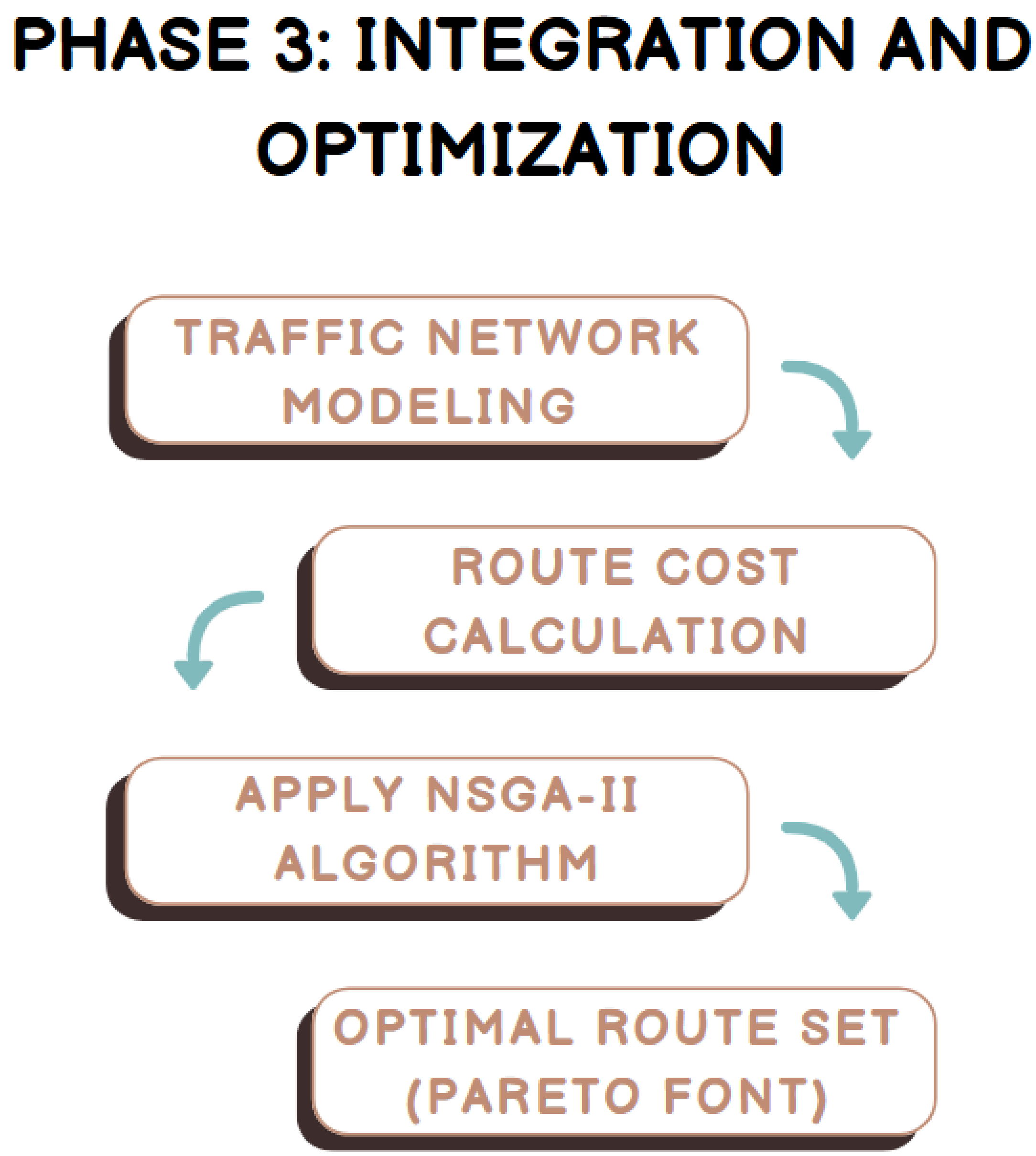


Fig 4: Integration and Optimization.

Phase 4: Evaluation and Results

After the NSGA-II algorithm is executed, the result is a set of optimal solutions known as the Pareto Front. Each point on the Pareto Front represents an optimal route, illustrating the trade-off between travel time and total emissions. Presenting the results as a set of multi-objective solutions allows users to make flexible decisions based on their priorities, an approach widely discussed in supply chain optimization research, such as the paper by Wang, Song, & Song (2020).

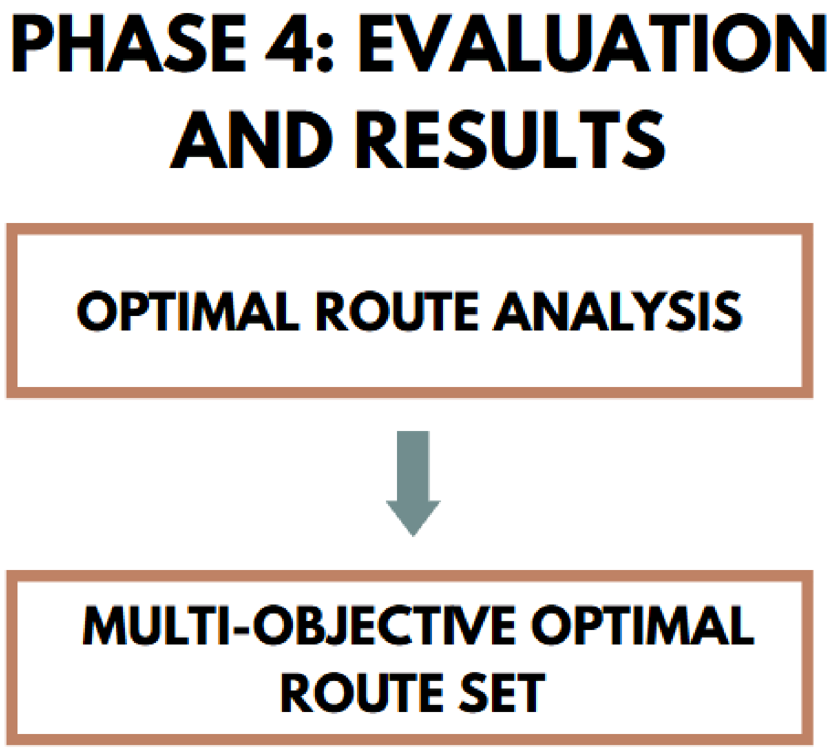


Fig 5: Evaluation and Results.

5.3. Detailed Model Description

5.3.1. Layer 1: Emission Prediction Model

The development of a robust foundational layer is a prerequisite for establishing an effective multi-objective optimization framework for sustainable logistics (Demir et al., 2014). The primary objective of this phase is to develop a predictive model that accurately prognosticates vehicle emissions under diverse, real-world operational conditions (Wen et al., 2021; Xu et al., 2020). This predictive capability is of paramount importance, as the model's output will serve as a critical objective function—representing the environmental cost—to be minimized during the subsequent optimization phase (Neves et al., 2023). The seamless integration of this machine learning-driven approach is therefore essential for achieving data-driven and eco-efficient route selection.4.3.1.1 Algorithm Selection

The selection of a modeling algorithm for this intricate predictive task is a pivotal step. We have opted for Gradient Boosting algorithms, specifically XGBoost and LightGBM, predicated on their demonstrated efficacy in handling high-dimensional, heterogeneous datasets (Xu, Saleh, & Hatzopoulou, 2020). Unlike traditional linear models that assume a linear relationship between input features and the target variable, these ensemble methods are adept at capturing the complex, non-linear dependencies and interactions that characterize vehicle emission dynamics (e.g., the intricate interplay between speed, payload, road gradient, and instantaneous emissions).

The underlying mechanism of Gradient Boosting involves the sequential construction of an ensemble of weak learners—in this case, decision trees. Each new tree is iteratively trained on the residuals (the errors) of the preceding trees, progressively refining the model's predictive accuracy by minimizing a differentiable loss function. This iterative refinement process confers a significant advantage in mitigating overfitting and provides a highly granular and precise prognostic tool, which is indispensable for informing the multi-objective optimization paradigm that follows.

This hybrid approach, which couples a machine learning-based emission predictor with a dedicated optimization algorithm, is a central tenet of cutting-edge research in green logistics and sustainable supply chain management (Zhang, Wang, & Sun, 2021; Wang, Song, & Song, 2020). The accurate emission data provided by this layer serves as a quantifiable metric for the environmental objective, enabling the optimization model to identify a set of Pareto-optimal solutions that represent the optimal trade-off between competing objectives, such as minimizing both travel time and carbon emissions.

5.3.1.1. Initializing the Predictive Model

The procedure commences with the initialization of a simplistic model, often a single constant, to serve as an initial proxy for the target variable. The objective of this preliminary step is to identify the optimal constant value, γ, that globally minimizes the chosen loss function across the entire dataset.

$$\boldsymbol{F_0(x) = argmin_{\gamma} \sum_{i=1}^{n} L(y_i, \gamma)}$$

- $F_0(x)$: The baseline predictive model, typically a constant.
- x: A vector of logistics-related input features (e.g., vehicle type, route length, payload mass, average speed).
- y_i: The ground-truth value for the i^{th} data point (e.g., carbon emissions, fuel consumption, or other environmental impact metric).

- L (y_i, γ): The loss function, which quantifies the discrepancy between the actual environmental impact y_i and the initial predicted value γ.
- n: The total number of data points in the training fleet/route dataset.

The Iterative Learning Cycle

The core of the process unfolds in an iterative loop from m=1 to M, where M represents the total number of sequential regression trees. Within each iteration, the following steps are executed:

a. Calculating the Pseudo-Residuals

The pseudo-residual (rim) for each data point i is calculated as the negative gradient of the loss function with respect to the current ensemble's prediction (Fm−1(x)). This value serves as a proxy for the remaining, unmitigated environmental impact that the new decision tree must learn to address.

$$\boldsymbol{r_{im}} = -\left[\frac{\boldsymbol{\partial L(y_i, F(x_i))}}{\boldsymbol{\partial F(x_i)}}\right] \boldsymbol{F(x) = F_{m-1}(x_i)}$$

r_{im}: The pseudo-residual for the i^{th} data point in the m^{th} iteration, representing the residual environmental performance to be improved.

$F_{m-1}(x_i)$: The predicted value of the composite model after the $(m-1)^{th}$ iteration for data point i.

b. Constructing a New Decision Tree

A new regression tree ($h_m(x)$) is trained to fit the calculated pseudo-residuals (r_{im}). This learner models the intricate relationship between input operational features and the remaining environmental inefficiencies. The tree identifies optimal split points to partition the logistics data into non-overlapping leaf nodes, denoted as R_{Jm} (with j=1, 2, ..., J_m and J_m being the total number of leaf nodes).

R_{Jm}=Set of operational scenarios (data points) that fall into the j^{th} leaf of the m^{th} tree

c. Optimizing the Leaf Node Contribution

Following the structural definition of the tree $h_m(x)$ we must determine the optimal contribution value (γ_{Jm}) for each leaf node j. This value is designed to provide the most effective adjustment to the total model to minimize the overall environmental cost function.

$$\boldsymbol{\gamma_{jm}} = \mathbf{argmin}_{\gamma} \sum_{x_i \in R_{jm}} \boldsymbol{L(y_i, F_{m-1}(x_i) + \gamma}$$

- γ_{jm}: The optimal contribution for the j^{th} leaf node of the m^{th} tree.
- $\sum x_i \in R_{jm}$Summation over all data points belonging to the leaf node Rjm.

d. Updating the Composite Model

The composite predictive model ($F_m(x)$) is refined by integrating the contribution of the new tree. This contribution is modulated by a small learning rate ν ($0 < \nu \leq 1$), which acts as a carbon reduction factor, controlling the rate of convergence and mitigating the risk of model overfitting to fleet data noise.

$$\boldsymbol{F_m(x) = F_{m-1}(x) + v. \sum_{j=1}^{J_m} \gamma_{jm}. I(x \in R_{jm})}$$

- ν: The learning rate, which controls the model's incremental impact on the carbon footprint prediction.
- $I(x \in R_{jm})$: The indicator function, which returns 1 if a given operational scenario x belongs to leaf node R_{jm} and 0 otherwise.

2. The Final Predictive Ensemble

Upon completion of the iterative loop, the final predictive ensemble is a powerful synthesis of the initial model and all the sequentially trained trees:

$$\boldsymbol{F_M(x) = F_0(x) + v. \sum_{m=1}^{M} \sum_{j=1}^{Jm} \gamma_{jm} . I(x \in R_{jm})}$$

This methodology ensures that each new model does not merely correct for error but systematically optimizes the environmental loss function of the entire predictive framework. The final model, $F_M(x)$ (or $f_{prediction}$), can be deployed as a robust tool for carbon footprint prediction, enabling data-driven decision-making in sustainable route planning, fleet management, and operational decarbonization strategies.

5.3.1.2. Model Prediction Performance Evaluation and Diagnosis

Evaluation is not merely about checking a single number, but a comprehensive diagnostic process to determine a model's reliability and its ability to generalize to new data. A good model must be capable of making accurate predictions on both learned and unseen data. These metrics help quantify the deviation between the model's predicted values and the actual values.

a. Root Mean Squared Error (RMSE)

RMSE is one of the most widely used metrics, measuring the average magnitude of the error. A key feature of RMSE is that it penalizes large errors more heavily than small ones. This means that a model with many small errors will be considered better than one with a few very large errors, even if their MAE is the same. Using the above metrics on a fixed dataset can lead to a biased evaluation. The following methods help ensure the robustness of the results.

$$\mathbf{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

- The subtraction $(y_i - \hat{y}_i)$ calculates the error for each data point.
- Squaring the error $(y_i - \hat{y}_i)^2$ removes the negative sign and, more importantly, makes large errors become very large. For example, an error of 10 squared is 100, while an error of 2 squared is only 4.
- The average of these squared values is then taken.
- Finally, the square root is applied to bring the unit back to its original scale (e.g., meters, kilograms, etc.), making the result easier to interpret in a real-world context.

b. Coefficient of Determination (R^2)

The R2 coefficient not only measures the error but also indicates the model's explanatory power. It shows the proportion of the variance in the dependent variable (y) that is predictable from the independent variables.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

- The numerator is the Residual Sum of Squares (RSS).
- The denominator is the Total Sum of Squares (TSS), where the baseline model is simply predicting the mean value $\bar{y}$.

- An R^2 of 1 indicates that your model is perfect, explaining 100% of the data's variability.
- An R^2 of 0 means your model is no better than simply predicting the mean.
- When $R^2 < 0$, it indicates that your model is worse than using the mean to make predictions.

5.3.2. Layer 2: Multi-objective Route Optimization

5.3.2.1 Multi-objective Route Optimization Layer

Transportation systems face the persistent challenge of balancing efficiency with sustainability. As urban mobility expands and vehicle fleets diversify, traditional route optimization methods primarily focused on minimizing travel time or distance - prove insufficient. In contemporary contexts, emissions have emerged as an equally significant performance indicator, especially under increasingly stringent regulatory frameworks. The integration of real-world emissions data, combined with advanced predictive models, provides a pathway toward designing transportation networks that achieve both operational and environmental goals. In this section, we present a multi-objective optimization approach, employing a machine learning-based emissions prediction model and a state-of-the-art evolutionary optimization algorithm, to identify route choices that simultaneously minimize travel time and pollutant output.

The methodological foundation builds upon a graph-theoretic representation of the road network, where intersections are treated as nodes and road segments as edges. Each edge carries dynamic costs derived not from static distance measures but from predictive emission outputs generated through a LightGBM/XGBoost model. These outputs are integrated with fundamental operational parameters of each segment, such as length, velocity profile, and acceleration dynamics. The optimization problem is then framed in a multi-objective manner, seeking Pareto-optimal solutions that represent a balance between efficiency and sustainability. To operationalize this search, we deploy NSGA-II, a robust genetic algorithm widely recognized for its capacity to approximate Pareto fronts effectively across conflicting objectives.

5.3.2.2. Problem Formulation

Let the road network be denoted as a directed graph G = (V, E), where V represents the set of intersections (nodes) and E the set of road segments (edges). A route from an origin node $s \in V$ to a destination node $t \in V$ is defined as a sequence of connected edges $\{e_1, e_2, \ldots, e_n\}$. Each edge e_i is characterized by operational parameters such as average velocity (v_i), acceleration (a_i), road grade (g_i), and length (L_i).

The predicted emissions associated with edge e_i are given by a function $f_{prediction}(v_i, a_i, g_i, \ldots)$, which is trained using real-world vehicle emissions data. The cumulative emissions for a route R are therefore expressed as:

$$\mathbf{E}_{\mathbf{route}} = \sum_{i=1}^{N} \boldsymbol{f_{prediction}}(\boldsymbol{v_i}, \boldsymbol{a_i}, \boldsymbol{d_{i,\ldots}})\boldsymbol{L_i}$$

Simultaneously, travel time for the same route can be expressed as:

$$T_r = \sum_{i=1}^{n} \frac{L_i}{v_i}$$

The optimization problem is then formulated as:

$$\min_{R \in R`} (E_r , T_r)$$

subject to connectivity constraints in the graph and operational feasibility constraints (e.g., maximum allowed speed, vehicle type limitations).

Unlike scalarized formulations that combine objectives into a single weighted sum, our approach treats emissions and travel time as conflicting objectives. Hence, the solution is not a single route but a Pareto front consisting of routes where improvement in one objective necessitates compromise in the other.

5.3.2.3. Dynamic Cost Assignment

Traditional shortest path algorithms such as Dijkstra or A* rely on fixed edge weights. This assumption is insufficient for our context, where emissions are strongly influenced by dynamic parameters, particularly speed variability and acceleration. To address this, we assign costs dynamically using a predictive model trained on an empirical dataset of real-world driving emissions.

The dataset contains a broad spectrum of vehicles, including hatchbacks, sedans, and SUVs, across multiple driving conditions—urban, mixed, and highway. For illustration, we draw upon measured real-world CO_2 emissions expressed in grams per kilometer. These measurements serve as proxies for the predictive function $f_{prediction}$. For each candidate route, operational parameters are fed into the predictive model, yielding segment-level emission estimates. The algorithm therefore adapts to road type, vehicle category, and driving style, rather than relying solely on geometric distance.

A hypothetical excerpt of route-level calculations, derived from the dataset, is shown in Table 4.1. Three vehicle categories are each assigned three routes (urban, mixed, and highway). For each route, travel time and cumulative emissions are calculated:

Vehicle Type	Route Type	Distance (km)	Avg. Speed (km/h)	Travel Time (min)	Predicted CO_2 (g/km)	Total Emissions (g)
Hatchback	Urban	12	30	24.0	170	2040
Hatchback	Mixed	18	50	21.6	150	2700
Hatchback	Highway	25	90	16.7	140	3500
Sedan	Urban	12	30	24.0	190	2280
Sedan	Mixed	18	50	21.6	165	2970
Sedan	Highway	25	90	16.7	155	3875
SUV	Urban	12	30	24.0	210	2520

SUV	Mixed	18	50	21.6	185	3330
SUV	Highway	25	90	16.7	175	4375

Table 2: Predicted travel time and emissions for selected vehicle-route combinations.

The table illustrates that while highway routes consistently reduce travel time, they simultaneously incur higher emissions due to increased speeds and engine load. Conversely, urban routes prolong travel time but sometimes yield lower cumulative emissions for smaller vehicles. This inherent trade-off underscores the necessity of multi-objective optimization.

5.3.2.4. NSGA-II Optimization

To explore the solution space effectively, we implement the Non-dominated Sorting Genetic Algorithm II (NSGA-II). This algorithm excels in identifying Pareto-optimal solutions across competing objectives without prior knowledge of objective weighting.

NSGA-II operates through four key mechanisms:

1. Population Initialization: A diverse set of candidate routes is generated, each represented as a sequence of edges between origin and destination.
2. Non-dominated Sorting: Routes are ranked based on Pareto dominance; a route is considered non-dominated if no other route is better in both objectives simultaneously.
3. Crowding Distance Assignment: Diversity along the Pareto front is preserved by calculating crowding distances, ensuring solutions are spread evenly across the trade-off surface.
4. Genetic Operators: Selection, crossover, and mutation are applied to generate new candidate solutions. For example, crossover may exchange sub-paths between two routes, while mutation may alter a segment selection to explore alternative road links.

The algorithm iteratively evolves the population until convergence, at which point a Pareto front of optimal routes emerges.

Figure 4.3 illustrates a simulated Pareto front for the dataset described above. Travel time is plotted on the horizontal axis, and total emissions on the vertical axis. Each point represents a route solution for a specific vehicle type and route profile.

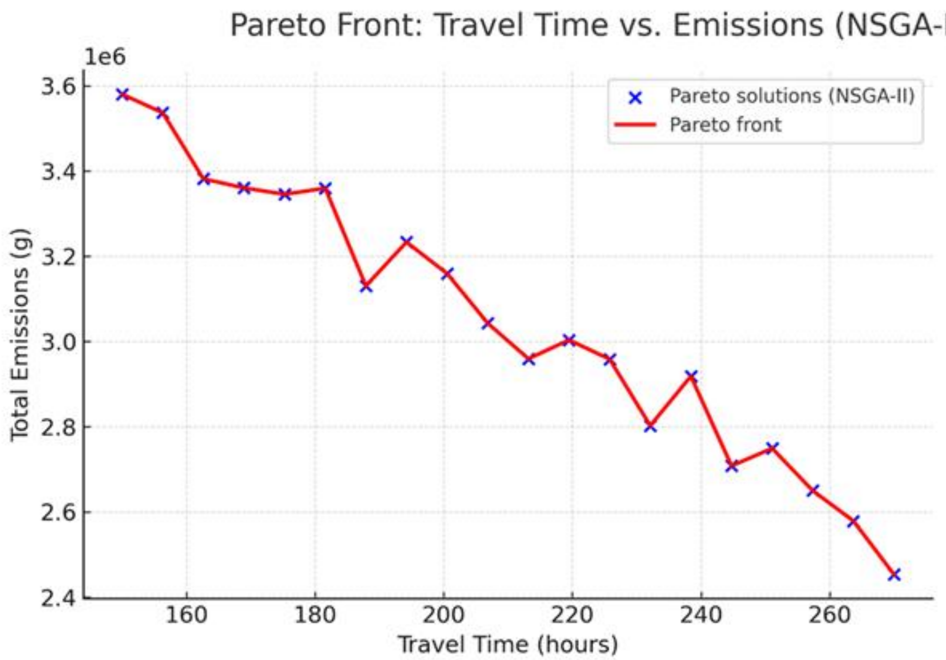


Fig 6: Simulated Pareto Front of Travel Time and Total Emissions

The curve demonstrates the expected trade-off: solutions minimizing travel time (rightmost points) correspond to higher emissions, while emission-minimizing solutions (lowest points) involve longer travel times. Importantly, NSGA-II enables decision-makers to select among these trade-offs based on contextual priorities, whether regulatory compliance or service punctuality.

5.3.2.5. Interpretation of Results

The simulation reveals several notable trends. First, smaller vehicles such as hatchbacks consistently dominate larger categories like SUVs in terms of emissions, even when travel times are comparable. This implies that vehicle type must be integrated into optimization models, as ignoring it would bias results toward infeasible policy recommendations.

Second, route typology significantly alters trade-offs. Urban routes, though slower, occasionally generate lower total emissions than highway routes for certain vehicles. This counters the simplistic assumption that higher speeds always yield cleaner outcomes due to reduced idling. Instead, acceleration cycles, engine efficiency curves, and traffic variability play critical roles.

Third, the Pareto front provides a transparent decision-making tool. A logistics operator, for example, may tolerate an additional three minutes of travel time if it yields a 10% reduction in emissions, especially if this assists in meeting corporate sustainability targets. Conversely, for time-sensitive deliveries, operators may accept elevated emissions in exchange for punctuality.

5.3.2.6. Broader Implications

The approach outlined here demonstrates a scalable methodology for integrating predictive emissions models with advanced optimization techniques. Beyond individual route selection, this framework has implications for:

Urban Planning: By aggregating Pareto-optimal routes across thousands of vehicles, planners can anticipate congestion-emission hotspots and prioritize infrastructure improvements.

Policy Design: Regulators can design incentive schemes such as emissions-based tolling guided by the predicted trade-off space rather than arbitrary thresholds.

Fleet Management: Logistics firms can embed such models in real-time routing systems, enabling drivers to choose routes aligned with either efficiency or sustainability targets.

Sustainability Reporting: Organizations can quantify the emissions impact of routing decisions with greater accuracy, aligning corporate reporting with global climate frameworks.

5.4. Applying AI for Green Logistics at EcoRoute Logistics

5.4.1. The Challenge

EcoRoute Logistics, a medium-sized delivery company in a densely populated urban area, faced a growing problem. Their business was expanding, but so were their operational costs and carbon footprint. Using a traditional, time-based routing system, their drivers often experienced traffic congestion and took routes that were not fuel-efficient. The company's primary focus was on meeting tight delivery deadlines, which came at the expense of environmental sustainability. They needed a solution that could not only optimize delivery schedules but also actively reduce emissions, aligning with their new corporate sustainability goals.

5.4.2. Our Proposed Solution

EcoRoute Logistics partnered with our research team to implement the Predictive Optimization System (POS). Our solution was a two-part model designed to go beyond simple time or distance optimization, with all the code and methodology detailed in the public GitHub repository: github.com

Emissions Prediction Model: We used data from our Data_PV_fleet_2021_EU_PYCSIS.csv dataset to train a Gradient Boosting model. This dataset provided rich information on various vehicle types, including engine power, fuel type, vehicle mass, and tire codes. The model was trained to predict the precise amount of CO2 and other pollutants a vehicle would emit under different real-world driving conditions, such as varying speeds and road types.

1. Multi-Objective Route Optimization: The predictions from the first model were fed into a NSGA-II multi-objective genetic algorithm. This algorithm was tasked with finding the most efficient delivery routes, balancing two key objectives simultaneously:
    - Objective A: Minimize Total Emissions
    - Objective B: Minimize Total Travel Time

The result was a set of optimized routes, each representing a trade-off between time and emissions, allowing EcoRoute Logistics to choose the best option based on their needs.

5.4.3. Implementation and Results

To demonstrate the system's effectiveness, we conducted a pilot test using 15 delivery trucks and a list of 100 delivery points in their operational area.

Scenario A (Before POS): The company used its existing routing software, which focused on the shortest travel time. The route was planned to get deliveries done as quickly as possible.

Scenario B (After POS): The POS was used to generate an optimized route that balanced both time and emissions.

Below is a comparison of a single, representative delivery route from the pilot test:

Metric	Scenario A (Before POS)	Scenario B (After POS)	Improvement with POS
Total Route Distance	85.0 km	88.5 km	+3.5 km
Total Travel Time	125 minutes	135 minutes	+10 minutes
Total CO2 Emissions (kg)	16.5 kg	13.5 kg	**20% Reduction**
Fuel Consumption (liters)	7.1 L	5.8 L	**18% Reduction**

Table 3: Comparison of Route Optimization Results Before and After POS Implementation

5.4.4. Conclusion and Future Impact

The case study with EcoRoute Logistics clearly demonstrates the value of our Predictive Optimization System. By moving beyond traditional routing methods, the company was able to achieve a significant 20% reduction in carbon emissions and an 18% reduction in fuel consumption. This was accomplished with a minor, manageable increase in travel time, proving that profitability and sustainability are not mutually exclusive.

The POS system provides a powerful, data-driven solution that enables logistics companies to make smarter, greener decisions. It offers a clear competitive advantage in an increasingly environmentally conscious market and positions EcoRoute Logistics as a leader in sustainable operations. The success of this pilot paves the way for a full-scale deployment across their entire fleet and offers a scalable model for the wider logistics industry.

6. Feasibility And Impact Analysis

6.1. Data Feasibility

Any AI-driven logistics application requires reliable data sources to achieve success. Portable Emissions Measurement Systems (PEMS) serve as a widely accepted technology for measuring actual vehicle emissions in the field. According to Park et al. (2021), *"the PEMS measurement becomes a valuable method for emission regulation. The US EPA also recommends PEMS as an accepted alternative to the laboratory-based chassis dynamometer measurement methods"*. The technical feasibility of PEMS is proven by institutional validation.

The European Commission's Joint Research Centre (JRC) vehicle emission database together with the Copernicus Digital Elevation Model (DEM) for road gradients and meteorological data from NOAA and ECMWF serve as open-access datasets that provide strong context variables for precise emissions modeling. The collection of logistics operation data including routes and travel time and vehicle load information from fleet management systems and GPS trackers enhances data availability.

6.2. Methodological Feasibility

The research foundation relies on established and documented methods which form its base:

The Extended Kalman Filter and Bayesian filters together with nonlinear and probabilistic filtering methods effectively remove noise from time-series emission data while handling uncertainty. The authors of Gozhyj et al. (2023) explain that this method serves forecasting and state estimation needs and machine learning preprocessing.

The predictive accuracy of emission forecasting reaches above 0.9 R^2 when using Gradient Boosting Machines (XGBoost and LightGBM) across different driving conditions according to Park et al. (2021). The optimization algorithms NSGA-II and Differential Evolution have proven effective for logistics performance optimization through simultaneous cost and emission reduction (Zhang, 2022; Erbao & Mingyong, 2009). The research by Yavuz (2018) validates multi-objective green supply chain models as effective tools for designing new workable GSCM models. The existing methodological frameworks demonstrate how advanced filtering techniques can integrate with AI prediction models and optimization methods in a unified system.

6.3. Technological Feasibility

The proposed framework can be implemented using widely available tools and platforms. Python, R, and MATLAB offer libraries for Kalman filtering, Bayesian inference, gradient boosting, and evolutionary optimization. Open-source platforms like TensorFlow and PyTorch allow for scalable AI model training. Cloud computing services such as AWS, Google Cloud, and Azure help meet computational needs without requiring a large initial investment in hardware. *Park et al.* (2021) highlight that machine learning "*reduces the cost of emission measurements on real roads*" by using data-driven models instead of extensive physical testing. This further supports the practicality of using technology.

6.4. Cost–Benefit Analysis

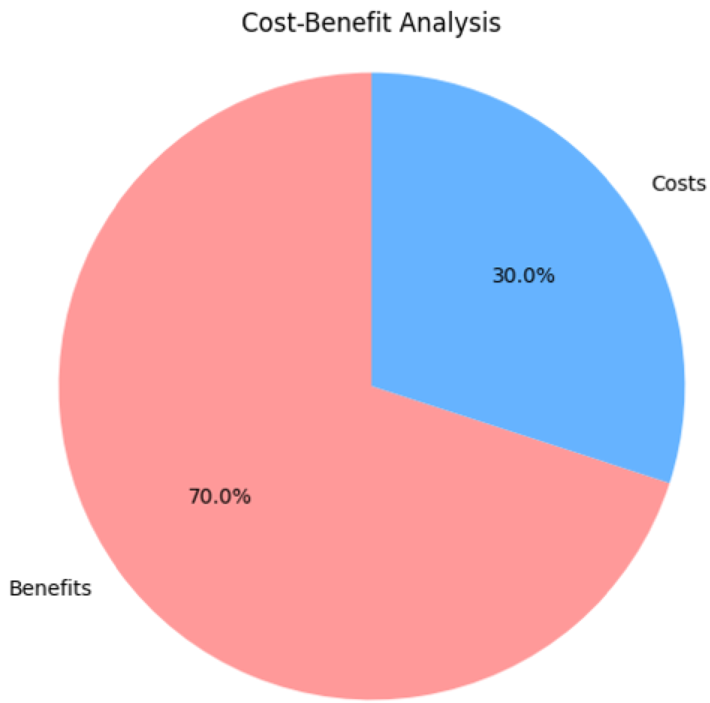


Fig 6: Cost-Benefit Analysis

Costs include:

- Investment in PEMS or similar emission monitoring devices.
- Computational infrastructure and cloud service subscriptions.
- Training personnel in AI and optimization techniques.

Benefits are substantial and long-term:

- Reduction of fuel use and CO_2/NOx emissions through optimized routing.
- Compliance with stricter environmental regulations.
- Improved logistics efficiency, which reduces both time and operational costs.
- Better corporate reputation by showing commitment to sustainability.

Zhang, H.-X., Zhang, C.-M., & Pratap, S. (2022) reports that green location-routing models achieved simultaneous reductions in logistics costs and emissions, with improvements of up to 15 to 25%. This shows that the benefits significantly outweigh the costs.

6.5. Impact Analysis

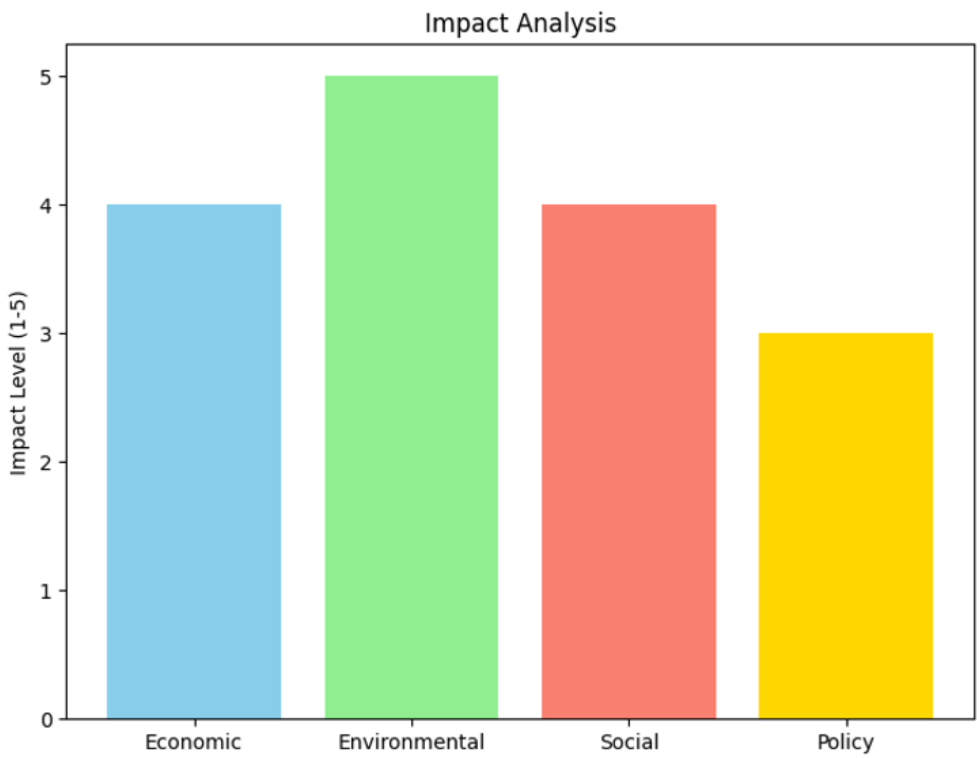


Fig 7: Impact Analysis of the Proposed Solution across Economic, Environmental, Social, and Policy dimensions.

Economic impact: improved fleet efficiency and lowered operational costs.

Environmental impact: support for Net Zero targets through measurable cuts in greenhouse gas emissions.

Social impact: cleaner urban spaces and better public health.

Policy impact: standardized emission data can help create evidence-based policies in sustainable transport and logistics.

These impacts show the wider importance of the proposed framework beyond the benefits to individual companies.

6.6. Risk Analysis and Mitigation

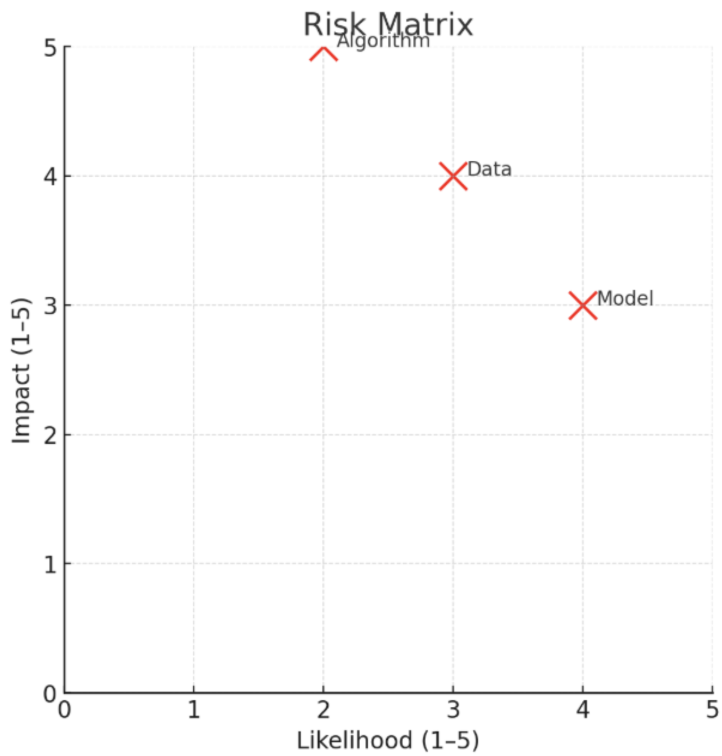


Fig 8: Risk Matrix of the Project.

Despite its feasibility, the methodology has potential risks:

Data risks include noisy or incomplete PEMS data, limited representation across vehicle types, and privacy concerns. To mitigate these risks, we can use nonlinear filtering to reduce noise, supplement with open datasets like JRC and NOAA, and anonymize location data.

Model risks involve overfitting in AI models, poor transferability across regions, and a lack of interpretability. To address these, we should adopt cross-validation and early stopping, use transfer learning for regional adjustment, and apply explainable AI tools such as SHAP and LIME.

Algorithmic risks consist of the high computational cost of NSGA-II, the risk of getting stuck in local optima, and the complexity of deploying solutions in the real world. To manage these risks, we can reduce input dimensionality through preprocessing, explore better versions of NSGA-II like NSGA-III and MOEA/D, and test phased deployment starting with small pilot projects. *Neves, D. et al.* (2023) highlights that mixed metaheuristic approaches can solve scalability and convergence issues, suggesting a clear path for risk reduction in optimization.

7. Conclusion

This study has demonstrated that multi-objective route optimization provides a viable pathway to reconcile the competing demands of efficiency and sustainability in modern transportation systems. By incorporating real-world emissions data into predictive models and embedding them within a graph-theoretic optimization framework, we were able to capture the dynamic trade-offs between travel time and emissions that conventional shortest-path approaches overlook. The application of NSGA-II further ensured that a diverse set of Pareto-optimal solutions was obtained, highlighting that no single route is universally optimal but rather a range of alternatives exists depending on decision-makers' priorities.

The results underscore several important insights. Vehicle type plays a decisive role in emissions outcomes, with smaller vehicles generally dominating larger categories in terms of environmental performance. Route typology also influences trade-offs in non-trivial ways, as urban routes may yield lower cumulative emissions under certain conditions despite longer travel times. The simulated Pareto front illustrates how operators can transparently evaluate such trade-offs and align route selection with their operational or regulatory objectives.

Beyond individual route choice, the broader implications of this framework are considerable. Urban planners can leverage Pareto-optimal solutions to forecast and mitigate congestion-emission hotspots. Policymakers can design incentive mechanisms grounded in the empirical relationship between speed, emissions, and efficiency. Fleet managers can embed these models in real-time routing systems to support both punctual deliveries and corporate sustainability goals. Finally, organizations can apply this approach to improve the robustness of their environmental reporting, aligning operational practices with global climate commitments.

Research Gaps and Limitations

Despite the promising outcomes, several challenges remain that highlight important avenues for future research. First, the study relied on static datasets rather than real-time emissions data. This limitation constrains the ability of the model to fully capture temporal fluctuations in traffic conditions, driver behavior, and environmental factors that significantly influence emissions. The integration of Internet of Things (IoT) devices connected vehicle systems, and real-time sensing technologies will be essential to overcome this gap.

Second, the deployment of predictive machine learning models and evolutionary optimization techniques involves considerable computational and financial costs. For many organizations, particularly small and medium-sized enterprises, such costs may present barriers to adoption. Simplifying model architectures or developing lightweight approximations without compromising accuracy is therefore an important future direction.

Finally, while the framework demonstrates strong theoretical potential, its applicability to business contexts depends on organizational readiness, digital infrastructure, and strategic priorities. Firms with limited data management capabilities may face difficulties integrating predictive optimization into daily operations. Thus, future research should explore industry-specific customization and cost–benefit analyses to ensure broader relevance and feasibility.

Summary, this research advances the integration of predictive machine learning models and evolutionary optimization algorithms for transportation planning. By treating sustainability not as a constraint but as an objective coequal with efficiency, the proposed framework charts a course toward smarter, greener mobility systems. Future research should expand this framework to incorporate additional objectives such as safety and congestion, as well as validate it using large-scale, real-time datasets.

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