The 18th Behavior Modeling Summer School

Sep. 21 – 23 , 2019 @ The University of Tokyo

Following Random utility theory

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

where

$F(\,)$ is a CDF of disturbances $(\varepsilon_1, \dots \varepsilon_J)$ (2)

$F_i(\,)$: $\partial F(\,) / \partial \varepsilon_i$; Partial derivative of $F(\,)$ with respect to ε_i.

the GEV is obtained from the following CDF

$$F(\,) = \exp(-G(e^{-\varepsilon_1}, \dots, e^{-\varepsilon_J}))$$

where G is a generating function.

Using equations (1) and (2) we get

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

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

this integral results in

$$P(i) = \frac{e^{V_i} \cdot G_i(e^{V_1}, \dots, e^{V_J})}{\mu G(e^{V_1}, \dots, e^{V_J})}$$

Basic inference and validation in discrete choice modeling

Giancarlos Troncoso Parady – The University of Tokyo

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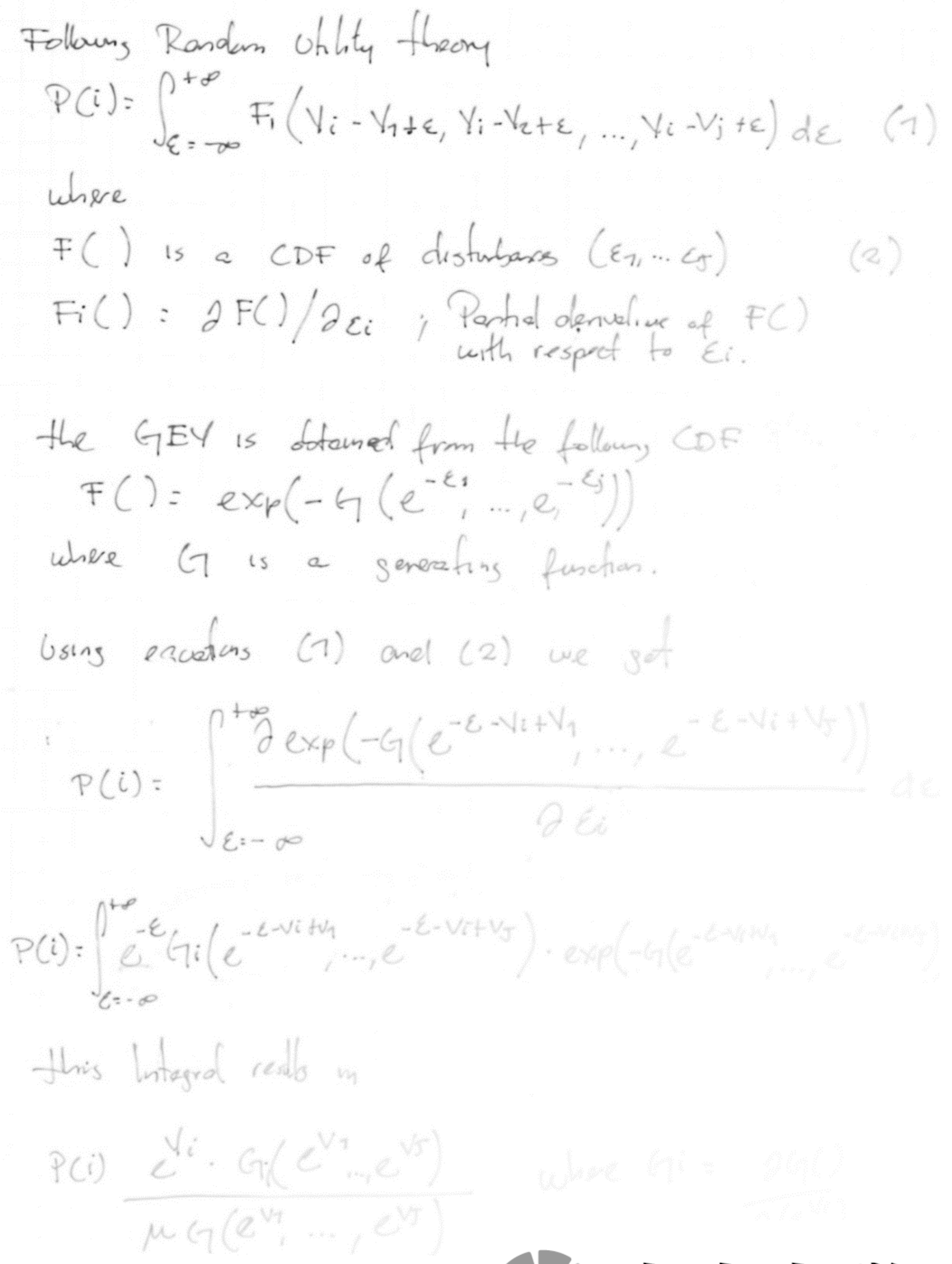

Basic inference discrete choice modeling

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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(β)	-347.4		
-2[LL(0)-LL(β)]	1371		
ρ^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

Hensher, David A., John M. Rose, and William H. Greene (2015)

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

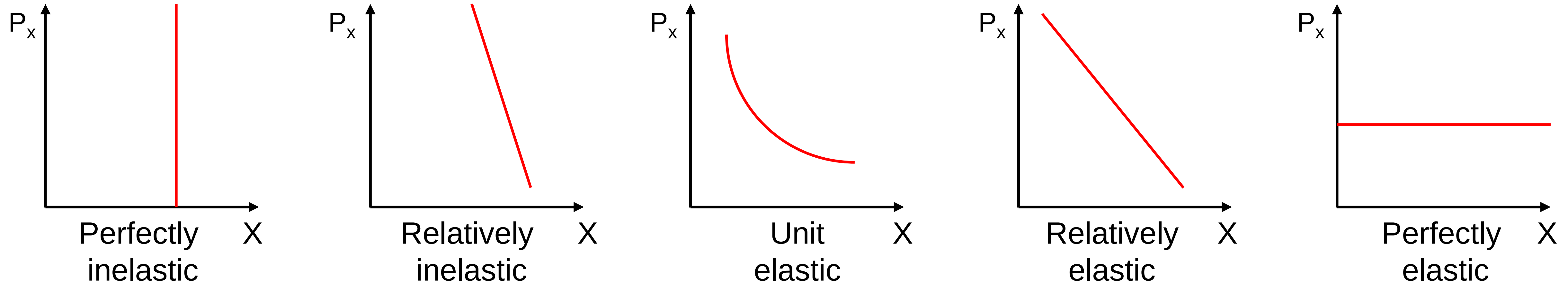
Where $\overline{P(i)}$ is the aggregate choice probability of alternative I, and $\hat{P}_{in}(i)$ is an estimated choice probability

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

Hensher, Rose, and Greene (2015)

Basic Inference in discrete choice models

Relation between elasticity of demand, change in price and revenue



Direct elasticity:

Perfectly inelastic	Relatively inelastic	Unit elastic	Relatively elastic	Perfectly elastic
1% increase in X results in a 0% decrease in P(i)	1% increase in X results in a less than 1% decrease in P(i)	1% increase in X results in a 1% decrease in P(i)	1% increase in X results in a more than 1% decrease in P(i)	1% increase in X results in a ∞ decrease in P(i)

Cross elasticity:

Perfectly inelastic	Relatively inelastic	Unit elastic	Relatively elastic	Perfectly elastic
1% increase in X results in a 0% increase in P(j)	1% increase in X results in a less than 1% increase in P(j)	1% increase in X results in no percent change in P(j)	1% increase in X results in a more than 1% increase in P(j)	1% increase in X results in a ∞ increase in P(j)

Hensher, Rose, and Greene (2015)

Basic Inference in discrete choice models

MNL: Marginal Effects

- **Direct marginal effects:** 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 effects:** 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.

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

Hensher, Rose, and Greene (2015)

Basic Inference in discrete choice models

MNL: Marginal Effects

- We can also calculate sample (aggregate) marginal effects we using e 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

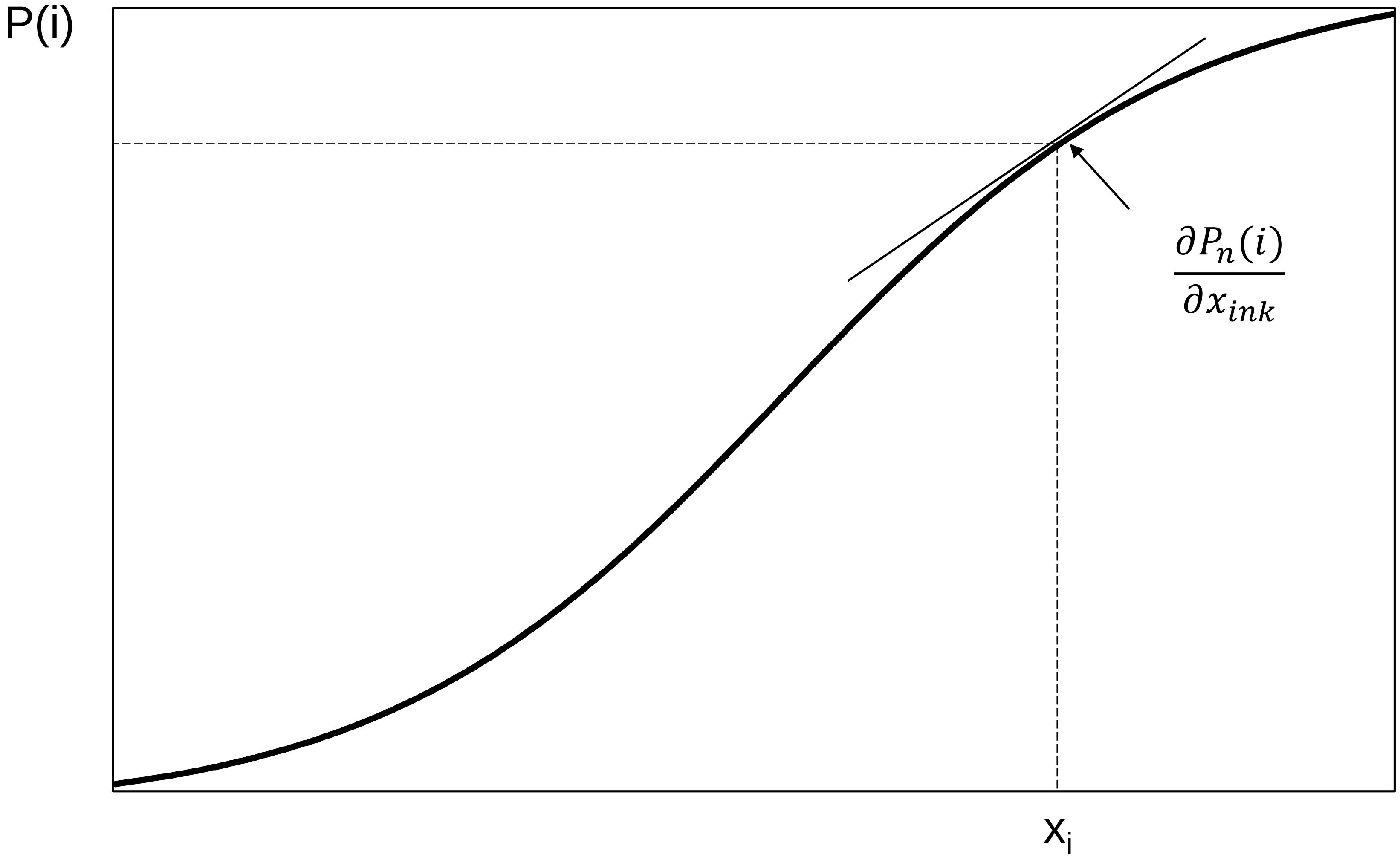
Where $\overline{P(i)}$ is the aggregate choice probability of alternative I, and $\hat{P}_{in}(i)$ is an estimated choice probability

- Marginal effects for dummy variables **do make sense** as we are talking about unit changes!

Hensher, Rose, and Greene (2015)

Basic Inference in discrete choice models

MNL: Marginal Effects



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

Hensher, David A., John M. Rose, and William H. Greene (2015)

Basic Inference in discrete choice models

Incremental Logit for prediction

- An alternative approach to using elasticities or marginal effects for prediction
- Prediction of changes in behavior based on existing choice probabilities

$$P'(i) = \frac{\exp(V_{in} + \Delta V_{in})}{\sum_{j \in C} \exp\left(V_{jn} + \Delta V_{jn}\right)}; \qquad where\ \Delta V_{in} = \sum_{k=1}^{K} \beta_k \Delta x_{ink}$$

Δx_{ink} is a marginal change in the k^{th} independent variable for alternative i and individual n

- In fact, for linear-in-parameter models we need not calculate the utilities again

$$P'(i) = \frac{\exp(V_{in} + \Delta V_{in})}{\sum_{j \in C} \exp\left(V_{jn} + \Delta V_{jn}\right)} = \frac{\mathrm{P}(i)\exp(\Delta V_{in})}{\sum_{j \in C} P(j) \exp\left(\Delta V_{jn}\right)}$$

Ben-Akiva and Lerman (1985)

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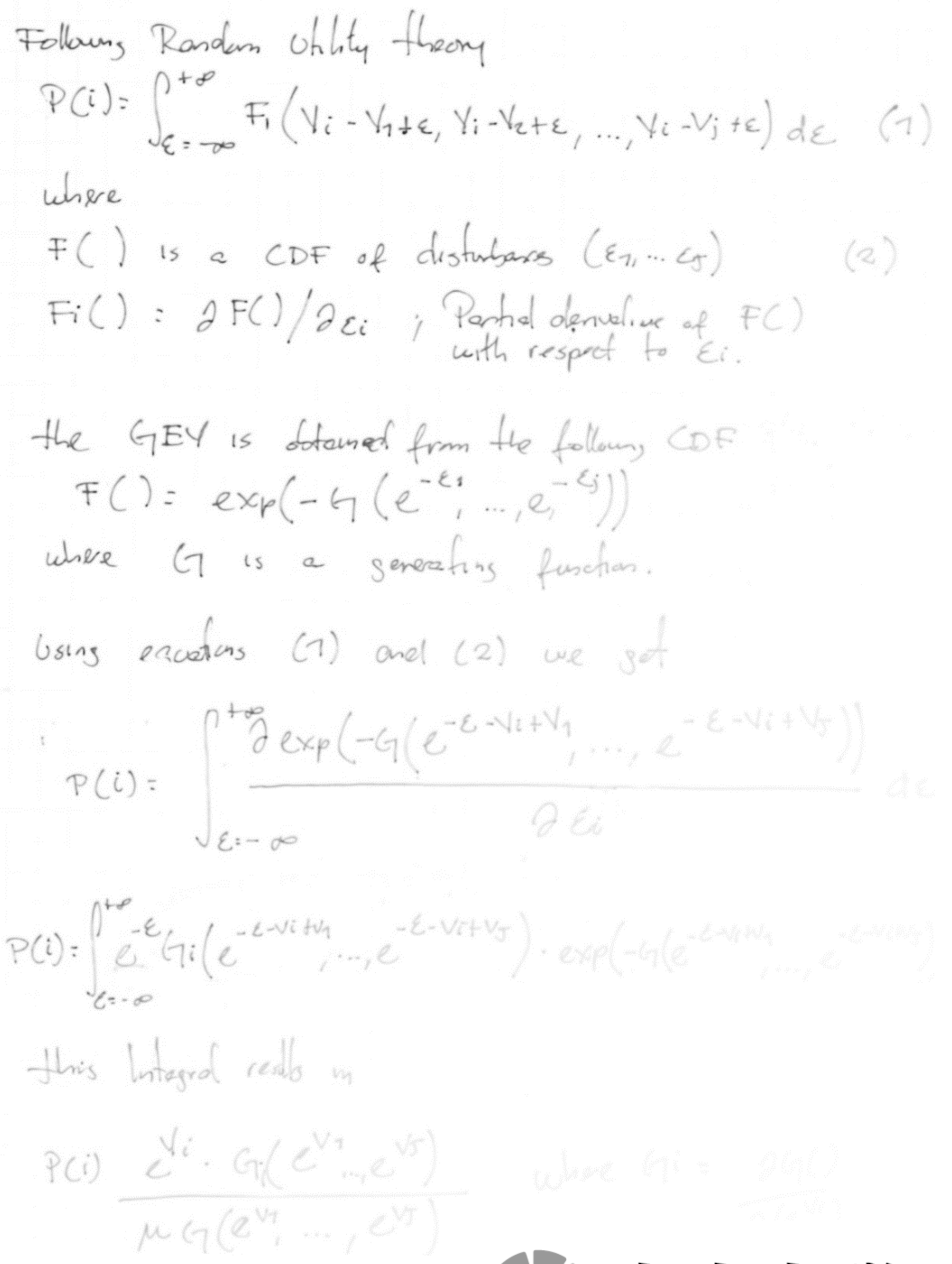

Validation practices in discrete choice modeling

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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.

(Ioannidis, 2005)

A credibility crisis in science and engineering?

What about the transportation field?

In practice:

Demand forecasting is the **“Achilles’ heel”** of the transport planning model (Banister, 2002)

Demand overestimation: **30% Highway trips**

35% Transit trips (UK, 1962 – 1972)

→ **Forecasts have not become more accurate (between 1969-1998).** (Flyvbjerg, kamris Holm, & Buhl, 2005)

Unlike the natural sciences

- Dependence on cross-section observational studies.
- Classic scientific hypothesis testing is more difficult.
- Underscores the need for proper validation practices.

> *“There is little tradition of confronting and confirming predictions of cross-sectional models with outcomes in either back-casting or detailed before-and-after studies”*
>
> (Boyce & William, 2015)

→ **While in practice, a feedback loop exists between forecast outputs and implementation results in the form of measurable forecasting errors, in academia such feedback loop rarely exists.**

Term definitions and research scope

- **Estimation:** *“the use of statistical analysis techniques and observed data to develop model parameters or coefficients”*

- **Calibration:** *“the adjustment of constants and other model parameters in estimated or asserted models in an effort to make the models replicate observed data for a base (calibration) year or otherwise produce more reasonable results”*

- **Validation:** *“the application of the calibrated models and comparison of the results against observed data”*. This comparison is done in terms of predictive ability.

Systemwide validation	Model level validation
More common in practice	More common in research

- **Sensitivity analysis:** At the individual model level, refers to the analysis of changes in outcomes given changes in input variables such as elasticities, marginal effects, etc. At the system level, it refers to the application of a model system using alternative input data or assumptions.

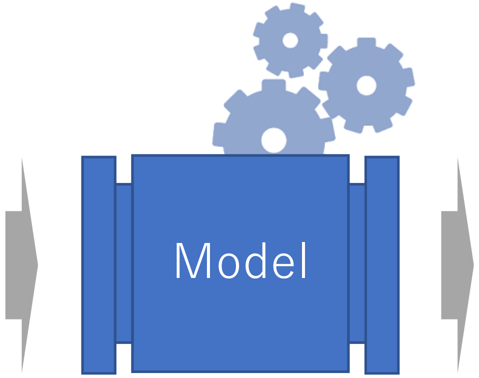
→ **Scope is limited to discrete choice models in the peer-reviewed transportation literature**

Cambridge Systematics (2010)

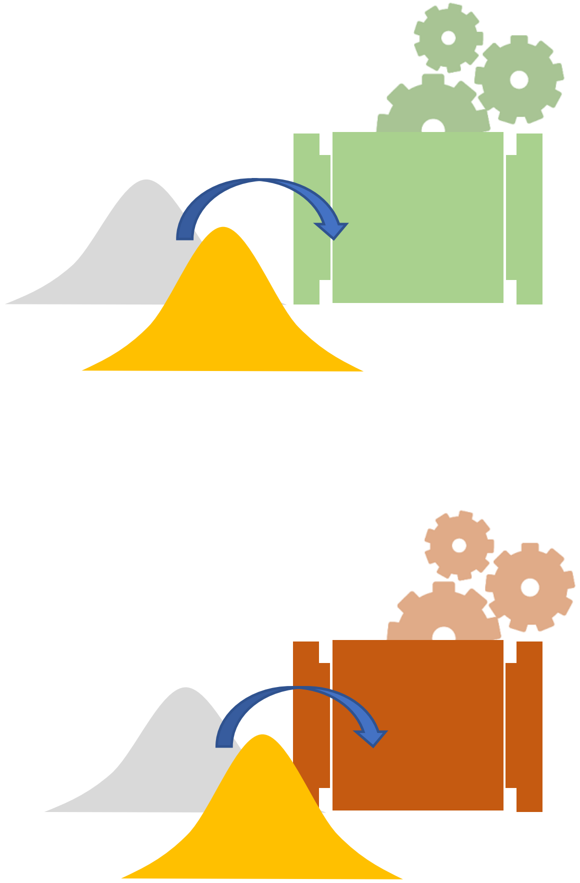
A general overview of model validation methods

Estimation and calibration

$\boldsymbol{x_a}, \boldsymbol{y_a}$

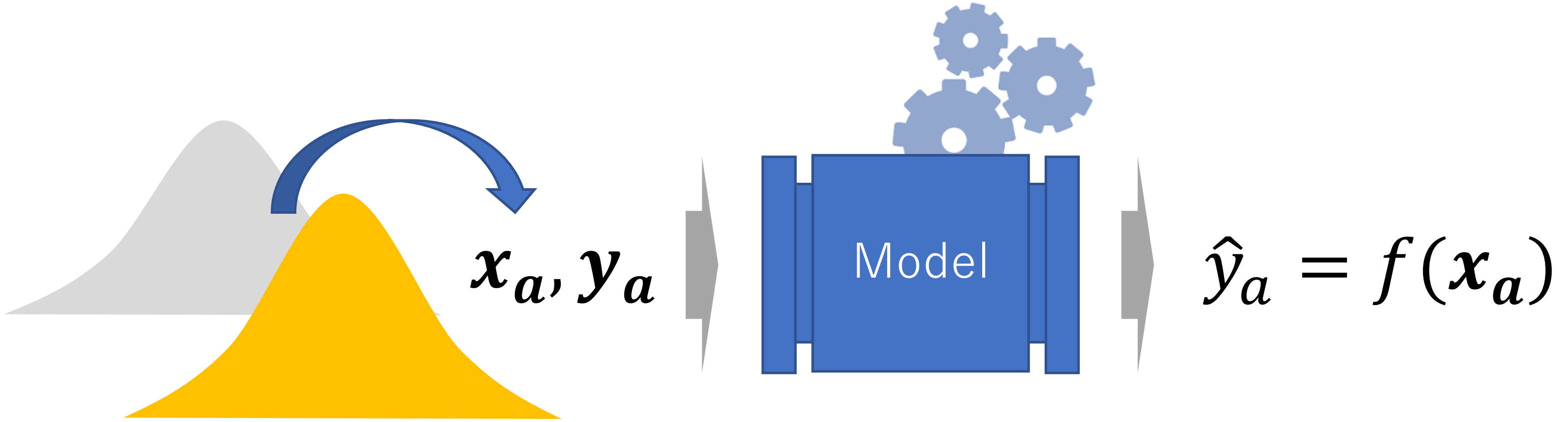


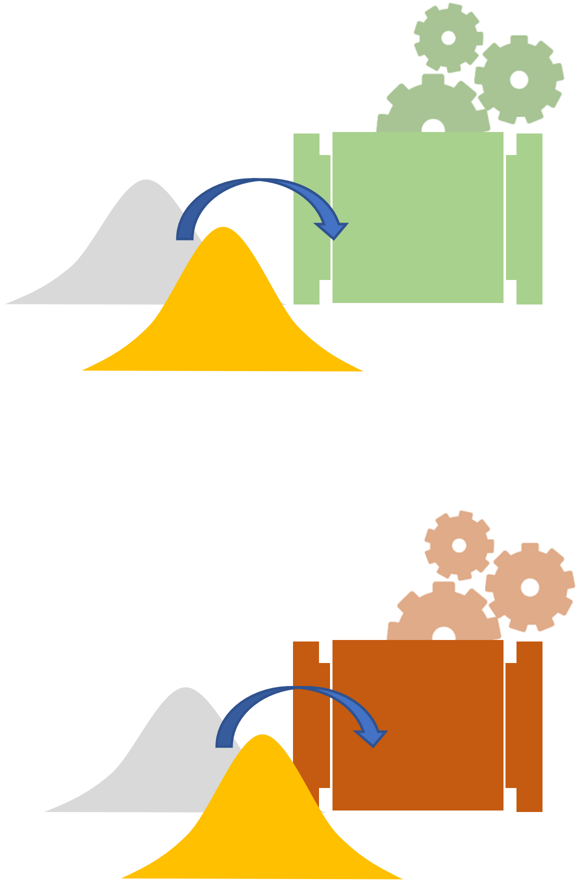
$\hat{y}_a = f(\boldsymbol{x_a})$



A general overview of model validation methods

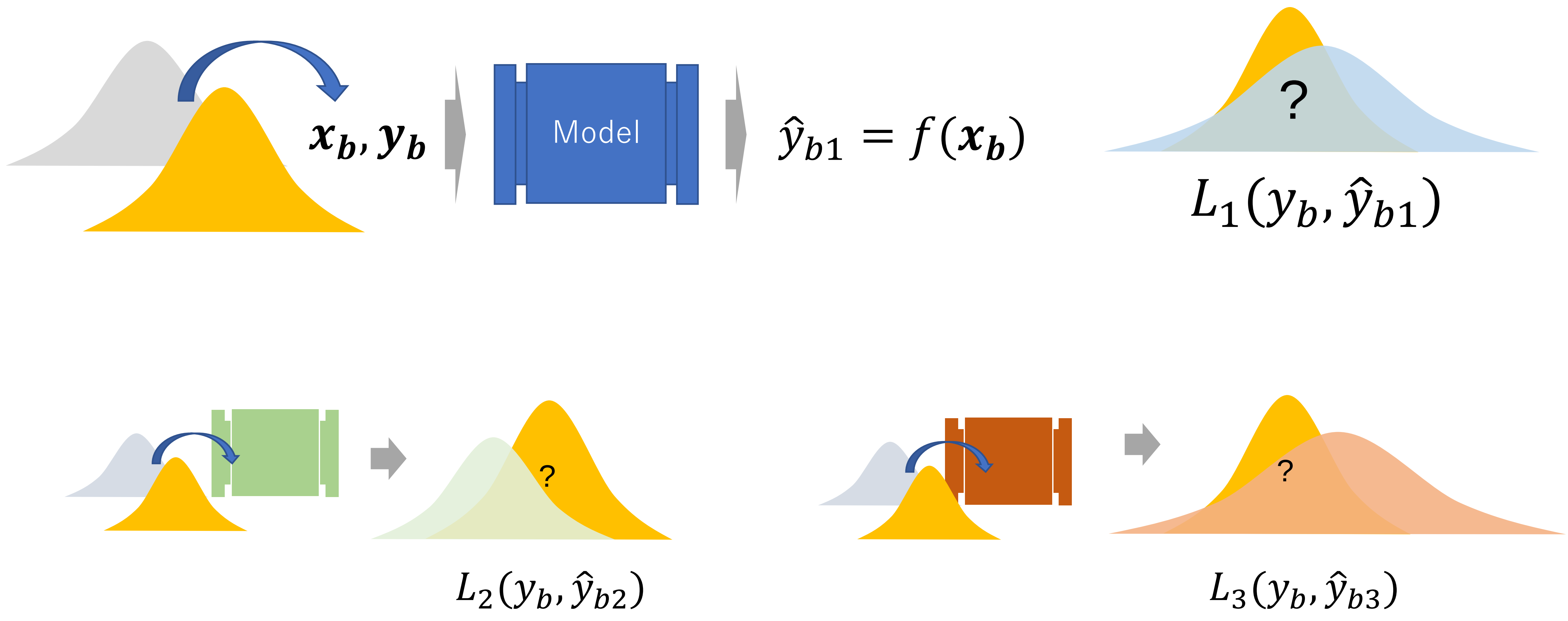
Estimation and calibration





A general overview of model validation methods

Validation



A general overview of model validation methods

Checking a model predictive ability

- Validation with:
  - An Independent sample from the same population ← Ideal, but limited by practical considerations
  - A subset of the same sample (holdout, cross-validation) ← Reduces overfitting risks, but still tied to the same data
- Within sample predictive check (Information criteria, etc.)

  - Over-optimistic since it uses the same data
  - Risk of overfitting
  - Asymptotic equivalence with cross validation relies on stronger distributional assumptions (Arlot & Celisse, 2009)

A general overview of model validation methods

Performance measures

Direct prediction accuracy measures

- Directly interpretable
- Objective indicator of the prediction accuracy of a model

Error-based measures

Likelihood-based measures

- Scores not directly interpretable
- Only meaningful in relative terms
- Useful for model selection

The best model among a set of models can still be a very bad model

Measure	Abbrv.
Predicted vs observed market outcomes	PVO
Percentage of correct predictions	FPR
% clearly right (t)	%CR
% clearly wrong (t)	%CW
% unclear (t)	%U
Fitting factor	FF
Maximum market share deviation	MSD
Correlation	Corr
Absolute percentage error	APE
Sum of square error	SSE
Root sum of square error	RSSE
Mean absolute error	MAE
Mean absolute percentage error	MAPE
Mean squared error	MSE
Root mean square error	RMSE
Brier Score	BS
χ^2 test	CHISQ
Log-likelihood	LL
Mean log-likelihood loss	MLLL
ρ^2, likelihood ratio test (LR), AIC	f(LL)

See Parady, Ory and Walker (2019) for specific details

Validation and reporting practices in the transportation literature

Using the Web of Science Core Collection maintained by Clarivate Analytics we reviewed validation and reporting practices in the transportation literature from the last 5 years (2014 to 2018). Articles were selected based on the following criteria:

- Peer-reviewed journal articles published between **2014 and 2018**
- Analysis uses **discrete choice models**
- Target choice dimensions are:

  Destination choice, Model choice and Route choice
- Web of Science Database fields are:

  Transportation; transportation science and technology; economics; civil engineering
- Research scope is limited to **land transport and daily travel behavior** (tourism, evacuation behavior, etc. were excluded)
- Articles use **empirical data** (Studies using numerical simulations only were excluded)
- Methodological papers only included if the use empirical data

Validation and reporting practices in the transportation academic literature

282 articles reviewed

91% reported a goodness of fit statistics

66% reported a policy-related inference

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

17% reported a validation measure

Validation Method	Abbrv.	Frequency	Percentage
Holdout validation	HOV	25	52.1%
Repeated learning testing cross validation	RLT	11	22.9%
Validation with independent sample from same population	ISV	7	14.6%
Validation with post-intervention data	PIDV	3	6.3%
K-fold cross validation	K-CV	1	2.1%
Other*	O	1	2.1%

*All indicators computed on calibration sample only

Validation and reporting practices in the transportation academic literature

Evaluation measure	Abbrv.	Frequency	% Studies
Log-likelihood	LL	16	33.3%
Percentage of correct predictions or First Preference Recovery	FPR	14	29.2%
Mean absolute error	MAE	6	12.5%
Mean log-likelihood loss	MLLL	6	12.5%
Predicted vs observed market outcomes	PVO	5	10.4%
Other functions of LL. ρ^2 , AIC, likelihood ratio test (LR)	f(LL)	4	8.3%
% clearly right (t)	%CR	3	6.3%
Mean absolute percentage error (MAPE)	MAPE	3	6.3%
Root mean square error	RMSE	3	6.3%
Absolute percentage error	APE	2	4.2%
Chi-square	CHISQ	2	4.2%
Sum of square error / Brier Score	SSE	1	2.1%
% clearly wrong (t)	%CW	1	2.1%
Mean squared error	MSE	1	2.1%
Maximum market share deviation	MSD	1	2.1%
Fitting factor	FF	1	2.1%
Correlation	Corr	1	2.1%
Brier Score	BS	1	2.1%

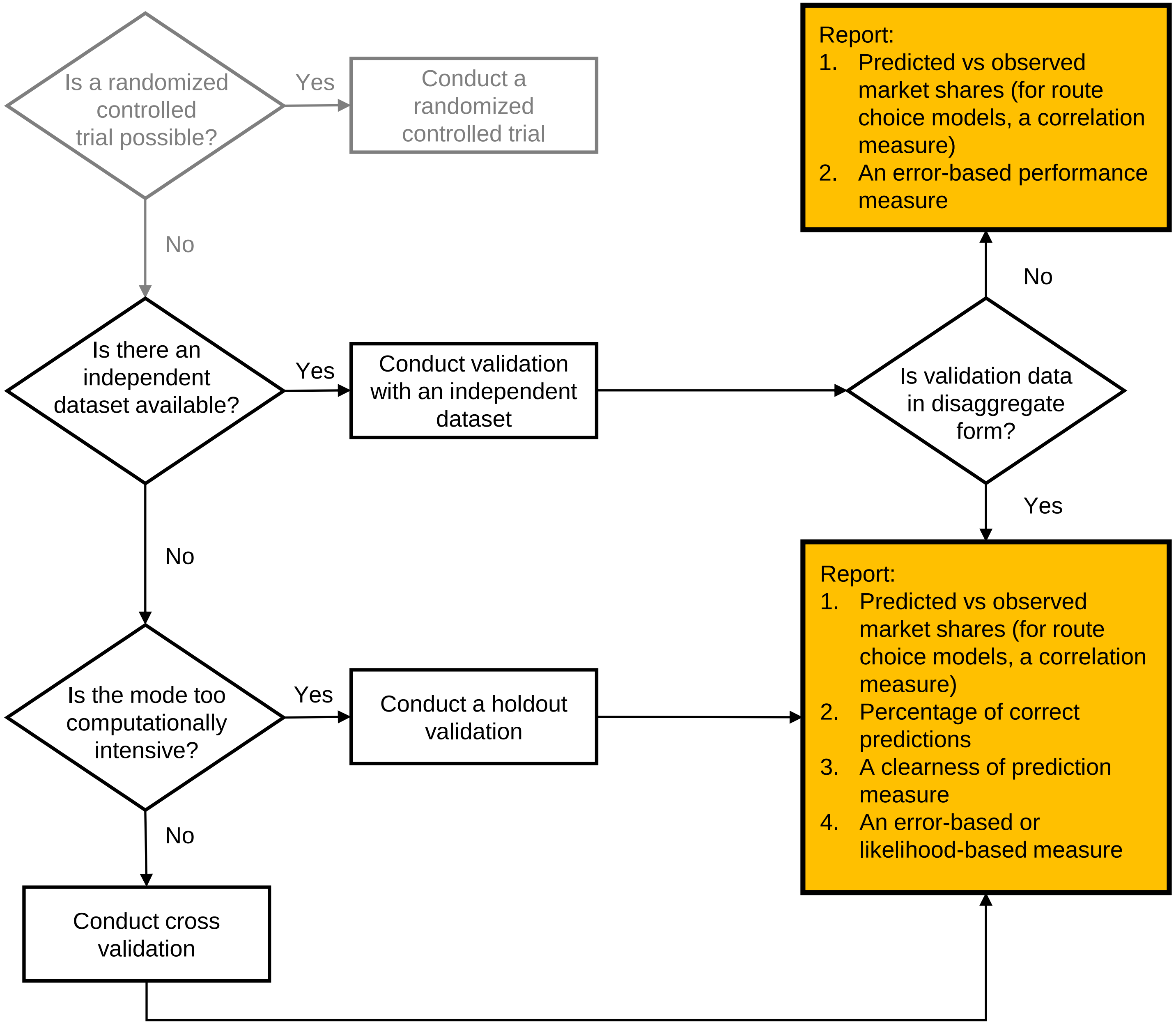
*Note that some studies reported more than one measure

73% of studies reported at least one likelihood-based measure

46% of studies reported at least one prediction accuracy measure

25% of studies reported at least one of both

Validation and reporting practices in the transportation academic literature



Recommended validation practices given available resources

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**.

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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. 2nd Edition.

3. Parady G., Ory, D., Walker, J. (2019) “The overreliance on statistical goodness of fit and under-reliance on empirical validation in discrete choice models: A review of validation practices in the transportation academic literature” Presented at the 6th International choice modelling conference, Kobe, Japan, August 19-21, 2019.

Following Random utility theory

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

where

$F(\ )$ is a CDF of disturbances $(\varepsilon_1, \dots \varepsilon_J)$ (2)

$F_i(\ )$: $\partial F(\ ) / \partial \varepsilon_i$; Partial derivative of $F(\ )$ with respect to ε_i.

the GEV is obtained from the following CDF

$$F(\ ) = \exp\left(-G\left(e^{-\varepsilon_1}, \dots, e^{-\varepsilon_J}\right)\right)$$

where G is a generating function.

Using equations (1) and (2) we get

$$P(i) = \int_{\varepsilon=-\infty}^{+\infty} \frac{\partial \exp\left(-G\left(e^{-\varepsilon - V_i + V_1}, \dots, e^{-\varepsilon - V_i + V_J}\right)\right)}{\partial \varepsilon_i} d\varepsilon$$

$$P(i) = \int_{\varepsilon=-\infty}^{+\infty} e^{-\varepsilon} G_i\left(e^{-\varepsilon - V_i + V_1}, \dots, e^{-\varepsilon - V_i + V_J}\right) \cdot \exp\left(-G\left(e^{-\varepsilon - V_i + V_1}, \dots, e^{-\varepsilon - V_i + V_J}\right)\right)$$

this Integral results in

$$P(i) = \frac{e^{V_i} \cdot G_i\left(e^{V_1}, \dots, e^{V_J}\right)}{\mu G\left(e^{V_1}, \dots, e^{V_J}\right)}$$

where $G_i = \partial G(\ ) / \partial e^{V_i}$

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

Type	Measure	Abbrv.	Equation	Notes
Direct predictive accuracy measure	Predicted vs observed outcomes	PVO	-	Simple comparison of predicted and observed outcomes (i.e. market shares, trips by mode, etc.). Usually in the form of a table or plot. No prediction accuracy statistics are calculated.
	Percentage of correct predictions or First Preference Recovery	FPR	$\frac{100}{N}\sum_{n=1}^{N}\hat{y}_n^c = y_n^c$	y_n^c is the observed choice made by individual n, and $\hat{y}_n^c$ is the choice with the highest predicted probability.
	% clearly right (t)	%CR	$\frac{100}{\mathrm{N}}\sum_{n=1}^{N}\hat{P}(y_n^c) > t$	$\hat{P}(y_n^c)$ is the estimated choice probability of the chosen alternative. $\hat{P}(y_n^{!c})$ is the estimated choice probability of an alternative other than the chosen one.
	% clearly wrong (t)	%CW	$\frac{100}{\mathrm{N}}\sum_{n=1}^{N}\hat{P}(y_n^{!c}) > t$	
	% unclear (t)	%U	100 – % $_{\text{clearly right}}$ (t) + % $_{\text{clearly wrong}}$ (t)	
	Fitting factor	FF	$\frac{1}{\mathrm{N}}\sum_{n=1}^{N}\hat{P}(y_n^c)$	$\hat{P}(y_n^c)$ is the estimated choice probability of the chosen alternative.
	Correlation	Corr	$\mathrm{corr}(s, \hat{s})$	Correlation between predicted and observed outcomes. s is a continuous aggregate outcome measure (i.e. train ridership, etc.)

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

Type	Measure	Abbrv.	Equation	Notes
Relative predictive accuracy measures	Absolute percentage error	APE	$100 \cdot \left\lvert \frac{\hat{s}_m - s_m}{s_m} \right\rvert$	M is the number of alternatives in the choice set. s_m is an aggregate outcome measure, such as the market share of alternative m (i.e. modal market share), choice frequency, etc. $\hat{P}(y_{nm})$ is the predicted probability that individual n chooses alternative m and y_{nm} is the actual outcome variable valued 0 or 1. In the particular case of a binary choice, the second summation sign disappears.
	Sum of square error	SSE	$\sum_{m=1}^{M} (\hat{s}_m - s_m)^2$	
	Root sum of square error	RSSE	$\sqrt{\sum_{m=1}^{M} (\hat{s}_m - s_m)^2}$	
	Mean absolute error	MAE	$\frac{1}{M} \sum_{m=1}^{M} \lvert \hat{s}_m - s_m \rvert$	
	Mean absolute percentage error	MAPE	$\frac{100}{M} \sum_{m=1}^{M} \left\lvert \frac{\hat{s}_m - s_m}{s_m} \right\rvert$	
	Mean squared error	MSE	$\frac{1}{M} \sum_{m=1}^{M} (\hat{s}_m - s_m)^2$	
	Root mean square error	RMSE	$\sqrt{\frac{1}{M} \sum_{m=1}^{M} (\hat{s}_m - s_m)^2}$	
	Brier Score	BS	$\frac{1}{\mathrm{N}} \sum_{n=1}^{N} \sum_{m=1}^{M} \left(\hat{P}(y_{nm}) - y_{nm}\right)^2$	
	χ^2 test	CHISQ	$\sum_{m=1}^{M} \frac{(f_m - E(f_m))^2}{E(f_m)}$	f_m is the observed choice frequency of alternative m, and $E(f_m)$ is the expected choice frequency

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

Type	Measure	Abbrv.	Equation	Notes
Relative predictive accuracy measures	Maximum market share deviation	MSD	$\max S$	S is the set of all market share deviations
	Log-likelihood	LL	$\sum_{n=1}^{N}\sum_{m=1}^{M} c_{nm} log \hat{P}(y_n)$	c_{nm} is a variable that takes value 1 if alternative m was chosen by individual n, and 0 otherwise.
	Mean log-likelihood loss	MLLL	$\frac{1}{\mathrm{R}}\sum_{r} -\frac{1}{VS_r} LL$	Where LL is the log-likelihood, VS is the size of the validation (holdout) sample r, and R is number of validation samples generated.
	ρ^2, likelihood ratio test (LR), AIC	f(LL)	$AIC = LL(\hat{\boldsymbol{\beta}}) - K$ $\rho^2 = 1 - \frac{LL(\hat{\boldsymbol{\beta}})}{LL(0)}$ $\rho^2 = 1 - \frac{AIC}{LL(0)}$ $LR = -2\left(LL(0) - LL(\hat{\boldsymbol{\beta}})\right)$	LL(0) is the log-likelihood when all parameters are zero. LL(β) is the maximized likelihood. K is the number of freely estimated parameters in the model.