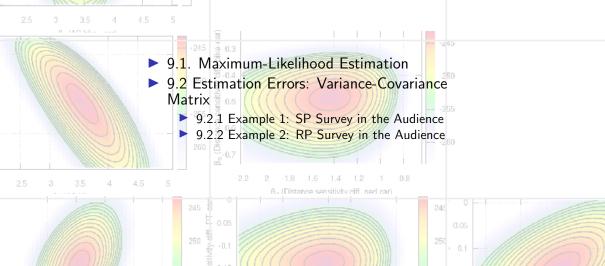
9: Inferential Statistics I of Discrete-Choice Models: Maximum-Likelihood Estimation



- The maximum-likelihood (ML) estimation is applicable for general stochastic models where the probabilities depend on a parameter vector β
- The goal is to maximize the likelihood function L(β), i.e., the probability that the model predicts all data points (y_n, x_n), n = 1, ..., N:

$$L(\boldsymbol{\beta}) = P(\hat{\boldsymbol{y}}_1(\boldsymbol{\beta}) = \boldsymbol{y}_1, \quad ..., \quad \hat{\boldsymbol{y}}_N(\boldsymbol{\beta}) = \boldsymbol{y}_N)$$

where $\hat{oldsymbol{y}}_n = \hat{oldsymbol{y}}(oldsymbol{x}_n)$ gives the model estimate for $oldsymbol{x}_n$

$$L(\boldsymbol{\beta}) = f_{\hat{\boldsymbol{y}}_1(\boldsymbol{\beta}),...,\hat{\boldsymbol{y}}_N(\boldsymbol{\beta})}(\boldsymbol{y}_1,...,\boldsymbol{y}_N)$$

- ? Verify that the density formulation is equivalent to the probability definition by requiring the model estimations to be in small intervals around the data instead of hitting the data exactly.
- I The multi-dimensional probability density f(.) is defined such that $dP = f_{\hat{y}_1,...,\hat{y}_N}(y)d^Ny$. Keeping d^Ny small and constant, dP and thus P is maximized if and only if f(.) is maximized.

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The ML method maximizes the likelihood function:

$$\hat{\boldsymbol{\beta}} = \arg \max_{\boldsymbol{\beta}} L(\boldsymbol{\beta})$$

Equivalently, and often better, one maximizes the log-likelihood:

$$\hat{\boldsymbol{\beta}} = \arg \max_{\boldsymbol{\beta}} \tilde{L}(\boldsymbol{\beta}), \quad \tilde{L}(\boldsymbol{\beta}) = \ln L(\boldsymbol{\beta})$$

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! Since, as a probability or probability density, L > 0 and the log function is defined and strictly monotonously increasing in this range. Since (i) in this case

$$x > y \Leftrightarrow f(x) > f(y)$$

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- ? Why it is possible to express $L(\beta)$ as a product?
- ! Since the random terms $\epsilon_n \sim i.i.dN(0, \sigma^2)$, particularly, they are *independent* from each other

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Probability to predict the chosen alternative i_n for a *single* decision n:

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ML estimation:

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Question

- ? Show that, in deriving the main ML result $\tilde{L} = \sum_n \sum_i y_{ni} \ln P_{ni}$, the random utilities need not to be uncorrelated between alternatives, only between choices
- ! Because of the exclusivity/completeness requirement for the alternatives, exactly one alternative can be chosen per decision so it is enough to maximize the corresponding probability (which, of course, depends on possible correlations)

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If there are no exogenous variables, we are left with just the ACs reflecting that people prefer certain alternatives over others for unknown reasons:

$$V_{ni} = \sum_{m=1}^{I-1} \beta_m \delta_{mi} \quad \text{or} \quad V_{ni} = \beta_i \text{ if } i \neq I, \ V_{nI} = 0$$

This **AC-only model** will be the "reference case" when estimating the model quality, e.g., by the **likelihood-ratio index**.

- ? Show that the estimated models gives probabilities $P_{ni} = P_i$ that are equal to the observed choice fractions N_i/N . (*Hint:* Lagrange multiplicators to satisfy $\sum_i P_i = 1$)
- ! we have $\tilde{L}(P) = \sum_n \ln P_{i_n} = \sum_i N_i \ln P_i$; maximize under the constraint $\sum_i P_i = 1$:

$$\frac{\mathrm{d}}{\mathrm{d}P_i} \left(\tilde{L}(\boldsymbol{P}) - \lambda (\sum_i P_i - 1) \right) \stackrel{!}{=} 0 \implies \frac{N_i}{P_i} = \lambda \implies P_i \propto N_i$$

? Based on this result $P_t = N_t/N_t$ give the parameters for the AC-only MNL and for the binary i.i.d. Probit model Logit: $P_t/P_t = N_t/N_t = \exp(\beta_t)$ (notice that *I* is the reference w/o AC)

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Exercise: simple binomial model with an AC and travel time

$$V_{ni} = \beta_1 \delta_{i1} + \beta_2 T_{ni}$$

Choice set	$T_{ped} = T_1 \ [min]$	$T_{bike} = T_2 [min]$	# chosen 1	# chosen 2
1	15	30	3	2
2	10	15	2	3
3	20	20	1	4
4	30	25	1	4
5	30	20	0	5
6	60	30	0	5

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β1

0

-0.05

-0.1

-0.15

-0.2

-0.25

-2

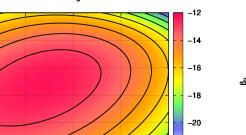
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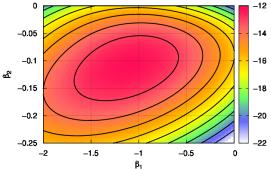


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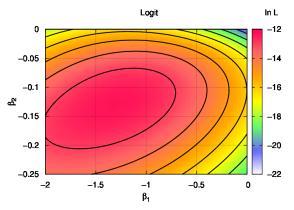
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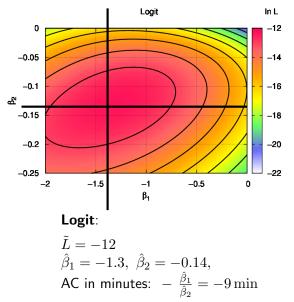
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$$V_{ni} = \beta_1 \delta_{i1} + \beta_2 T_{ni}$$

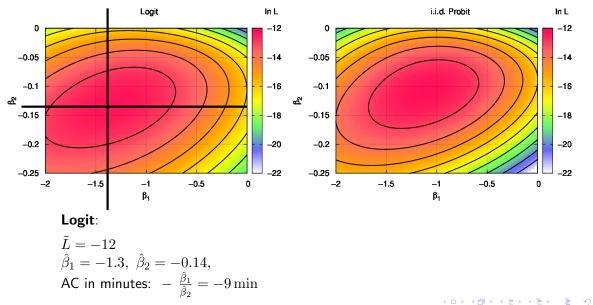


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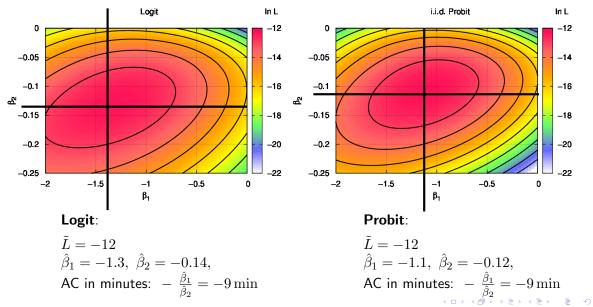
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II. Numerical solution

- Generally, we have a nonlinear optimization problem.
- For parameter-linear utilities, we know for the MNL that a maximum exists and is unique.
- Standard methods of nonlinear optimization are possible:
 - Newton's and quasi-Newton method: Fast but may be unstable
 - Gradient/steepest descent methods: slow but reliable
 - Broyden-Fletcher-Goldfarb-Shanno (BFGS) or Levenberg-Marquardt algorithm combining gradient and Newton methods. Such methods are used in many software packages

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 - genetic algorithms if the objective function landscape is complicated (nonlinear utilities).

Special case: estimating the MNL

The special structure of the MNL with parameter-linear utilities, $V_{ni} = \sum_{m} \beta_m X_{mni}$ allows for an intuitive formulation of the estimation problem:

The observed and modeled **property sums** sums of the factors X for a given parameter m should be the same

$$X_m^{\mathsf{MNL}} = X_m^{\mathsf{data}},$$
$$\sum_{n,i} x_{mni} P_{ni}(\hat{\boldsymbol{\beta}}) = \sum_{n,i} x_{mni} y_{ni} = \sum_n x_{mni_n}$$

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 $\mathsf{MNL} \ \mathsf{model}, \ V_{ni} = \beta_1 T_{ni} + \beta_2 C_{ni} + \beta_3 g_i \delta_{i1} + \beta_4 \delta_{i1}, \ g_{\text{O}} = 0, \ g_{\text{Q}} = 1:$

• $X_1 = T$: Total travel time for the chosen alternatives:

$$T^{\mathsf{MNL}} = \sum_{n,i} P_{ni}(\boldsymbol{\beta}) T_{ni}, \quad T^{\mathsf{data}} = \sum_{n,i} y_{ni} T_{ni} = \sum_{n} T_{ni_n}$$

• $X_2 = C$: Total money spent by the decision makers:

$$C^{\mathsf{MNL}} = \sum_{n,i} P_{ni}(\boldsymbol{\beta}) C_{ni}, \quad C^{\mathsf{data}} = \sum_{n,i} y_{ni} C_{ni} = \sum_{n} C_{ni_n}$$

► $X_3 = N_{1, \mathbf{p}}$: number of woman choosing alternative 1:

$$N_{1,\mathbf{P}}^{\mathsf{MNL}} = \sum_{n} P_{n1}(\boldsymbol{\beta})g_{n}, \quad N_{1,\mathbf{P}}^{\mathsf{data}} = \sum_{n} y_{n1}g_{n}$$

 \blacktriangleright $X_4 = N_1$: total number of persons choosing alternative 1:

$$N_1^{\mathsf{MNL}} = \sum_n P_{n1}(\beta), \quad N_1^{\mathsf{data}} = \sum_n y_{n1}$$

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► $X_3 = N_{1,2}$ number of woman choosing alternative 1:

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• $X_4 = N_1$: total number of persons choosing alternative 1:

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9.2 Estimation Errors: Variance-Covariance Matrix

Since the log-likelihood is maximized at $\hat{oldsymbol{eta}}$, we have

$$\frac{\partial \tilde{L}}{\partial \boldsymbol{\beta}} = 0 \ \Rightarrow \ \tilde{L}(\boldsymbol{\beta}) \approx \tilde{L}_{\max} + \frac{1}{2} \Delta \boldsymbol{\beta}^T \cdot \mathbf{H} \cdot \Delta \boldsymbol{\beta}, \quad \Delta \boldsymbol{\beta} = \boldsymbol{\beta} - \hat{\boldsymbol{\beta}}$$

with the (negative definite) Hessian $H_{lm} = \frac{\partial^2 \tilde{L}(\beta)}{\partial \beta_l \ \partial \beta_m} \Big|_{\beta = \hat{B}}$

Compare $L(\beta)$ near its maximum with the density f(x) of the general multivariate normal distribution with variance-covariance matrix Σ :

$$\begin{split} L(\boldsymbol{\beta}) &= L_{\max} \exp\left(\frac{1}{2}\Delta \boldsymbol{\beta}^T \cdot \mathbf{H} \cdot \Delta \boldsymbol{\beta}\right), \\ f(\boldsymbol{x}) &= \left((2\pi)^M \mathsf{Det} \boldsymbol{\Sigma}\right)^{-1/2} \; \exp\left(-\frac{1}{2} \boldsymbol{x}' \boldsymbol{\Sigma}^{-1} \, \boldsymbol{x}\right) \end{split}$$

Identify $\Delta\beta$ with x, the sought-after variance-covariance matrix V with Σ , and assume the asymptotic limit (higher than quadratic terms in $\tilde{L}(\hat{\beta})$ negligible): \Rightarrow

$$\mathbf{V} = \operatorname{Cov}(\hat{\boldsymbol{\beta}}) = E\left[\left(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}\right)\left(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}\right)'\right] \approx -\mathbf{H}^{-1}(\hat{\boldsymbol{\beta}})$$

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Fisher's information matrix

The variance-covariance matrix is related to **Fisher's information matrix** \mathcal{I} :

$$\mathcal{I} = \mathbf{V}^{-1} = -\mathbf{H}, \quad I_{lm} = -\frac{\partial^2 \hat{L}(\hat{\boldsymbol{\beta}})}{\partial \beta_l \ \partial \beta_m}$$

Roughly speaking, information is missing uncertainty, so the higher the main components of *I*, the lower the main components of V

Cramér-Rao inequality: A lower bound for the variance-covariance matrix is the inverse of Fisher's information matrix => The ML estimator is asymptotically efficient

Comparison with the OLS estimator $V_{OLS} = 2\sigma^2 H_{SSE}^{-1}$ of regression models:

$$\mathcal{I} = -\mathbf{H} = \mathbf{H}_{SSE}/(2\sigma^2) = \mathbf{X}'\mathbf{X}/\sigma^2$$

The negative Hesse matrix of $\tilde{L}(\beta)$ is proportional to the Hesse matrix of the regression SSE $S(\beta)$.

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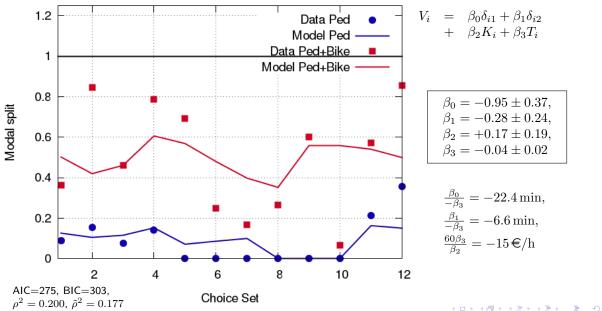
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9.2.1 Example 1 from past lecture: SP Survey in the Audience WS18/19 (red: bad weather, W = 1)

Choice Set	Alt. 1: Ped	Alt. 2: Bike	Alt. 3: PT/Car	Alt 1	Alt 2	Alt 3
1	30 min	20 min	20 min+0€	1	3	7
2	30 min	20 min	20 min+2€	2	9	2
3	30 min	20 min	20 min+1€	1	5	7
4	30 min	20 min	30 min+0€	2	9	3
5	50 min	20 min	30 min+0€	0	9	4
6	50 min	30 min	30 min+0€	0	3	9
7	50 min	40 min	30 min+0€	0	2	10
8	180 min	60 min	60 min+2€	0	4	11
9	180 min	40 min	60 min+2€	0	9	6
10	180 min	40 min	60 min+2€	0	1	14
11	12 min	8 min	10 min+0€	3	5	6
12	12 min	8 min	10 min+1€	5	7	2

Model specification for Model 1 of the past lecture



Likelihood and log-likelihood function for varying cost (β_2) and time (β_3) sensitivities

$$V_{i} = \beta_{0}\delta_{i1} + \beta_{1}\delta_{i2} + \beta_{2}K + \beta_{3}T$$

$$\int_{0}^{4} \frac{\beta_{0}}{\beta_{0}} \frac{1}{\beta_{0}} + \beta_{1}\delta_{i2} + \beta_{2}K + \beta_{3}T$$

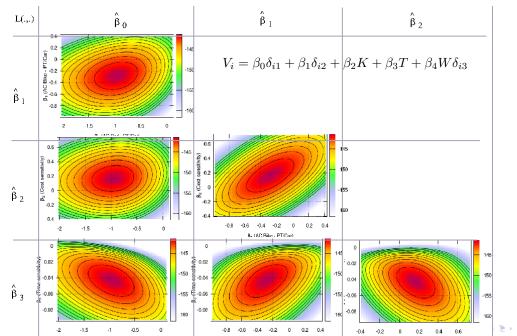
$$\int_{0}^{4} \frac{\beta_{0}}{\beta_{0}} \frac{1}{\beta_{0}} + \beta_{1}\delta_{12} + \beta_{2}K + \beta_{3}T$$

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$$\int_{0}^{4} \frac{\beta_{0}}{\beta_{0}} + \beta_{1}\delta_{12} + \beta_{1}\delta_{$$

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Log-likelihood function in parameter space

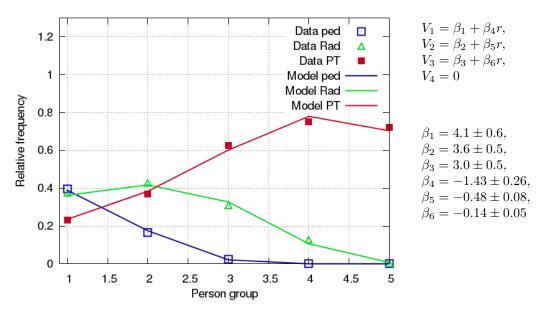


9.2.2 Example 2: RP Survey in the Audience

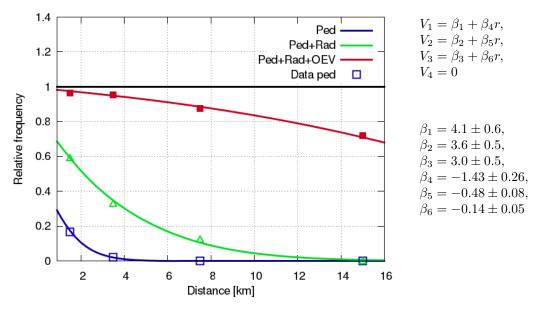
Distance classes for the trip home to university (cumulated till 2018) Weather: good

Distance	Class- center	Choice Alt. 1: ped	Choice Alt. 2: bike	Choice Alt. 2: PT	Choice Alt. 3: car
0-1 km	0.5 km	17	16	10	0
1-2 km	1.5 km	9	23	20	2
2-5 km	3.5 km	2	27	55	4
5-10 km	7.5 km	0	7	42	7
10-20 km	12.5 km	0	0	18	7

Revealed Choice: fit quality

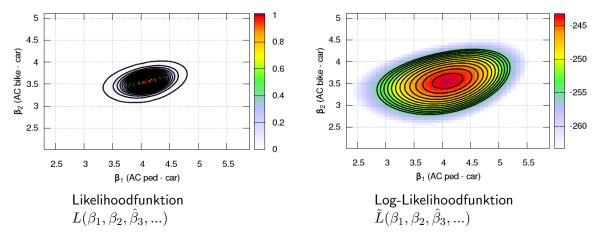


Revealed Choice: Modal split as a function of distance



Likelihood and Log-Likelihood as $f(\beta_1, \beta_2)$

$$V_i = \sum_{m=1}^{3} \beta_m \delta_{m,i} + \sum_{m=1}^{3} \beta_{m+3} r \delta_{m,i}$$



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