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THEORY-GUIDED NEURAL NETWORK FOR AGENT-BASED MODELING AND SIMULATION

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ABSTRACT

Recently, constructing ABS from detailed and large amounts of behavioral data and a statistical model have been attracted attention. However, it is difficult to utilize such models for assessing social policies because of a lack of behavioral data under the policies. In this paper, we propose a new training framework based on theory-guided neural network, which trains neural networks taking advantage of theoretical knowledge.

1 INTRODUCTION

Agent-based simulation (ABS) has been actively developed and used in the field of urban design and urban transportation management. In addition, detailed and large amounts of urban data, such as image recognition data and GPS data, has become easier to be collected. In recent years, statistical models, such as hidden markov models or a recurrent neural network, have been attracted attention as methods for constructing ABS from detailed and large amounts of behavioral data (Baeder et al. 2019). However, it is difficult to utilize the models for assessing social policies because of a lack of behavioral data under the policies. For example, if we want to find optimal expressway discount for congestion reduction, we need behavioral data under various expressway toll for the modeling, but it is hardly available.

In physics, there are notable works called theory-guided neural network, where researchers investigate how to construct statistical models utilizing theoretical knowledge. For example, Daw et al. (2017) succeeded in constructing a neural network model consistent with physics theory through training the model to minimize violation of physics laws in addition to training error. Their core idea is to use a loss function defined by

$$L = E(\hat{Y}, Y) + \lambda P(\hat{Y}). \tag{1}$$

$\hat{Y}$ is a model prediction when a feature vector, X, inputs to the model. Y is a ground truth for X. $E(\cdot)$ denotes training error function calculating inconsistency between the prediction and the ground truth. $P(\cdot)$ denotes penalty function that calculates physical inconsistency in the output structure. λ is a hyper-parameter deciding relative importance of the training error and the penalty. Theory-guided neural network can generate models that is consistent with physics theory by training the models to minimize equation (1).

However, it is difficult to apply the previous penalty function to the agent modeling because there are few obvious input-output relationships in the agent modeling. Our challenge is to construct a novel training framework for agent-based simulations based on theory-guided neural network.

2 METHOD

Our method introduces a new penalty function that calculates a penalty by comparing multiple outputs, which inspired by a control experiment in psychology. We propose a loss function defined by

$$L = E(\hat{Y}, Y) + \lambda P(\hat{Y}, \hat{Y}'). \tag{2}$$

In the agent modeling, the input vector X is social data when action(s) Y is obtained. $\hat{Y}$ is model prediction when X inputs to the model. X' is a synthetic data that is generated from X and only different in a parameter related to interested policy, e.g., price of train is 5 dollar in X but 2 dollar in X', and $\hat{Y}'$ is model prediction for X'. In equation (2), $P(\cdot)$ evaluates whether variation from output $\hat{Y}$ to output $\hat{Y}'$ is consistent with the rational choice theory.

Figure 1 is an example of the loss calculation using a series of behavioral data. Whole training procedure is as follows. 1) Generating a synthetic input vector, X', from a original real data ,X, which is only different in a parameter related to interested policy. 2) Getting predictions $\hat{Y}$ from inputting X to the model and a prediction $\hat{Y}'$ from inputting X' to the model. Then, checking whether inequality relation between $\hat{Y}$ and $\hat{Y}'$ is consistent with a theory. 3) Executing 1) and 2) for all of data included in the training data set and calculating percentage of data that violates the theory as penalty. Then, training the model to minimize the loss function that consists of training error and the penalty (equation (2)).

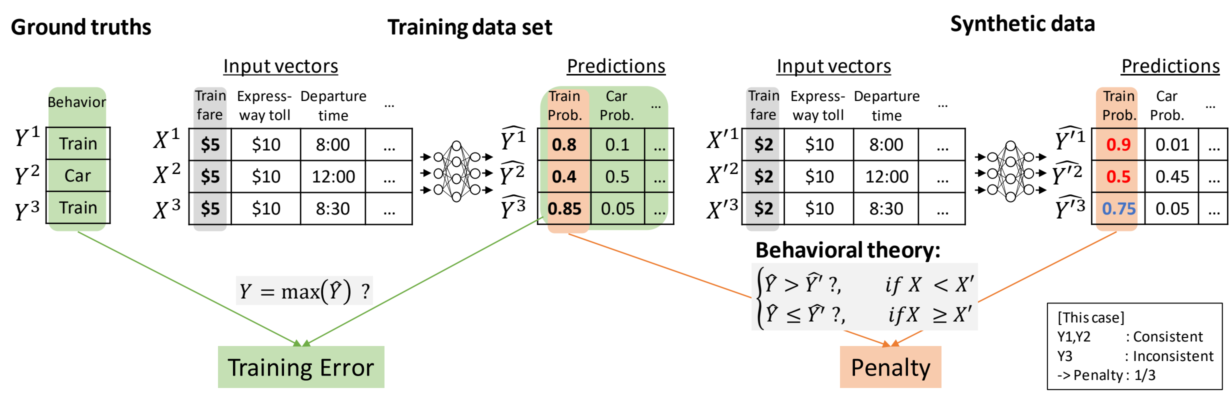

Figure 1: The loss function: training error is calculated based on inconsistency between the ground truth and the maximum probability behavior; penalty is calculated based on whether variation of target behavior probability is consistent with the theory (whether the train probability increases linked with decrease of the train fare). The input vectors are variety of social data when each behavioral result was observed. The predictions are a set of probabilities of the behaviors.

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