

# The 20<sup>th</sup> Behavior Modeling Summer School

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## Basic inference and validation in discrete choice modeling

Giancarlo Parady – The University of Tokyo

Following Random Utility theory

$$P(i) = \int_{\epsilon=-\infty}^{+\infty} F_i(V_i - V_1 + \epsilon, V_i - V_2 + \epsilon, \dots, V_i - V_j + \epsilon) d\epsilon \quad (1)$$

where

$F(\cdot)$  is a CDF of disturbances  $(\epsilon_1, \dots, \epsilon_j)$  (2)

$F_i(\cdot) = \partial F(\cdot) / \partial \epsilon_i$  ; Partial derivative of  $F(\cdot)$  with respect to  $\epsilon_i$ .

The GIEV is obtained from the following CDF

$$F(\cdot) = \exp(-G(e^{-\epsilon_1}, \dots, e^{-\epsilon_j}))$$

where  $G$  is a generating function.

Using equations (1) and (2) we get

$$P(i) = \int_{\epsilon=-\infty}^{+\infty} \frac{\partial \exp(-G(e^{-\epsilon - V_1 + V_1}, \dots, e^{-\epsilon - V_i + V_j}))}{\partial \epsilon_i} d\epsilon$$

$$P(i) = \int_{\epsilon=-\infty}^{+\infty} e^{-\epsilon} G_i(e^{-\epsilon - V_1 + V_1}, \dots, e^{-\epsilon - V_i + V_j}) \cdot \exp(-G(e^{-\epsilon - V_1 + V_1}, \dots, e^{-\epsilon - V_i + V_j})) d\epsilon$$

This integral reads in

$$P(i) = \frac{e^{V_i} \cdot G_i(e^{V_1}, \dots, e^{V_j})}{\sum_k G_k(e^{V_1}, \dots, e^{V_j})} \quad \text{where } G_i = \frac{\partial G(\cdot)}{\partial \ln V_i}$$

# Basic inference discrete choice modeling

Following Random Utility theory

$$P(i) = \int_{\epsilon=-\infty}^{+\infty} F_i(V_i - V_j + \epsilon, V_i - V_k + \epsilon, \dots, V_i - V_j + \epsilon) d\epsilon \quad (1)$$

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$F(\cdot)$  is a CDF of disturbances  $(\epsilon_1, \dots, \epsilon_j)$  (2)

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$$P(i) = \int_{\epsilon=-\infty}^{+\infty} e^{-\epsilon} G_i(e^{-\epsilon - V_i + V_j}, \dots, e^{-\epsilon - V_i + V_j}) \cdot \exp(-G(e^{-\epsilon - V_i + V_j}, \dots, e^{-\epsilon - V_i + V_j})) d\epsilon$$

This integral results in

$$P(i) = \frac{e^{V_i} \cdot G_i(e^{V_j}, \dots, e^{V_j})}{\sum_k G(e^{V_k}, \dots, e^{V_k})} \quad \text{where } G_i = \frac{\partial G(\cdot)}{\partial \ln V_i}$$

# Why is inference important ?

When talking about policy, **Size matters!**

- Ask not whether there is an effect, ask how big is it?
- Is the effect big enough to make a policy successful?
- Is the effect big enough to make invest millions of dollars?
- 64.6% of studies in the transportation field report some sort of policy-relevant inference analysis (Parady, Ory and Walker, 2021)

# Why is inference important ?

Variable name	Coefficient	S.E.	t statistic
Auto constant	1.45	0.393	3.70
In-vehicle time (min)	-0.0089	0.0063	-1.42
Out-of-vehicle time (min)	-0.0308	0.0106	-2.90
Auto out-of-pocket cost (c)	-0.0115	0.0026	-4.39
Transit fare	-0.0070	0.0038	-1.87
Auto ownership (specific to auto mode)	-0.770	0.213	3.16
Downtown workplace (specific to auto mode)	-0.561	0.306	-1.84
Number of observations	1476		
Number of cases	1476		
LL(0)	-1023		
LL( $\beta$ )	-347.4		
-2[LL(0)-LL( $\beta$ )]	1371		
$\rho^2$	0.660		
$\bar{\rho}^2$	0.654		

Table adapted from Ben-Akiva and Lerman (1985)

← Magnitudes are not directly interpretable. We can only interpret the effect direction, or use them to calculate utilities, and choice probabilities

**To make some sense of these parameters we must calculate elasticities or marginal effects**

# Basic Inference in discrete choice models

## MNL: Logit Elasticities (Point elasticities)

- **Direct elasticity:** measures the **percentage change in the probability** of choosing a particular alternative in the choice set with respect to a given **percentage change** in an attribute of that same alternative.

$$E_{x_{ink}}^{P(i)} = \frac{\partial P_n(i)}{\partial x_{ink}} \cdot \frac{x_{ink}}{P_n(i)} = [1 - P_n(i)] x_{ink} \beta_k$$

- **Cross-elasticity:** measures the **percentage change in the probability** of choosing a particular alternative in the choice set with respect to a given **percentage change** in a competing alternative.

$$E_{x_{jnk}}^{P(i)} = \frac{\partial P_n(i)}{\partial x_{jnk}} \cdot \frac{x_{jnk}}{P_n(i)} = -P_n(j) x_{jnk} \beta_k$$

← Because of IIA, cross-elasticities are uniform across all alternatives

# Basic Inference in discrete choice models

## MNL: Logit Elasticities (Point elasticities)

- The elasticities shown before are **individual elasticities (Disaggregate)**
- To calculate sample (aggregate) elasticities we use the **probability weighted sample enumeration** method:

$$E_{x_{ink}}^{\overline{P(i)}} = \frac{\sum_{n=1}^N \hat{P}_n(i) E_{x_{ink}}^{P(i)}}{\sum_{n=1}^N \hat{P}_n(i)}$$

Sample direct elasticity

$$E_{x_{jnk}}^{\overline{P(i)}} = \frac{\sum_{n=1}^N \hat{P}_n(i) E_{x_{jnk}}^{P(i)}}{\sum_{n=1}^N \hat{P}_n(i)}$$

Sample cross-elasticity

Where  $\overline{P(i)}$  is the aggregate choice probability of alternative  $I$ , and  $\hat{P}_{in}(i)$  is an estimated choice probability

- Uniform cross-elasticities do not necessarily hold at the aggregate level
- Also note that elasticities for dummy variables are **meaningless!**

# Basic Inference in discrete choice models

## NL: Logit Elasticities (Point elasticities)

$$P(j) = \frac{e^{V_j/\tau}}{e^{IV(i)}} \cdot \frac{e^{\tau IV(i)}}{\sum_{i=1}^I e^{\tau IV(i)}} \quad \leftarrow \text{NL RUM2 specification}$$

### Direct Elasticity

When alternative  $j$  does not belong to any nest

$$E_{x_{jnk}}^{P(j)} = [1 - P_n(j)] x_{jnk} \beta_k$$

When alternative  $j$  belongs to nest  $i$

$$E_{x_{jnk}}^{P(j)} = \left[ (1 - P_n(j)) + \left( \frac{1}{\tau} - 1 \right) (1 - P(j|i)) \right] x_{jnk} \beta_k$$

### Cross Elasticity

When alternatives  $j$  and  $j'$  belong to different nests

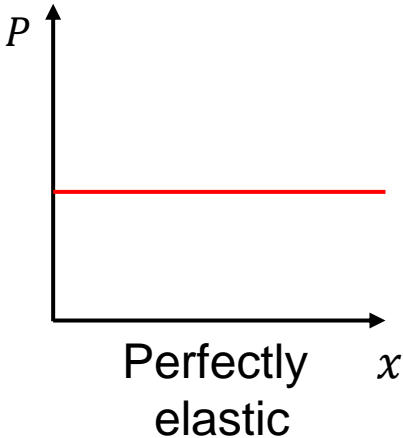
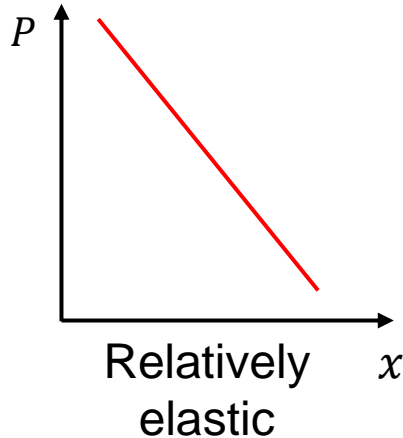
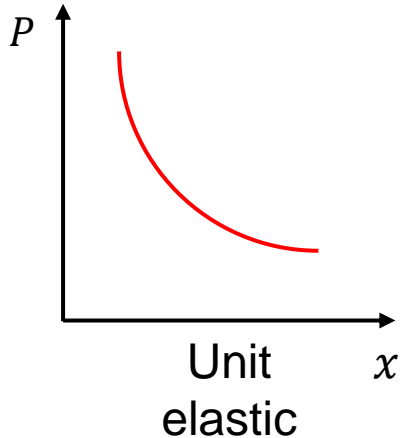
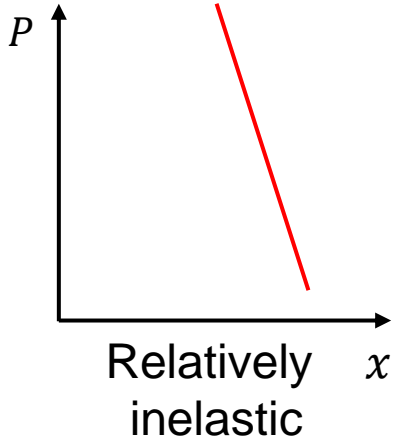
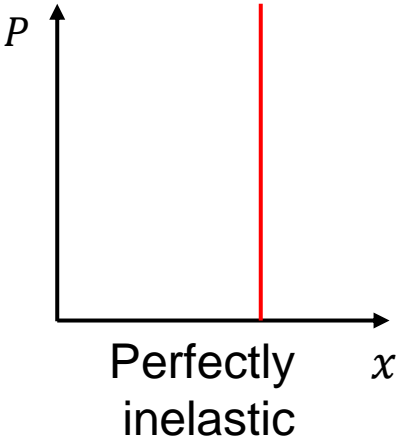
$$E_{x_{j'nk}}^{P(j)} = -P_n(j') x_{j'nk} \beta_k$$

When alternatives  $j$  and  $j'$  belong to the same nest

$$E_{x_{j'nk}}^{P(j)} = - \left[ P_n(j') + \left( \frac{1}{\tau} - 1 \right) P(j'|i) \right] x_{j'nk} \beta_k$$

# Basic Inference in discrete choice models

## Relation between elasticity of demand, change in price and revenue



**Direct elasticity:**

1% increase in  $x_i$  results in a 0% decrease in  $P(i)$

1% increase in  $x_i$  results in a less than 1% decrease in  $P(i)$

1% increase in  $x_i$  results in a 1% decrease in  $P(i)$

1% increase in  $x_i$  results in a more than 1% decrease in  $P(i)$

1% increase in  $x_i$  results in a  $\infty$  decrease in  $P(i)$

**Cross elasticity:**

1% increase in  $x_j$  results in a 0% increase in  $P(i)$

1% increase in  $x_j$  results in a less than 1% increase in  $P(i)$

1% increase in  $x_j$  results in no percent change in  $P(i)$

1% increase in  $x_j$  results in a more than 1% increase in  $P(i)$

1% increase in  $x_j$  results in a  $\infty$  increase in  $P(i)$

Adapted from Hensher, Rose, and Greene (2015)



# Basic Inference in discrete choice models

## MNL: Marginal Effects

- **Direct marginal effect:** measures the **change in the probability** (absolute change) of choosing a particular alternative in the choice set with respect to a **unit change** in an attribute of that same alternative.

$$M_{x_{ink}}^{P(i)} = \frac{\partial P_n(i)}{\partial x_{ink}} = P_n(i)[1 - P_n(i)]\beta_k$$

- **Cross-marginal effect:** measures the **change in the probability** (absolute change) of choosing a particular alternative in the choice set with respect to a **unit change** in a competing alternative.

$$M_{x_{jnk}}^{P(i)} = \frac{\partial P_n(i)}{\partial x_{jnk}} = P_n(i)(-P_n(j)\beta_k)$$

# Basic Inference in discrete choice models

## MNL: Marginal Effects

- We can also calculate sample (aggregate) marginal effects using the **probability weighted sample enumeration** method:

$$M_{x_{ink}}^{\overline{P(i)}} = \frac{\sum_{n=1}^N \hat{P}_n(i) M_{x_{ink}}^{P(i)}}{\sum_{n=1}^N \hat{P}_n(i)}$$

Sample direct marginal effect

$$M_{x_{jnk}}^{\overline{P(i)}} = \frac{\sum_{n=1}^N \hat{P}_n(i) M_{x_{jnk}}^{P(i)}}{\sum_{n=1}^N \hat{P}_n(i)}$$

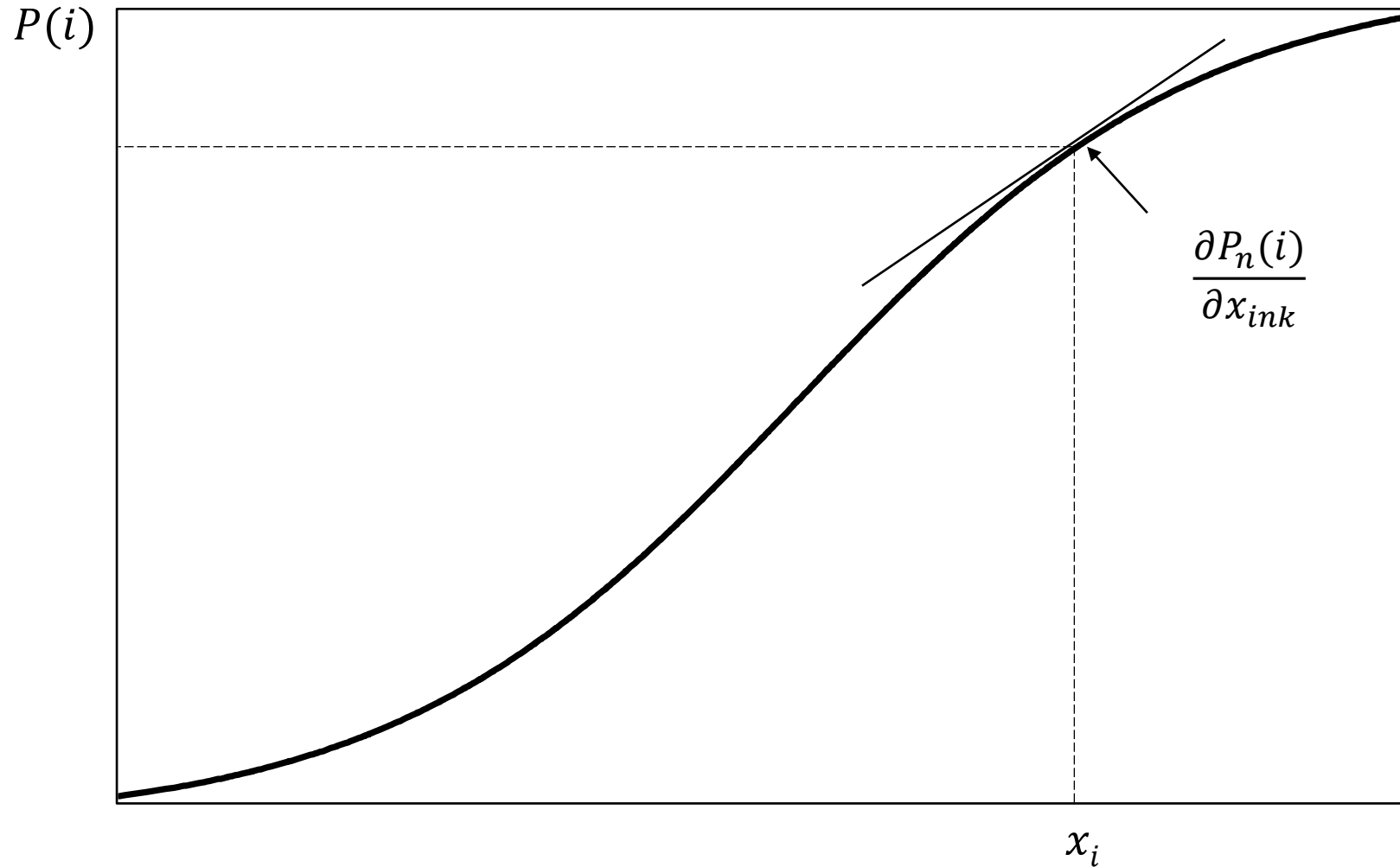
Sample cross-marginal effect

Where  $\overline{P(i)}$  is the aggregate choice probability of alternative  $i$ , and  $\hat{P}_n(i)$  is an estimated choice probability

- Marginal effects for dummy variables **do make sense** as we are talking about unit changes, **but a different procedure is necessary to estimate marginal effects.**

# Basic Inference in discrete choice models

## MNL: Marginal Effects



Marginal effects as the slopes of the Tangent lines to the cumulative probability curve

# Basic Inference in discrete choice models

## MNL: Marginal Effects

Calculating marginal effects for dummy variables

Calculated via simulation:

1. Set the values of the variable of interest to 0
2. Estimate base predictions (at the individual level)
3. Set the values of the variable of interest to 1
4. Estimate new predictions (at the individual level)
5. Calculate marginal effects by taking the mean of the difference in individual predictions

# Validation practices in discrete choice modeling

Following Random Utility theory

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This integral results in

$$P(i) = \frac{e^{V_i} \cdot G_i(e^{V_j}, \dots, e^{V_l})}{\sum_k e^{V_k} \cdot G_k(e^{V_j}, \dots, e^{V_l})} \quad \text{where } G_i = \frac{\partial G(\cdot)}{\partial \ln V_i}$$

# A credibility crisis in science and engineering?

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See original article here:

M. Baker, D. Penny (2016) [Is there a reproducibility crisis?](#) Nature, 533  
(7604) pp. 452-454

# A credibility crisis in science and engineering?

**Most published research findings are likely to be false** due to factors such as lack of power of the study, small effect sizes, and great flexibility in research design, definitions, outcomes and methods.



*Focused on experimental studies*

(Ioannidis, 2005)

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In the transportation field

## Unlike the natural sciences

- Dependence on cross-section observational studies
- Classic scientific hypothesis testing is more difficult
- Impact evaluation of policies drawn based on model-based academic research is rarely conducted
- No feedback in terms of how right or how wrong are these models and the policy recommendations derived from them
- **These issues underscore the need for proper validation practices**

# Term definitions

**Predictive accuracy:** The degree to which predicted outcomes match observed outcomes.

**Predictive accuracy is a function of :**

- **Calibration:** The degree to which predicted probabilities match the relative frequency of observed outcomes.
- **Discrimination ability:** The ability of a model or system of models to discriminate between those instances with and without a particular outcome.



# Term definitions

**Generalizability:** The ability of a model, or system of models to maintain its predictive accuracy in a different sample.

**Generalizability of a model is a function of :**

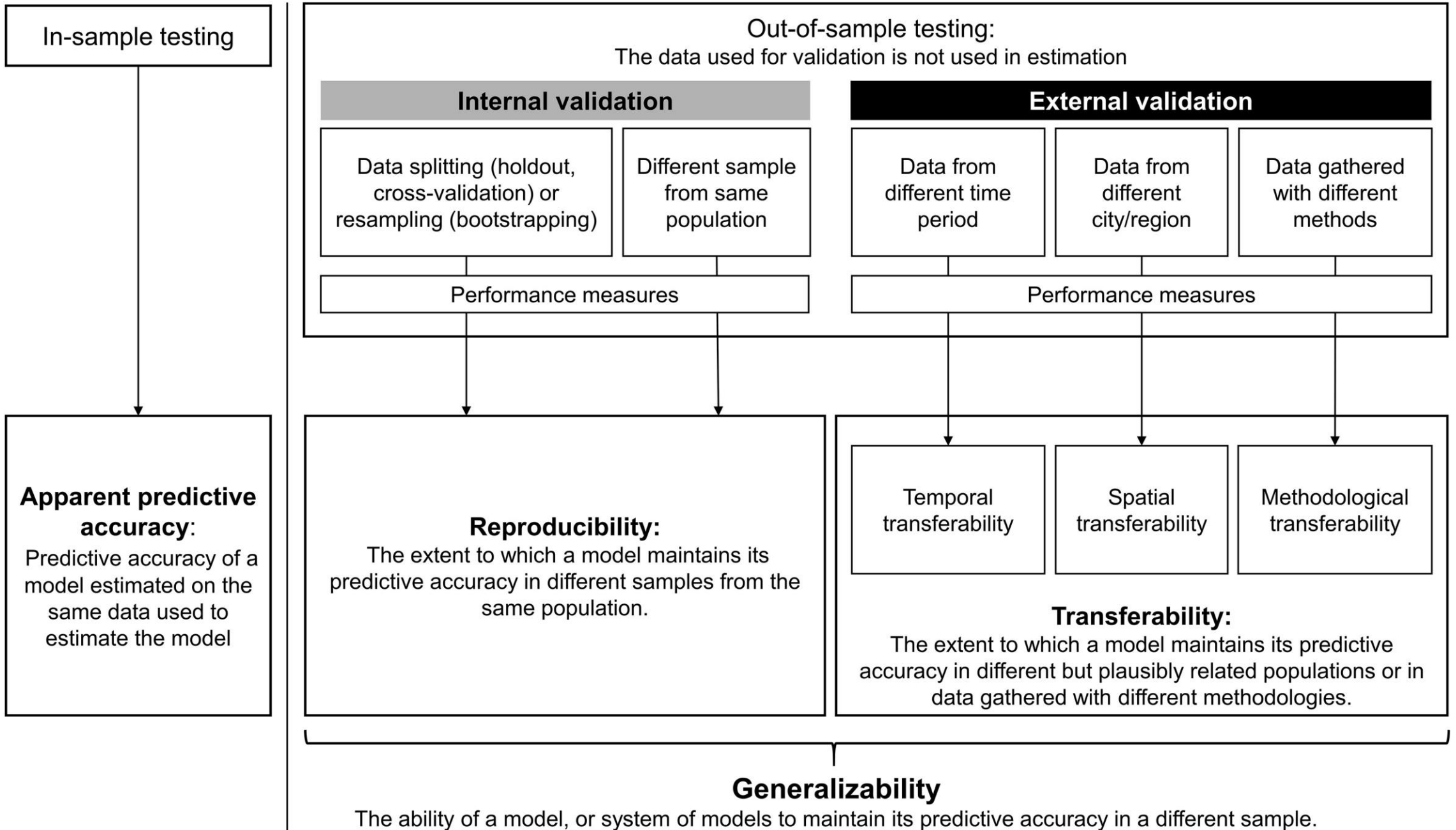
- **Reproducibility:** The extent to which a model or system of models maintains its predictive ability in different samples from the same population.
- **Transferability:** The extent to which a model or system of models maintains its predictive ability in samples from different but plausibly related populations or in samples collected with different methodologies (sometimes called transportability.)

# Term definitions

**Model validation:** The evaluation of the generalizability of a statistical model.

## Types of model validation :

- **Internal validation:** The evaluation of the reproducibility of a model.
  - Data splitting, resampling methods
  - Different sample from the same population
- **External validation:** The evaluation of the transferability of a model.
  - Temporal transferability
  - Spatial transferability
  - Methodological transferability



# A brief introduction to internal validation

- **Internal validation:** The evaluation of the reproducibility of a model.
- Due to the high costs of data collection the most common approaches are
  - **Data splitting (Holdout validation, Cross validation)**
  - **Resampling methods (Bootstrapping)**

# A brief introduction to internal validation (data splitting methods)

**Holdout validation:** Dataset is randomly split into an estimation dataset and a validation dataset.

Estimation data

Validation data

For illustration purposes, let us define  $Q[y_n, \hat{y}_n]$  as a measure of prediction correctness for the  $n$ th instance, for the binary choice case as:

$$Q[y_n, \hat{y}_n] = \begin{cases} 0 & \text{if } y_n = \hat{y}_n \\ 1 & \text{if } y_n \neq \hat{y}_n \end{cases}$$

where  $y_n$  is the observed outcome, and  $\hat{y}_n$  is the predicted outcome for instance  $n$ .

The holdout estimator is

$$HOV = \frac{1}{N_v} \sum_{n_v=1}^{N_v} Q[y_{n_v}, \hat{y}_{n_v}^e]$$

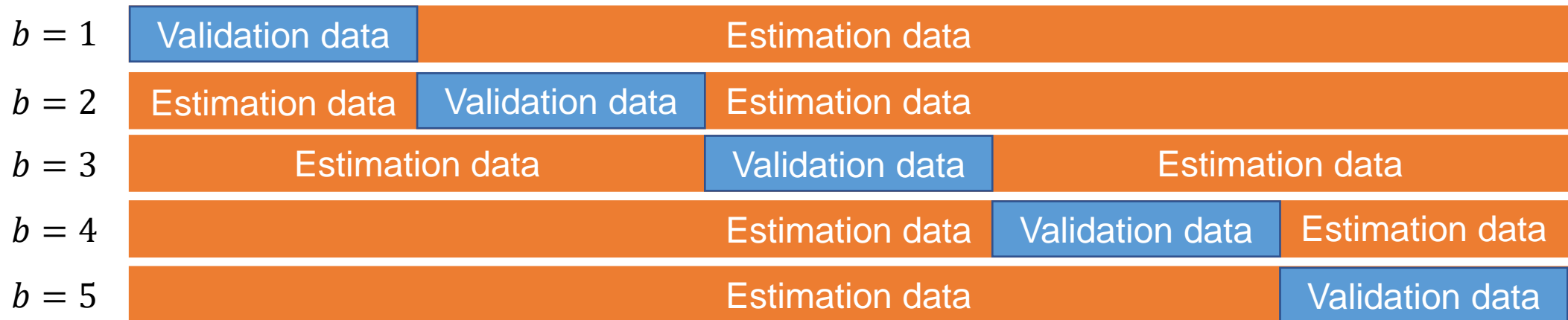
where  $\hat{y}_{n_v}^e$  is the predicted outcome for instance  $n$  in sample  $v$ , using the model estimated with sample  $e$ , and  $N_v$  is the validation sample size.

## A brief introduction to internal validation (data splitting methods)

**Cross-validation:** When the holdout process is repeated multiple times, thus generating a set of randomly split estimation-validation data pairs, we refer to the validation procedure as cross-validation (CV).

$$CV = \frac{1}{B} \sum_b HOV_b$$

where  $B$  is the number of estimation-validation data pairs generated and is the holdout estimator for set  $b$ .



A 5-fold cross validation illustration

# A brief introduction to internal validation (data splitting methods)

## Cross-validation : Commonly used methods

$$CV = \frac{1}{B} \sum_b HOV_b$$

- Cross-validation **methods differ from one another in the way the data is split.**
- When the data splitting considers all possible estimation sets of size , the splitting is **exhaustive**, otherwise the splitting is **partial**. (Arlot and Celisse, 2009)。

## Exhaustive splitting methods

- **Leave-one-out** : estimation set size is  $N_e = N - 1$ , and  $B = N$ . The model is fitted leaving out one instance per iteration, and the outcome of that single instance is predicted based on the estimated model.
- **Leave-p-out** :  $N_e = N - p$ . The model is fitted leaving out p-instances per iteration, and the outcome of the remaining instances is predicted based on the estimated model.

# A brief introduction to internal validation (data splitting methods)

## Cross-validation : Commonly used methods

$$CV = \frac{1}{B} \sum_b HOV_b$$

- Cross-validation **methods differ from one another in the way the data is split.**
- When the data splitting considers all possible estimation sets of size , the splitting is **exhaustive**, otherwise the splitting is **partial**. (Arlot and Celisse, 2009)。

## Partial splitting methods (lower calculation cost)

- **K-fold cross-validation:** data is partitioned into  $K$  mutually-exclusive subsets of roughly equal size, and  $B=K$ .
- **Repeated learning-testing:** a  $B$  number of randomly-split estimation-validation pairs are generated. This method is also called repeated holdout validation.



# A brief introduction to internal validation (data splitting methods)

## Performance measures

### Market share comparison

- Easy to execute
- Does not provide a quantitative measure to evaluate the level of agreement between predictions and observations

Image removed due to copyright issues  
See original article here:

Hasnine, M. S. and Habib, K. N. (2018) '[What about the dynamics in daily travel mode choices? A dynamic discrete choice approach for tour-based mode choice modelling](#)', Transport Policy. Elsevier Ltd, 71(August), pp. 70–80. doi: 10.1016/j.tranpol.2018.07.011.

# A brief introduction to internal validation (data splitting methods)

## Performance measures

Percentage of correct predictions: the alternative with the highest probability is defined as the predicted choice. However,

### Model A :

- **Alt. A: 0.34 \***
- Alt. B: 0.33
- Alt. C: 0.33

### Model B :

- **Alt. A: 0.50 \***
- Alt. B: 0.30
- Alt. C: 0.20

### Model C :

- **Alt. A: 0.90 \***
- Alt. B: 0.05
- Alt. C: 0.05

\* Observed choice

Cannot discriminate differences in estimated probabilities.

A measure that accounts for “clearness” of prediction is necessary.

# A brief introduction to internal validation (data splitting methods)

## Performance measures

### Clearness of prediction:

**Percentage of clearly right choices:** *“the percentage of users in the sample whose observed choices are given a probability greater than threshold  $t$  by the model”*

$$\%CR = \frac{100}{N_v} \sum_{n_v=1}^{N_v} CR_{n_v} \quad \text{where} \quad CR_{n_v} = \begin{cases} 1 & \text{if } \hat{P}(y_{n_v}^e) > t \\ 0 & \text{otherwise} \end{cases}$$

**Percentage of clearly wrong choices:** *“the percentage of users in the sample for whom the model gives a probability greater than threshold  $t$  to a choice alternative differing from the observed one”*

$$\%CW = \frac{100}{N_v} \sum_{n_v=1}^{N_v} CW_{n_v} \quad \text{where} \quad CW_{n_v} = \begin{cases} 1 & \text{if } \hat{P}(!y_{n_v}^e) > t \\ 0 & \text{otherwise} \end{cases}$$

$\hat{P}(!y_{n_v}^e)$  is the estimated choice probability of an alternative other than the chosen one.

# A brief introduction to internal validation (data splitting methods)

## Performance measures

### Clearness of prediction: defining threshold $t$

- To be meaningful, the threshold  $t$  must be “considerably larger” than  $c^{-1}$ , where  $c$  is the choice set size.
- Values used in the literature:
  - Binary model :  $t = 0.9$  (de Luca and Di Pace, 2015)
  - Trinary model :  $t = 0.5$  (Glerum, Atasoy and Bierlaire , 2014)

Image removed due to copyright issues  
See original article here:

de Luca, S. De and Cantarella, G. E. (2009)  
[‘Validation and comparison of choice models’](#), in Saleh, W. and Sammer, G. (eds)  
Travel Demand Management and Road  
User Pricing: Success, Failure and  
Feasibility. Ashgate publications, pp. 37–58.

**See appendix for a list of commonly used indicators**

# Validation and reporting practices in the transportation academic literature

**226** articles reviewed by Parady, Ory and Walker (2021)

**92%** reported a goodness of fit statistics

**64.6%** reported a policy-related inference

Marginal effects, elasticities, odds ratios, value of time estimates, marginal rates of substitution, and policy scenario simulations

**18.1%** reported a validation measure

**Table 3**

Internal validation methods reported in the literature by frequency.

Method	Abbvr.	Frequency	Percentage
Holdout validation	HOV	18	56.3%
Repeated learning-testing	RLT	8	25.0%
Validation against an independent sample	IS	4	12.5%
Repeated K-fold cross-validation	R-K-CV	1	3.1%
Other sample splitting methods	SS-O	1	3.1%

# Towards better validation practices in the field

## ■ Make model validation mandatory:

- Non-negotiable part of model reporting and peer-review in academic journals for any study that provides policy recommendations.
- Cross-validation is the norm in machine learning studies.

## ■ Share benchmark datasets:

- A fundamental limitation in the field is the lack of benchmark datasets and a general culture of sharing code and data.

## ■ Incentivize validation studies:

- Lot of emphasis on theoretically innovative models.
- Encourage submissions that focus on proper validation of existing models and theories.

## ■ Draw and enforce clear reporting guidelines:

- In addition to detailed information of survey characteristics such as sampling method, discussion on representativeness of the data, validation reporting is required.
- Efforts to improve reporting are well documented in other fields (i.e. STROBE statement (von Elm et al., 2007))

**Wait a minute...**

*“I’m not validating my model because I’m not trying to build a predictive framework. I’m trying to learn about travel behavior”*

**The more orthodox the type of analysis** conducted (such as the dimensions of travel behavior covered in this study), **the stronger the onus of validation.**

**Wait a minute...**

*“Does every study that uses a discrete choice model  
should be conducting validation?”*

In short, yes. At the very least, **any article that makes policy recommendations should be subject to proper validation** given the dependence of the field on cross-section observational studies, and the lack of a feedback loop in academia.



**Wait a minute...**

*“Is what we learn about travel behavior from coefficient estimation less valuable if not conducted?”*

There is a myriad of reasons why some **skepticism is warranted** against any particular model outcome. the most obvious one being model overfitting.

# Finally

**Better validation practices will not solve the credibility crisis** in the field, but it's a step in the right direction.

Model validation is **no solution to the causality problem** in the field, but we want to underscore that **the reliance on observational studies inherent to the field demands more stringent controls to improve external validity of results.**

## References:

1. Ben-Akiva, M. E., Lerman, S. R. (1985). Discrete choice analysis: theory and application to travel demand. MIT press.
2. Hensher, D. A., Rose, J. M., & Greene, W. H. (2015). Applied choice analysis: a primer. Cambridge University Press. 2<sup>nd</sup> Edition.
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6. Glerum, A., Atasoy, B. and Bierlaire, M. (2014) 'Using semi-open questions to integrate perceptions in choice models', Journal of Choice Modelling. Elsevier, 10(1), pp. 11–33. doi: 10.1016/j.jocm.2013.12.001.
7. Hasnine, M. S. and Habib, K. N. (2018) 'What about the dynamics in daily travel mode choices? A dynamic discrete choice approach for tour-based mode choice modelling', Transport Policy. Elsevier Ltd, 71(August), pp. 70–80. doi: 10.1016/j.tranpol.2018.07.011.

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$$F(\cdot) = \exp(-G(e^{-\epsilon_1}, \dots, e^{-\epsilon_j}))$$

where  $G$  is a generating function.

Using equations (1) and (2) we get

$$P(i) = \int_{\epsilon=-\infty}^{+\infty} \frac{\partial \exp(-G(e^{-\epsilon - V_i + V_j}, \dots, e^{-\epsilon - V_i + V_l}))}{\partial \epsilon_i} d\epsilon$$

$$P(i) = \int_{\epsilon=-\infty}^{+\infty} e^{-\epsilon} G_i(e^{-\epsilon - V_i + V_j}, \dots, e^{-\epsilon - V_i + V_l}) \cdot \exp(-G(e^{-\epsilon - V_i + V_j}, \dots, e^{-\epsilon - V_i + V_l})) d\epsilon$$

This integral results in

$$P(i) = \frac{e^{V_i} \cdot G_i(e^{V_j}, \dots, e^{V_l})}{\sum_k e^{V_k} \cdot G_k(e^{V_j}, \dots, e^{V_l})} \quad \text{where } G_i = \frac{\partial G(\cdot)}{\partial \ln e^{V_i}}$$

# Appendix: Definition of model validation performance measures reported in the literature

Parady, Ory & Walker (2021)

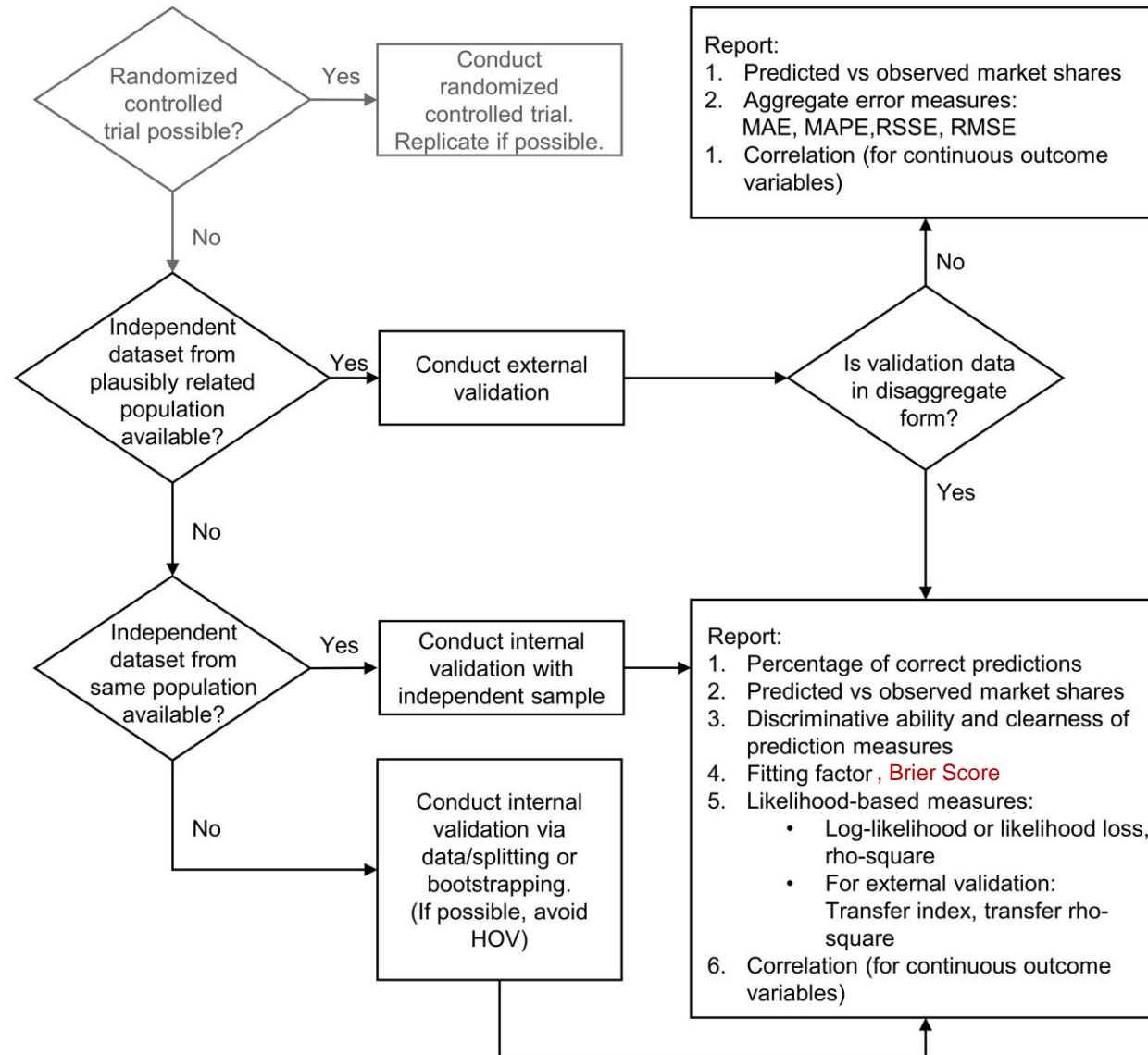
Index	Type	Formula	Notes
<b>Mean absolute percentage error</b> 平均絶対誤差率	MAPE <i>Absolute</i>	$\frac{100}{M} \sum_{m=1}^M \left  \frac{\hat{s}_{v,m}^e - s_{v,m}}{s_{v,m}} \right $	M is the number of alternatives in the choice set.
<b>Root sum of square error</b> 二乗平方根誤差和	RSSE <i>Relative</i>	$\sqrt{\sum_{m=1}^M (\hat{s}_{v,m}^e - s_{v,m})^2}$	$s_{v,m}$ is an aggregate outcome measure in sample $v$ , such as the market share of alternative $m$ (i.e. modal market share), choice frequency, etc.
<b>Mean absolute error</b> 平均絶対誤差	MAE Aggregate: Relative Disaggregate: Absolute	$\frac{1}{M} \sum_{m=1}^M  \hat{s}_{v,m}^e - s_{v,m} $	$\hat{s}_{v,m}^e$ is an aggregate outcome measure in sample $v$ , such as the market share of alternative $m$ , predicted from model estimated on sample $e$ .
<b>Mean squared error</b> 平均二乗誤差	MSE Aggregate: Relative Disaggregate: Absolute	$\frac{1}{M} \sum_{m=1}^M (\hat{s}_{v,m}^e - s_{v,m})^2$	$\hat{P}(y_{n_v,m}^e)$ is the predicted probability that individual $n$ chooses alternative $m$ , predicted from model estimated on sample $e$ .
<b>Root mean square error</b> 二乗平均平方根誤差	RMSE Aggregate: Relative Disaggregate: Absolute	$\sqrt{\frac{1}{M} \sum_{m=1}^M (\hat{s}_{v,m}^e - s_{mv})^2}$	$y_{nm}$ is the actual outcome variable valued 0 or 1.
<b>Brier Score</b> ブライアスコア	BS <i>Absolute</i>	$\frac{1}{N_v} \sum_{n_v=1}^{N_v} \sum_{m=1}^M (\hat{P}(y_{n_v,m}^e) - y_{n_v,m})^2$	

# Appendix: Definition of model validation performance measures reported in the literature

Parady, Ory & Walker (2021)

Index	Type	Formula	Notes	
<b>Log-likelihood</b> 対数尤度	LL	Relative	$LL_v(\hat{\beta}^e)$	$LL_{v,r}(\hat{\beta}^e)$ is log-likelihood of the model estimated on data $e$ applied to the validation data $v_r$ .
<b>Log-likelihood loss</b> 対数尤度損失	LLL	Absolute	$\frac{1}{R} \sum_r -\frac{1}{N_{v,r}} \sum_{n_{v,r}} LL_{v,r}(\hat{\beta}^e)$ $\forall 1 \leq r \leq R$	$N_{v,r}$ is the size of the validation (holdout) sample $r$ , and $R$ is number of validation samples generated.
<b>Rho-square</b> $\sigma^2$	RHOSQ	Absolute	$\rho^2 = 1 - \frac{LL_v(\hat{\beta}^e)}{LL_v(\mathbf{0})}$	$LL_v(\mathbf{0})$ is log-likelihood of the model when all parameters are zero for data $v$ .
<b>Transfer rho-square</b> 移転 $\sigma^2$	T- RHOSQ	Relative	$\rho_{transfer}^2 = 1 - \frac{LL_v(\hat{\beta}^e)}{LL_v(\mathbf{MS}^v)}$	$LL_v(\hat{\beta}^v)$ is the likelihood of the model estimated on the validation data $v$ .
<b>Transfer index</b> 移転指標	TI	Pass/Fail	$\frac{LL_v(\hat{\beta}^e) - LL_v(\mathbf{MS}^v)}{LL_v(\hat{\beta}^v) - LL_v(\mathbf{MS}^v)}$	$LL_v(\mathbf{MS}^v)$ is a base model estimated on validation data $v$ (i.e. market share model.)
<b>Transferability test statistic</b> 移転性検定統計量	TTS	Relative	$-2 \left( LL_v(\hat{\beta}^v) - LL_v(\hat{\beta}^e) \right)$	$\rho_{local}^2$ is the local rho-square of the model.
<b><math>\chi^2</math> test</b>	CHISQ	Pass/Fail	$\sum_{m=1}^M \frac{(f_m - E(f_{v,m}^e))^2}{E(f_{v,m}^e)}$	$f_m$ is the observed choice frequency of alternative $m$ in sample $v$ , and $E(f_{v,m}^e)$ is the expected choice frequency predicted from model estimated on sample $e$ .

# Appendix: Validation and reporting practices in the transportation academic literature



Heuristic to select validation method given available resources and recommended performance measures to report

## Appendix: Validation and reporting practices in the transportation academic literature

**Table 4**

Predictive accuracy performance measures reported in the literature by frequency.

Performance measure	Abbrev.	Frequency	Percentage
Log-likelihood/log-likelihood loss	LL/LLL	19	46.3%
Percentage of correct predictions or First Preference Recovery	FPR	10	24.4%
Predicted vs observed market outcomes	PVO	10	24.4%
Mean absolute error	MAE	6	14.6%
Root mean square error	RMSE	4	9.8%
Error/Percentage error/Absolute percentage error	E/PE/APE	3	7.3%
Rho-Square	RHOSQ	3	7.3%
Transfer index	TI	2	4.9%
% clearly right (t)	%CR	1	2.4%
Brier Score	BS	1	2.4%
Chi-square	CHISQ	1	2.4%
Concordance index	C	1	2.4%
Correlation	CORR	1	2.4%
Fitting factor	FF	1	2.4%
Mean absolute percentage error	MAPE	1	2.4%
Sum of square error	SSE	1	2.4%
Transferability test statistic	TTS	1	2.4%
All other measures specified in <a href="#">Table 1</a>	–	0	0%
Other measures not specified in <a href="#">Table 1</a>	–	3	7.3%

Very similar measures are reported jointly.