

## Up-scaling Agent-Based Discrete-Choice Transportation Models using Artificial Neural Networks

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1 **ABSTRACT**

2 Agent based models (ABMs) can be used for simulating consumer transportation discrete choices,  
3 while incorporating the effects of heterogeneous agent behaviors and social influences. However,  
4 the application of ABMs at large-scales may be computationally prohibitive (*e.g.*, for millions of  
5 agents). In an attempt to harness the modeling capabilities of ABMs at large scales, we develop a  
6 recurrent artificial neural network (ANN) to replicate nonlinear spatio-temporal discrete choice  
7 patterns produced by a spatially-explicit ABM with social influence. This particular ABM has been  
8 developed to model consumer decision making between purchasing a Prius-like hybrid or plug-in  
9 hybrid electric vehicle (PHEV) for a given geographic region (*e.g.*, city or town). Our goal is to see if  
10 an ANN trained at the city scale can operate as a “fast function approximator” to estimate nonlinear  
11 dynamic response functions (*e.g.*, fleet distribution, environmental attitudes, etc.) based on city-  
12 wide attributes (*e.g.*, socio-economic distributions). Recurrent feedback connections were added to  
13 the ANN to leverage the temporal history and correlations and improve forecasts in time. Outputs  
14 from the city-scale ABM, run for a variety of population sizes and initial and input conditions, were  
15 used to train and test the ANN. Initial results suggest the ABM may be replaced by ANNs that  
16 interact with each other and other agents (*e.g.*, manufacturing agents) to investigate PHEV  
17 penetration at the national scale.

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## 51 INTRODUCTION AND MOTIVATION

52 Regulatory actions by federal, state and local governments can play a critical role in influencing the  
53 transportation energy market. Due to the high degree of interdependency between various  
54 governing market factors, it is difficult to predict the market consequences and sensitivity to any  
55 given regulatory change.

56 Discrete choice decision models are commonly used to study transportation and travel  
57 phenomena, including vehicle choice behavior (1), hybrid choice behavior (2), and travel mode and  
58 destination choice (3). Agent based models (ABMs) with social influence are capable of modeling  
59 nonlinear spatio-temporal discrete choice patterns. ABMs have been used as an alternative  
60 methodology to model discrete-choice decisions in applications like driver route choice (4) and  
61 pedestrian walking behavior (5). Incorporating social influences in an agent-based discrete choice  
62 models make them more representative of real-world decision-making process (6), but drastically  
63 elevates the complexity of the simple binary choice model (7). While ABMs have proven useful for  
64 modeling behavior in complex systems (8) and demonstrate utility in the field of transportation (9),  
65 they can require large amounts of computation when implementing complicated decision with  
66 numerous agents.

67 The ABM in this work (10) has been developed to simulate the consumer discrete-choice  
68 decision process between purchasing a hybrid or plug-in hybrid (PHEV) vehicle type for a given  
69 demographic region (*e.g.*, city or town), with given socioeconomic characteristics. As a proof of  
70 concept, our ABM model uses synthetic data to reveal the importance of social influence on the  
71 vehicle purchasing behavior of its agents. However, this consumer discrete-choice model with  
72 numerous agents requires an alternative modeling strategy to replicate the behavior of the ABM  
73 when considering regulatory policies across scales larger than individual towns or cities (*e.g.*, larger  
74 than the state level).

75 In this research, we use an artificial neural network (ANN) to learn the dynamic behavior of  
76 the socially-influenced agent-based discrete-choice model and map its behavior for a wide range of  
77 synthetic demographic regions (towns) and socioeconomic characteristics. The ANN, operates as a  
78 fast function approximator, and requires recurrent feedback connections to allow outputs at one  
79 time step to be used as inputs for the next time step. We look to answer the question: can a simple  
80 ANN be used to replicate the behavior of a complex agent-based consumer discrete choice model  
81 with social influence? If proven successful, these ANNs will be surrogates for the ABM in a national-  
82 scale simulation that investigates alternative policies to influence PHEV fleet penetration.

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## 84 BACKGROUND

85 Artificial neural networks (ANNs) are nonparametric statistical tools that can be viewed as  
86 universal approximators (11). They were developed as large parallel-distributed information  
87 processing systems in attempt to model the learning processes of the human brain. Many different  
88 types of ANN have been introduced over the years for problems in pattern recognition and function  
89 approximation. ANNs specialize in mapping nonlinear relationships given extremely large datasets  
90 (12). They have a relatively simple computational architecture, which makes them extremely  
91 powerful and computationally efficient. The ANN known as feedforward backpropagation (FFBP)  
92 has been used in numerous transportation modeling studies, for example, predicting travel time  
93 under transient traffic conditions (13), among others. However, FFBP does have some drawbacks,  
94 namely it can become trapped in local minima, requires optimization of parameters (*e.g.*, number of  
95 hidden layers and nodes, the learning coefficient and momentum) and can take extended periods of  
96 training to converge to an adequate solution.

97 In this work, we use a generalized regression neural network (GRNN) to forecast discrete  
98 consumer choices using socioeconomic, social influence and market condition descriptors as inputs.  
99 The GRNN has many advantages. It relaxes many of the assumptions required by traditional  
100 parametric statistical methods (*e.g.*, does not require an assumption of multivariate normality;

101 allows binary or categorical data). Unlike the FFBP network, the GRNN has one-pass training and  
102 guaranteed convergence. In transportation studies, the GRNN has been used to forecast daily trip  
103 flows (14), predict the hazardousness of intersection approaches (15), model travel mode choice  
104 (16), predict CO<sub>2</sub> fluxes (17), predict real-time driver fatigue (18) and real-time video traffic  
105 modeling (19,20).

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## 107 **METHODS**

### 108 **Agent Based Model**

109 When selecting a vehicle to purchase, real-world consumers may compare a variety of  
110 characteristics, including fuel efficiency, seating and cargo capacity, safety, reliability, brand-loyalty,  
111 public perception, etc. Our model currently assumes that our agents are the subset of *new* vehicle  
112 consumers who have already narrowed their choice down to a less-expensive Prius-like hybrid and  
113 a higher-premium Prius-like PHEV.

114 Since PHEVs are not yet available in the commercial marketplace, we based PHEV price  
115 premiums, battery recharge requirements, electric assist ranges, and mileage with and without  
116 electric assist, from reported specifications for the Hymotion PHEV conversion kit for the Prius  
117 (21). The hybrid's fuel economy is 45 mpg while the PHEV's is 105 mpg when running on all-  
118 electric mode (45 mpg otherwise), with an all-electric range of 35 miles and 5.5 hour charging time  
119 at 5 kWh. We assume otherwise identical specifications and features between the two vehicles with  
120 only gas mileage and price premium differing.

121 Several major assumptions have been made in the development of our ABM to simplify the  
122 modeled processes. Our goal was not to exactly model real-world vehicle purchasing behavior, but  
123 rather to grossly approximate it and investigate the impact of social influence and regulatory  
124 policies. Here, we present a brief overview of the ABM; for more details, please refer to Pellon et al.  
125 (10).

126 Each agent represents a single vehicle consumer (not a household) and drives only one car  
127 (with no specification of vehicle purpose). Agents' socioeconomic characteristics are drawn  
128 randomly from distributions based on National Household Travel Survey (NHTS) data (22),  
129 including annual driving distance and durations of vehicle ownership. Agents are randomly  
130 distributed, yet clustered in space with an urban center and four suburban peripheral town-  
131 centers. Agents with similar annual salary have been loosely clustered in space using a 2-D turning  
132 bands method (23). Several agent attributes (*e.g.*, age, driving distance, number of years they  
133 typically own a vehicle, and willingness to consider adopting the new PHEV technology) are also  
134 positively or negatively correlated to salary, in varying degrees. The threshold for willingness to  
135 consider new PHEV technology was initialized so that roughly one half of new car buyers were  
136 willing to consider being PHEV early-adopters, consistent with recent survey results that indicated  
137 that 46% of potential consumers reported that they were some chance they might purchase a  
138 PHEV, depending on the price premium (24).

139 Agents have specified social and spatial neighbors that make up their social and  
140 geographical networks. The spatial network is defined on the physical proximity of the agents,  
141 while the social network is based on physical proximity and similar socioeconomic characteristics.  
142 These networks affect the agents' decision-making process, as agents look in their networks to see  
143 what vehicles other agents currently own; in addition, agents' attitudes can be influenced by other  
144 agents in their social networks. Heterogeneity in agent locations, social networks and driving  
145 distances cause different agents to be exposed to different vehicle fleets. The proportion of PHEVs  
146 within an agent's observed fleet influences their willingness to consider adopting this new  
147 technology. This "threshold" concept is found to be a very important feature in social influence  
148 models (7; 25).

149 Agents stochastically decide when to purchase a vehicle based on their current vehicle's  
150 age, the number of years they expect to own a car and how much more attractive a new vehicle is

151 compared with their current vehicle. Once an agent decides to purchase a vehicle, they compare  
152 the relative financial costs and environmental benefits to determine whether the PHEV (assuming  
153 their threshold has been met) or hybrid vehicle best suits their needs, and then purchase the best  
154 vehicle for their circumstance. This process is repeated every year, for all agents over the 15 year  
155 simulation time period.

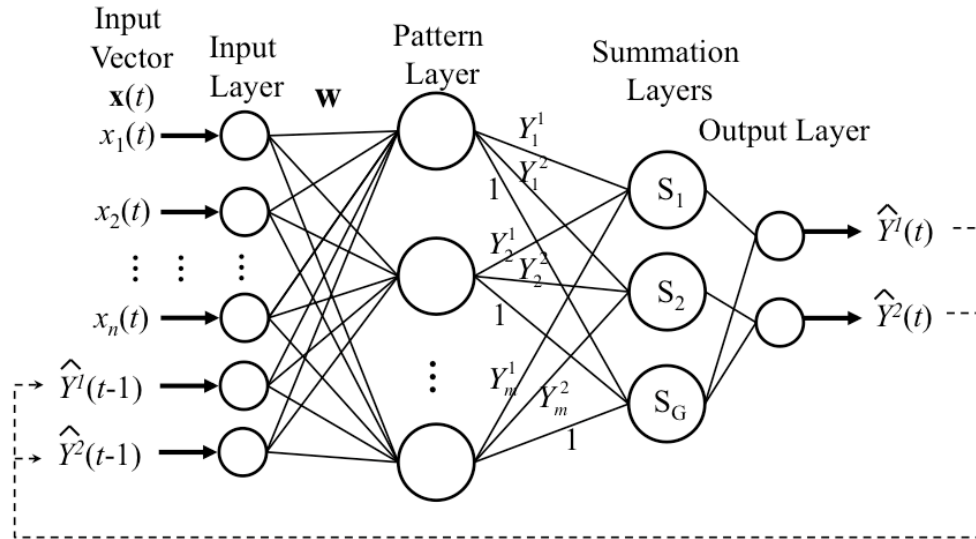
156 In addition to agents deciding to purchase vehicles, some of their internal characteristics  
157 are updated every year. For example, their environmental attitude (or greenness) and the time  
158 period over which they compute potential fuel savings may both be increased by social influence,  
159 depending on their social susceptibility. Greenness is a weighting factor ranging between 0 and 1  
160 that determines how much an agent values the perceived environmental benefits of the PHEV (in  
161 this paper, proportion of gas saved by the PHEV relative to the HEV) vs. the perceived financial  
162 benefits of the HEV (proportion of cost savings of the HEV relative to the PHEV); a greenness value  
163 of 0 implies the decision is based solely on perceived financial benefits. In estimating relative costs,  
164 some agents ignore potential fuel savings and simply look at the price premium of the PHEV, some  
165 also compute projected fuel costs over a period of 1 year, and others compute projected fuel costs  
166 over the entire duration for which they anticipate owning their next car. Thus, some agents are  
167 more forward-thinking than others, and these agents can influence others in their social network to  
168 become more forward-thinking (i.e., to consider projected fuel costs over longer periods), resulting  
169 in interesting dynamics in discrete-choice behavior. Note that if an agent's projected fuel savings  
170 exceed the PHEV price premium and the PHEV will be thus perceived as the cheaper vehicle, the  
171 agent will purchase the PHEV, regardless of their greenness value (assuming their threshold has  
172 been met). See (10) for more details.

173 Our model assumes there is no shortage of either vehicle type (i.e., no waiting period).  
174 There are several additional exogenous inputs: PHEV price premium as well as future projections of  
175 gas prices and current national electricity prices (26).

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### 177 **Generalized Regression Neural Network**

178 Developed as a nonlinear, non-parametric extension of multiple linear regression, the GRNN is a  
179 memory-based network capable of estimating continuous variables (27). The GRNN consists of four  
180 layers: input, pattern, summation, and output (Figure 1). Each layer is fully connected to the  
181 adjacent layers by a set of weights between the nodes. Some output,  $\hat{Y}(t)$ , is predicted based on a  
182 set of input variables,  $\mathbf{x}$ , defined by some non-linear function  $Y = f(\mathbf{x})$ , captured by the training data.  
183 Training data consist of a set of input vectors,  $\mathbf{x}$ , and corresponding output,  $Y$  (input-output pairs).  
184 For this application, we use the algorithm to predict two output variables ( $Y^1$  and  $Y^2$ ), which  
185 represent median greenness and proportion of PHEVs in a given town, respectively.



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**Figure 1. Architecture of a general regression neural network with recurrent feedback connections for two outputs variables  $Y^1$  and  $Y^2$ .**

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The user specifies the number of nodes in the input layer by determining what predictor variables best represent the system being modeled. The pattern layer has one node for each of the  $m$  training patterns. The weights on the left side of the pattern layer nodes store (e.g., are set equal to) the input training vectors,  $\mathbf{x}$ . Each node in the pattern layer is connected to the summation layer nodes,  $S_1$ ,  $S_2$  and  $S_G$ . The weights linking the pattern layer nodes with summation nodes  $S_1$  and  $S_2$  store the model outputs for the two variables being predicted (e.g.,  $Y_i^1$ ,  $Y_i^2$ ) for all input-output training patterns ( $i=1, 2, \dots, m$ ). The weights from the pattern layer nodes to summation node  $S_G$  are set equal to 1.

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Once the weights are set, the GRNN may predict each of the two outputs. A new input vector for which a prediction is desired,  $\mathbf{x}$ , is presented to the pattern layer. The Euclidean distance is computed between the input vector and all pattern weight vectors,  $\mathbf{w}_i$  where  $i=1, 2, \dots, m$  as:  $D_i^2 = (\mathbf{w}_i - \mathbf{x})^T (\mathbf{w}_i - \mathbf{x})$ . The distance,  $D_i^2$ , is passed to the summation layers and a prediction for variable  $\hat{Y}^1$  is computed as:

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$$\hat{Y}^1 = \frac{S_1}{S_G} = \frac{\sum_{i=1}^m Y_i^1 \exp\left(-\frac{D_i^2}{2\sigma^2}\right)}{\sum_{i=1}^m \exp\left(-\frac{D_i^2}{2\sigma^2}\right)},$$

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where  $\sigma^2$  is a smoothing parameter that is pivotal for estimating  $\hat{Y}^1$  (this process is also executed for predicting  $\hat{Y}^2$ ). Large values of  $\sigma^2$  smooth the regression surface and produce estimates that approach the sample mean; while small values produce a surface with greater chance of discontinuity resulting in nearest neighbor estimates. Intermediate values of  $\sigma^2$  produce well behaved estimates that approximate the joint probability density function of  $\mathbf{x}$  and  $Y$  (27). The prediction,  $\hat{Y}^1$ , is a weighted average of all stored response observations ( $\hat{y}_1^1, \hat{y}_2^1, \dots, \hat{y}_m^1$ ), where each response is weighted exponentially according to its Euclidean distance from input vector  $\mathbf{x}_i$  (the same computations are computed for output variable  $\hat{Y}^2$ ).

In addition, the GRNN has been modified to allow for recurrent feedback connections (dashed line of Figure 1). Recent predictions for  $\hat{Y}^1$  and  $\hat{Y}^2$ , are passed back to the input layer and

213 used to predict  $\hat{Y}^1$  and  $\hat{Y}^2$  at the next time step. For more detail, please refer to Besaw et al. (28).  
 214 The GRNN algorithm described in this work was written in MatLab V. 7.4.0.287 (R2007a).  
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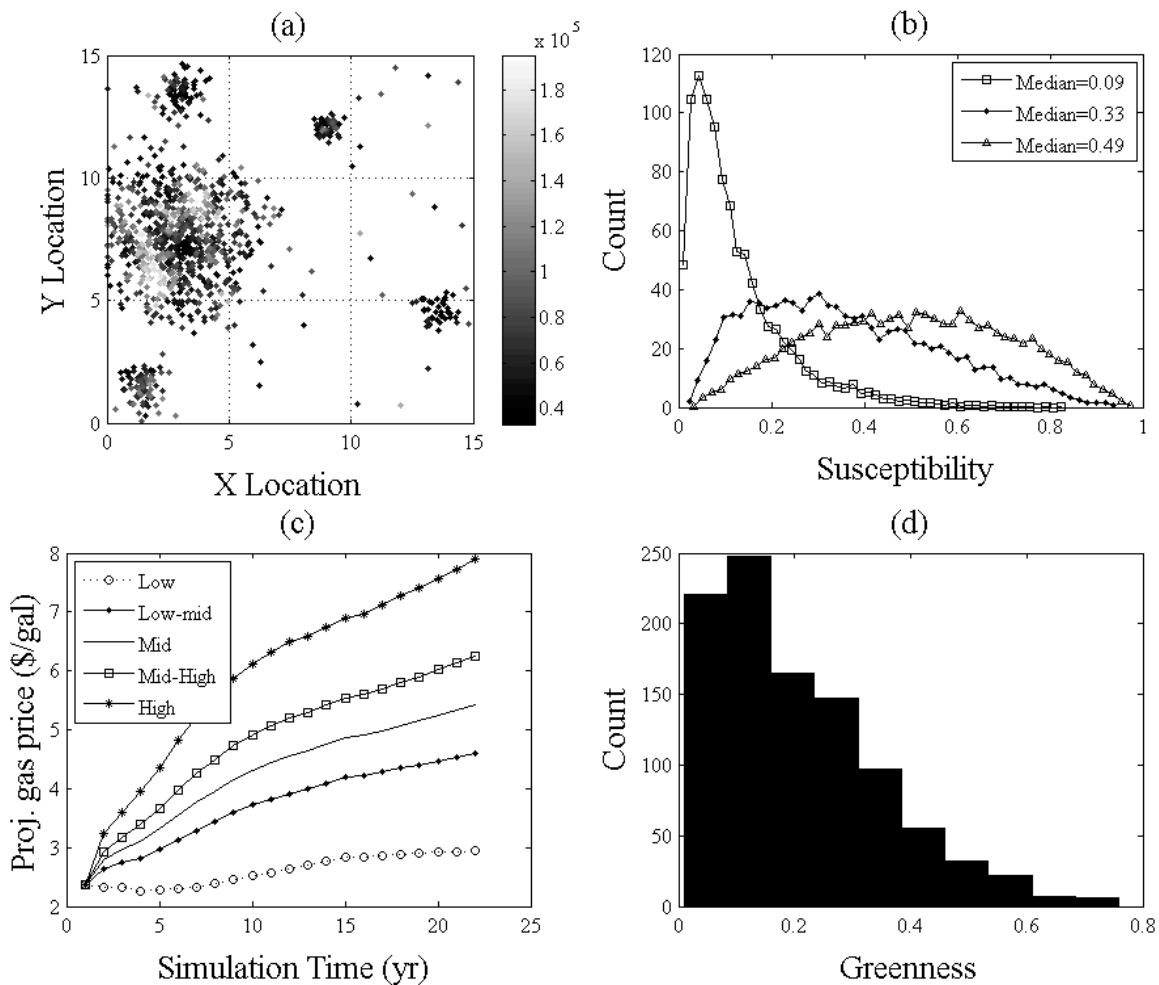
### 216 **ABM and GRNN implementations**

217 The ABM was run under several scenarios to provide a range of town socioeconomic and vehicle  
 218 fleet distributions (Table 1). Prior experimentation revealed similar ABM trends when run for  
 219 10,000 or 1,000 agents. To save on computation, our scenarios use 1,000 agents. The hypothetical  
 220 region of interest consisted of one larger (population of 726 agents) and 4 smaller towns  
 221 (populations ranging from 55 to 79 agents) (Figure 2a). The socioeconomic distributions of these  
 222 areas were generated pseudo-randomly, different from town to town and included spatial cross-  
 223 correlation of salary and other inter-attribute correlation. Agents in the respective towns had  
 224 different social networks based on the proximity of neighboring agents and their socioeconomic  
 225 characteristics. In addition, the ABM simulations use 10 initial random seeds to account for  
 226 potential stochastic noise in the results.

227 **Table 1. List of ABM parameters that were varied during the generation of training, validation and**  
 228 **prediction datasets.**

Model Parameter	Training & Validation Dataset	Prediction Dataset
Median Social Susceptibility	[0.01, 0.09, 0.33, 0.49]	[0.17, 0.45]
Proj. Gas Price	Low, Medium, High	Low-mid, Mid-High
PHEV Price Premium	\$5k, \$10k, \$15k	\$7k, \$13k
Town Identification	1, 2, 3, 4, 5	1, 2, 3, 4, 5
Region Population	1,000	1,000
Initial Random Seeds	1 to 10	1 to 10

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 230 For this proof-of-concept, the agent thresholds for social susceptibility varied from 0 to 1,  
 231 making a broad distribution of potential early adopters and non-conformists. Social susceptibility  
 232 distributions were stochastically generated between 0 (not socially susceptible) to 1 (very  
 233 susceptible). The medians of these distributions were varied to generate agent populations with  
 234 large susceptibility variations (Table 1 and Figure 2b). Agent initial greenness distributions were  
 235 also stochastically generated but remained statistically similar between scenarios. Exogenous  
 236 model inputs (*i.e.*, projected gas prices (Figure 2c) and PHEV price premium) were also varied to  
 237 produce representative scenarios. U.S. Energy Information Administration (26) provided  
 238 reasonable projections of high and low gas prices (medium was the average of high and low).  
 239 Different PHEV-premiums were used to investigate the potential impact of price incentives.  
 240 Greenness was stochastically initialized to range from 0 to 1, with an initial median value of  
 241 approximately 0.17; as shown for a representative distribution in Figure 2d.



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243 **Figure 2. (a) Spatial coordinates of agents and their annual income shown in grayscale. (b) Example**  
 244 **distributions of social susceptibilities with different medians. (c) Fifteen year projections of gas**  
 245 **prices (high and low data from EIA). (d) Representative distribution of agents' initial greenness.**

246 Descriptive statistics (median and interquartile range) of the ABM simulations were  
 247 computed at each time step for the numerous agent distributions. These were then averaged over  
 248 the 10 random seeds for each town and simulation setup. This resulted in a total of 4,320 different  
 249 town simulations used to train the GRNN (comprising a 15-year time series when PHEVs are  
 250 introduced in year 2). As is typical in ANN applications, this dataset was separated into training  
 251 and validation datasets. The training dataset comprised 3,000 town simulations (~80%) to set the  
 252 GRNN weights. The validation dataset was comprised of the remaining 1,320 town simulations  
 253 (~20%) and was used to optimize the GRNN smoothing parameter  $\sigma^2$  (via trial and error).

254 GRNN inputs include many of the socioeconomic descriptors incorporated in the ABM,  
 255 including a statistical descriptors agents' age, income and social susceptibilities, PHEV thresholds,  
 256 driving distances and car replacement age. In addition exogenous inputs include projected gas  
 257 prices, and PHEV-price premium. All inputs were normalized such that their minimum and  
 258 maximum values were 0 and 1 respectively. Outputs from the GRNN are statistical descriptors of  
 259 agent greenness (median) and the proportion of the fleet that are PHEVs in a particular town. As



260 this is a recurrent GRNN, these outputs are fed back into the GRNN and used as inputs in the next  
261 time step.

262 To generate the prediction dataset, an entirely new spatial distribution of agents and their  
263 corresponding socioeconomic characteristics were generated (Table 1). Other initial model  
264 parameters were changed as well, including: social susceptibility, projected gas prices and PHEV-  
265 premium. Again, descriptive statistics were computed for each town at every time step and  
266 averaged over the 10 random seeds. This combination of parameters resulted in prediction  
267 scenarios that were similar to, yet significantly different from, those upon which the GRNN was  
268 trained.

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## 270 **RESULTS AND DISCUSSION**

271 We have summarized the accuracy of the GRNN predictions for both the validation and prediction  
272 datasets (Table 2) for both PHEV penetration and one of the changing agent attributes (greenness).  
273 We have used the coefficient of determination ( $R^2$ ), and in some cases the root-mean-square error  
274 (RMSE) between the GRNN predictions and the ABM results as accuracy metrics. The means and  
275 standard deviations of  $R^2$  are computed for each town over the given number of scenarios. The  
276 optimized smoothing parameter ( $\sigma^2=0.004$ ) was used to predict PHEV fleet proportion and  
277 greenness in each of the five towns for 171 validation and 16 prediction scenarios.

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### 279 **GRNN predictions of ABM PHEVs and greenness**

280 Although the time horizon over which individual agents projected fuel costs for prospective  
281 vehicles was allowed to vary dynamically due to social influence, current implementation of the  
282 GRNN does not feed this back as a recurrent input. Despite this known source of error, the  
283 coefficients of determination for the validation dataset (Table 2) show that the GRNN was able to  
284 map the general behavior of the discrete-choice ABM. When predicting PHEV-fleet proportion and  
285 greenness in the validation dataset, the GRNN was most accurate when predicting larger towns  
286 (*e.g.*, towns 1 and 3, Table 2). The GRNN predictions were least accurate in town 4 (PHEV average  
287 and standard deviation of  $R^2$  were 0.57 and 0.33) where the number of agents was least.

288 The GRNN performed better when predicting PHEV fleet proportion than when predicting  
289 greenness in all validation scenarios. In addition, there exist large amounts of variability between  
290 the coefficients of determinations computed in the validation dataset (for both PHEV and  
291 greenness). These effects are most likely caused by the large variation of social susceptibility in the  
292 training and validation datasets (Table 1). Figure 2c provides a visual comparison of some of these  
293 distributions. When social susceptibilities are so drastically different, the trajectories of the  
294 greenness, and to a lesser extent PHEV fleet proportion, are very different. It appears there may  
295 have been too much variation in our distributions of social susceptibility in the training and  
296 validation datasets that limited the GRNNs ability to accurately learn all of the 3,000 scenarios.  
297 Future experiments will add the distribution of time horizons for fuel cost projections as a  
298 recurrent input into the GRNN to see if this improves the situation.

299 The  $R^2$ 's computed for the predictions dataset indicate the GRNN has successfully learned  
300 the relationships from the training dataset (including the influence of social influence/networks)  
301 and was able to accurately predict PHEV fleet proportion and greenness. The scenarios used for  
302 prediction were generated using entirely new datasets with respect to the projected gas prices,  
303 PHEV price premium, spatial distribution and social susceptibility (Table 1). However, we did not  
304 introduce as much variation in the social susceptibility as was introduced in the training and  
305 validation datasets (medians of 0.17 and 0.45).

306 As a result, for the particular scenarios presented here, the GRNN was more accurate  
307 predicting on the prediction dataset than on the validation dataset. The estimated PHEV-fleet  
308 proportion in the validation and prediction datasets had  $R^2$ 's of 0.8 and 0.97 respectively (0.75 and

309 0.87 for greenness). Similar to the validation dataset, we predicted PHEV-fleet proportion more  
 310 accurately than greenness in the prediction dataset, 0.97 and 0.87 respectively. The greater  
 311 accuracies are most likely due to the less variable distributions of social susceptibility used in the  
 312 prediction dataset.

313 **Table 2. Table of summary statistics for the coefficient of determination ( $R^2$ ) computed for the**  
 314 **validation and prediction datasets (a mean  $R^2$  of 1.0 indicates the ANN predictions perfectly match**  
 315 **the ABM results).**

Output Variable	Dataset	Statistic	Town 1	Town 2	Town 3	Town 4	Town 5	All Towns
Number of Agents	Validation & Prediction	Mean	74	66	726	55	79	1000
	PHEV-Fleet Proportion	Validation (n=171)	Mean $R^2$	0.89	0.83	0.88	0.57	0.83
Prediction (n=16)		Std. Dev. $R^2$	0.22	0.34	0.24	0.33	0.25	0.28
		Mean $R^2$	0.97	0.98	0.99	0.94	0.96	0.97
Std. Dev. $R^2$		0.02	0.01	0.01	0.03	0.02	0.02	
Greenness	Validation (n=171)	Mean $R^2$	0.85	0.82	0.87	0.47	0.76	0.75
		Std. Dev. $R^2$	0.27	0.31	0.24	0.29	0.29	0.28
	Prediction (n=16)	Mean $R^2$	0.83	0.74	0.97	0.89	0.91	0.87
		Std. Dev. $R^2$	0.09	0.06	0.01	0.04	0.01	0.04

316  
 317 **Further analysis into two prediction scenarios**

318 To further highlight the GRNN capabilities to learn the behavior of this discrete-choice ABM, we  
 319 have selected two scenarios (call them I and II) from our possible 16 prediction scenarios and  
 320 plotted the time-series of PHEV proportion and greenness for towns 2, 3 and 4. The social  
 321 susceptibility distribution was with only parameter that varied between scenario I and II (Table 3).

322 Scenarios I and II demonstrate several different ABM phenomena that we would like our  
 323 GRNN to be able to replicate, including: differential rates of PHEV adoption, different final adoption  
 324 proportion as well as linear and non-linear dynamics of adoption. These interesting dynamics have  
 325 arisen out of the different distributions of social susceptibility used in these two scenarios. The time  
 326 series plots provided below assume the PHEV was been introduced in year 0 (with year -1 being  
 327 our initial model conditions).

328 **Table 3. Parameter values for the two representative scenarios I and II.**

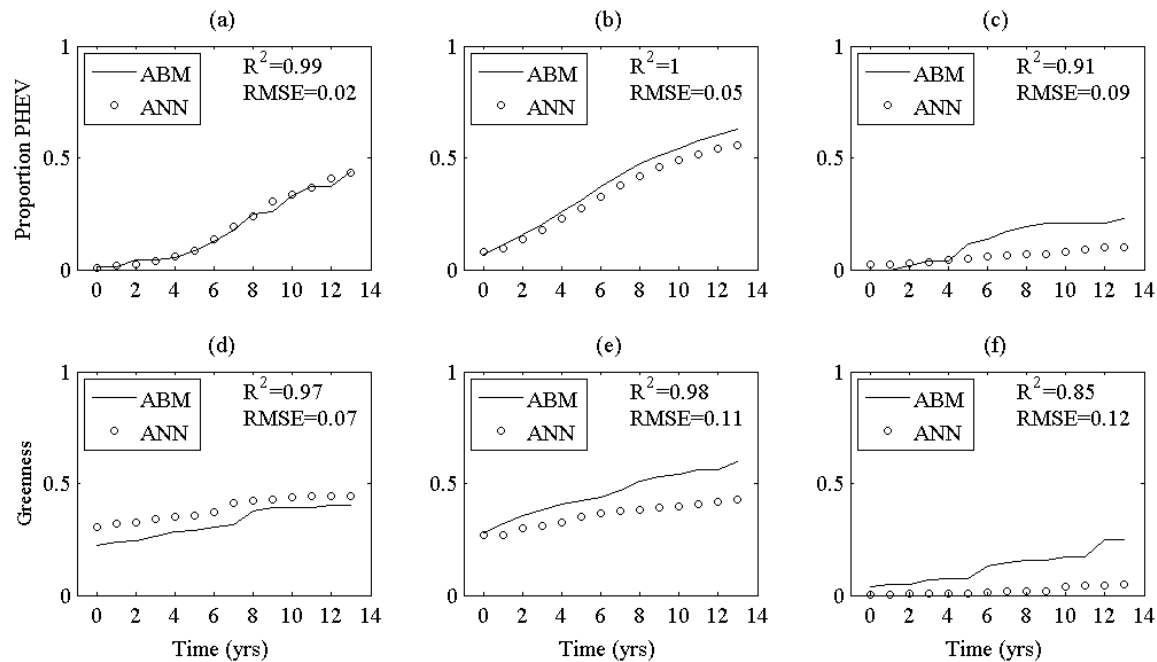
Parameter	Scenario I	Scenario II
PHEV premium	\$13k	\$13k
Social Susceptibility Median	0.17	0.45
Proj. Gas Price	Low-mid	Low-mid
Representative Simulation	Figure 3	Figure 4

329  
 330 In scenario I, we observe that roughly 50% of the agents in towns 2 and 3 (Figures 3a and  
 331 3b) have adopted PHEVs. Due to the low economic status of agents in town 4 (Figure 3c), a much  
 332 lower fraction of these agents have adopted PHEV. These three towns have different PHEV  
 333 adoption trajectories. In town 2 (Figure 3a) we see highly nonlinear behavior. There is slow  
 334 adoption at first, followed by an increased rate of adoption. In town 3 (Figure 3b), the adoption  
 335 rate remains fairly constant over the simulation. Finally, town 4 (Figure 3c) shows a nonlinear  
 336 jump in adoption.

337 The GRNN accurately predicts the time-series of PHEV adoption for towns 2 and 3 ( $R^2$  of  
 338 0.99 and 1, respectively). This is encouraging because one trajectory is nonlinear while the other is  
 339 linear. The GRNN does relatively poor when predicting the PHEV-fleet proportion for town 4. As in

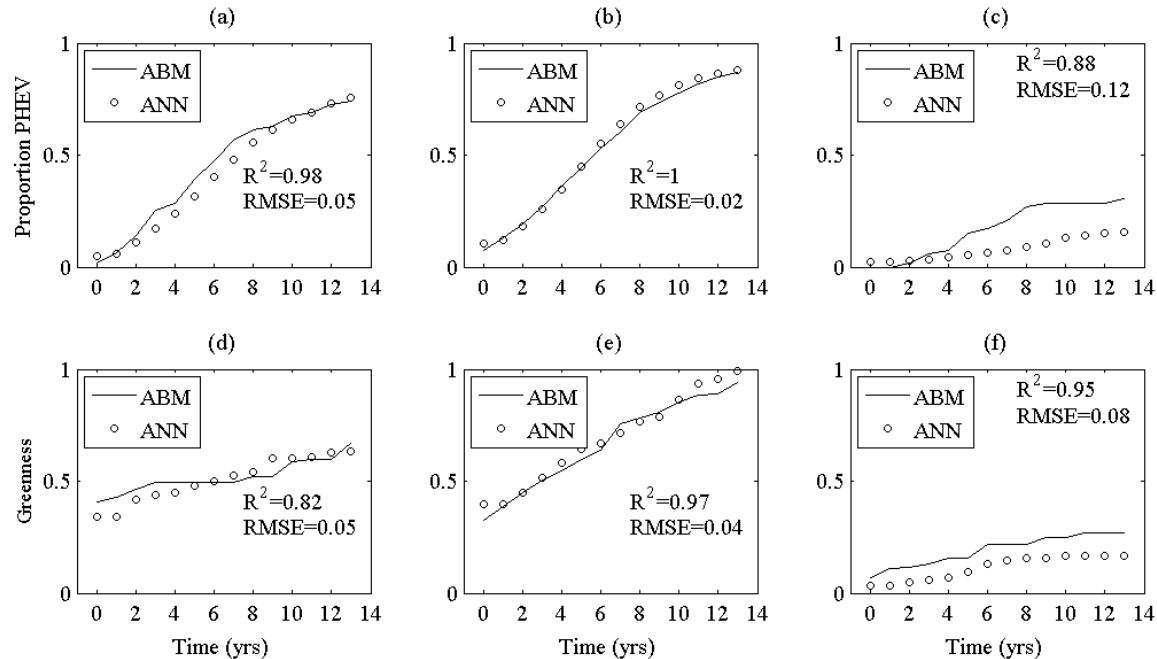
340 the training and validation dataset, town 4 continues to be the least well predicted of the five towns  
 341 (Table 2). However, results demonstrate the GRNN has learned both linear and nonlinear dynamics  
 342 of this ABM.

343 As illustrated with the training and validation datasets, the GRNN does not predict  
 344 greenness (Figures 3d, 3e and 3f) as well as it predicts PHEV-fleet proportion. In Town 2, the  
 345 GRNN accurately predicts greenness ( $R^2=0.97$ ). However, the coefficients of determination and  
 346 RMSE show that the GRNN does not predict greenness in towns 3 and 4 very well. This is most  
 347 likely due to the high variability of social susceptibility in the training dataset, upon which  
 348 greenness is primarily based.



349  
 350 **Figure 3. Representative GRNN predictions (for scenario I in which the PHEVs are adopted by**  
 351 **~50% of the consumer agents). GRNN predictions of PHEV fleet proportion versus time for (a)**  
 352 **town 2, (b) town 3 and (c) town 4. (d-f) GRNN predictions of greenness for towns 2, 3 and 4**  
 353 **respectively.**

354 In scenario II, we observe a greater proportion of the agents adopting PHEVs in towns 2 and  
 355 3 (Figures 4a and 4b). Fewer PHEVs were adopted by town 4 (Figure 4c), indirectly due to its low  
 356 annual incomes (Figure 2a, rightmost town) which were correlated with longer vehicle ownership  
 357 times and higher PHEV adoption thresholds. We see non-linear adoption rates in towns 2 and 3.  
 358 Adoption is relatively slow initially, but increases with time. In this scenario, the GRNN again  
 359 accurately predicts PHEV-fleet proportion for towns 2 and 3 ( $R^2$  of 0.98 and 1 respectively). The  
 360 GRNN greenness predictions for towns 2 and 3 are more accurate than scenario I indicating that the  
 361 GRNN may be slightly biased, as well as more accurate, when predicting using larger social  
 362 susceptibility medians. This could be remedied easily using more training scenarios with lower  
 363 social susceptibility medians and by allowing the time horizon for fuel cost projections, which are  
 364 also affected by social susceptibility, to be recurrent.



365

366 **Figure 4. Representative GRNN predictions (for scenario II in which the PHEVs are adopted by**  
 367 **~80% of the consumer agents). GRNN predictions of PHEV fleet proportion versus time for (a)**  
 368 **town 2, (b) town 3 and (c) town 4. (d-f) GRNN predictions of greenness for towns 2, 3 and 4**  
 369 **respectively.**

370 Scenarios I and II present a good examples of the impact of social influence and networks on  
 371 the discrete-choice ABM. In scenario I, the social susceptibility distribution was skewed left causing  
 372 the general population to be less influenced by their social network (median = 0.17). Conversely,  
 373 the social susceptibility distribution of scenario II was less skewed (median = 0.45), resulting in  
 374 agents that were more influenced by their social network. The PHEV-fleet proportion curves of  
 375 scenario II (greater social influence) had a larger number of PHEVs adopted in towns 2 and 3 than  
 376 in scenario I (roughly 50% and 80% respectively). This is due to the difference in contribution of  
 377 social influence in the two scenarios.

378 The predictions for these two scenarios show the GRNN was able to accurately predict  
 379 PHEV-fleet proportion under these two different conditions (less and more social susceptibility).  
 380 This is an important contribution of this work; because accurate predictions of PHEV adoption will  
 381 allow us to use the GRNNs as a surrogate for the ABM when predicting PHEV adoption under many  
 382 different types of scenarios. It also demonstrates that the GRNN has been able to learn the  
 383 importance of social influence and networks generated by the ABM.

384 These two scenarios demonstrate the GRNN has learned and accurately predicted  
 385 important ABM phenomena, including: differential rates of PHEV adoption, different final adoption  
 386 proportion, as well as, linear and non-linear dynamics of adoption.

387

### 388 Computational Speedup

389 The speed of computation is another important consideration of this work. Our objective is to use  
 390 the GRNN as a surrogate for the ABM for large-scale simulations (*e.g.*, nation scale). To be a viable  
 391 surrogate, the GRNN must be computationally faster than the ABM for large-scale simulations.

392 The ABM scales super linearly with increasing number of agents ( $N$ ). This is due to the  
 393 large amounts of computation performed at every time step for every agent. The ABM takes: 11.5  
 394 seconds for 1000 agents, 70 seconds for 10000 agents, and continues to rise. Example

395 computations include the threshold to consider purchasing a PHEV based on social and geographic  
396 networks (which scale super linearly with  $N$ ). Because of this super linear scaling, performing large  
397 scale simulations with the ABM may not be feasible. However, as demonstrated previously, the  
398 GRNN is capable of learning the non-linear dynamics of the discrete-choice ABM.

399 The production of the GRNN training and validation datasets also scale non-linearly with  $N$ ,  
400 due to the same computations discussed above. It took approximately 24 hours to produce the  
401 training and validation dataset (4,320 scenarios) used in this proof-of-concept. However once  
402 these datasets are developed, the GRNN takes relatively little time to train (~4 hours in this work).  
403 Once the GRNN is trained, it takes very little time to run (~0.4 seconds for any number of agents),  
404 no matter how large of a town or city is being simulated. This is due to the fact that the GRNN must  
405 only march through 15 time steps, independent of the town's population. Thus, the major time  
406 required for the GRNN is the production of the training and validation datasets by the ABM. Thus,  
407 for the 4,320 scenarios (each with 1000 agents) in this small demonstration comparable timings for  
408 the ABM and ANN are 13.8 hours versus 0.48 hours, respectively.

409 These demonstration timings were generated on a 3 GHz Intel Core 2 Duo processor with  
410 3 GB of RAM running MatLab V. 7.3.0.267 (R2006b).

411

412

### 413 **CONCLUSIONS AND FUTURE WORK**

414 This work was originally conceived based on the premise that the GRNN can operate as a fast  
415 function approximator of a discrete-choice agent-based transportation model with social networks  
416 and influences. For training and validation, we produced a large dataset that exhibited spatio-  
417 temporal dynamics of this simplified consumer vehicle choice ABM. The inclusion of social  
418 influence introduced through social networks, adoption thresholds and susceptibility resulted in  
419 nonlinear agent behavior.

420 This proof-of-concept GRNN has proven capable of learning the spatio-temporal dynamics  
421 of the discrete-choice ABM with social influence. By incorporating a recurrent feedback connection,  
422 the easy-to-train GRNN was able to adequately replicate the behavior of ABM at the town scale.  
423 Adding in additional recurrency for other dynamically changing attributes (in this case, time  
424 horizon for fuel cost projections) is expected to improve results even further. Although it does take  
425 significant amounts of time to generate the training and validation datasets and optimize the  
426 GRNN's smoothing parameter, once trained, it operates as a fast function approximator that  
427 demonstrated tremendous speedup time relative to the ABM. The combined effects of accurate  
428 approximation and dramatic speedup will allow us to simulate large-scale dynamics more  
429 computationally efficiently than running a large-scale ABM.

430 In order to investigate potential regulatory policies that can influence the adoption of  
431 PHEVs (*e.g.*, price incentives, rebates) a large-scale model is currently under development. This  
432 large-scale model incorporates additional types of agents (*e.g.*, vehicle manufacturing and  
433 electricity producing agents). With the GRNN able to operate as a surrogate of the consumer ABM,  
434 GRNNs representing neighboring towns will interact with each other and with other large-scale  
435 agents. With this framework, we can explore potential regulatory policies that may impact the  
436 decisions and behavior of large-scale agents.

437

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