Using Deep Neural Network to Analyze Travel Mode Choice with Interpretable Economic Information: An Empirical Example

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Abstract
Recently deep neural network (DNN) has been increasingly applied to microscopic demand analysis. While DNN often performs with higher predictive accuracy than traditional multinomial logit (MNL) model, it is unclear whether we can obtain interpretable economic information from DNN-based choice model beyond prediction accuracy. This paper seeks to provide an empirical method of numerically extracting valuable economic information such as choice probability, probability derivatives (or elasticities), and marginal rates of substitution such as value of time. Using a stated preference survey collected in Singapore, we find that when the economic information is aggregated over population or ensembled over models, the DNN models are able to reveal roughly S-shaped choice probability curves, inverse bell-shaped driving probability derivatives regarding costs and time, and reasonable median value of time (VOT). However at the disaggregate level, choice probability curves of DNN models can be non-monotonically decreasing with costs and highly sensitive to the particular estimation; derivatives of choice probabilities regarding costs and time can be positive at some region; VOT can be infinite, undefined, zero, or arbitrarily large. Some of these patterns can be seen as counter-intuitive, while others can potentially be regarded as advantages of DNN for its flexibility to reflect certain behavior peculiarities. These patterns broadly relate to two theoretical challenges of DNN, irregularity of its probability space and large estimation errors. Overall, this study provides a practical guidance of using DNN for demand analysis with two suggestions: First, researchers can use numerical methods to obtain behaviorally intuitive choice probabilities, probability derivatives, and reasonable VOT. Second, given the large estimation errors and irregularity of the probability space of DNN, researchers should always ensemble either over population or individual models to obtain stable economic information.

Keywords: Deep Neural Network, Machine Learning, Travel Mode Choice, Interpretability
1. Introduction

Multinomial logit (MNL) models have been used to examine individual decision making for decades with wide applications to economics, marketing, transportation, environmental engineering, etc. [1] [2]. But there is an emerging trend of using machine learning models, particularly deep learning models, to analyze individual decisions. Deep neural network (DNN) empirically performed the best out of 17 families of 179 classifiers for two-alternative choices in 121 different datasets [3]. It also outperformed traditional MNL in transportation specific tasks, such as travel mode choice, automobile ownership, and route choice [14] [6] [15]. However, so far the DNN applications to travel choice analysis exclusively focus on the comparison of prediction accuracy, and DNN is criticized as a "black-box" model lacking interpretability. While Wang and Zhao (2018) discussed the utility interpretation of DNN and introduced one numerical method for its interpretability, the performance and the specific procedures of the numerical method in real datasets are not demonstrated [7]. With the popularity of deep learning models and the urgency of interpreting model results, how researchers could extract reliable economic information from a prediction-driven DNN becomes an important question in practice.

To fill the research gap, this study seeks to demonstrate how to use DNN-based models to analyze individual travel mode choice in a real data set for interpretation purposes. Since DNN can be seen as a high-dimensional MNL model with complex and nonlinear feature transformation [7], we can numerically compute choice probabilities, probability derivatives \(^1\), and marginal rate of substitution (MRS) based on the utility interpretation of DNN. This study focuses on the derivatives of probabilities with respect to costs and time and value of time (VOT) as one concrete example of MRS. We examine the economic information aggregated over population and models as well as the disaggregate information for specific estimation and individuals and visualize how choice probabilities, probability derivatives and VOT vary with travel attributes. We find that aggregate-level economic information based on DNN is reasonable and intuitive, while disaggregate-level information can be counter-intuitive, due to the high-dimensionality and the irregularity of the DNN models.

This study provides a set of practical guidance on how to extract economic information from DNN for behavioral and policy analysis. First, researchers can numerically compute choice probabilities and other economic information, which are largely consistent with our behavioral intuition. Second, given the large estimation errors and irregularity of the probability space of DNN, researchers should always ensemble either over population or individual models to obtain stable economic information. Particularly, ensembled models can smoothen choice probabilities and probability derivatives, and aggregate VOT numbers are much more reasonable than disaggregate values at the individual level. These suggestions are important for DNN-based demand analysis, because so far the majority of DNN applications in travel demand analysis tend to use single training result and disregard interpretable economic information contained in DNN models. Overall, we emphasize the interpretability of DNN-based choice models distinct from the sole prediction focus of prior DNN applications in travel demand analysis. Economic information can be numerically computed without involving individual parameters as an intermediate step,

\(^1\) An alternative focus is elasticity. But we opt for probability derivatives because probability derivatives retain unit information in input X, which help intuitive understanding. Since the formula of probability derivatives \(\partial P/\partial x\) is quite similar to \((\partial P/P)/(\partial x/x)\), our main findings should hold for elasticity as well.
which is an end-to-end approach in line with the practice of machine learning modeling.

The paper is structured as following. Section 2 reviews relevant studies. Section 3 briefly connects the utility interpretation of MNL to DNN, discusses data, and provides numerical methods to compute economic information. Section 4 presents the application of DNN to one stated preference travel survey and computes the economic information. Section 5 concludes the paper.

2. Literature Review

In the field of travel demand analysis, MNL models have been used for decades to analyze various types of choices such as travel mode choice, travel frequency, travel scheduling, destination and origin choices, route choice, and choice of using new transit lines [14] [8] [3]. MNL models have also been applied to activity choices from long-term to short-term decisions, including choice of working places, residential locations, and car ownership in the long run; and trips for various trip purposes in the short run [9] [10] [11].

Classic MNL models provide a set of important information for economic analysis [1] [2]. The interpretable components in MNL include choice prediction, choice probabilities, probability derivatives, and marginal rate of substitutes, all of which are based on the utility interpretation of the choice models and are critical to understand behavior and analyze policies. Average choice probabilities represent market shares, which can then be used to analyze market power [1]. Elasticity of travel demand regarding price and time influences the efficacy of changing behavior through the change of monetary and time costs [12]. VOT, as one important instance of MRS, is the basis for the cost benefit analysis: to translate the time saving to dollar value to quantify the benefit of the transportation projects [12]. Overall, while prediction accuracy is important in choice modeling, other economic information is also critical for researchers to understand the models and to use them for policy and marketing analysis.

In recent years, researchers started to use machine learning models to analyze individual choices in the transportation field. For instance, Karlaftis and Vlahogianni (2011) [13] summarized 86 studies in six transportation fields to which NN models were applied. Cantarella et al. (2005) found that NN has a better performance than logit models in predicting travel mode choice [14]. Three studies used NN to predict traffic flows with specifically designed NN architectures in order to capture the spatio-temporal correlation in traffic flow data [15] [16] [17]. Xiao et al. (2016) used NN to detect trip purposes from smartphone-based data to suggest that smartphone-based travel surveys could complement conventional travel surveys when DNN is used [18]. Other studies used deep learning approaches to predict traffic accidents, travellers’ decision rules, and driving behaviors [19] [20] [21], or compared neural network, support vector machine, decision trees, and random forest to baseline MNL model in predicting travel behavior [22] [23] [24]. All of these studies found that DNN could outperform traditional statistical models and replicate realistic scenarios well. However, nearly all of these studies focused solely on the comparison of prediction accuracy. One recent paper by Wang and Zhao (2018) introduced utility interpretation to DNN and discussed a numerical method of interpreting DNN modeling results based on a simulated dataset [7]. But it is unclear whether researchers can use the numerical method to extract reliable and interpretable economic information from DNN based on real datasets. It is also unclear what specific procedures researchers should follow to interpret DNN-based choice models [7].
The exclusive focus on the prediction accuracy of DNN models is understandable since machine learning models mainly aim to achieve high capacity for prediction. However, recent studies started to investigate how to extract interpretable information from machine learning models. For instance, visualization of images was used to interpret the outcomes of convolutional neural networks (CNN) [25]. Ribeiro et al. (2016) [26] presented the idea of fitting local data points by LIME and SP-LIME to make specific data points interpretable. Studies took gradients with respect to input vectors to form a salience map to analyze how outputs are influenced by input features [27]. In fact, computing the derivatives of outputs with respect to inputs is one common way to interpret machine learning models.

The comprehensive understanding of the DNN models remains challenging because of several theoretical difficulties. First, researchers still lack understanding of the probability field and the partition of input space. Probability field of the input space refers to the field that uses input features as coordinates and uses choice probabilities (soft labels) as measurement at each point; and partition of the input space refers to the input space partitioned by choices (classes). Since DNN has highly nonlinear feature transformation and high dimensional parameters, the probability field and the partition of input space can have very irregular shapes. This problem relates to the discussions about DNN robustness, adversarial training, and cybersecurity concerns of using DNN [28]. In sharp contrast to the irregular probability field of DNN, MNL models have very regular properties: the features are partitioned by a hyperplane, and orthogonal directions in the probability field of input space are monotonic and smooth [2], i.e., choice probabilities regarding input variables is monotonic and smooth. For example, the probability of choosing car monotonically decreases as driving costs increase. But as we will show later, this feature is not guaranteed in the DNN models.

The second challenge of DNN germane to this study is its large estimation errors due to the high dimensionality. The large number of parameters in DNN pose threats to its ability to generalize [30]. The key inequality in Vapnik (1999) [31] shows that when model capacity is very high, particularly the ratio between VC dimension and sample size is very high, generalization errors cannot be well bounded by empirical error in a probabilistic manner. Hence the principle of structural risk minimization, or practically regularization, is important in reducing generalization errors in high dimensional models [31]. Practically, $\ell_p$ norm penalties, explicit domain constraint on parameters, and parameter sharing are common regularization tools. This trade-off between estimation and approximation errors is coined in many different names, such as bias-variance trade-off or underfitting vs. overfitting [32]. These two theoretical difficulties, irregular probability field and large estimation errors, are highly relevant to our empirical results, to which we will turn.

3. Setup for Empirical Analysis

3.1. Utility Interpretation

Wang and Zhao (2018) recognize that the inputs into the last softmax activation functions of DNN can be seen as utilities. In fact, the utility interpretation emerges naturally when we treat DNN as an extension of MNL with complex feature transformation. The details of the relationship and trade-off between MNL and DNN are presented in [7]. Figure 1 shows the feedforward DNN we will use in this study. This DNN uses choice of

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[2] We assume that features are not transformed before being fed into the MNL models.
five travel modes as target variables $Y$. When the last activation layer in DNN is softmax function, the choice probabilities take the form:

$$P_{nk} = \frac{e^{V_{nk}}}{\sum_j e^{V_{nj}}}$$

in which $V_{nj}$ is the deterministic utility from a discrete choice model perspective. Compared to a simple MNL model, the difference here is that $V_{nj}$ has a more complex functional form:

$$V_{nj} = (g^m_j \circ g^{m-1} \circ \ldots \circ g^2 \circ g^1)(x)$$

in which each $g_i = ReLU(w^T_i x + b_i)$ is the linear plus rectified linear unit (ReLU) transformation of one hidden DNN layer, and $g^m_j$ is the transformation of the last hidden layer into the utility of alternative $j$. Each hidden layer $g_i()$ is more complex than a simple MNL model, in which only one linear transformation is applied to input features with identifiable utility specification.

3.2. Numerical Computation of Economic Information

With the utility interpretation as the connection between MNL and DNN, we can numerically compute choice prediction, choice probabilities, probability derivatives, and MRS, as summarized in Table 1. The second column in Table 1 summarizes how we computed the economic information numerically; the third column is the formula used in MNL model. In MNL model, the estimations of individual parameters ($\hat{w}$) are needed to compute probability derivatives and MRS. In contrast, because these parameters are not identifiable in the DNN models, we opt to compute probability derivatives and MRS numerically.

3.3. Dataset

This study used a stated preference (SP) survey conducted in Singapore in July 2017. In total, 2,073 respondents participated, and each respondent answered in seven choice
Table 1: Formula to Numerically Compute the Four Types of Economic Information, adopted from Wang and Zhao (2018)

| Economic Information       | Numerical Computation in DNN | Formula in MNL |
|----------------------------|------------------------------|----------------|
| Choice Predictions         | \(\hat{y}_n\)               | \(\hat{y}_n\) |
| Choice Probabilities       | \(\hat{P}_{nk}\)            | \(\hat{P}_{nk}\) |
| Probability Derivatives    | \(\frac{\partial \hat{P}_{nk}}{\partial x_{ni}}\) | \(P_{nk}(1 - P_{nk})\hat{w}_i\) |
| MRS                       | \(\frac{\partial P_{nk}}{\partial x_{ni}}\) | \(\hat{w}_i/\hat{w}_j\) |

scenarios varying by the availability and attributes of travel mode alternatives. We selected only the choice scenarios in which all travel modes were available and the final dataset included 8,418 observations (individuals*scenarios). The target choice variable \(Y\) was travel mode, including five alternatives: walking, buses, ride sharing, autonomous vehicle, and driving. The explanatory variables included 25 individual-specific and alternative-specific variables, such as income, education, gender, driving costs, driving time, among others. The survey started with questions about the home and working locations of respondents and their current travel mode. The revealed preference information was used to generate the SP scenarios. The SP survey followed the standard method of orthogonal design. Each attribute took three levels of values with the medium equal to the value reported by the respondent so that the values were realistic and readily understandable to participants, and the other two levels were adjusted by multiplying the medium value by certain constants. All participants reported their socioeconomic information in the last section of the survey.

We split the data into training, validation, and testing sets, with a ratio of 6 : 2 : 2, associated with 5,050 : 1,684 : 1,684 observations for each. Training set was used for training each single model; validation set was used to train hyperparameters and select models; testing set was used for final analysis after the model selection and parameter training. Due to the non-convexity of empirical risk minimization in DNN, each training on a fixed dataset can generate different model parameters. Therefore, our study uses fifty rounds of estimation for each single model with fixed hyperparameter. Note that the unstability in estimation does not exist in traditional MNL model because its ERM is convex. This method of splitting full dataset into training, validation, and testing sets is also different from the way of using data in MNL models (splitting into training and testing sets)\(^3\).

4. Empirical Results

After briefly discussing the hyperparameter training as the first step, this section will present the results of choice probabilities, probability derivatives, and VOT. In the discussion of probability derivatives and VOT, we use as example the choice of driving, driving costs and in-vehicle travel time. The discussion includes a limited comparison to the MNL model, although the main focus is the analysis of DNN-based choice modeling itself.

\(^3\)A more comprehensive approach is to use cross-validation. But to save computational cost, we did not use it in this study. The purpose of using cross-validation is to identify a robust model with high prediction accuracy that does not vary with sampling process. This is different from our focus on interpretability in this paper.
4.1. Hyperparameter Training

Hyperparameter training and architecture design are the first step in training a deep learning model. We used the hyperparameters suggested by standard practices [33] [34], and tuned them manually. The DNN uses eight fully connected hidden layers, 100 neurons for each hidden layer, ReLU activation functions in hidden layers, and Softmax activation function in the last layer. It uses cross-entropy loss function, Glorot initialization, Adam optimization with default learning rate 0.001, early stopping as regularization, $L_1$ norm regularization with very weak strength $\lambda = 1e^{-50}$, dropout rates equal to 0.01, and minibatch size = 50.

Hyperparameter training and architecture design of DNN are very complicated issues. The space of hyperparameter training is a mixture of integer and continuous variables. There are many ways to perform a more comprehensive and systematic hyperparameter searching and architecture design, such as using reinforcement learning or Bayesian methods [35] [38] [39]. However, this study focuses on how to interpret economic information from one or several DNN models, rather than how to choose final DNN models out of multiple candidates. We simply acknowledge that hyperparameter training and architecture design are important steps when using DNN for choice analysis.

4.2. Choice Probabilities

Figure 2 describes the relationship between probabilities of choosing driving and driving cost (left figure) and in-vehicle time (right figure). The grey and color curves are the results of fifty separate estimations, out of which we will highlight the five color curves for discussions. The dash curve is from one ensembled model averaged over 38 estimations. Only 38 models out of the total 50 models are used because the other 12 models generate entirely unreasonable results (when travel time goes to infinity, the probability of choosing to drive should not be large) and are discarded. All the curves are generated by varying driving costs and in-veh travel time, while holding other variables at the levels of the population mean. We report several important findings.

The majority of the choice probability curves are intuitive and reasonable, resembling the standard S-shaped curve from MNL model. For driving cost, in nearly all the estimations, people have close-to-one probabilities to choose to drive when driving cost is close to zero and close-to-zero probabilities to choose driving when the cost becomes large. For in-vehicle travel time, this observation holds for the majority of the 50 estimations. When driving costs are between about $7 and $20 or in-vehicle travel time is between about 20 and 80 minutes, the mode choice demonstrates a clear trade-off between driving and other four modes. The ensembled model results in an intuitive and reasonable profile of choice probability with respect to travel attributes, even though we do not give any a priori knowledge to the model.

While the choice probability curve of the ensembled model behaves well, any particular individual estimation in Figure 2 may not: the DNN-based choice models may have non-monotonic choice probabilities and are highly sensitive to estimations. First, the driving probabilities are not monotonically decreasing regarding time and costs at certain regions. In terms of driving costs, the driving probabilities in Estimation 10 increase

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4 Since we used early stopping as regularization, the total number of training epochs does not matter that much.

5 Our manual hyperparameter searching shows that even 0.01 regularization strength could reduce prediction accuracy, so we chose to use no regularization at all.
when the driving costs are below 5 dollars, so do those in Estimation 9 when the driving costs are larger than 20 dollars. A more dramatic example is the driving probability with respect to in-vehicle travel time based on Estimations 17: the driving probability increase when the driving time is larger than 80 minutes. Second, even conditioning on the same hyperparameter and the same dataset, each estimation of DNN gives us different results.

For instance, while most of the curves describing the relationship between driving probabilities and driving costs have similar and reasonable shape, the exact ranges vary with estimations. Estimation 1 suggests that driving probabilities start to drop at about $7 and approaches zero at about $17, while Estimation 2 suggests that driving probabilities start to drop at about $12 and approaches zero at about $15. It is important to note that the prediction accuracy itself does not help identify these irregular patterns. In fact, the average prediction accuracy of the 38 valid models is 0.567, while that of the 12 invalid ones is 0.566, nearly the same.

The two properties of non-monotonic decrease and high sensitivity to estimations are exactly associated with the two theoretical challenges of DNN: irregularity of its probability fields and large estimation errors. Since these curves of choice probabilities are a subset of the whole probability field of DNN, non-monotonically decreasing choice probabilities reveal the irregularity of the whole probability field. In addition, the high sensitivity to estimations shows the high estimation errors of DNN. To fully address these problems, researchers need to have better understanding about the geometry of the input space, partition by classification tasks, generalization of DNN models, and their robustness. In fact, these theoretical challenges have triggered heated discussions [28].

We can evaluate this non-monotonically decreasing choice probabilities in two opposite views. The first is to treat it as a problem. In general people should not be more likely to choose one alternative when its cost increases. Accordingly we chose only 38 models of
the total of 50 for the ensembled model. Researchers need to find ways within the DNN framework to retain the monotonicity property. The second is to evaluate the irregular shapes of choice probabilities as an opportunity because DNN framework is less restrictive in terms of the relationship between choice probabilities and input variables. For instance, the true probability curves may not follow a S-shape and the result in Estimation 31 could be realistic for certain individuals in certain scenarios—people may behave irrationally in certain feature space. It may also be the case that choice probability curves do not change in a smooth way in reality and DNN captures these patterns due to its flexibility.

If the irregularity of DNN is treated as problems, one method of improving DNN models is model ensemble, as shown by the dash lines in Figure 2. The two dash lines are the results from an ensembled model averaged across 38 estimations. Compared to each individual estimation, the ensembled model is more monotonic and smoother. The driving probabilities with respect to both cost and time in the ensembled model are well behaved, similar to a typical S-shaped curve in the MNL model but not exactly the same. Theoretically it is not a surprise that the ensembled models behave better because model ensemble reduces the variance of the models. It is particularly effective for the models with large variance such as DNN.

4.3. Probability Derivatives

Figure 3 visualizes the probability derivatives of driving with respect to driving costs and in-vehicle travel time based on the fifty estimations. Again we only vary driving costs and time, holding all other variables constant at the population mean. The fifty grey curves are individual estimations; dash curves are ensembled models; five color curves correspond to those in Figure 2. The standard formula of probability derivatives in MNL models is \( \frac{\partial P_{ni}}{\partial x_{ni}} = P_{ni}(1 - P_{ni}) \cdot (\frac{\partial V_{ni}}{\partial x_{ni}}) \), which has an inverse bell-shape and all negative values. Intuitively, people are not sensitive to price changes when price is close to zero or infinity, but are sensitive to the changes when price is close to some tipping point. This pattern holds for most of our DNN estimations. Each curve of probability derivatives has some peak values resembling the peak of inverse bell-shaped curve of standard MNL model.

The two irregular patterns of non-monotonically decreasing choice probabilities and sensitivity to estimation, as identified in Figure 2, also apply to the individual probability derivatives in Figure 3. More specifically, when choice probabilities are locally increasing, the probability derivatives at those regions are positive. Sometimes the probability derivatives are unreasonably large at certain regions. For instance, Estimation 34 suggests that one dollar increase from $7 to $8 triggers about 80% probability decrease of driving.

The probability derivatives based on the ensembled model are smoother and the values are more reasonable: the probability derivatives of the ensembled model is always negative and the two dash curves are close to bell-shape but not exactly. It suggests that model ensemble should be used in DNN-based choice analysis, not only for the benefit of its higher prediction accuracy, but also for its higher regularity than individual estimations.

The probability derivatives aggregated over population are quite reasonable and even stable across estimations. Figure 4 shows the average probability derivative values of the population from 50 estimations and the distributions are closely centered around the mean values. The mean value of driving probability derivatives with respect to costs

\[ ^{6} \] We have removed the models that are implausible.
is $-2.9\%$, which is not far from the max of $-2.2\%$ and the min of $-3.5\%$. Similarly, the average probability derivatives with respect to travel time is $-0.87\%$, which is also close to the max of $-0.65\%$ and the min of $-1.14\%$. While the raw parameters in DNN models do not follow the central limit theory, Figure 4 suggests that some aggregate values, such as the average probability derivatives, could have a shape similar to the Gaussian distribution, or at least some distribution with the concentrated shape. Future research should explore the question about the sampling or estimation distribution of the interpretable information in the DNN-based choice models.

4.4. Marginal Rate of Substitution: Value of Time (VOT)

The aggregate values of VOT over population are reasonable while the individual-specific values are highly unstable. In our study, VOT in driving was computed by using the ratio of driving probability derivatives with respect to driving costs and in-vehicle travel time. Figure 5 shows the distribution of aggregate VOT over 50 estimations. The numbers are intuitive and quite close to prior studies. The average VOT value over the 50 estimations is $13.3$ per hour, and the distribution resembles a normal distribution with the standard deviation of $1.8$ per hour. The Gaussian-like shape may not be an accident if the two distributions of probability derivatives are both Gaussian. But without further evidence, we cannot conclude that the Gaussian-like shape always happens in the DNN-based choice models. However at the individual level, the VOT can have many patterns due to the fact that it was computed as the ratio of two numbers. Basically the

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7 We hesitate about the term here. A traditional term is sampling distribution, which reflects the intuition of repeated sampling resulting in the distribution of estimators, while here the source of randomness is not sampling but the estimation procedure, such as stochastic gradient descent. Hence Figure 4 is not exactly the sampling distribution, but can be regarded as estimation distribution.

8 We computed the aggregate values after dropping NaN and Inf values of VOTs.

9 Continuous mapping theory shows that the VOT can be approximated as a Gaussian distribution when the denominator and nominator are both Gaussian.
problems identified in the choice probabilities and probability derivatives propagate here. Table 2 provides some VOT examples of ten observations from five estimations. The VOT numbers could be undefined, infinite, negative values, or extremely large numbers in each estimation.\(^{10}\)

As a summary, the overall shapes and the economic information derived from the DNN-based choice models are reasonable when the information is aggregate over population or ensembled across models, but there exist very diverse or even irregular patterns at

\(^{10}\)When the denominator equals to zero, VOT numbers are undefined; when the denominators are very close to zero, VOT numbers become infinite; when the denominators are close to zero but not too small, VOT numbers are relatively large but do not explode.
Table 2: VOT of Ten Individuals Across Five Estimations

| Observation | Estimation 1 | Estimation 2 | Estimation 3 | Estimation 4 | Estimation 5 |
|-------------|--------------|--------------|--------------|--------------|--------------|
| 1           | 79.838       | -3.460       | inf          | -11.576      | Nan          |
| 2           | -31.351      | 37.617       | 12.017       | 396.456      | -156.103     |
| 3           | 19.581       | 4.968        | 0.000        | 3.548        | 0.000        |
| 4           | 24.034       | -14.908      | 0.000        | -218.849     | -2.722       |
| 5           | 25.930       | 12.729       | 61.461       | 19.460       | 26.349       |
| 6           | Nan          | 14.516       | Nan          | Nan          | Nan          |
| 7           | -4.230       | 13.306       | 4.810        | 36.917       | 11.177       |
| 8           | -39.056      | -37.460      | 0.000        | 191.611      | 34.173       |
| 9           | -31.490      | 48.218       | -8.265       | 16.499       | 119.235      |
| 10          | -9.992       | 1776.807     | 5.011        | 16.649       | 284.394      |

certain regions of probability fields or for certain individuals. Prediction accuracy itself does not help identify these irregular patterns. A model selected only based on prediction accuracy may misguide researchers to choose a model that does not make behavioral sense. To solve the problems, researchers need to better address DNN’s theoretical problems, irregular probability fields and large estimation errors.

4.5. Comparison to MNL Model

While the focus of this paper is not the comparison, we present some results from the MNL model as a reference. A standard form of MNL model was estimated with linear combination of alternative-specific and individual-specific variables forming the utility function. The prediction accuracy of the MNL model in the training set is 0.453 and that in the testing set is 0.451, compared to 0.89 and 0.567, respectively, of the DNN models. The prediction accuracy of the DNN model is higher than MNL model, which is expected and consistent with prior studies. The 11 percentage point improvement of prediction accuracy seems large, which can be attributed to both the advantage of using DNN models and the specific dataset. The big gap between the accuracy in the training set and testing test echoes our discussion concerning the high-dimensionality of DNN and the necessity of regularization in DNN.

Another finding is that the probability derivatives of driving regarding time and cost based on the MNL model is not far from what we obtained through DNN. Based on a simulation based on the MNL model, we find that the probability derivatives regarding driving cost and time are $-2.2\%$ and $-0.8\%$, compared to $-2.9\%$ and $-0.87\%$, the average values from the DNN-based choice model. Accordingly, the VOT based on MNL is also close to that based on DNN. Note that it is impossible to argue whether DNN or MNL better approaches the true VOT or probability derivatives based on these evidences since we don’t know the ground truth.

5. Conclusion and Discussion

This study seeks to use a DNN-based choice model to examine the classical travel mode choice decisions with an emphasis on interpretability. Built upon Wang and Zhao (2018), this paper numerically computes the key economic information, including choice probabilities, probability derivatives, and VOT by using one real dataset from Singapore travel survey.

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11 We skipped the report of the modeling result here for simplicity
We summarize our findings as follows. First, the DNN-based choice models generate reasonable economic information at the aggregate level either through model ensemble or population average. They obtain roughly S-shaped choice probability curves and inverse bell-shaped probability derivatives. Driving probability derivatives regarding costs and time, aggregated over population and models, are reasonable: 2.9% and 0.87%. The average VOT is $13.29/hour, which is also reasonable. Compared to the individual estimations, the ensemble models have more regular shapes in terms of their choice probabilities and probability derivatives. Second, the individual models based on DNN have diverse and even irregular patterns at certain regions of input space and that the results are highly sensitive to estimations. Driving probabilities regarding costs and time may not be monotonically decreasing and are sensitive to estimations. As a result, probability derivatives could be positive at certain region, and the VOT could be undefined, infinite, negative, or unreasonably large. Some of these patterns can be treated as problems because they are against our behavioral assumptions but others can be treated as examples of DNN’s flexibility to capture diverse human behavior in reality. Overall we demonstrate that it is feasible to develop an empirical method of prediction-driven DNN models and extract interpretable and reliable economic information from real datasets.

The diverse and irregular patterns at the disaggregate levels of DNN-based choice model relate to two theoretical challenges: irregularity of probability fields and high estimation errors in DNN. These are generic challenges, neither domain-specific nor data-specific. Different from the regular choice probability field of MNL model, the choice probability field of DNN model is theoretically ambiguous. As a result, the choice probability curves as a subspace of the whole choice probability field are not as regular as those monotonically decreasing choice probabilities in the MNL models. Further theoretical work in DNN is needed to resolve these challenges, particularly concerning its statistical properties and geometric intuition.

However, it is important to note that DNN does not necessarily lead to irregular shapes of choice probabilities and large estimation errors. The two theoretical challenges have been well known for many years and there exist many ways to mitigate them, one of which is model ensemble. $L_2$ regularization can also make models smoother since it shrinks parameters. With better hyperparameters, DNN architectures, and regularization methods, many problems about DNN can be mitigated and the prediction accuracy of DNN can be further boosted. In our study, we only used the basic approach of building DNN, by choosing eight DNN layers with 100 neurons in each layer without the thorough neural architecture search, and selecting one group of hyperparameters without searching through the whole hyperparameter space. This study is far from exhausting the arsenal of the DNN techniques.

Extensions of this paper include research based on other types of datasets, other coefficients of choice models, and other choice scenarios beyond travel mode choice. Future studies should seek to provide other practical methods to mitigate the two problems of irregularity of probability space and large estimation errors. The numerical method should not be the only way to make DNN interpretable and we expect other ideas to combine
domain-specific knowledge and generic-purpose DNN. The post-hoc numerical method allows researchers to apply the deep learning tools to traditional choice analysis, but in the reverse direction, researchers can use utility theories to enrich the design of machine learning models. We briefly presented the sampling distributions of economic information from DNN, and noticed that they may have a Gaussian-like form. Further studies should explore whether some sampling distributions exist for the economic information derived from the DNN-based choice models. More simulation-based research can also be helpful in understanding the trade-off between estimation and approximation errors. Our study is only about statistical association, but it will be interesting to see efforts on causal relationship of DNN in choice modeling. In summary, given the power of deep learning models and the richness of decision-making theories, we believe the interaction between utility-based choice analysis and DNN will be a fertile research area.

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