September 21-23, 2019 The 18th Summer Course for Behavior Modeling in Transportation Networks @The University of Tokyo

Urban science and behavioral informatics with AI/machine learning Application of AI for travel behavior modelling in urban networks

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Problem setting

- Standard logit model: $P_{ij} = \frac{\exp(V_{ij})}{\sum_{j'=1}^{J} \exp(V_{ij'})}$
- The conventional form of V_{ij} :
 - Linear approximation (rooted to the Taylor's theorem)
 - Also known as a linear-in-parameter model
- Problem at hand:
 - Is there any better way to determine the functional form?
 - Obviously, taking into account the non-linearlity of V_{ij} would improve the goodness-of-fit.
 - What is the cost of doing that?

Problem setting

• Can we understand the non-linear transformation of V_{ij} logically?

Example: contribution of travel time to mode/route choice model



Problem setting

• In what context we may NOT need to explain the impacts of each factor logically?

Example: contribution of eye movement to the speed choice



Adapted from Wang et al. (2019)

Contents

- 1. Logically explainable non-linear transformation
- 2. Spline-based non-linear transformation
- 3. NN (Neural network)-based non-linear transformation

Advanced discrete choice models

[based on Hato (2002)]



Castillo, E., Menendez, J.M., Jimenez, P., Rivas, A. (2008) Closed form expressions for choice probabilities in the Weibull case. Transportation Research Part B 42, 373-380.

Chikaraishi, M., Nakayama, S. (2016) Discrete choice models with qproduct random utilities, Transportation Research Part B

LOGICALLY EXPLAINABLE NON-LINEAR TRANSFORMATION

Nonlinearity of V_{ij}

(2) Difference in systematic utility



Distribution/linearity: an example

(1) Difference in distribution assumption



Distribution/linearity: an example



(See Castillo et al. (2008) for elegant explanations)

q-product random utility



- Preliminaries: q-generalization (Tsallis, 2009)
 - Generalized Boltzmann–Gibbs statistical mechanics
 - The core concept is the so-called Tsallis entropy, where the "q-generalization" plays a central role

q-logarithm:
$$\ln_q(x) \coloneqq \frac{x^{1-q} - 1}{1-q} \quad \lim_{q \to 1} (\ln_q(x)) = \ln(x)$$

q-exponential:
$$\exp_q(x) \coloneqq [1 + (1-q)x]^{\frac{1}{1-q}} \quad \lim_{q \to 1} (\exp_q(x)) = \exp(x)$$

q-product:
$$x \bigotimes_q y \coloneqq [x^{1-q} + y^{1-q} - 1]^{\frac{1}{1-q}} \quad \lim_{q \to 1} (x \bigotimes_q y) = xy$$

Some properties:

 $\ln_q \left(\exp_q(x) \right) = x, \quad \ln_q \left(x \otimes_q y \right) = \ln_q(x) + \ln_q(y)$ 11

Generalization of logit and weibit



q-generalized random term

q-generalized reverse Gumbel distribution

$$f_{ij}(x) = g_{ij}(y) \left| \frac{dy}{dx} \right| = \frac{1}{\theta_i x^{q_i}} \exp\left(\frac{\ln_{q_i}(x) - \ln_{q_i}(\mu_{ij})}{\theta_i}\right) \exp\left(-\exp\left(\frac{\ln_{q_i}(x) - \ln_{q_i}(\mu_{ij})}{\theta_i}\right)\right)$$



Behavioral implication

- Risk attitude
 - ✓ $\ln_{q_i}(\mu_{ij})$ is an isoelastic utility function (also known as a power utility function), which has been widely used in economics
 - ✓ This gives the parameter q_i a clear behavioral meaning: q_i is equivalent to the Arrow–Pratt measure of relative risk aversion when imposing Gumbel distribution on its error component

$$R(\mu_{ij}) = -\mu_{ij} \frac{\partial^2 \ln_{q_i} (\mu_{ij}) / \partial \mu_{ij}^2}{\partial \ln_{q_i} (\mu_{ij}) / \partial \mu_{ij}} = q_i$$

Behavioral implication

• Example



Other choice models with nonlinearity transformation



Swait, J., 2001. A non-compensatory choice model incorporating attribute cutoffs. *Transportation Research Part B: Methodological 35, 903-928*.

Li, B. (2011) The multinomial logit model revisited: A semiparametric approach in discrete choice analysis. Transportation Research Part B 45, 461-473.

SPLINE-BASED NON-LINEAR TRANSFORMATION

Choice probability

Li (2011) shows that we can derive a number of discrete choice models under different error tem distributions:

$$P_{ij} = \theta \alpha_{ij} \int_{z \in \Omega_i} \exp[-\alpha_{i0} \exp(\theta z)] \exp(\theta z) dz$$
$$= \frac{\alpha_{ij}}{\alpha_{i0}} = \frac{\alpha_{ij}}{\Sigma_{j' \in C_i} \alpha_{ij'}} = \frac{H(V_{ij})}{\Sigma_{j' \in C_i} H(V_{ij'})} = \frac{\exp(S(\beta \mathbf{x_{ij}}))}{\Sigma_{j' \in C_i} \exp(S(\beta \mathbf{x_{ij}}))}$$

Table 2

The variance-stabilizing transformations, mean functions, and sensitivity functions for some distributions in family (1).

	Variance-stabilizing transformation $h(t)$	Mean function $H(t)$	Sensitivity function $S(t)$
Exponential	$\theta^{-1}\log(t)$	t^{-1}	$-\log(t)$
Pareto	$\theta^{-1}\log\{\log(t)\}$	t/(t-1)	$\log(t) - \log(t-1)$
Type II generalized logistic	$\theta^{-1}\log\{\log[1 + \exp(t)]\}$	$\psi^{-1}(\psi(1) - \psi(t))$	$\log\{\psi^{-1}(\psi(1) - \psi(t))\}$
Gompertz	$\theta^{-1}\log\{\exp(\theta t)-1\}$		
Rayleigh	$\theta^{-1}\log(t^2)$	$\pi/(2t^2)$	$-2\log(t)$
Weibull	$\log(t)$	$\{\Gamma(1+1/\theta)/t\}^{ heta}$	$-\theta \log(t)$
Gumbel	t	$\exp(-\gamma - \theta t)$	- heta t

The above equation indicates the choice of error term distribution would be equal to the choice of non-linear transformation of systematic utility. (as we already confirmed)

Semi-parametric discrete choice models

Semi-parametric approach (such as P-splines approach) can be used as an approximation of any base distribution.



Fig. 2. The estimated sensitivity function S(t) for the train data.

Fig. 3. The estimated sensitivity function S(t) for the bus data.

Emergence of Deep Learning

Limitations of linear-in-parameter model

- No consideration of non-linearity
- No consideration of interactions among variables
- **Possible solutions** (Goodfellow et al., 2016)
 - 1. Theory-driven (e.g., assuming noncompensatory, using BPR function, etc.)
 - 2. Use Kernel, Splines, etc.
 - Learn the function from the data (e.g., deep learning) → produce more accurate results in many cases

Sifringer, B., Lurkin, V., Alahi, A., 2018. Enhancing Discrete Choice Models with Neural Networks. 18th Swiss Transport Research Conference, Monte Verità, May 16–18.

DISCRETE CHOICE WITH NEURAL NETWORK

Background and objective

• RUM model vs neural network

- Advantage of RUM model
 - Interpretability of the results.
- Advantage of neural network
 - Better goodness-of-fit

• Objective

 Bringing the predictive strength of Neural Networks, a powerful machine learning-based technique, to the field of Discrete Choice Models (DCM) without compromising interpretability of these choice models.

RUM model and neural network (NN)

Discrete choice model as a Random Utility Maximization (RUM) model

Utility function:
$$U_{in} = \beta_1 x_{1in} + ... + \beta_d x_{din} + \varepsilon_{in}$$
 $\forall i \in C_n$
= $V_{in} + \varepsilon_{in}$

Choice probability: $P(i|C_n) = P(U_{in} > \max_{j \neq i}(U_{jn})) = \frac{\exp(V_{in})}{\sum_{j \in C_n} \exp(V_{jn})}$

(negative) log-likelihood: $LL = -\sum_{n=1}^{N} \sum_{i \in C_n} y_{in} \log[P(i|C_n)]$

A discrete choice model from the perspective of neural network

Softmax activation function: $(\sigma(\mathbf{V}_n))_i = \frac{\exp(V_{in})}{\sum_{j \in C_n} \exp(V_{jn})}$

Cross-entropy: $H_n(\sigma, \mathbf{y}_n) = -\sum_{i \in C_n} y_{in} \log[(\sigma(\mathbf{V}_n))_i]$

The conventional MNL can be seen as a neural network model with a simple network structure.

Discrete Choice Model with NN

Utility function with non-linear component:

$$\begin{aligned} \mathbf{U}_{n} &= \boldsymbol{\beta} \boldsymbol{\chi}^{T} + \mathbf{u}_{n} + \boldsymbol{\varepsilon}_{n} \\ & \text{Linear-in-parameters component component (via NN)} \\ & \mathbf{U}_{n} &: \{U_{1n}, U_{2n}, ..., U_{In}\} \\ & \boldsymbol{\beta} &: \text{A vector of parameters (1 \times d)} \\ & \boldsymbol{\chi} &: \text{A set of explanatory variables (I \times d)} \\ & \mathbf{u}_{n} &= \psi(\mathbf{Q}) \end{aligned}$$

where \mathbf{Q} is the ensemble of input features, and, ψ is the function defined by multiple neural network layers and their corresponding activation functions.

Discrete Choice Model with NN

Non-linear component

Linear-in-parameters component



Empirical analysis

- Dataset
 - Swissmetro dataset (Bierlaire et al., 2001)
 - A stated preference data on mode choice
 - 10700 entries from 1190 individuals
- Linear-in-parameters component:

Variable		Alternative			
		Car	Train	Swissmetro	
ASC	Constant	Car-Const		SM-Const	
TT	Travel Time	B-Time	B -Time	B -Time	
Cost	Travel Cost	B-Cost	B-Cost	B-Cost	
Freq	Frequency		B-Freq	B-Freq	
GA	Annual Pass		B-GA	B-GA	
Age	Age in classes		B-Age		
Luggage	Pieces of luggage	B-Luggage			
Seats	Airline seating			B -Seats	

Empirical analysis

- Non-linear component:
 - 1. Travel purpose: Discrete value between 1 to 9 (Business, leisure, travel,...)
 - 2. First class: 0 for no or 1 for yes if passenger is a first class traveler in public transport
 - **3. Ticket**: Discrete value between 0 to 10 for the ticket type (Oneway, half-day, ...)
 - **4. Who**: Discrete value between 0 to 3 for who pays the travel (self, employer, ...)
 - 5. Male: Traveler's gender, 0 for female and 1 for male
 - 6. Income: Discrete value between 0 to 4 concerning the traveler's income per year
 - 7. Origin: Discrete value defining the canton in which the travel begins
 - 8. Dest: Discrete value defining the canton in which the travel ends

Multinomial Logit as Benchmark

Table 2: MNL parameter values

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	<i>t</i> -stat	<i>p</i> -value
1	ASC_{Car}	1.20	0.183	6.58	0.00
2	ASC_{SM}	1.19	0.182	6.53	0.00
3	β_{age}	0.175	0.0512	3.41	0.00
4	β_{cost}	-0.00690	0.000577	-11.97	0.00
5	β_{freq}	-0.00704	0.00116	-6.09	0.00
6	β_{GA}	1.54	0.168	9.17	0.00
7	$\beta_{luggage}$	-0.113	0.0479	-2.36	0.02
8	β_{seats}	0.432	0.115	3.76	0.00
9	β_{time}	-0.0129	0.000842	-15.34	0.00

Number of observations = 7234

 $\mathcal{L}(\hat{\beta}) = -5766.705$

Hybrid model (1)

Table 3: Hybrid Model parameter values

				Robust		
	Parameter		Coeff.	Asympt.		
	number	Description	estimate	std. error	<i>t</i> -stat	<i>p</i> -value
	1	ASC_{Car}	0.0652	0.179	0.37	0.71
	2	ASC_{SM} .	0.327	0.171	1.92	0.06
	3	β_{age}	0.376	0.0464	8.12	0.00
	4	β_{cost}	-0.0141	0.000595	-23.63	0.00
Unused Features	5	β_{freq}	-0.00807	0.00123	-6.55	0.00
	6	β_{GA}	0.130	0.181	0.72	0.47
	7	$\beta_{luggage}$	0.0153	0.0505	0.30	0.76
	8	β_{seats}	0.207	0.106	1.95	0.05
	9	β_{time}	-0.0157	0.000952	-16.53	0.00
	10	β_{NN}	1.24	0.0524	23.74	0.00

Number of observations = 7234

$$\mathcal{L}(\hat{\beta}) = -5008.996$$

Note: Statistical properties of the parameters are obtained through Biogeme (Bierlaire, 2009)

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Simplified hybrid model (2)

Table 4: Hybrid model containing only values of greater interest

				Robust		
Parameter			Coeff.	Asympt.		
nui	number	Description	estimate	std. error	<i>t</i> -stat	<i>p</i> -value
	1	AS C _{Car}	0.966	0.0977	9.89	0.00
Unused Features	2	ASC_{SM}	1.13	0.0941	11.97	0.00
16 Dense Layer 3 New terms u _{in}	3	β_{cost}	-0.0165	0.000666	-24.71	0.00
	7 4	β_{freq}	-0.00820	0.00129	-6.38	0.00
	5	β_{time}	-0.0171	0.000853	-20.05	0.00
	6	β_{NN}	1.25	0.0854	14.65	0.00
Number of observations = 7234						
$\mathcal{L}(\hat{\beta}) = -4894.539$						
All remaining variables are used here						

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Conclusions & future works

Conclusions:

 Combining the advantage of linear-in-parameters RUM model and the advantage of neural network where highly non-linear impacts of explanatory variables

Future works:

- The selection of hyper parameters (it would change the results)
- Possibility of using the model for long-term demand forecasting (cross-validation may not be enough)
- Possibility of using different NN components (e.g., convolutional NN, recurrent NN, etc.)

Comparison of key parameters

Table 6: Parameter ratio comparison

Parameter	MNL	Hybrid	Simple Hybrid	
β_{cost}	100.0%	204.3%	239.1%	
β_{freq}	100.0%	114.6%	116.5%	
β_{time}	100.0%	121.7%	132.5%	
Value of Time	0.54	0.89	0.96	
Value of Frequency	0.98	1.75	2.01	
Final Log-Likelihood	-5766.71	-5009.00	-4894.54	
Number or parameters	9	10	6	

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