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Empirical study of the effects of physics-guided machine learning on freeway traffic flow modelling: model comparisons using field data

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ABSTRACT

Recent studies have shown the successful implementation of classical model-based approaches (e.g. macroscopic traffic flow modelling) and data-driven approaches (e.g. machine learning – ML) to model freeway traffic patterns, while both have their limitations. Even though model-based approaches could depict real-world traffic dynamics, they could potentially lead to inaccurate estimations due to traffic fluctuations and uncertainties. In data-driven models, the acquisition of sufficient high-quality data is required to ensure the model performance. However, many transportation applications often suffer from data shortage and noises. To overcome those limitations, this study aims to introduce and evaluate a new model, named as physics-guided machine learning (PGML), that integrates the classical traffic flow model (TFM) with the machine learning technique. This PGML model leverages the output of a traffic flow model along with observational features to generate estimations using a neural network framework. More specifically, it applies physics-guided loss functions in the learning objective of neural networks to ensure that the model not only consists with the training set but also shows lower errors on the known physics of the unlabelled set. To illustrate the effectiveness of the PGML, this study implements empirical studies with a real-world dataset collected from a stretch of I-15 freeway in Utah. Experimental study results show that the proposed PGML model could outperform the other compatible methods, including calibrated traffic flow models, pure machine learning methods, and physics unguided machine learning (PUML).

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Traffic state estimation; physics-guided machine learning; macroscopic traffic flow modelling; neural networks

1. Introduction

Accurate traffic information plays an important role in transportation management systems, which helps travelers plan their trips, allows transportation agencies to take actions to mitigate traffic congestion, and therefore promotes a more efficient and safer driving environment (Lv et al. 2014; Ma et al. 2015; J. Wang, Chen, and He 2019). Giving accurate and

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timely traffic information has always been complicated because of the stochastic nature of the traffic patterns. In the literature, traffic state (i.e. flow, speed, and density) estimation (TSE) is a method that can infer traffic information using partially observed and noisy data from traffic sensors on the roadway system (Seo et al. 2017), which is the best way to tackle the limitation of observed data.

Input data and estimation approaches are two essential parts of TSE (Xiao, Wei, and Liu 2018). Regarding the technologies used for data collection, traffic data can be grouped into stationary data and probe data. In practice, stationary data can be easily retrieved because it is collected by fixed traffic detectors (e.g. inductive loops and radar detectors) on freeways. Each stationary detector counts the number of vehicles that pass every minute and detects the speed of each vehicle. However, the data is only available at the locations with the stationary detector installed. Probe data is a sample of information collected from vehicle navigation systems, cell phone applications, and fleet vehicles (Z. Zhang, Yuan, and Yang 2020). Compared to stationary data, probe data can provide traffic information (e.g. speed and flow) on variable locations of statewide highways but are very likely to be biased because of the low penetration rate (e.g. 3%).

In terms of the estimation approaches, previous studies have shown that model-based and data-driven models are commonly used (Seo et al. 2017). The basic logic is that these approaches can be used as prior knowledge of partial traffic observations to simulate traffic dynamics, capture data noises, and predict unobserved traffic states. More specifically, model-based approaches rely on physics principles to study traffic dynamics over space and time. In the early stages, the fundamental diagram of traffic flow was discovered by borrowing concepts from the fluid mechanism (Yuan et al. 2021). Following the same line, macroscopic traffic flow models were developed with the conservation law and momentum equation, and a set of kinematic wave models were also formulated (Seo et al. 2017). However, most models require great efforts to calibrate parameters and are challenging to apply to noisy and biased traffic data because they were derived under some ideal theoretical assumptions. In general, model-based approaches can be classified into two categories: (a) continuous models, such as the Lighthill-Whitham-Richards (LWR) model (Lighthill and Whitham 1955; Richards 1956), the Payne–Whitham (PW) model (Payne 1971; Whitham 1975), and the Aw-Rascle-Zhang (ARZ) model (Aw and Rascle 2000; H. M. Zhang 2002); and (b) discretised models, which were presented to simulate traffic states of subsegments and time intervals because of their tremendous computational efficiency. METANET (Papageorgiou, Blosseville, and Hadj-Salem 1989), a discrete PW-like TSE model, has been successfully applied by many studies (Y. Wang and Papageorgiou 2005; Y. Wang, Papageorgiou, and Messmer 2007, 2008; Z. Zhang, Yuan, and Yang 2020). The advantages of model-based approach include: (1) it can estimate accurate traffic state with less input data; (2) it has high explanatory power; and (3) it can be directly implemented on traffic operations. However, the model-based method may require plenty of time to select and calibrate the models based on different scenarios. In some applications, calibrating a model requires a tremendous amount of data.

With the development of data collecting, processing, and computation technologies recently, data-driven approaches such as ML models have been widely developed and implemented for TSE because they have the following benefits: (1) do not require clear theoretical assumptions, and (2) low computational cost. Hence, ML models are prevailing in utilising big data for TSE in recent years (Duan et al. 2016; Li, Li, and Li 2013;

Ni and Leonard 2005; Polson and Sokolov 2017a, 2017b; Tak, Woo, and Yeo 2016; Tan et al. 2013, 2014; Tang et al. 2015; Y. Wu et al. 2018; Yin, Murray-Tuite, and Rakha 2012; Yuan et al. 2021; Z. Zhang and Yang 2020; Z. Zhang, Yuan, and Yang 2020). However, the performance of ML models depends on high-quality data due to their data-driven nature. The deficiency of ML models includes: (a) scarce and insufficient training data to train the model, (b) training data contains noisy/error information, (c) the pattern of test data is different from the training set, and (d) the results of ML models are difficult to interpret because they are developed as 'black boxes'.

Figure 1 summarises the existing research gaps and the proposed solutions. Herein, model-based approaches are usually constructed with strong prior knowledge, require great effort in parameter calibrations, and are difficult to capture data uncertainties, even though they can present the underlying mechanisms of traffic flow. Data-driven approaches such as ML models do not require clear theoretical assumptions, but their performance depends heavily on data quality and the model results are unexplainable. Therefore, recognising the advantages and deficiencies of model-based and data-driven approaches, this research aims to develop an innovative framework, named as physics-guided machine learning (PGML). More specifically, the PGML framework could incorporate physics knowledge into loss functions to help ML models capture generalisable dynamic patterns, in consistent with established traffic physics laws. Figure 2 shows the proposed PGML model can leverage the advantages of both model-based and data-driven approaches by making efficient use of traffic data and existing physics relationships in traffic flow, where the *x*-axis measures the use of traffic data and *y*-axis measures the use of traffic physics models. This study makes significant contributions to the literature from the following perspectives: (a) compared with traditional physics models, the PGML can use the ML portion to capture the uncertainties in estimation and greatly reduces the effort required to calibrate parameters; (b) compared to pure ML models, the PGML is more resistant to data limitation as valuable knowledge from physics models can help guide the ML training process; and (c) the model results are more interpretable by learning parameters with physics meanings. This research is expected to bridge the gap between the research

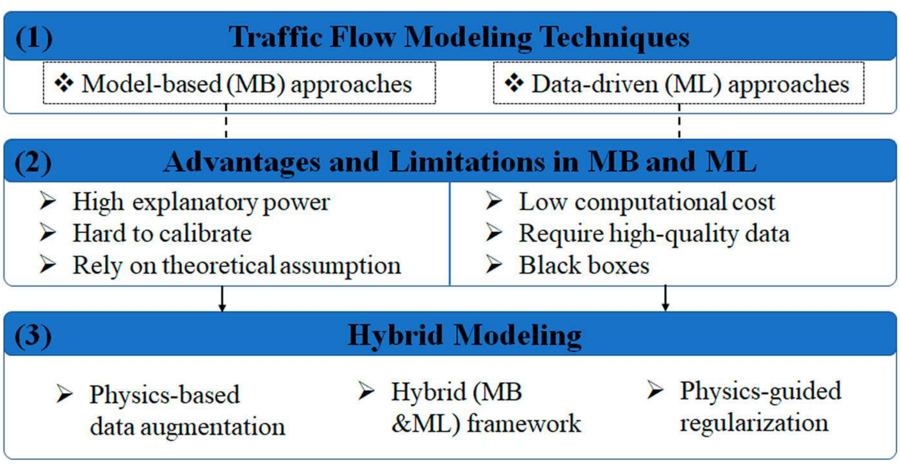


Figure 1. Hybrid modelling in traffic flow modelling domian.

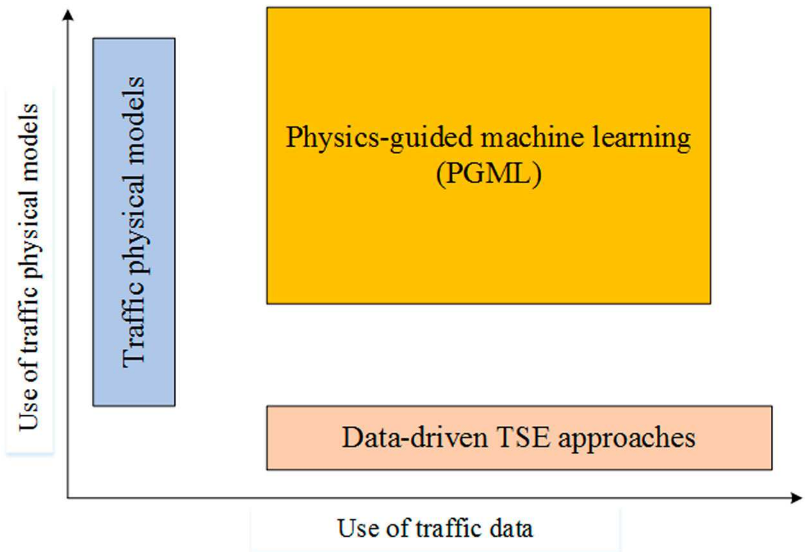


Figure 2. A presentation of model-based, data-driven, and PGML TSE approaches.

of transportation theoretical foundations and data-driven approaches proposed by the innovative hybrid TSE framework.

The rest of this paper is organised as follows. Section 2 reviews existing studies related to TSE and estimation methods. In Section 3, traffic flow fundamentals and a macroscopic TSE model are introduced. The PGML framework and physics-guided loss function are presented in Section 4. Section 5 implements the case study on the real-world data from interstate freeway I-15. The last section summarises the key findings and future research directions.

2. Literature review

2.1. Classical traffic flow model

The importance and controllability of highways in transportation systems make TSE a vital fundamental task of highway traffic management systems. In the early stages, macroscopic traffic flow was found to be similar to hydrodynamic theory (Seo et al. 2017). Based on that finding, the fundamental diagram was defined as the relationship between traffic speed, flow, and density. The fundamental diagram is one of the most basic concepts in traffic flow theory, which is described in Equations (1)–(2).

$$v = V(\rho) \tag{1}$$

$$q = \rho V(\rho) \tag{2}$$

where V represents the speed-density fundamental diagram.

According to the fundamental diagram, macroscopic traffic flow models were developed using partial differential equations (PDE) to represent the aggregated traffic behaviour. The traffic flow models can be generally classified into continuous models and discretised models. The Lighthill–Whitham–Richards (LWR) model (Lighthill and Whitham 1955;

Richards 1956) is a continuous first-order model and can be formulated in Equations (3)–(4).

$$\partial_t \rho + \partial_x(\rho v) = 0 \tag{3}$$

$$v = V(\rho) \tag{4}$$

The LWR model succeeds in mimicking simple traffic conditions (e.g. traffic jam and shockwave) but it cannot reproduce more complicated traffic phenomena well.

To tackle such limitations, the well-known second-order PW model (Payne 1971; Whitham 1975) was developed by adding the momentum equation to capture complex traffic behaviour. The PW model is formulated as Equations (5)–(6), where Equation (6) is the momentum equation.

$$\partial_t \rho + \partial_x(\rho v) = 0 \tag{5}$$

$$\partial_t v + v\partial_x v = -\frac{V - V(\rho)}{\tau} - \frac{c_0^2}{\rho}\partial_x(\rho) \tag{6}$$

where τ is the relaxation time and c_0^2 is a parameter related to driver anticipation. Papageorgiou, Blosseville, and Hadj-Salem (1989) proposed a discrete PW-like TSE model, named METANET, which is an extension of PW model. It can reproduce complex traffic phenomena but does not require tremendous computation efforts at a certain level.

2.2. Pure data-driven approach

In recent decades, more researchers began using data-driven methods (e.g. statistical and ML methods) for TSE with the advancement of data collecting, processing, and computation technologies. In the existing literature, Support Vector Machine (SVM) (J. Wang and Shi 2013; Z. Zhang and Yang 2020; Z. Zhang, Yuan, and Yang 2020) and Random Forest (RF) (Hamner 2010; Leshem and Ritov 2007; D. Wang et al. 2016; Z. Zhang and Yang 2020; Z. Zhang, Yuan, and Yang 2020) have a great ability to capture the stochastic characteristics of traffic flow. SVM models can effectively model time series and regression problems since they estimate the regression based on a number of kernel functions that can convert the lower-dimensional data into a higher-dimensional feature space through a nonlinear relationship and then execute linear regression within this space (Smola and Schölkopf 2004). The effectiveness of SVM-based models for time series and regression problems in the transportation field has been approved by several existing studies (Asif et al. 2013; C.-H. Wu, Ho, and Lee 2004; Y. Zhang and Liu 2009). The RF model (Breiman 2001) can reduce variance by combining a set of 'weak' learners, which can overcome the over-fitting problem through Breiman's 'bagging' idea as it randomly selects features. The RF has been widely implemented to predict traffic state (Hamner 2010; Leshem and Ritov 2007; Z. Zhang and Yang 2020; Z. Zhang, Yuan, and Yang 2020). Moreover, the Artificial Neural Network (ANN) is also considered as an effective method for TSE and traffic state prediction because it can deal with multi-dimensional data, flexible model structure, strong generalisation, learning ability, and adaptability (Karlaftis and Vlahogianni 2011). Compared with traditional statistical methods, ANN can effectively work with missing and noisy inputs since it doesn't have underlying assumptions (Karlaftis and Vlahogianni 2011). Many existing studies have shown that ANN has a strong ability to predict traffic state (Taylor and Meldrum 1995; Van

Lint, Hoogendoorn, and Zuylen 2005; Zeng et al. 2008; Z. Zhang and Yang 2020; Z. Zhang, Yuan, and Yang 2020). In addition, graph neural networks (GNNs) have been conducted in recent years and obtained superior performance in traffic state modelling for nested urban networks (Jiang and Jiayun 2022).

However, the performance of those models would be significantly reduced when the training data is too scarce and the pattern of testing data is geographically far away from the training set. In addition, the results of ML models are challenging to interpret because they are developed as 'black boxes'.

2.3. Hybrid physics machine learning

Both model-based approaches and data-driven approaches have their advantages and drawbacks. Model-based approaches can simulate traffic dynamics and predict unobserved spatiotemporal traffic states with a limited amount of traffic observations. Data-driven approaches are prevailing in capturing the stochastic characteristics of traffic flow based on a massive amount of historical data. The estimation methodology and the data quality are the two essential parts in TSE (Xiao, Wei, and Liu 2018). Hence, to overcome the limitation of both types of approaches, data expansion, data fusion, and hybrid approaches were developed in the literature. Those hybrid concepts can partially combine the advantages of different data sources and different methods (Z. Zhang, Yang, and Yang 2023). The hybrid data-driven and model-based approaches for traffic time estimation and forecasting were implemented and evaluated by a group of studies (Allström et al. 2016; Anusha, Anand, and Vanajakshi 2012; Hofleitner, Herring, and Bayen 2012; Kumar et al. 2017; Sharmila, Velaga, and Kumar 2019; You and Kim 2000; Yu et al. 2010; Z. Zhang, Yuan, and Yang 2020; Zhu et al. 2018). Furthermore, other studies (Willard et al. 2021b) point out that a variety of methodologies are needed to integrate physics theory into ML models in different subjects and applications because of different forms of scientific knowledge in various disciplines. This paper further indicated that feeding the output of a physics model as input into an ML model is one direct and effective way to combine the physics model and ML models.

2.4. Physics-guided machine learning

Scientific problems usually exhibit high complexity because physics variables vary with spatial and temporal on different scales. Standard ML models usually fail to generalise to scenarios not experienced in training data because they tend to fail to capture spatiotemporal relationships, especially in the case of incomplete data. Hence, people started to integrate physics knowledge into the loss functions to help ML models capture generalisable dynamic patterns that are consistent with known physical laws. Daw et al. (2017) stated that physics-guided machine learning (PGML) is one of the most effective ways to make ML models align with physical laws by integrating physical constraints into the loss function of ML models. Recently, the effectiveness of PGML models in improving the performance of standard ML methods in various fields has been recognised (Daw et al. 2017; Doan, Polifke, and Magri 2019; Jia et al. 2018; Kahana et al. 2020; Yang and Perdikaris 2018; L. Zhang et al. 2018). In transportation field, physics informed machine learning (PIML) developed by Huang and Shaurya (2022) and Shi et al. (2021), refers to training an ML model to solve for TSE problem while respecting the physics law inside of continuous traffic flow model, such as LWR and LWR, given by general nonlinear partial differential equations (PDE). Hence, these models only work for continuous TSE problem. To tackle this problem, this paper attempts to propose a PGML that integrates the physics law from the METANET model to solve the discrete TSE problem, which could speed up the estimation process.

In summary, a hybrid framework that integrates physics knowledge and data-driven methods with low computational cost for discrete TSE problem is still lacking. This paper focuses on filling the gap by proposing an ANN-based PGML model for TSE.

3. Fundamentals and review of macroscopic TSE models

To facilitate the convenience of reference, Table 1 provides a concise summary of the key notations used in the proposed PGML model.

As an existing influential study, Papageorgiou, Blosseville, and Hadj-Salem (1989) developed a discrete macroscopic traffic flow model, METANET, which conceptually subdivides the target freeway segment into n subsegments with a unit length of ΔL (500 m). Figure 3 shows the template freeway segment. For each subsegment i, the mean density, $d_i(k)$, can be determined by the difference between the input and output flows by Equation (7).

$$d_i(k+1) = d_i(k) + \frac{T}{\lambda_i \Delta L}[q_{i-1}(k) - q_i(k) + r_i(k) - s_i(k)] \tag{7}$$

The departure flow is assumed to be a portion of the flow at the segment in Equation (8). The ramp flow is captured by the sensors installed at the ramps.

Table 1. Key notations of proposed PGML model.

Notation	Definition
$\mathcal{D}$	the training data set
$\mathcal{S}$	stationary data points
$\mathcal{T}$	traffic flow model data points
$\mathcal{Y}$	target values
i	the index of sub-sections of a freeway segment
j	the index of the physics data points in the data set
k	the index of the time step
m	the number of observations on each segment
n	the number of segments on the highway
$q_i(k)$	the total flow at the end of segment i
r_i	the inflow of vehicles at on-ramps
s_i	the outflow of vehicles at off-ramps
λ_i	number of lanes in subsegment i
$u_i(k)$	the average speed at segment i
u_f	the free-flow speed
a	the exponent of the stationary speed equation
$\beta_i(k)$	the departure rate
ΔL	the segment length at the segment
$d_i(k)$	the density at the end of segment i
d_{cr}	the critical density
τ, γ, κ	positive physics model parameters
α	hyper-parameter of empirical error in the loss function
β	hyper-parameter of physics inconsistency in the loss function
λ	hyper-parameter of structural error in the loss function
$\boldsymbol{X}$	the data input vectors of size $n * m$
$\mathbf{Y}_{\text{phy}}$	traffic physics inconsistency vectors of size $n * m$
$\widehat{Y}$	the model estimation vectors of size $n * m$
$\mathbf{Y}$	the data output vectors of size $n * m$

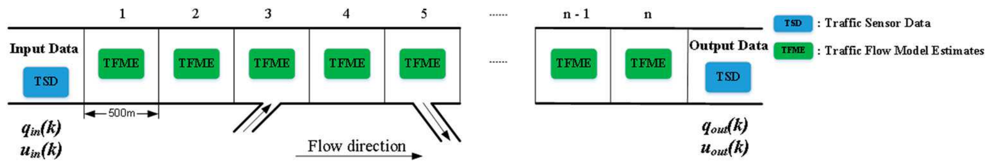


Figure 3. Freeway stretch example.

$$s_i(k) = \beta_i(k) \times q_{i-1}(k) \tag{8}$$

For dynamically updating the average speed, $u_i(k)$, a well-developed equation proposed by the METANET model (Papageorgiou, Blosseville, and Hadj-Salem 1989) is adopted by Equation (9).

$$\begin{aligned} u_i(k+1) = u_i(k) + \frac{\Delta T}{\tau}[V_i(d_i(k)) - u_i(k)] + \frac{\Delta T}{L_i} u_i(k)(u_{i-1}(k) - u_i(k)) \\ - \frac{\gamma_i \Delta T}{\tau \Delta L} \frac{d_{i+1}(k) - d_i(k)}{d_i(k) + \kappa} - \frac{\delta \Delta T}{\Delta L \lambda_i} \frac{r_i(k), u_i(k)}{d_i(k) + \kappa} \end{aligned} \tag{9}$$

where $V[d_i(k)]$ is the static speed for segment i at time k with respect to the density $d_i(k)$:

$$V[d_i(k)] = u_f \exp\left[-\frac{1}{a}\left(\frac{d_i(k)}{d_{cr}}\right)^a\right] \tag{10}$$

Also, the relationship between flow, density, and speed is given by Equation (11):

$$q_i(k) = d_i(k) u_i(k) \lambda_i \tag{11}$$

where Equations (7)–(11) are the conservation equation, dynamic speed equation, stationary speed equation, and flow equation, respectively; $\tau, \gamma, \kappa, d_{cr}, u_f, a$ are positive model parameters which are given the same values for all segments. Using the traffic flow and speed from traffic sensors at upstream and downstream stations, on-ramps, and off-ramps, one can directly use Equations (7)–(11) to estimate the traffic speed evolution on the target freeway section.

4. Physics-guided machine learning algorithm

Let $\mathcal{D}$ denote the set of freeway segments i at various time step k: $\mathcal{D} = \{x_{i,k} \mid i \in [0, n], \forall k \in [0, t]\}$ (k denotes the time interval (5-min)). Let $\mathcal{S}$ and $\mathcal{T}$ be two subsets of $\mathcal{D}$, as $\mathcal{D} = \mathcal{S} \cup \mathcal{T}$. $\mathcal{S} = \{x^S_{i,k} \mid i = 1, \ldots, n_S\}$ is composed of the observed traffic information from stationary sensors. $\mathcal{T} = \{x^T_{j,k} \mid i = 1, \ldots, n_T\}$ is composed of generated TFM estimates based on the upstream and downstream stationary data $[x^S_{1,k}, x^S_{n,k}]$. Then, the training data for PGML model consist of (1) stationary data points is denoted by $\mathcal{S} = \{x^S_{i,k} \mid i = 1, \ldots, n_S\}$; (2) TFM data points $\mathcal{T} = \{x^T_{j,k} \mid i = 1, \ldots, n_T\}$; and (3) target values $\mathcal{Y} = \{y_{i,k} \mid i = 1, \ldots, n_S\}$ (i.e. the true traffic states at the stationary points), where i and j are the indexes of stationary points and TFM data points. $\mathcal{S}$ and $\mathcal{Y}$ have the same index i in the case of the target value $\mathcal{Y}$ paired with stationary point $\mathcal{S}$. In experiments, the stationary data points are usually limited by the availability of traffic sensors (e.g. probe and sensor detectors). Hence, the traffic state can be observed only in limited locations. An estimation method is needed to infer the unknown traffic state in locations without traffic sensors installed. In this study, the traffic flow model is utilised to construct traffic state for those locations based on limited traffic information from $\mathcal{S}$, named TFM data points $\mathcal{T}$. The input of TFM includes speed and flow from upstream, off-ramp, on-ramp, and downstream segments. Then, unobserved traffic states could be estimated by TFM for all segments by Equation (12). In particular, the METANET model is chosen as the traditional TFM model to estimate traffic speeds and flows for target locations. Detailed procedures of the METANET model are shown in Equations (7)–(11).

$$\begin{bmatrix} x_{1,1}^{s} & q_{i,1}^{on} & q_{i,1}^{off} & x_{n,1}^{s} \\ x_{1,2}^{s} & q_{i,2}^{on} & q_{i,2}^{off} & x_{n,2}^{s} \\ \vdots & \vdots & \vdots & \vdots \\ x_{1,t}^{s} & q_{i,t}^{on} & q_{i,t}^{off} & x_{n,t}^{s} \end{bmatrix}_{t\times 4} \xrightarrow{TFM} \begin{bmatrix} x_{1,1}^{T} & x_{2,1}^{T} & \cdots & x_{n,1}^{T} \\ x_{1,2}^{T} & x_{2,2}^{T} & \cdots & x_{n,2}^{T} \\ \vdots & \vdots & \vdots & \vdots \\ x_{1,t}^{T} & x_{2,t}^{T} & \cdots & x_{n,t}^{T} \end{bmatrix}_{t\times n} \tag{12}$$

TFM data points could overcome both location and measurement limitations, which also can reflect the real traffic physics truth. The parameters of traffic flow models need to be calibrated by the ground truth data and this process is similar to the training process of machine learning. The TFM model can offer available data for a freeway segment based on the upstream and downstream traffic information. However, the output of TFM may include incomplete information of the target traffic state because of simplified or missing information in $\mathcal{T}$. Hence, the PGML model is constructed with an ML portion based on the output from TFM. Figure 4 presents the framework of the proposed PGML model for TSE, which includes two key steps: (1) build up a hybrid physics neural network, termed as HP-NN, and (2) substitute the HP-NN output into a traffic physical law to obtain the physics inconsistency on target freeway segments and develop a physics-based loss function. Then, the model training process would be guided by the new loss function. The basic logic of the proposed PGML for TSE is presented in Algorithm 1. The unobserved traffic states can be estimated by PGML using Equation (16), based on the samples in Equations (13)–(15). Herein, the input $\mathbf{X}$ represents time t, distance d, on-ramp flow q^{on}, off-ramp flow q^{off}, TFM speed u^{T} and flow q^{T}, the $\mathbf{Y}_{phy}$ represents the traffic physics inconsistency in flow and speed, the output $\mathbf{Y}$ represents the corresponding vector of flow and speed. The $\mathbf{Y}_{phy}$ are used as a guide, making the estimation of PGML more consistent with the traffic

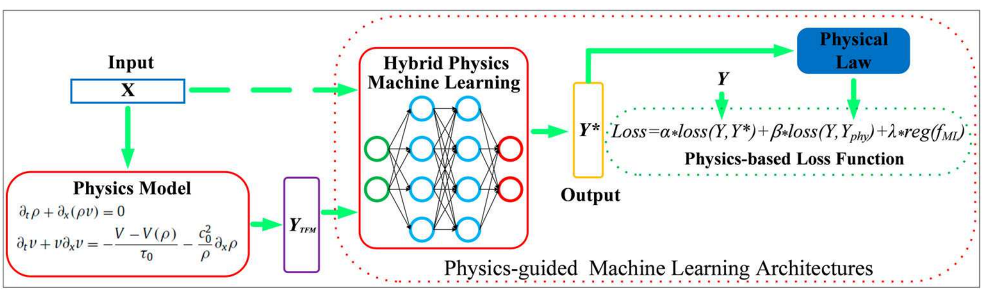


Figure 4. The Diagram of Physics-guided Machine Learning (PGML) model, $\mathbf{Y}$ refers to the observed stationary values, $\mathbf{Y}^{\star}$ refers to the predicted value, and $\mathbf{Y}_{phy}$ refers to the physics value on the intermediate subsegment.

physics knowledge. The detailed calculation procedures of traffic physics inconsistency are described in the following section.

Algorithm 1 PGML algorithm

Results: Estimated traffic states

Pick a freeway segment with point data available at upstream and downstream stations
Set the length of each sub-segment to 500 m
Run TFM to produce estimates for all sub-segments: $[x^s_{1,t}, x^s_{n,t}] \xrightarrow{TFM} [x^s_{1,t}, x^s_{2,t}, \ldots, x^s_{n,t}]$
for sub-segment $i = 1, \ldots, n$ **do**
    if sub-segment i without point data **then**
        Group the TFM estimates and point data of its nearby sensor stations: $[t_{n,t}, d_{n,t}, q^{\text{on}}_{n,t}, u^{\text{off}}_{n,t}, q^{\text{phy}}_{n,t}, u^{\text{phy}}_{n,t}] \Rightarrow [q_{n,t}, u_{n,t}]$
        Build up physics-based loss function: $PGLoss = \alpha * \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}(x^S_{i,k} - \widehat{Y})^2 + \beta * \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}|Y^{\text{phy}}_{i,k} - \widehat{Y}| + \lambda * R(f)$
        Train PGML model with the grouped dataset.
        Use the trained model to estimate traffic state for sub-segment i: $\hat{f} = \left[\mu^{(q)}(X)\&\mu^{(u)}(X)\right]^T_{2\times 1}$
    end if
end for

$$\mathbf{X} = \begin{bmatrix} x_1 & x_2 & \ldots & x_n \end{bmatrix}^T = \begin{bmatrix} t_{1,1} & d_{1,1} & q^{\text{on}}_{1,1} & q^{\text{off}}_{1,1} & u^T_{1,1} & q^T_{1,1} \\ t_{1,2} & d_{1,2} & q^{\text{on}}_{1,2} & q^{\text{off}}_{1,2} & u^T_{1,2} & q^T_{1,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ t_{1,t} & d_{1,t} & q^{\text{on}}_{1,t} & q^{\text{off}}_{1,t} & u^T_{1,t} & q^T_{1,t} \\ t_{2,1} & d_{2,1} & q^{\text{on}}_{2,1} & q^{\text{off}}_{2,1} & u^T_{2,1} & q^T_{2,1} \\ t_{2,2} & d_{2,2} & q^{\text{on}}_{2,2} & q^{\text{off}}_{2,2} & u^T_{2,2} & q^T_{2,2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ t_{2,t} & d_{2,t} & q^{\text{on}}_{2,t} & q^{\text{off}}_{2,t} & u^T_{2,t} & q^T_{2,t} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ t_{n,t} & d_{n,t} & q^{\text{on}}_{n,t} & q^{\text{off}}_{n,t} & u^T_{n,t} & q^T_{n,t} \end{bmatrix}_{(n\times t)\times 6} \tag{13}$$

$$\mathbf{Y} = \begin{bmatrix} y_1 & y_2 & \ldots & y_n \end{bmatrix}^T = \begin{bmatrix} u_{1,1} & q_{1,1} \\ u_{1,2} & q_{1,2} \\ \vdots & \vdots \\ u_{1,t} & q_{1,t} \\ u_{2,1} & q_{2,1} \\ u_{2,2} & q_{2,2} \\ \vdots & \vdots \\ u_{2,t} & q_{2,t} \\ \vdots & \vdots \\ u_{n,t} & q_{n,t} \end{bmatrix}_{(n\times t)\times 2} \tag{14}$$

$$\mathbf{Y}_{\text{phy}} = \begin{bmatrix} y_1^{\text{phy}} & y_2^{\text{phy}} & \dots & y_n^{\text{phy}} \end{bmatrix}^T = \begin{bmatrix} u_{1,1}^{\text{phy}} & q_{1,1}^{\text{phy}} \\ u_{1,2}^{\text{phy}} & q_{1,2}^{\text{phy}} \\ \vdots & \vdots \\ u_{1,t}^{\text{phy}} & q_{1,t}^{\text{phy}} \\ u_{2,1}^{\text{phy}} & q_{2,1}^{\text{phy}} \\ u_{2,2}^{\text{phy}} & q_{2,2}^{\text{phy}} \\ \vdots & \vdots \\ u_{2,t}^{\text{phy}} & q_{2,t}^{\text{phy}} \\ \vdots & \vdots \\ u_{n,t}^{\text{phy}} & q_{n,t}^{\text{phy}} \end{bmatrix}_{(n\times t)\times 2} \tag{15}$$

$$\hat{\mathbf{f}} = \begin{bmatrix} \mu^{(q)}(X) & \mu^{(u)}(X) \end{bmatrix}_{2\times 1}^T \tag{16}$$

4.1. Physics-guided machine learning model structure

In this study, a basic ANN is utilised to regress the traffic state, $\mathbf{Y}$. The relationship between the input features, $\mathbf{X}$, and target prediction, $\widehat{Y}$ for a fully connected neural network with m hidden layers can be described as:

$$\mathbf{z}_1 = W_1^k\mathbf{X} + \mathbf{b}_1 \tag{17}$$

$$\mathbf{z}_i = W_i^k\mathbf{X} + \mathbf{b}_i, \quad \forall\, i \in [2, m] \tag{18}$$

$$\mathbf{a}_i = f(\mathbf{z}_i), \quad \forall\, i \in [1, m] \tag{19}$$

$$\widehat{Y} = W_{m+1}^k\mathbf{a}_l + \mathbf{b}_{m+1}, \quad \forall\, i \in [2, m] \tag{20}$$

where $\{W_i, b_i\}_1^{m+1}$ denotes the weight and bias parameters in hidden and output layers; f is the activation function in hidden layers.

The proposed PGML uses the ANN as base machine learning model with hybrid data, which combines the observed data and TFM estimates as the input to train the neural network. Hence, the PGML can also be termed as a physics-guided neural network (PGNN). The structure of The PGNN is depicted in Figure 5. The PGNN not only uses additional TFM estimates as input, but also adds the traffic physics knowledge as additional term in the loss function so that it can guide the entire training process. The loss function of PGML is termed as a physics-guided loss function.

4.2. Physics-guided loss function

The objective of the training procedure of pure machine learning model is to minimise the empirical loss of its model estimations, $\widehat{\mathbf{Y}}$, to maintain low model complexity as follows:

$$Loss = \frac{1}{N}\sum_{i=1}^{n}(\widehat{Y} - Y)^2 \tag{21}$$

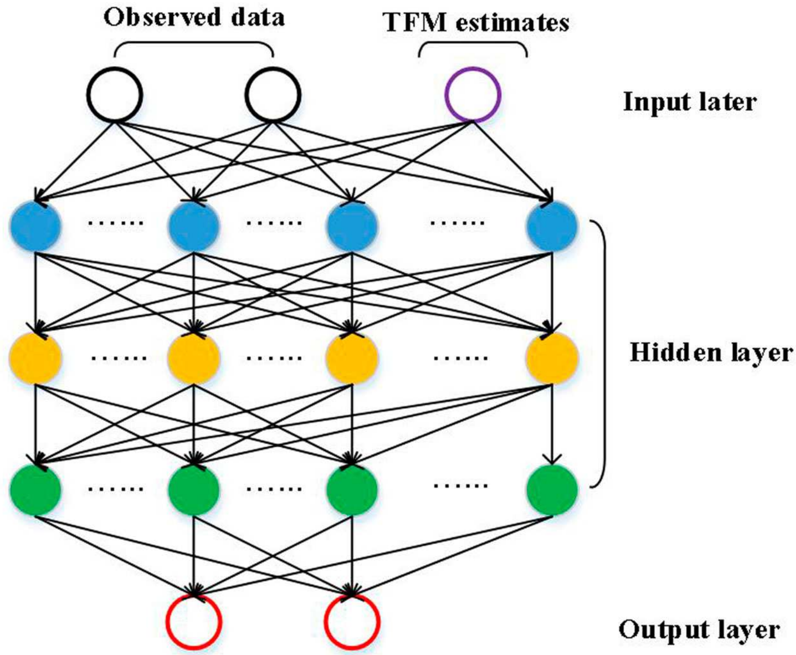


Figure 5. The deep structure for PGNN.

TSE problems often involve a high degree of complexity because of relationships between physics variables (e.g. flow, density, and speed) are varying spatially and temporally at different scales. Those relationships are usually difficult to be captured directly by the training data, using pure-ML models. Hence, the proposed PGML framework will offer a new solution to model the stochastic correlations between traffic states by incorporating physics knowledge into loss function. The corresponding physics-based loss function would convert physics constraints into the ANN loss function, which is one of the most efficient methods to make model estimations consistent with physics laws (Willard et al. 2021a). The physics-guided loss function is described as:

$$PGloss = \alpha * \underbrace{Loss(\widehat{Y}, Y)}_{\textit{empirical error}} + \beta * \underbrace{Loss(\widehat{Y}, Y_{\text{phy}})}_{\textit{physical inconsistency}} + \lambda * \underbrace{R(f)}_{\textit{structural error}} \tag{22}$$

where the training $Loss(\widehat{Y}, Y)$ measures the empirical error (e.g. MSE) between labels Y and predictions $\widehat{Y}$; $Loss(\widehat{Y}, Y_{\text{phy}})$ denotes the physics inconsistency (also termed as physics-based loss) that aims to keep the consistency between predictions and physics laws. $R(f)$ denotes the model structural error that measures the model complexity; α, β, and λ represent the trade-off hyper-parameters of empirical error, physics inconsistency, and structural error respectively. The detailed description of how to establish the physics-based loss is as follows.

Traffic physics relationships inside of TFM could be used to build up physics inconsistency for target segments once the traffic information of upstream and downstream segments is available. Figure 6 illustrates the detailed procedures of calculating the physics inconsistency by traffic physics law. An algorithmic description of physics inconsistency is

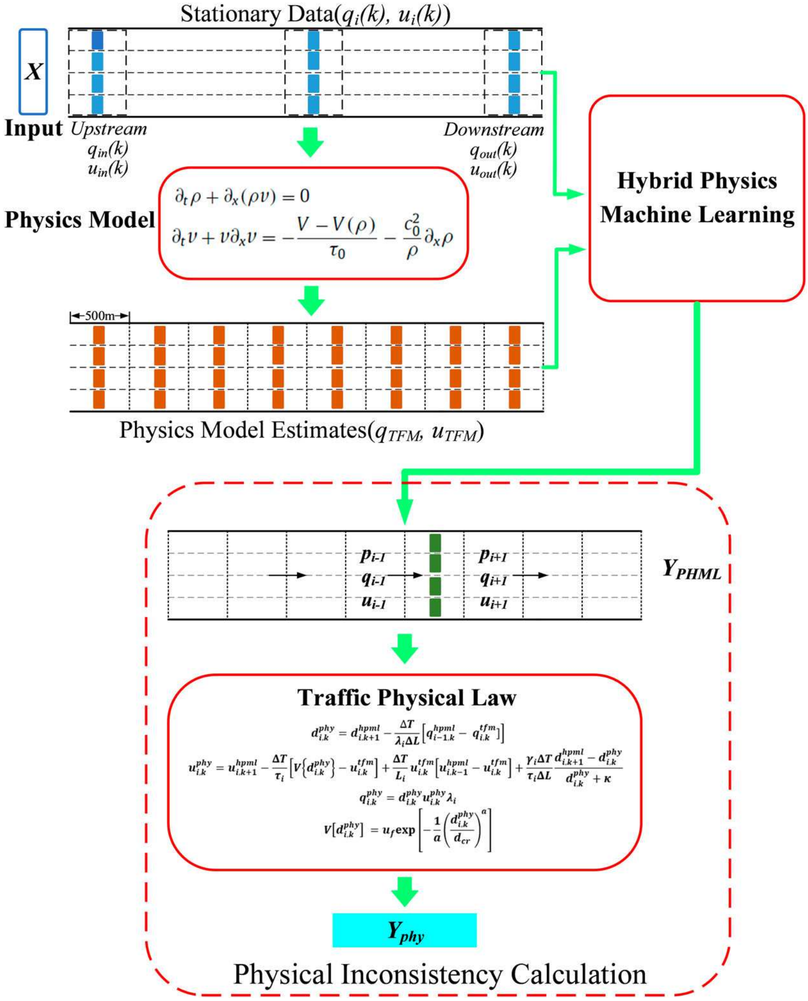


Figure 6. The diagram of physics inconsistency calculation.

presented in Algorithm 2. The preliminary traffic state estimates of all segments have been obtained by TFM and HPML model. Then, those estimates are used to construct the physics inconsistency by traffic physics law. The utilised traffic physics law is a converted form of TFM, which is introduced as:

$$d_{i,k}^{\text{phy}} = d_{i,k+1}^{\text{hpml}} - \frac{\Delta T}{\lambda_i \Delta L}\left[q_{i-1,k}^{\text{hpml}} - q_{i,k}^{T}\right] \tag{23}$$

$$u_{i,k}^{\text{phy}} = u_{i,k+1}^{\text{hpml}} - \frac{\Delta T}{\tau_i}\left[V\{d_{i,k}^{\text{phy}}\} - u_{i,k}^{T}\right] + \frac{\Delta T}{L_i} u_{i,k}^{T}\left[u_{i,k-1}^{\text{hpml}} - u_{i,k}^{T}\right] + \frac{\gamma_i \Delta T}{\tau_i \Delta L}\frac{d_{i,k+1}^{\text{hpml}} - d_{i,k}^{\text{phy}}}{d_{i,k}^{\text{phy}} + \kappa} \tag{24}$$

$$q_{i,k}^{\text{phy}} = d_{i,k}^{\text{phy}} u_{i,k}^{\text{phy}} \lambda_i \tag{25}$$

$$V[d_{i,k}^{\text{phy}}] = u_f \exp\left[-\frac{1}{a}\left(\frac{d_{i,k}^{\text{phy}}}{d_{cr}}\right)^a\right] \tag{26}$$

where $d_{i,k}^{\text{phy}}$, $u_{i,k}^{\text{phy}}$, and $q_{i,k}^{\text{phy}}$ are values of physical laws;$u_{i,k}^{T}$ and $q_{i,k}^{T}$ denotes TFM estimates from TFM; and $d_{i,k+1}^{\text{hpml}}$, $q_{i-1,k}^{\text{hpml}}$, and $u_{i,k-1}^{\text{hpml}}$ denote HPML predictions.

Algorithm 2 Traffic physics law algorithm

Results: physics inconsistency

Set the length of each sub-segment to 500 m
for sub-segment i **do**
    Run TFM model: $[x_{1,t}^s, x_{n,t}^s] \xrightarrow{TFM} [x_{1,t}^s, x_{2,t}^s, \ldots, x_{n,t}^s]$
end for
Group the training dataset: $[t_{n,t}, d_{n,t}, q_{n,t}^{\text{on}}, q_{n,t}^{\text{off}}] \Rightarrow [q_{n,t}, u_{n,t}]$
for sub-segment $i = 1, \ldots, n$ **do**
    if sub-segment i without point data **then**
        Train HPML model with grouped dataset: $Loss = \alpha * Loss(\widehat{Y}, Y) + \lambda * R(f)$
        Use the trained HPML model to estimate traffic state for sub-segment i, $[u_{n,t}^{\text{hpml}}, q_{n,t}^{\text{hpml}}]$
    end if
end for
for sub-segment $i = 1, \ldots, N$ **do**
    $Y_{i,k}^{\text{phy}} = \begin{cases} u_{i,k}^{\text{phy}} = u_{i,k+1}^{\text{hpml}} - \frac{\Delta T}{\tau_i}\left[V\{d_{i,k}^{\text{phy}}\} - u_{i,k}^{T}\right] + \frac{\Delta T}{L_i} u_{i,k}^{T}\left[u_{i,k-1}^{\text{hpml}} - u_{i,k}^{T}\right] \\ \qquad + \frac{\gamma_i \Delta T}{\tau_i \Delta L} \frac{d_{i,k+1}^{\text{hpml}} - d_{i,k}^{\text{phy}}}{d_{i,k}^{\text{phy}} + \kappa} \\ q_{i,k}^{\text{phy}} = d_{i,k}^{\text{phy}} u_{i,k}^{\text{phy}} \lambda_i \end{cases}$
    calculate $\Delta_{i,k} = |Y_{i,k}^{\text{phy}} - \widehat{Y}|$
end for
physics violations: $PHY.Loss(\widehat{Y}) = \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}\Delta_{i,k}$
Physics-guided loss function: $PGLoss = \alpha * \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}(x_{i,k}^{S} - \widehat{Y})^2 + \beta * \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}|Y_{i,k}^{\text{phy}} - \widehat{Y}| + \lambda * R(f)$

Physics value for all target segments could be computed by Equations (23)–(26) with both TFM and HPML model estimates. To ensure model estimates comply with traffic flow physics laws, Y_{phy} , this research first calculates the difference between physics values and model estimates during time-step k at segment i:

$$\Delta_{i,k} = |Y_{i,k}^{\text{phy}} - \widehat{Y}| \tag{27}$$

A positive value of $\Delta_{i,k}$ can be viewed as a violation of physics laws at segment i during time-step k. Hence, the mean of physics violations across all observations can be considered as an additional term in the physics-based loss function:

$$PHY.Loss(\widehat{Y}) = \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}\Delta_{i,k} \tag{28}$$

Adding the term into the original ANN loss function, the physics-guided loss function can be expressed as:

$$PGLoss = \alpha * \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}(x_{i,k}^{S} - \widehat{Y})^2 + \beta * \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}|Y_{i,k}^{\text{phy}} - \widehat{Y}| + \lambda * R(f) \tag{29}$$

where $x_{i,k}^{S}$ denotes the ground truth from stationary data; $Y_{i,k}^{\text{phy}}$ denotes the physical values (e.g. flow and speed) from converted TFM.

Note that the selection of hyper-parameters, α and β, can affect the performance of PGML. To reduce the number of hyper-parameters to be calibrated or optimised, the physics-based loss function could be simplified as:

$$J(\rho) = \rho * \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}(x_{i,k}^{S} - \widehat{Y})^2 + \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}|Y_{i,k}^{\text{phy}} - \widehat{Y}| + \lambda * R(f) \tag{30}$$

where ρ equals α/β. To optimise the value of ρ, a stochastic approximation approach is developed as:

$$\rho* = \arg\min J(\rho) \tag{31}$$

Then, the optimal value, ρ^*, could be obtained by the iterative process:

$$\rho_{k+1} = \rho_k - \frac{J(\rho_k + \delta_k e_i) - J(\rho_k - \delta_k e_i)}{2\delta_k} \tag{32}$$

where, δ_k is a small positive number that decreases with the iteration index, k; and e_i is the unit vector in the searching process.

4.3. Problem statement summary of PGML model for TSE

This subsection briefly summarises the PGML model for TSE problem. For a discrete spatiotemporal traffic state points $\mathcal{D} = \{x_{i,k} \mid i \in [0, n], \ \forall\, k \in [0, t]\}$, given limited observation points $\mathcal{S}$, the fully-covered estimated traffic state can be obtained by TFM:

$$\{x_{i,k}^{s} \mid i = 1, \ldots, n_s\} \xrightarrow{\text{traffic flow model}} \{x_{j,k}^{T} \mid i = 1, \ldots, n_T\} \tag{33}$$

Then the data set are ready for PGML as below:

$$\begin{cases} \mathcal{D} = \{x_{i,k}^{s} \mid i = 1, \ldots, n_s\} \\ \mathcal{Y} = \{y_{i,k}^{s} \mid i = 1, \ldots, n_s\} \in \mathcal{D} \\ \mathcal{T} = \{x_{i,k}^{T} \mid i = 1, \ldots, n_T\} \in \mathcal{D} \end{cases} \tag{34}$$

With the design of PGML model based on a neural network, the loss function include three parts: (a) empirical error between prediction $\widehat{Y}$ on $\mathcal{S}$ and label values $\mathcal{Y}$; (b) physics inconsistency between predictions $\widehat{Y}$ and physics values Δ, and (c) structural error that measures the model complexity. Then a general PGML for TSE is to solve the problem:

$$\min J(\rho) = \frac{\rho}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}(x_{i,k}^{S} - \widehat{Y})^2 + \frac{1}{n*m}\sum_{i=1}^{n}\sum_{k=1}^{m}|Y_{i,k}^{\mathrm{phy}} - \widehat{Y}| + \lambda * R(f) \tag{35}$$

5. Experimental study with field data

5.1. Case setting

To evaluate the effectiveness of the proposed PGML framework, field data are obtained from a stretch of interstate freeway I-15 (mileposts 299.68 – 304) in Salt Lake City, Utah. The studied freeway stretch is presented in Figure 7, where the observed data are available at the stations, indicated by blue and yellow icons, and the probe data can be collected over the entire segment. Seven blue icons (three detectors located on normal segments, two detectors located on off-ramps, and two detectors located on on-ramps) represent the detectors for training and the three yellow icons (one detector located on a normal segment, one detector located on an off-ramp segment, and one detector located on an on-ramp segment) represent the detectors for testing.

Data from the Performance Measurement System (PeMS) and Utah ClearGuide databases managed by the Utah Department of Transportation (UDOT) are used for model development and evaluations. The PeMS traffic information is collected by detectors installed every few miles along the freeway. Each detector counts the number of vehicles that pass every minute and detects the speed of each vehicle. Stationary point data is only available at the locations with detectors installed, but it can provide more precise traffic information. Probe speed data collected from the Clearguided database that is the estimated information collected from vehicle navigation systems, cell phone applications, and fleet vehicles. The probe data have a relatively low resolution because of the low penetration rate (e.g. 3%) of probe vehicles. but it can provide full-field speed information on

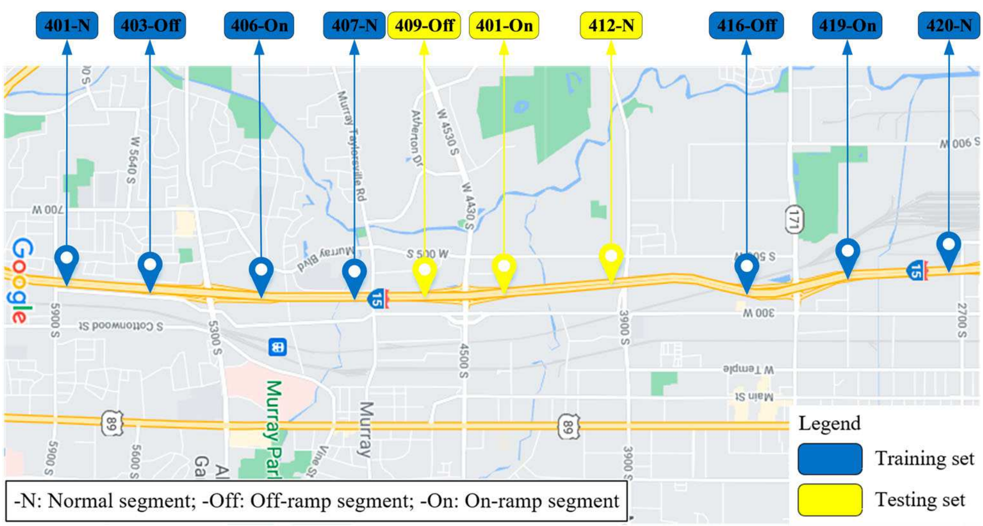
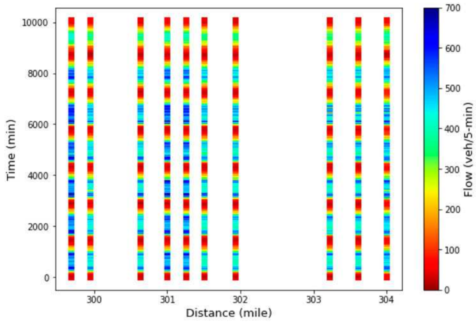
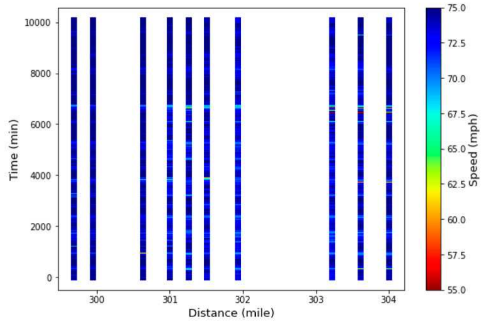


Figure 7. The deployment of freeway corridor and stations.



(a)



(b)

Figure 8. Sample data in the studied cases. (a) Observed flow. (b) Observed speed.

statewide freeways. The real-time traffic data and roadway geometry design information can be retrieved by the public online. For model evaluation, the time range of the data used is between January 4, 2021, and January 10, 2021. There are 288 observations per detector per day because the data is collected every 5-min. PeMS data with 5-min time intervals are widely utilised for TSE by many existing studies (Duan et al. 2016; Xu et al. 2020; Yuan et al. 2021; Z. Zhang and Yang 2020; Z. Zhang, Yuan, and Yang 2020). All obtained stationary point data, including both flow and speed information from stationary detectors, are shown in Figure 8. Notably, such data are collected from stationary traffic detectors and are only available in limited locations. In this research, two cases with different datasets are analysed for model evaluations: (1) Physics unguided neural network (termed PUNN) that utilises hybrid spatiotemporal information and the TFM data as input and treats observed traffic state as the label; and (2) physics-guided neural network (termed as PGNN) that uses spatiotemporal information and the TFM data as the input and treats observed traffic state as the label. Three benchmark machine learning models (e.g. RF, SVM, and ANN) and PUNN are utilised for evaluating the PGML performance.

In this study, the calibrated initial METANET model parameters are listed in Table 2. The performance of the proposed system for TSE is evaluated and compared by three common statistical indicators, including root meaning square Error (RMSE), mean absolute percentage error (MAPE), and mean absolute error (MAE), which are defined in Equations (36)–(38):

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\hat{y} - y_i)^2} \tag{36}$$

$$MAPE = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\hat{y} - y_i}{y_i}\right| * 100\% \tag{37}$$

$$MAE = \frac{1}{N}\sum_{i=1}^{N} \mid \hat{y} - y_i \mid \tag{38}$$

where y_i is the observed traffic speed and flow and $\hat{y}$ is the estimated traffic speed and flow.

Table 2. The parameters of traffic flow model.

Parameter	Value
n	9
λ_i	4
ΔT	1/360 (h)
u_f	120 (km/h)
γ	35 (km^2/h)
ΔL	0.5 (km)
δ	1.4
τ	0.05 (h)
α	1.4324
d_{cr}	36.85 (veh/km)
κ	13 (veh/k)m)

5.2. Results analysis

5.2.1. Estimation results on normal segment

Table 3 summarises the TSE results from TFM, pure-ML models, PUNN, and PGNN of normal freeway segment. Among all three pure-ML models, the lowest flow RMSE, MAPE, and MAE are 95.30 vehicles/5-minutes, 26.09%, 65.86 vehicles/5-minutes, respectively, and the lowest speed RMSE, MAPE, and MAE are 2.56 mph, 2.04%, and 1.38 mph, respectively, while TPM can generate lower RMSE, MAPE, and MAE of both flow and speed estimates. It yields a 2.40 mph of RMSE, a 1.91% of MAPE, and 1.30 mph of MAE for speed and a 56.28 vehicles/5-minutes of RMSE, a 14.80% of MAPE, and 38.14 vehicles/5-minutes of MAE for flow, while TPM can generate lower RMSE, MAPE, and MAE of both flow and speed estimates. These results indicate that pure-ML cannot reach an acceptable estimation accuracy with limited information. It demonstrates that the TPM data could be a fully covered traffic information for ML model training. Hence, the PGNN is developed for TSE problem with TFM data as an additional information. PGNN generates a 1.90 mph of RMSE, a 1.64% of MAPE, and 1.17 mph of MAE for speed and a 40.96 vehicles/5-minutes of RMSE, a 10.81% of MAPE, and 27.85 vehicles/5-minutes of MAE for flow. This finding indicates that TSE accuracy by PGNN is within an acceptable range. To further confirm this finding, Table 4 shows the improvement percentage of TSE results from TFM, PUNN, and PGNN. Compared with the results from TFM and the best pure-ML model (ANN), the RMSE, MAPE, and MAE are improved by PUNN. It indicates that TFM estimates can be valid additional training variables to improve TSE accuracy. Furthermore, The PGNN is the most effective model for TSE because the PGNN obtains the largest improvement. Figure 9 show the comparison of estimated flow and speed by TFM, pure-ML models, PUNN, and PGNN with ground truth. It can be clearly seen

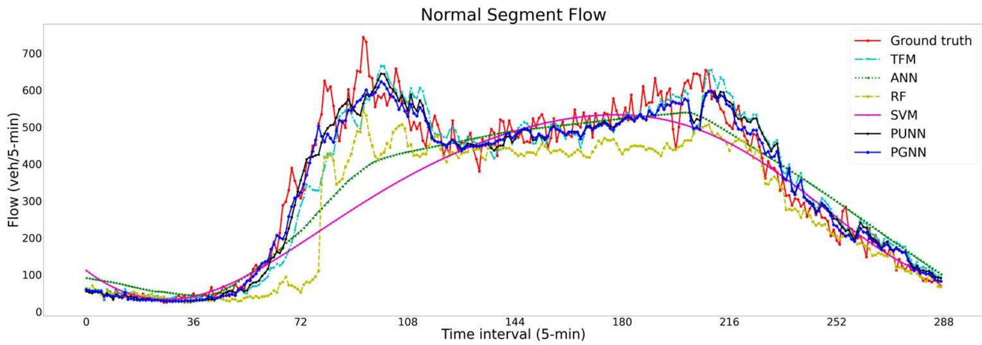
Table 3. Estimation results of on freeway normal segment.

Models	Flow RMSE	Flow MAPE	Flow MAE	Speed RMSE	Speed MAPE	Speed MAE
TFM	56.28	14.80%	38.14	2.40	1.91%	1.30
SVM	106.73	26.09%	68.08	2.56	2.04%	1.38
RF	103.25	26.50%	71.19	2.80	2.57%	1.78
ANN	95.30	31.17%	65.86	2.68	2.43%	1.68
PUNN	45.10	12.46%	31.82	2.38	1.74%	1.17
PGNN	40.96	10.81%	27.85	1.90	1.64%	1.17

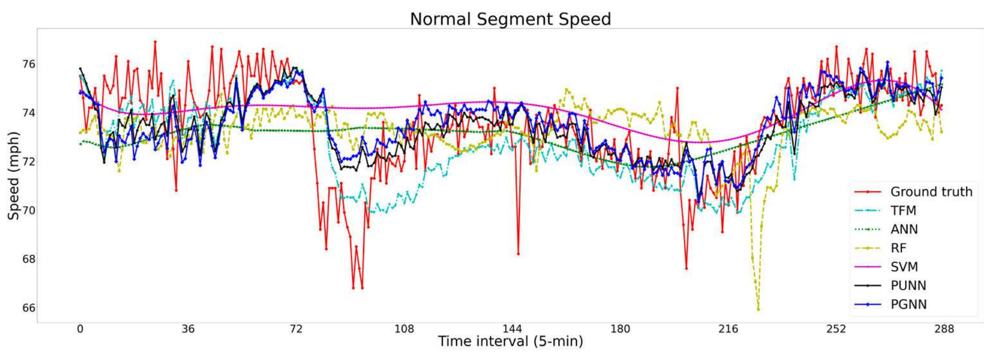
Note: Flow: veh/5-min; Speed: mph.

Table 4. The performance improvement of TFM and PGNN compared with pure-ML.

Models	Flow RMSE	Flow MAPE	Flow MAE	Speed RMSE	Speed MAPE	Speed MAE
TFM	40.94%	52.52%	42.09%	10.45%	21.40%	22.62%
PUNN	52.68%	60.03%	11.19%	11.2%	28.40%	30.36%
PGNN	57.02%	65.32%	57.71%	29.10%	32.51%	30.36%



(a) Estimated flow of normal segment



(b) Estimated speed of normal segment.

Figure 9. TSE estimates vs. ground truth on normal segment. (a) Estimated flow of normal segment and (b) Estimated speed of normal segment.

that the line of PGNN better fits the ground truth, which demonstrates that PGNN could accurately estimate speed and flow. To further confirm this finding, the TSE results obtained by PGNN are compared to the observed data. In Figure 10, the estimation results will be seen as fitting the ground truth well if the coefficient of the trend line is close to one and the intercept is close to zero. In this case, the coefficient is 0.95 and the intercept is 11.49 for flow estimation, and the coefficient is 0.36 and the intercept is 47.33 for speed estimation. It proves that PGML could achieve relatively higher TSE accuracy.

To further illustrate the variation of MAPEs of different models, Figure 11 shows the violin plots of MAPEs on the test set by different models. In each 'violin', its margin shows the Gaussian distribution of the dataset, and a box plot is drawn inside. In Figure 11, it is noted

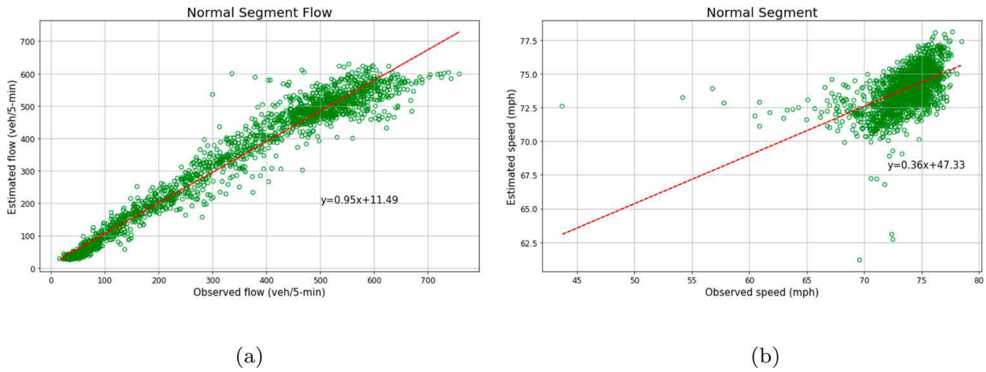


Figure 10. Estimated flow and speed by PGML vs. ground truth on normal segment. (a) Estimated flow of normal segment and (b) Estimated speed of normal segment.

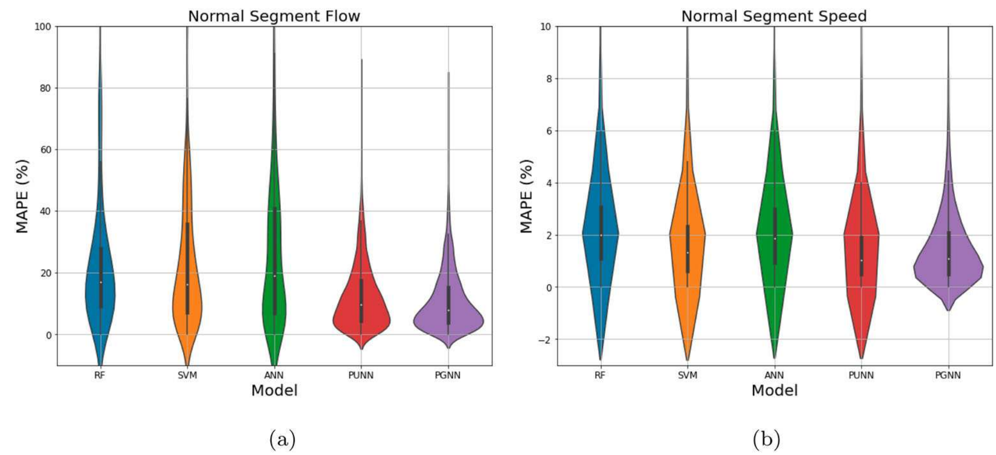


Figure 11. MAPE distribution of different models on test set of normal segment. (a) MAPE of estimated flow and (b) MAPE of estimated speed.

that PGNN generally has a lower MAPE value. All results proved that PGNN could perform well for flow and speed estimation and especially for flow estimation.

5.2.2. Estimation results on on-ramp and off-ramp segment

Tables 5–6 show the TSE results from TFM, pure-ML models, PUNN, and PGNN of freeway on-ramp and off-ramp segments. Compared with Table 3, the conclusion can be reached that the performance of pure-ML models on on-ramp and off-ramp segments is better than normal segments. The RMSE, MAPE, and MAE for both flow and speed of PGNN on on-ramp and off-ramp segments are lower than those for normal segments. It indicates that PGNN also performs better on on-ramp and off-ramp segments. Compared TSE results from TFM, pure-ML, and PUNN, the RMSE, MAPE, and MAE for both flow and speed of PGNN are greatly decreased, especially for the flow. It indicates that TSE accuracy can be significantly enhanced by PGNN on normal, on-ramp, and off-ramp segments. Figure 12 show the comparison of estimation results of TFM, pure-ML, PUNN, and PGNN with ground truth on on-ramp and off-ramp segments. The lines of TFM, pure-ML, and pure-ML with probe

Table 5. Estimation results of on freeway on-ramp.

Models	Flow RMSE	Flow MAPE	Flow MAE	Speed RMSE	Speed MAPE	Speed MAE
TFM	64.47	21.74%	51.12	1.92	2.02%	1.46
SVM	72.74	24.89%	50.20	1.99	2.17%	1.56
RF	50.82	20.01%	33.66	3.85	2.81%	2.03
ANN	55.08	26.91%	40.83	2.22	2.39%	1.72
PUNN	35.04	11.71%	24.03	1.82	1.99%	1.44
PGNN	31.37	11.38%	21.78	1.41	1.44%	1.04

Note: Flow: veh/5-min; Speed: mph.

Table 6. Estimation results of on freeway off-ramp.

Models	Flow RMSE	Flow MAPE	Flow MAE	Speed RMSE	Speed MAPE	Speed MAE
TFM	40.01	12.73%	26.82	2.04	1.98%	1.44
SVM	57.95	26.53%	41.70	2.00	1.67%	1.19
RF	52.00	20.37%	34.71	2.64	1.92%	1.37
ANN	55.87	24.06%	40.68	2.23	1.96%	1.41
PUNN	34.99	12.86%	23.89	1.75	1.54%	1.10
PGNN	31.98	11.23%	21.90	1.69	1.46%	1.05

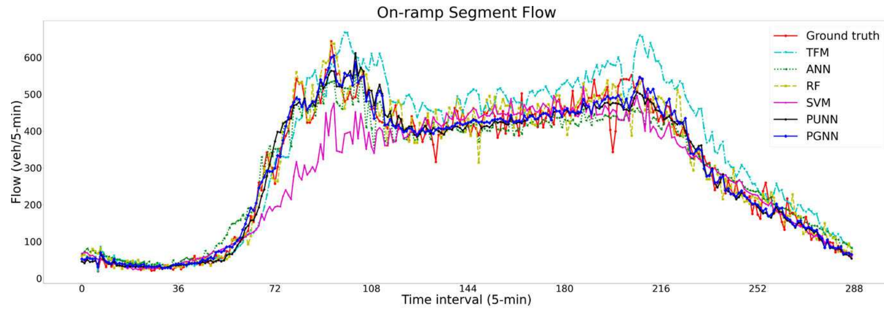
Note: Flow: veh/5-min; Speed: mph.

do not fit the ground truth well. It can be clearly seen that the line of PGNN better fits the ground truth, which indicates that PGNN also performs well on the on-ramp and off-ramp segments. It further demonstrates that PGNN could reach an acceptable TSE accuracy on all segments. To further confirm this finding, the TSE results obtained by PGNN are compared to the observed data in Figure 13. For the on-ramp segment, the coefficient is 0.97 and the intercept is 9.81 for flow estimation, and the coefficient is 0.56 and the intercept is 32.69 for speed estimation. For the off-ramp segment, the coefficient is 0.97 and the intercept is 13.04 for flow estimation, and the coefficient is 0.40 and the intercept is 43.89 for speed estimation. All results proved that PGNN could perform well for flow and speed estimation and especially for flow estimation. Overall, the PGNN could reach an acceptable TSE accuracy on all segments.

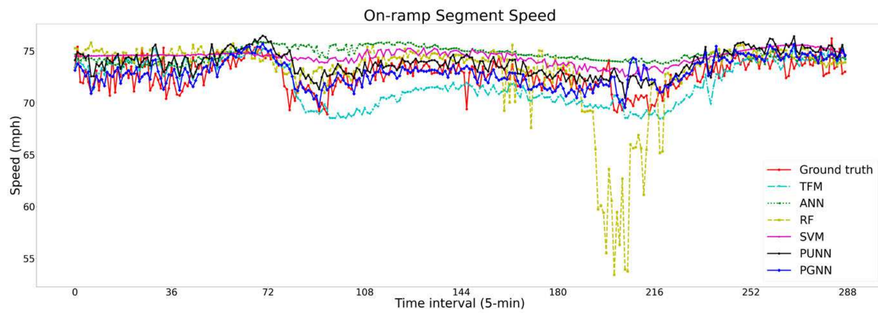
The performance of different models in peak hours and off-peak hours are also compared in Figure 14. Peak hours include six hours (7 am – 10 am and 4 pm – 7 pm) and off-peak hours include eighteen hours (midnight – 7 am, 10 am – 4 pm, and 7 pm – midnight). As shown in the figure, the pure-ML model produces very high RMSEs, especially in peak hours. The RMSEs of all PUNN and PGNN models are lower than the pure-ML model and PGNN obtains the lowest RMSEs in both peak and off-peak hours on normal, on-ramp, and off-ramp segments. It indicates that the PGML models could obtain better estimation accuracy for both flow and speed under low traffic volume conditions on freeways. The PGNN model performance degradation during peak hours may be due to traffic congestion or traffic crashes.

6. Conclusions and future research directions

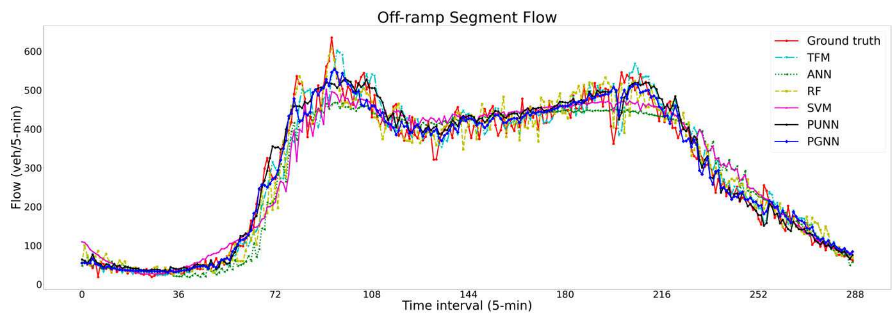
The quality of TSE directly affects the effectiveness of traffic control and the efficiency of intelligent transportation systems (ITSs) operations. Recently, classical model-driven approaches and data-driven approaches have been successfully deployed in TSE. However, model-driven approaches could potentially yield inaccurate estimation and data-driven



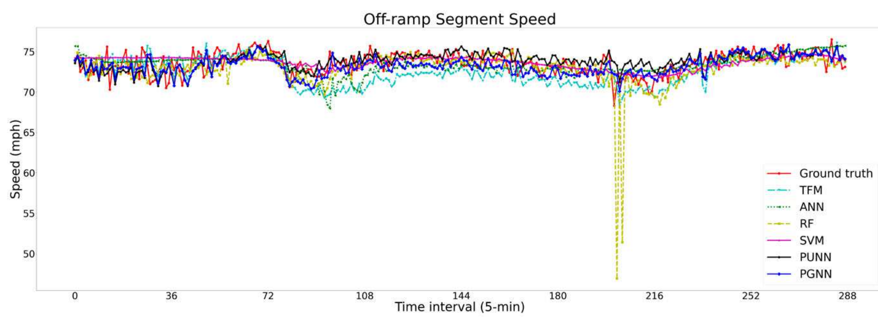
(a) Estimated flow of on-ramp segment.



(b) Estimated speed of on-ramp segment.



(c) Estimated flow of off-ramp segment.



(d) Estimated speed of off-ramp segment.

Figure 12. TSE estimates vs. ground truth on on-ramp and off-ramp segments. (a) Estimated flow of on-ramp segment. (b) Estimated speed of on-ramp segment. (c) Estimated flow of off-ramp segment and (e) Estimated speed of off-ramp segment.

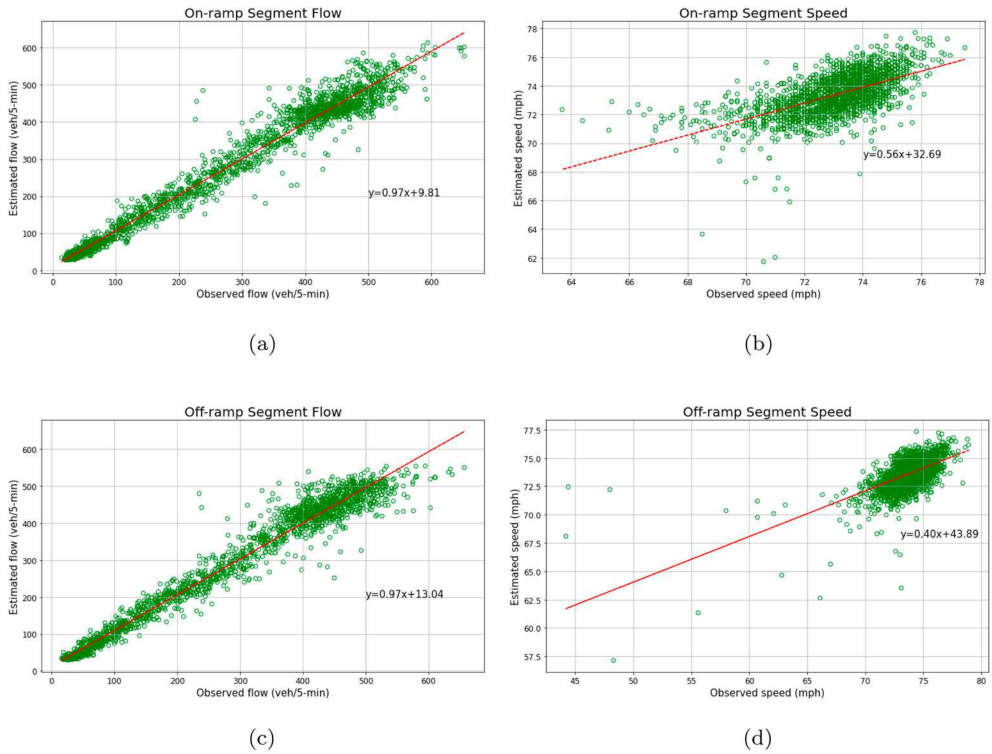
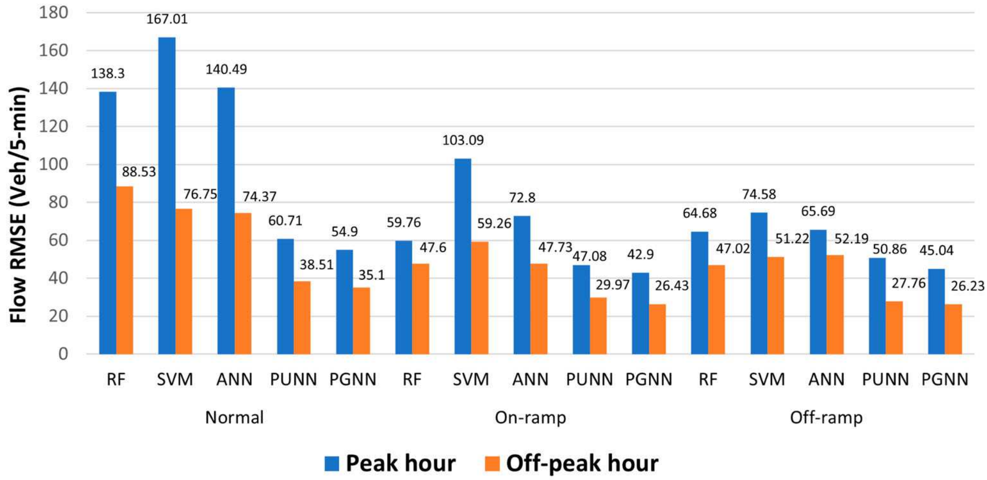


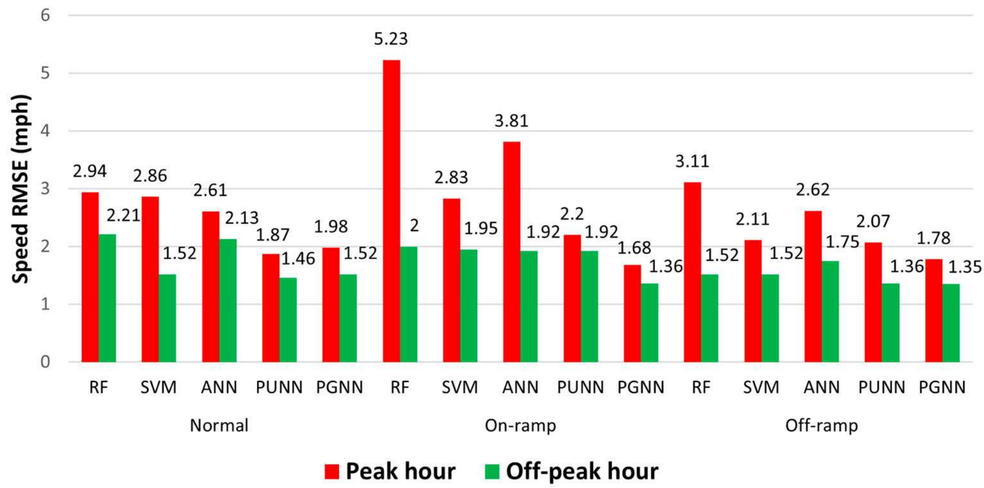
Figure 13. Estimated speed and flow by PGML vs. ground truth on on-ramp and off-ramp segments. (a) Estimated flow of on-ramp segment. (b) Estimated Speed of on-ramp segment. (c) Estimated Flow of off-ramp segment and (d) Estimated Speed of off-ramp segment.

approaches require a massive amount of data to train the model. To overcome these limitations, this study develops an innovative physics-guided machine learning (PGML) that combines the classical traffic flow model with the machine learning model (neural network) to improve TSE accuracy. The PGML framework incorporates physics knowledge into loss functions to help ML models capture generalisable dynamic patterns consistent with established traffic physics laws. More specifically, the application of physics-based loss functions in the learning objective of neural networks in our PGML framework ensures that the model predictions will not only show lower errors on the training set but also have scientific consistency with the known physics on the unlabelled set.

To test the effectiveness of the proposed PGML approach for coping with the problems of freeway traffic flow modelling, this paper conducted empirical studies on a real-world dataset collected from a stretch of I-15 freeway in Utah. Research results indicate that the proposed PGML framework performed better than the previous compatible methods, including the calibrated traffic physics model and the pure machine learning methods, especially in terms of estimation accuracy and input robustness. The proposed PGML approach can offer high-resolution, wide-coverage, and accurate traffic state information with limited traffic sensor data. The research findings provide the basis for future research if they have the same research concern. This work will help transportation agencies find better countermeasures to mitigate traffic congestion, improve traffic operation efficiency



(a) RMSE of flow.



(b) RMSE of speed.

Figure 14. The pure-ML, PUNN, and PGNN model performance comparison between peak hour and off-peak hour. (a) RMSE of flow and (b) RMSE of speed.

and safety, and help travelers preplan and schedule routes. The proposed PGML approach, which combines machine learning models with a traffic physics-based model, could potentially lead to a revolution in ITS development and significantly reduce the amount of money required for traffic detectors. This research will indeed help build up the era of big data for transportation.

The effectiveness of the proposed PGML approach has been proven. However, the PGML traffic state estimation still needs additional study. In particular, a more efficient machine learning algorithm and traffic physics-based model and its application on urban freeway networks are worth studying. The proposed PGML approach benefits other transportation-related applications such as missing data imputation and validating traffic detector data.

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