# BIOGEME: a free package for the estimation of discrete choice models

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# BIOGEME: a free package for the estimation of discrete choice models

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**Abstract**

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# 1 Introduction

Discrete choice models in general, and random utility models in particular, have been extensively used in several fields of applications for the last three decades. The theoretical derivation of these models is well documented in the literature (Luce, 1959, McFadden, 1981, Ben-Akiva and Lerman, 1985, Anderson et al., 1992, Hensher and Johnson, 1981, Horowitz et al., 1986, Bierlaire, 1998, Ben-Akiva and Bierlaire, 1999). Recently, new sophisticated models have been proposed in the literature. Among them, two main categories can be identified: Generalized Extreme Value models, and mixed logit models.

Generalized Extreme Value (GEV) models have been proposed 25 years ago by McFadden (1978). It is actually a family of models, consistent with random utility theory. Since then, only a few members have been exploited, the Multinomial Logit model and the Nested Logit model being the most popular (Ben-Akiva and Lerman, 1985). Recently, research on the Cross-Nested logit model (Small, 1987, Vovsha, 1997, Vovsha and Bekhor, 1998, Ben-Akiva and Bierlaire, 1999, Papola, 2000, Bierlaire, 2001, Wen and Koppelman, 2001, Swait, 2001) has extended the number of GEV models used in practice. Also, Daly (2001) and Bierlaire (2002) have proposed new theoretical results providing an operational representation of GEV models.

Mixed or hybrid logit models (Ben-Akiva and Bolduc, 1996,McFadden and Train, 1997,Bhat, 2001,Ben-Akiva et al., 2002) combine different model structures into a richer framework. A Mixed GEV model can be roughly described as a GEV model containing random parameters, which are normally distributed.

The level of sophistication of these models enables to capture a wide range of situations. The price to pay is their rather complicated formulation, and the lack of appropriate estimation procedure. For example, Vovsha (1997) proposes a heuristic procedure for the estimation of Cross-Nested Logit models, which appears not to be valid.

Biogeme (**BI**erlaire's **O**ptimization package for **GE**V **M**odels **E**stimation) is an open source package designed to estimate a wide variety of random utility models, based on state-of-the-art optimization algorithms. The motivation for developing Biogeme is to provide researchers with an appropriate and efficient tool enabling to explore new models, focusing on their specification without worrying about the estimation part. In this paper, we describe the general design of the Biogeme package, and we illustrate the capabilities of Version 0.6.

## 2 Random utility models

A random utility model is designed to forecast the choice of an individual $n$ among a finite and discrete set of alternatives $C_n$. The main assumption is that each individual associates a quantity, called *utility*, to each alternative in $C_n$, and selects the alternative with the highest utility. The utility associated by individual $n$ to alternative $i$, denoted by $U_{in}$ is a random variable such that

$$U_{in} = V_{in} + \varepsilon_{in} \tag{1}$$

where $V_{in} \in \mathbb{R}$ is the deterministic, or systematic, component of the utility, and $\varepsilon_{in}$ is a random term. If $z_{in}$ is a vector of attributes of alternative $i$ for individuals $n$, and $S_n$ is a vector of socio-economical characteristics for individual $n$, we have

$$V_{in} = V_{in}(\beta, z_{in}, S_n), \tag{2}$$

where $\beta$ is a vector of unknown parameters to be estimated. For simplification, it is common practice to merge $z_{in}$ and $S_n$ into a vector of attributes, denoted by $x_{in}$. Therefore, we have a simpler formulation

$$V_{in} = V_{in}(\beta, x_{in}) \tag{3}$$

The probability that individual $n$ selects alternative $i$ is given by

$$P(i|C_n) = P(U_{in} \geq U_{in} \ \ \forall j \in C_N). \tag{4}$$

In order to obtain an operational choice model, specific assumptions must be made about the functional form of $V_{in}$ and the distribution of $\varepsilon_{in}$. We briefly review the assumptions which are relevant for the Biogeme package.

The most common functional form adopted for $V_{in}$ is a linear-in-parameters defintion, that is

$$V_{in} = \sum_j \beta_j x_{inj}. \tag{5}$$

Less common in the literature, nonlinear formulations may also be used. The Box-Tukey transform of attributes is a typical example, that is

$$V_{in} = \sum_j \beta_j \frac{(x_{inj} + \alpha_{inj})^{\lambda_{inj}} - 1}{\lambda_{inj}}. \tag{6}$$

where $x_{inj} + \alpha_{inj}$ must be non negative, $\alpha_{inj}$ and $\lambda_{inj}$ are unknown parameters to be estimated. Box-Tukey transforms allow to capture a wide range of non-linearities. Indeed, in addition to the obvious exponential transformation of the attributes, linear ($\lambda_{inj} = 1$) and logarithm ($\lambda_{inj} = 0$) transformations are interesting special cases.

Before discussing the assumptions about the distribution of $\varepsilon_{in}$, we analyze the mean and the variance of the random variable. The mean can be considered as a specific parameter of the utility function (called *Alternative Specific Constant*), capturing a bias toward that alternative. In that case, $\varepsilon_{in}$ is decomposed into

$$\varepsilon_{in} = \beta_i^0 + \tilde{\varepsilon}_{in} \tag{7}$$

so that the expectation of $\tilde{\varepsilon}_{in}$ can be set to any arbitrary value, typically zero. Therefore, if an alternative specific constant is included in the utility function, the mean can be assumed to be zero without loss of generality.

The case of the variance is discussed by first noting that

$$P(U_{in} \geq U_{in}) = P(\nu U_{in} \geq \nu U_{in}) \quad \forall \nu > 0.$$

Therefore, using $U_{in} = V_{in} + \varepsilon_{in}$ or $\nu U_{in} = \nu V_{in} + \nu \varepsilon_{in}$ yields to the exact same probability model. As

$$\mathrm{Var}(\nu U_{1n}) = \nu^2 \mathrm{Var}(U_{1n}),$$

the choice of $\nu$ determines the variance. Therefore, the variance of the random parameter is directly linked to its scale, and can be arbitrarily imposed. $\nu = 1$ is a typical choice.

The above discussion is valid only for a given individual. It is important to realize that assuming constant mean and variance over the population may be a strong and irrealistic assumption. In most applications, those quantities are different for various groups of the population. The variations of the mean across the population are captured by dummy parameters associated with socio-economic characteristics. Variations of the variance (or, equivalently, of the scale parameter $\nu$) are more complicated to capture, as they introduce a nonlinearity in the utility function. If we consider a heterogeneous population composed of identified groups, the utility of each group is scaled by a different factor. In that case, if individual $n$ belongs to group $g_n$, we generalize (5) as

$$V_{in} = \nu_{g_n} \sum_j \beta_j x_{inj}. \tag{8}$$

and (6) as

$$V_{in} = \nu_{g_n} \sum_j \beta_j \frac{(x_{inj} + \alpha_{inj})^{\lambda_{inj}} - 1}{\lambda_{inj}}, \tag{9}$$

where $\nu_{g_n}$ is the unknown scale parameter associated with group $g_n$, to be estimated. A typical example is when Revealed Preference (RP) data are combined with Stated Prefenrece (SP) data (Ben-Akiva et al., 1994,Ben-Akiva and Morikawa, 1990). Note that (5), (6) and (8) are special cases of (9), where some parameters are set to fixed values. Whatever the assumptions about the distribution of $\varepsilon_{in}$, Biogeme allows to estimate parameters $\beta$, $\lambda$, $\alpha$ and $\nu$ in (9) from the data, if they are identifiable.

In the literature, there are typically two families of models, based on two types of assumptions about the error term $\varepsilon_{in}$. The *Probit* family assumes that $\varepsilon_{in}$ captures the sum of many independent sources of errors, and invokes the central-limit theorem to assume that $\varepsilon_{in}$ follows a normal distribution. The *Generalized Extreme Value* (GEV) family, assumes that $\varepsilon_{in}$ captures the largest of many independent sources of errors and, consequently, has an Extreme Value distribution (Gumbel, 1958).

The Generalized Extreme Value (GEV) model has been derived from the random utility paradigm by McFadden (1978). This general model consists of a large family of models that include the Multinomial Logit, the Nested Logit and the Cross-Nested Logit models. The probability of choosing alternative $i$ within the choice set $C$ of a given choice maker is

$$P(i|C) = \frac{y_i \frac{\partial G}{\partial y_i}(y_1,\ldots,y_J)}{\mu G(y_1,\ldots,y_J)} \tag{10}$$

where $J$ is the number of available alternatives, $y_i = e^{V_i}$, $V_i$ is the deterministic part of the utility function associated to alternative $i$, and $G$ is a $\mu$-GEV function. A $\mu$-GEV function is a differentiable function defined on $\mathbb{R}^J_+$ with the following properties:

1. $G(y) \geq 0$ for all $y \in \mathbb{R}^J_+$,
2. $G$ is homogeneous of degree $\mu > 0$, that is $G(\lambda y) = \lambda^\mu G(y)$, for $\lambda > 0$,
3. $\lim_{y_i \to +\infty} G(y_1,\ldots,y_i,\ldots,y_J) = +\infty$, for each $i = 1,\ldots,J$,
4. the $k$th partial derivative with respect to $k$ distinct $y_i$ is non-negative if $k$ is odd and non-positive if $k$ is even that is, for any distinct indices $i_1,\ldots,i_k \in \{1,\ldots,J\}$, we have

$$(-1)^k \frac{\partial^k G}{\partial x_{i_1}\ldots\partial x_{i_k}}(x) \leq 0, \ \forall x \in \mathbb{R}^J_+. \tag{11}$$

Although this condition is never stated in the literature, it is also required that $G(x) \neq 0$.

The homogeneity of $G$ and Euler's theorem give

$$P(i|C) = \frac{e^{V_i + \ln G_i(\ldots)}}{\sum_{j=1}^{J} e^{V_j + \ln G_j(\ldots)}}, \tag{12}$$

where $G_i = \frac{\partial G}{\partial y_i}$. This is equivalent to assume that the joint distribution of the error terms $\varepsilon_1, \ldots, \varepsilon_J$ is

$$F(\varepsilon_1, \ldots, \varepsilon_J) = e^{-G(e^{-\varepsilon_1}, \ldots, e^{-\varepsilon_J})} \tag{13}$$

The Multinomial Logit (MNL) model is a member of this model family with

$$G(y) = \sum_{i=1}^{J} y_i^{\mu}. \tag{14}$$

where $\mu > 0$. The Nested Logit (NL) model is also a member of the GEV family. Contrarily to the MNL, the NL includes $M + 1$ parameters, where $M$ is the number of nests. The generating function is

$$G(y; \mu_1, \ldots, \mu_M) = \sum_{m=1}^{M} \left( \sum_{i \in C_m} y_i^{\mu_m} \right)^{\frac{\mu}{\mu_m}} \tag{15}$$

where $C_m$ is the set of alternatives belonging to nest $m$. It complies with the GEV conditions if $\mu_m \geq \mu > 0$, for all $m$.

The Cross-Nested Logit (CNL) model is also a member of the GEV family. Several formulations have been proposed in the literature (Small, 1987, Vovsha, 1997, Ben-Akiva and Bierlaire, 1999, Papola, 2000, Wen and Koppelman, 2001). They are all based on the same formulation, and vary with regard to the parameters that are kept fixed. A detailed analysis of this model, including the elasticities, have been recently proposed by Wen and Koppelman (2001). However, they call it the *generalized nested logit*. The generating function proposed by Ben-Akiva and Bierlaire (1999), with $M(J + 1) + 1$ parameters, where $M$ is the number of nests, is given by

$$G\left(y; \mu_1, \ldots, \mu_M, (\alpha_{jm})_{j=1,\ldots,J}^{m=1,\ldots,M}\right) = \sum_{m=1}^{M} \left( \sum_{j=1}^{J} \alpha_{jm} y_j^{\mu_m} \right)^{\frac{\mu}{\mu_m}}. \tag{16}$$

Bierlaire (2001) has shown that the following conditions are sufficient for (16) to comply with the GEV conditions:

1. $\mu_m \geq \mu > 0$, $m = 1, \ldots, M$,

2. $\alpha_{jm} \geq 0$, $j = 1, \ldots, J$, $m = 1, \ldots, M$,

3. $\sum_m \alpha_{jm} > 0$, $j = 1, \ldots, J$.

The Network GEV (NGEV) model, proposed by Bierlaire (2002), and based on a model formulation by Daly (2001), is a general representation of GEV models, based on a network structure. A parameter is associated with each node and each arc of this network. We refer the reader to Bierlaire (2002) for more details.

Thanks to Denis Bolduc, Biogeme v0.6 is also able to estimate Logit Kernel models with error components. A Logit-Kernel model is such that the utility function of an alternative is

$$U_i = V_i + \sum_{j=1}^{p} \sigma_j \nu_j + \varepsilon_i \tag{17}$$

where $\sigma_j$ are unknown parameters to be estimated, and $\nu_j$ are normal random variables $N(0,1)$.

In the rest of the paper, we denote by $\beta$ the unknown parameters associated with the utility function (that is, parameters $\beta$, $\lambda$, $\alpha$ and $\nu$ in (9)), and by $\gamma$ the unknown parameters associated with a specific GEV model (that is, parameters $\mu_m$ in the NL, CNL and NGEV models, and parameters $\alpha_{im}$ in the CNL and NGEV models).

# 3 Maximum likelihood estimation

The estimation of unknown parameters by maximum likelihood is a standard technique. An observation $k$ consists in a set of values for the set of attributes $x_{in}$, denoted $x_{in}^k$, and an observed choice. The attributes are associated both with the individual $n$ and the alternative $i$. The probability for the model to reproduce the observed choice is given by $P_{in}^k(\beta,\gamma) = P_{in}(\beta,\gamma,x_{in}^k)$, where $P_{in}$ is the probability function corresponding to the model under consideration (like (10) for the GEV model). If a sample of $K$ observations is available, the probability for the model to reproduce the whole sample is called the *likelihood*, and is given by

$$\mathcal{L}^*(\beta,\gamma) = \prod_{k=1}^{K} P_{in}^k(\beta,\gamma). \tag{18}$$

The maximum likelihood estimators $\hat{\beta}$ and $\hat{\gamma}$ are given by

$$(\hat{\beta}, \hat{\gamma}) = \operatorname{argmax}_{\beta,\gamma} \mathcal{L}(\beta, \gamma), \tag{19}$$

where

$$\mathcal{L}(\beta, \gamma) = \ln \mathcal{L}^*(\beta, \gamma) = \sum_{k=1}^{K} \ln P_{in}^k(\beta, \gamma) \tag{20}$$

is the log-likelihood function. In some cases, the observations are weighted in order to adjust their relative importance in the sample according to their relative importance in the population. In that case, a weight $\omega_k$ is associated with each observation, and the log-likelihood function is then

$$\mathcal{L}(\beta, \gamma) = \sum_{k=1}^{K} \omega_k \ln P_{in}^k(\beta, \gamma) \tag{21}$$

Problem (19) is a nonlinear programming problem, usually non concave. Moreover, it is sometimes necessary (and most of the time useful) to impose constraints on $\beta$ and $\gamma$. For example, the condition $\mu_m \geq \mu$ is necessary for the validity of the NL and CNL models. Also, normalisation conditions may be imposed on the parameters. Note that Biogeme allows to impose bound constraints, linear equality and inequality constraints, and nonlinear equality constraints on the parameters.

Biogeme contains three different optimization algorithms. CFSQP is a C implementation of the FSQP optimization algorithm developed by E.R. Panier, A.L. Tits, J.L. Zhou, and C.T. Lawrence (see Lawrence et al., 1997). SolvOpt (Solver for local optimization problems) by Kuntsevich and Kappel (1997) implements a version of a minimization method with space dilation by Shor (1985). And DONLP2 is a sequential equality constrained quadratic programming method, developed by Spellucci (n.d.). The algorithm is described by Spellucci (1998a) and Spellucci (1998b).

All those algorithms identify a local optimum of (19). In the (rare) cases where the objective function is concave, and the constraints are convex, the local optimum is also global.

## 3.1 Comparison

We provide in Table 1 a comparison of the final log-likelihood for the models available on the website, and the time it took to estimate them with CFSQP, DONLP2 and SOLVOPT on a Dell Inspiron 8200 running Linux RedHat 7.3. Entries with **** correspond to failure of convergence of the algorithm. The examples are describe in Bierlaire (2003). We provide here some comments about the results.

- CFSQP is most of the time the fastest algorithm, followed by DONLP2 and finally by SOLVOPT, the slowest of the three.
- Biogeme may be significantly slower for general NGEV, as it does not exploit the special structure of the model.
- On the difficult problem number 10, CFSQP was much slower than DONLP2 with the CNL version (`EX10`), and did not even converge after 1000 iterations on the NGEV version (`NGEV10`).
- For Logit Kernel models (examples `EX13` to `EX18`) the final log-likelihood may vary from one estimation to the next, as the normally distributed random variables are simulated based on a Monte-Carlo procedure.

# 4 Biogeme Packages

BIOGEME is a freeware designed for the development of research in the context of discrete choice models in general, and of GEV models in particular. All information relative to BIOGEME is maintained at

`http://roso.epfl.ch/biogeme`

where a detailed tutorial is available (Bierlaire, 2003). We cite here the main features of the packages.

BIOGEME has been developed on Linux, but a Windows version is available. With the distribution of Biogeme, there are two additional utilities. Bioroute helps preparing the input files for Biogeme in the context of a route choice analysis, and Biosim is designed to perform simulations with a given model. Biogeme is invoked by the following command

```
biogeme model_name sample_file
```

If the name of the model is `mymodel`, say, Biogeme reads the following files:

- a file containing the parameters controlling the behavior of Biogeme: `mymodel.par`,
- a file containing the model specification: `mymodel.mod`,
- a file containing the data: `sample.dat`,

and generates the following output files:

- a file reporting the results of the estimation: `mymodel.rep`,
- the same file in HTML format: `mymodel.html`,
- a file containing the specification of the estimated model, in the same format as the model specification file: `mymodel.res`,
- a file containing some statistics on the data: `mymodel.sta`.

For most users, the parameter file is edited only to select a specific optimization algorithm. The data file contains in its first line a list of labels corresponding to the available data, and that each subsequent line contains the exact same number of numerical data, each row corresponding to an observation. The model specification file is based on a syntax designed to define a wide range of models, with several sections. We enumerate here the most important sections.

**Section [Beta ]** Each line of this section corresponds to a parameter $\beta$ in (9). Five entries must be provided for each parameter: its name, a default value, a lower bound and an upper bounds on the valid values and a binary status, specifying if the value of the parameter must be estimated or kept at its default value. Note that this section is independent of the specific model to be estimated, as it captures only the deterministic part of the utility function. Here is an example.

```
[Beta]
// Name Value        LowerBound    UpperBound     status
ASC1    -5.22e-02       -1.0          1.0           0
ASC2          0.0       -1.0          1.0           1
ASC3    -4.06e-01       -1.0          1.0           0
ASC4          0.0       -1.0          1.0           1
BETA1   -2.06e-02       -1.0          1.0           0
BETA2   -2.19e-02       -1.0          1.0           0
```

**Section [Utilities ]** For each alternative in the model, the following information must be provided in this section: the numerical identifier of the alternative, the name of the alternative, the availability condition and the linear-in-parameter utility function. For example,

```
[Utilities]
//Id Name  Avail linear-in-parameter expression
 100 Alt1 avail1 BETA_COST * COST1 + BETA_TIME * TIME1 + ASC1 * one
 200 Alt2 avail2 BETA_COST * COST2 + BETA_TIME * TIME2 + ASC2 * one
 300 Alt3 avail3 BETA_COST * COST3 + BETA_TIME * TIME3 + ASC3 * one
 400 Alt4 avail4 BETA_COST * COST4 + BETA_TIME * TIME4
```

where lines starting by `//` are ignored by Biogeme and used for comments.

**Section [Box-Cox ]** Each line of this section corresponds to a parameter $\lambda$ in (9). The following entries must be provided: the name of the attribute $x_{inj}$, a default value, a lower bound and an upper bounds on the valid values and a binary status, specifying if the value of the parameter must be estimated or kept at its default value.

**Section [Box-Tukey ]** Each line of this section corresponds to a parameter $\alpha$ in (9). The following entries must be provided: the name of the attribute $x_{inj}$, a default value, a lower bound and an upper bounds on the valid values and a binary status, specifying if the value of the parameter must be estimated or kept at its default value.

**Section [Expressions ]** In this section are defined all expressions appearing either in the availability conditions or in the utility functions of the alternatives. If the expression is readily available from the data file, it can be omitted in the list. It is especially useful to tests alternative model specifications (like nonlinear effects) without modifying the data file.

**Section [Choice ]** The user provides here the formula to compute the identifier of the chosen alternative in the data file. Typically, a "`choice`" entry will be available directly in the file, but any formula can be used to compute it.

**Section [Weight ]** The user provides here the formula to compute the weights $\omega_k$ in (21). Ideally, the sum of the weights should be equal to the total number of observations, although it is not required.

**Section [Group ]** The user provides here the formula to compute the group ID of the observed individual. Typically, a "`group`" entry will be available directly from the data file, but any formula can be used to compute it. A different scale parameter $\mu_{g_n}$ will be estimated for each group.

**Section [Scale ]** Each line of this section corresponds to a parameter $\nu_{g_n}$ in (9), one per group. The following entries must be provided: the group number, a default value, a lower bound and an upper bound on the valid values and a binary status, specifying if the value of the parameter must be estimated or kept at its default value.

**Section [Model ]** Selects the GEV model. Valid entries are `$MNL` for Multinomial Logit model, `$NL` for single level Nested Logit model, `$CNL` for Cross-Nested Logit model (in the sense described in Ben-Akiva and Bierlaire (1999)), `$NGEV` for Network GEV model, and `$LK` for Logit Kernel model.

**Section [NLNests ]** This section is relevant only if the `$NL` option has been selected. Each row of this section corresponds to a nest. The following entries are required: the nest name, a default value, a lower bound and an upper bound on the valid values of the nest parameter $\mu_m$, and a binary status, specifying if the value of the parameter must be estimated or kept at its default value. And finally, the list of alternatives belonging to the nest. Similar sections must be defined if a CNL or a NGEV model are to be estimated.

**Section [ConstraintNestCoef ]** In this section, the user can constraint nests parameters to be equal, with the following syntax.

```
NEST_A = NEST_B
```

**Section [ConstantProduct ]** In this section, the user may constrain the product of two coefficients to a given value. The syntax for the constraint $\beta_1\beta_2 = 3.1415$ is

```
[ConstantProduct]
  BETA1    BETA2  3.1415
```

**Section [Ratios ]** The user defines here the ratio of parameters that must be computed. Typically, the value of time is the ratio for the time paraeter by the cost parameter.

**Section [LinearConstraints ]** In this section, the user can define a list of linear constraints, in one of the following syntaxes:

1. Formula = number,
2. Formula $\leq$ number,
3. Formula $\geq$ number.

For example, the constraint

$$\sum_i \mathrm{ASC}_i = 0.0$$

is written

```
ASC1 + ASC2 + ASC3 + ASC4 + ASC5 + ASC6 = 0.0
```

and the constraint

$$\mu \leq \mu_j$$

is written

```
MU - MUJ <= 0.0
```

or

```
MUJ - MU >= 0.0
```

**Section [NonLinearEqualityConstraints ]** In this section, the user can define a list of nonlinear equality constraints of the form

$$h(x) = 0.0.$$

The section must contain a list of functions $h(x)$. For example, the constraint

$$\alpha_{a1}^{\mu_a} + \alpha_{b1}^{\mu_b} = 1$$

is written

```
[NonLinearEqualityConstraints]
ALPHA_A1 ^ MU_A  + ALPHA_B1 ^ MU_B - 1.0
```

**Section [LogitKernelSigmas ]** Each line of this section corresponds to a $\sigma$ parameter associated with the normal terms in the utility functions for the Logit Kernel (17). Note that the sign of the parameter is meaningless, so it is good practice to specify symmetric bounds (that is, lower bound is the opposite of the upper bound).

**Section [LogitKernelFactors ]** This section defines the factors of the Logit Kernel model. For each factor, the name of the associated parameter and the ID of the associated alternative must be specified.

The report file (`mymodel.rep`) contains the results of the maximum likelihood estimation of the model.

- The estimated value of the $\beta$ parameters, with the associated standard error and the $t$-test. A star (`*`) is appended if the $t$-test fails, according to a threshold specified by the use in the parameter file (default threshold: 1.96).
- The estimated value of the $\mu$ parameter, with the associated standard error and the $t$-test.
- The estimated value of the GEV model parameters, with the associated standard error and the $t$-test. Note that the $t$-test is computed to compare the estimated value both to 0 and 1.
- The estimated value of the scale parameters, with the associated standard error and the $t$-test. Note that the $t$-test is computed to compare the estimated value to 1.
- A covariance/correlation analysis of pairs of estimated $\beta$ parameters, sorted according to the $t$-test value.

A list of examples is available from the BIOGEME webpage, and are commented in Bierlaire (2003).

The package Biosim is invoked exactly like Biogeme, with the exact same input file. But instead of performing a parameter estimation, it uses the default value for each parameter, performs a sample enumeration and produces a Gnuplot file allowing for a graphical display of the model sensitivity. The output file `mymodel.enu` contains the result of the sample enumeration. For each observation in the sample, the following results are provided:

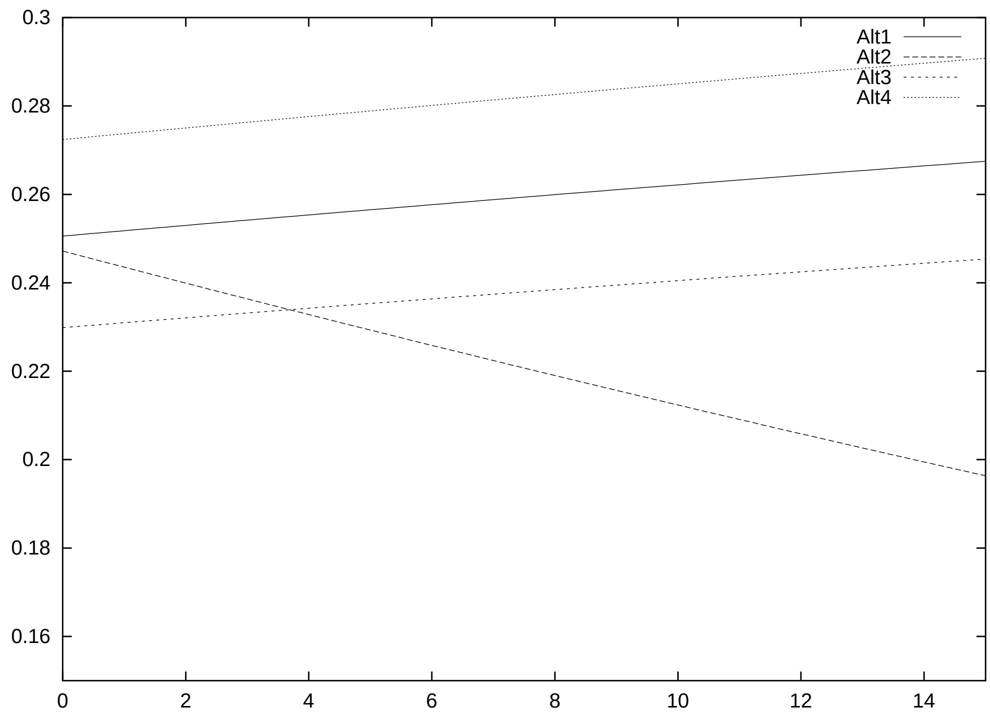


Figure 1: Example of a Gnuplot output

1. The choice actually reported in the sample file;
2. The probability given by the model for the chosen alternative;
3. For each alternative, the probability given by the model;
4. A list of simulated choice, based on random draws using the model.

The file `mymodel.gp` is an input file for the Gnuplot. It allows to graphically analyze the sensitivity of the model to modifications of one attribute (see, for instance, Figure 1).

Finally, the package Bioroute is used in the context of route choice analysis. Indeed, the explicit enumeration of paths may be cumbersome when specifying route choice models. Moreover, computing the size of the paths for Path-Size models (Ben-Akiva and Bierlaire, 1999, Ramming, 2001) or the cross-nested coefficients for the link-nested logit model (Vovsha and Bekhor, 1998) is tedious and subject to errors. The utility `BioRoute` is designed to help the analyst. Bioroute takes as input a full description of the network, and prepares the files needed by

Biogeme, that is the model specification file and the sample file. After Bioroute has been used, it is important to edit the generated specification file.

# 5 Future developments

Biogeme is in continuous developement. Biogeme 0.7 will be able to estimate general nonlinear utility functions, and *Mixed GEV models*. Mixed GEV models are a generalization of Mixed Logit models, also called Hybrid Loigt or Logit Kernel models (see McFadden and Train, 1997, Ben-Akiva et al., 2001, Bhat, 2001, Ben-Akiva et al., 2002). This is a major step that will allows a vast variety of models to be estimated, including the heteroscedastic model, the factor analytic with fixed loadings, the error component formulation and the general autoregressive process (see Ben-Akiva and Bierlaire, 1999, Walker, 2001 and Ben-Akiva et al., 2001). All these efforts are motivated by the same objective: provide researchers and practitionners with flexible tools to investigate a wide range of discrete choice models.

# 6 Appendix: derivatives

In addition to the programming burden, a major effort in developping packages for model estimation is the computation of the derivatives required by the optimization packages. We provide in this appendix the derivatives used in Biogeme for log-likelihood estimation of Multinomial, Nested and Cross-Nested logit models.

The log-likelihood function is defined by (21). The derivatives are trivially defined as

$$\frac{\partial \mathcal{L}}{\beta} = \sum_{k=1}^{K} \frac{\partial \ln P^k_{in}(\beta,\gamma)}{\partial \beta} \tag{22}$$

and

$$\frac{\partial \mathcal{L}}{\gamma} = \sum_{k=1}^{K} \frac{\partial \ln P^k_{in}(\beta,\gamma)}{\partial \gamma}. \tag{23}$$

Denoting by $i$ the chosen alternative, $V$ the $J$ utilities, $\gamma$ the $\ell$ model parameters, and $\nu$ the scale parameter, we have

$$P(i, V_1, \ldots, V_J, \gamma_1, \ldots, \gamma_\ell, \nu, \mu) = \frac{e^{\nu V_i + \ln G_i(e^{\nu V_1}, \ldots, e^{\nu V_J}, \gamma_1, \ldots, \gamma_\ell, \mu)}}{\sum_j e^{\nu V_j + \ln G_j(e^{\nu V_1}, \ldots, e^{\nu V_J}, \gamma_1, \ldots, \gamma_\ell, \mu)}}$$

and

$$
\begin{aligned}
\ln P(i, V_1, \ldots, V_J, \gamma_1, \ldots, \gamma_\ell, \nu, \mu) &= \nu V_i \\
&+ \ln G_i(e^{\nu V_1}, \ldots, e^{\nu V_J}, \gamma_1, \ldots, \gamma_\ell, \mu) \\
&- \ln \left( \sum_j e^{\nu V_j} G_j(e^{\nu V_1}, \ldots, e^{\nu V_J}, \gamma_1, \ldots, \gamma_\ell, \mu) \right).
\end{aligned}
$$

The derivatives with respect to $\beta_k$ are given by

$$
\frac{\partial}{\partial \beta_k} \ln P = \nu \frac{\partial V_i}{\partial \beta_k} + \frac{1}{G_i} \sum_{j=1}^{J} \frac{\partial G_i}{\partial x_j} e^{\nu V_j} \nu \frac{\partial V_j}{\partial \beta_k} - \frac{1}{\Delta} \sum_j e^{\nu V_j} \left( \nu \frac{\partial V_j}{\partial \beta_k} G_j + \sum_{n=1}^{J} \frac{\partial G_j}{\partial x_n} e^{\nu V_n} \nu \frac{\partial V_n}{\partial \beta_k} \right)
$$

where

$$
\Delta = \sum_j e^{\nu V_j} G_j.
$$

Note that we do not assume here that the $V_j$ are linear-in-parameters, so that $\partial V_j / \partial \beta_k$ may be not trivial.

The derivatives with respect to the model parameters $\gamma_k$ are given by

$$
\frac{\partial}{\partial \gamma_k} \ln P = \frac{1}{G_i} \frac{\partial G_i}{\partial \gamma_k} - \frac{1}{\Delta} \sum_j e^{\nu V_j} \frac{\partial G_j}{\partial \gamma_k}.
$$

The derivative with respect to the homogeneity parameter $\mu$ is given by

$$
\frac{\partial}{\partial \mu} \ln P = \frac{1}{G_i} \frac{\partial G_i}{\partial \mu} - \frac{1}{\Delta} \sum_j e^{\nu V_j} \frac{\partial G_j}{\partial \mu}
$$

In general, the parameter $\mu$ is constraint to 1. However, Biogeme allows to estimate it if the user desires to do so. Therefore, the derivatives are necessary.

The derivative with respect to the scale parameter $\nu$ is given by

$$
\frac{\partial}{\partial \nu} \ln P = V_i + \frac{1}{G_i} \frac{\partial G_i}{\partial \nu} - \frac{1}{\Delta} \frac{\partial \Delta}{\partial \nu}
$$

where

$$
\frac{\partial G_i}{\partial \nu} = \sum_j V_j e^{\nu V_j} \frac{\partial G_i}{\partial x_j}
$$

and

$$
\frac{\partial \Delta}{\partial \nu} = \sum_j \left( V_j e^{\nu V_j} G_j + e^{\nu V_j} \frac{\partial G_j}{\partial \nu} \right).
$$

The GEV generating function for the MNL model is given by (14). We have

$$
\frac{\partial G}{\partial y_i} = G_i = \mu y_i^{\mu - 1},
$$

and

$$\frac{\partial G}{\partial \mu} = \sum_{i=1}^{n} y_i^{\mu} \ln(y_i).$$

The second derivatives are

$$\frac{\partial^2 G}{\partial y_i \partial y_j} = \begin{cases} \mu(\mu-1) y_i^{\mu-2} & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$

and

$$\frac{\partial^2 G}{\partial x_i \partial \mu} = (\mu \ln x_i + 1) x_i^{\mu-1}.$$

The GEV generating function for the NL model is given by (15). We have

$$\frac{\partial G}{\partial y_i} = \mu y_i^{\mu_{m_i}-1} \left( \sum_{j \in C_{m_i}} y_j^{\mu_{m_i}} \right)^{(\frac{\mu}{\mu_{m_i}}-1)}$$

where $m_i$ is the (unique) nest containing alternative $i$, and

$$\frac{\partial G}{\partial \mu} = \sum_{m=1}^{M} \frac{1}{\mu_m} \left( \sum_{i \in C_m} y_i^{\mu_m} \right)^{\frac{\mu}{\mu_m}} \ln \left( \sum_{i \in C_m} y_i^{\mu_m} \right).$$

The partial derivative with respect to one structural parameter $\mu_m$ is

$$\frac{\partial G}{\partial \mu_m} = \frac{\mu}{\mu_m} (\sum_{i \in C_m} y_i^{\mu_m})^{\frac{\mu}{\mu_m}-1} (\sum_{i \in C_m} y_i^{\mu_m} \ln(y_i)) - \frac{\mu}{\mu_m^2} (\sum_{i \in C_m} y_i^{\mu_m})^{\frac{\mu}{\mu_m}} \ln(\sum_{i \in C_m} y_i^{\mu_m}).$$

We have now the second partial derivative with respect to two variables $i$ and $j$. If $i = j$, we have

$$\frac{\partial^2 G}{\partial y_i^2} = \frac{\partial G_i}{\partial y_i} = \mu(\mu_m - 1) y_i^{(\mu_m-2)} (\sum_{i \in C_m} y_i^{\mu_m})^{(\frac{\mu}{\mu_m}-1)} + \mu(\mu - \mu_m) y_i^{(2\mu_m-2)} (\sum_{i \in C_m} y_i^{\mu_m})^{(\frac{\mu}{\mu_m}-2)}$$

If $i \neq j$ and $i, j \in C_m$, we have

$$\frac{\partial^2 G}{\partial y_i \partial y_j} = \frac{\partial G_i}{\partial y_j} = \mu(\mu - \mu_m) y_i^{\mu_m-1} y_j^{\mu_m-1} (\sum_{i \in C_m} y_i^{\mu_m})^{(\frac{\mu}{\mu_m}-2)}$$

If $i \in C_m$ and $j \notin C_m$, we have

$$\frac{\partial^2 G}{\partial y_i \partial y_j} = \frac{\partial G_i}{\partial y_j} = 0$$

The second partial derivative with respect to one variable and $\mu$ is given by

$$\frac{\partial^2 G}{\partial y_i \partial \mu} = \frac{\partial G_i}{\partial \mu} = y_i^{\mu_m - 1} (\sum_{i \in C_m} y_i^{\mu_m})^{\frac{\mu}{\mu_m} - 1} \left( 1 + \frac{\mu}{\mu_m} \ln (\sum_{i \in C_m} y_i^{\mu_m}) \right)$$

We have now the second partial derivative with respect to one structural parameter $\mu_m$ and one variable $y_i$. If $i \in C_m$, we have

$$\frac{\partial^2 G}{\partial y_i \partial \mu_m} = \frac{\partial G_i}{\partial \mu_m} = \mu \Gamma_m^{\frac{\mu}{\mu_m} - 1} y_i^{\mu_m - 1} \ln y_i + \mu y_i^{\mu_m - 1} \Gamma_m^{\frac{\mu}{\mu_m} - 1} \left( \frac{\frac{\mu}{\mu_m} - 1}{\Gamma_m} \sum_j y_j^{\mu_m} \ln y_j - \frac{\mu}{\mu_m^2} \ln \Gamma_m \right),$$

where

$$\Gamma_m = \sum_{j \in C_m} y_j^{\mu_m}.$$

If $i \notin C_m$ we have

$$\frac{\partial^2 G}{\partial y_i \partial \mu_m} = \frac{\partial G_i}{\partial \mu_m} = 0.$$

The GEV generating function for the CNL model is given by (16). We have

$$G_i = \frac{\partial G}{\partial y_i} = \mu \sum_m \alpha_{im} y_i^{\mu_m - 1} \left( \sum_j \alpha_{jm} y_j^{\mu_m} \right)^{\frac{\mu}{\mu_m} - 1}.$$

The partial derivative with respect to $\mu$, the homogeneity factor is

$$\frac{\partial G}{\partial \mu} = \sum_m \frac{1}{\mu_m} \Gamma_m^{\frac{\mu}{\mu_m}} \ln(\Gamma_m)$$

where

$$\Gamma_m = \sum_{j \in C_m} \alpha_{jm} y_j^{\mu_m}. \tag{24}$$

The partial derivative with respect to one nest parameter $\mu_m$ is

$$\frac{\partial G}{\partial \mu_m} = \frac{\mu}{\mu_m} \Gamma_m^{\frac{\mu}{\mu_m} - 1} \left( \sum_{j \in C_m} \alpha_{jm} y_j^{\mu_m} \ln(y_j) \right) - \frac{\mu}{\mu_m^2} \Gamma_m^{\frac{\mu}{\mu_m}} \ln(\Gamma_m)$$

and with respect $\alpha_{im}$ is

$$\frac{\partial G}{\partial \alpha_{im}} = \frac{\mu}{\mu_m} \Gamma_m^{\frac{\mu}{\mu_m} - 1} y_i^{\mu_k}$$

where $\Gamma_m$ is defined by (24). We write now the second partial derivative with respect to two variables $y_i$ and $y_j$. If $i = j$, we have

$$\frac{\partial^2 G}{\partial y_i^2} = \frac{\partial G_i}{\partial y_i} = \sum_m \frac{\mu}{\mu_m} \Gamma_m^{\frac{\mu}{\mu_m} - 2} \alpha_{im} \mu_m y_i^{\mu_m - 2} ((\frac{\mu}{\mu_m} - 1) \alpha_{im} \mu_m y_i^{\mu_m} + \Gamma_m (\mu_m - 1))$$

and if $i \neq j$, we have

$$\frac{\partial^2 G}{\partial y_i \partial y_j} = \frac{\partial G_i}{\partial y_j} = \sum_m \mu_m \mu(\frac{\mu}{\mu_m} - 1)\alpha_{im}\alpha_{jm}\Gamma_m^{\frac{\mu}{\mu_m}-2} y_i^{\mu_m - 1} y_j^{\mu_m - 1}$$

where

$$\Gamma_m = \sum_{j \in C_m} \alpha_{jm} y_j^{\mu_m}.$$

The second partial derivative with respect to one variable $y_i$ and $\mu$ is

$$\frac{\partial^2 G}{\partial y_i \partial \mu} = \frac{\partial G_i}{\partial \mu} = \sum_m \Gamma_m^{\frac{\mu}{\mu_m}-1} \alpha_{im} y_i^{\mu_m - 1}(1 + \frac{\mu}{\mu_m}\ln(\Gamma_m))$$

where $\Gamma_m$ is defined by (24). The second partial derivative with respect to one nest parameter $\mu_m$ and one variable $y_i$ is

$$\begin{aligned}
\frac{\partial^2 G}{\partial y_i \partial \mu_m} = \frac{\partial G_i}{\partial \mu_m} = & - \frac{\mu}{\mu_m}\Gamma_m^{\frac{\mu}{\mu_m}-1} \alpha_{im} y_i^{\mu_m - 1} \\
& - \frac{\mu^2}{\mu_m^2}\Gamma_m^{\frac{\mu}{\mu_m}-1} \ln(\Gamma_m)\alpha_{im} y_i^{\mu_m - 1} \\
& + \frac{\mu}{\mu_m}\Gamma_m^{\frac{\mu}{\mu_m}-1} \alpha_{im} y_i^{\mu_m - 1} \\
& + \mu\Gamma_m^{\frac{\mu}{\mu_m}-1} \alpha_{im} y_i^{\mu_m - 1} \ln(y_i),
\end{aligned}$$

and the second partial derivative with respect to $\alpha_{jk}$ and one variable $y_i$ is

$$\frac{\partial^2 G}{\partial y_i \partial \alpha_{ik}} = \mu y_i^{\mu_k - 1} \Gamma_k^{\frac{\mu}{\mu_k}-1} \left(1 + \alpha_{ik}(\frac{\mu}{\mu_k} - 1)\Gamma_k^{-1} y_i^{\mu_k}\right)$$

and, if $i \neq j$,

$$\frac{\partial^2 G}{\partial y_i \partial \alpha_{jk}} = \mu \alpha_{ik} y_i^{\mu_k - 1}(\frac{\mu}{\mu_k} - 1)\Gamma_k^{\frac{\mu}{\mu_k}-2} y_j^{\mu_k}$$

where $\Gamma_m$ is defined by (24).

Finally, we provide the derivatives of (9) with respect to the parameters. As the scale parameter $\nu$ has already been addressed above, we consider here

$$V(\beta, \lambda, \alpha) = \beta\frac{(x + \alpha)^\lambda - 1}{\lambda}$$

where the indices have been dropped for clarity. We have also

$$\lim_{\lambda \to 0} V(\beta, \lambda, \alpha) = \beta \ln(x + \alpha).$$

The derivatives are

$$\frac{\partial V}{\partial \beta} = \frac{(x+\alpha)^{\lambda} - 1}{\lambda},$$

$$\frac{\partial V}{\partial \lambda} = \frac{\beta}{\lambda^2} \left(1 + (x+\alpha)^{\lambda}(\lambda \ln(x+\alpha) - 1)\right),$$

$$\lim_{\lambda \to 0} \frac{\partial V}{\partial \lambda} = \frac{\beta}{2} \ln^2(x+\alpha)$$

and

$$\frac{\partial V}{\partial \alpha} = \beta(x+\alpha)^{\lambda-1}.$$

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| Example | $\mathcal{L}^*$ | Time CFSQP | Time DONLP2 | Time SOLVOPT |
|---|---|---|---|---|
| EX00 | -1582.56 | 00:00:01 | 00:00:03 | 00:00:08 |
| NGEV00 | -1582.56 | 00:00:20 | 00:00:25 | 00:01:58 |
| EX01 | -1582.56 | 00:00:01 | 00:00:02 | 00:00:08 |
| NGEV01 | -1582.56 | 00:00:20 | 00:00:27 | 00:01:54 |
| EX02 | -1582.56 | 00:00:02 | 00:00:02 | 00:00:09 |
| NGEV02 | -1582.56 | 00:00:20 | 00:00:27 | 00:02:03 |
| EX03 | -1578.25 | 00:00:02 | 00:00:02 | 00:00:15 |
| NGEV03 | -1578.25 | 00:00:22 | 00:00:26 | 00:03:31 |
| EX04 | -1587.30 | 00:00:02 | 00:00:02 | 00:00:18 |
| NGEV04 | -1587.30 | 00:00:22 | 00:00:26 | 00:03:59 |
| EX05 | -1586.09 | 00:00:03 | 00:00:03 | 00:00:09 |
| NGEV05 | -1586.09 | 00:00:57 | 00:01:07 | 00:03:30 |
| EX06 | -691.937 | 00:00:05 | 00:00:06 | 00:00:16 |
| NGEV06 | -691.937 | 00:01:22 | 00:01:39 | 00:03:37 |
| EX07 | -690.833 | 00:00:07 | 00:00:11 | 00:00:20 |
| NGEV07 | -690.833 | 00:01:29 | 00:03:21 | 00:03:51 |
| EX08 | -688.665 | 00:00:07 | 00:00:08 | 00:00:48 |
| NGEV08 | -688.665 | 00:01:23 | 00:03:30 | 00:10:55 |
| EX09 | -691.21 | 00:00:10 | 00:00:13 | 00:01:07 |
| NGEV09 | -691.21 | 00:02:18 | 00:03:08 | 00:11:57 |
| EX10 | -658.205 | 00:23:42 | 00:03:23 | **** |
| NGEV10 | -658.205 | **** | 00:10:21 | |
| EX11 | -691.935 | 00:00:53 | 00:01:05 | 00:15:23 |
| NGEV11 | -691.935 | 00:09:07 | 00:14:43 | |
| EX12 | -662.619 | 00:00:10 | 00:01:36 | 00:30:22 |
| NGEV12 | -662.619 | 00:05:03 | 00:07:36 | |
| EX13 | -652.219 | 00:02:55 | 00:05:03 | 00:09:19 |
| EX14 | -676.072 | 00:03:25 | 00:05:49 | 00:11:53 |
| EX15 | -655.517 | 00:04:26 | 00:06:32 | 00:12:47 |
| EX16 | -657.651 | 00:05:00 | 00:08:43 | 00:13:46 |
| EX17 | -655.519 | 00:03:39 | 00:08:47 | 00:10:03 |
| EX18 | -685.451 | 00:04:55 | 00:07:30 | 00:14:15 |

Table 1: Comparison of the examples