Monte-Carlo integration with PythonBiogeme

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SERIES ON BIOGEME

The package PythonBiogeme (biogeme.epfl.ch) is designed to estimate the parameters of various models using maximum likelihood estimation. It is particularly designed for discrete choice models. In this document, we investigate some aspects related to Monte-Carlo integration, which is particularly useful when estimating mixtures choice models, as well as choice models with latent variables. We assume that the reader is already familiar with discrete choice models, with PythonBiogeme, and with simulation methods, although a short summary is provided. This document has been written using PythonBiogeme 2.4, but should remain valid for future versions.

1 Monte-Carlo integration

Monte-Carlo integration consists in approximating an integral with the sum of a large number of terms. It comes from the definition of the expectation of a continuous random variable. Consider the random variable X with probability density function (pdf) $f_X(x)$. Assuming that X can take any value in the interval [a,b], where $a \in \mathbb{R} \cup \{-\infty\}$ and $b \in \mathbb{R} \cup \{+\infty\}$, the expected value of X is given by

$$E[X] = \int_{a}^{b} x f_X(x) dx. \tag{1}$$

Also, if $g: \mathbb{R} \to \mathbb{R}$ is a function, then

$$E[g(X)] = \int_{a}^{b} g(x)f_{X}(x)dx.$$
 (2)

The expectation of a random variable can be approximated using simulation. The idea is simple: generate a sample of realizations of X, that is generate R draws x_r , $r=1,\ldots,R$ from X, and calculate the sample mean:

$$E[g(X)] \approx \frac{1}{R} \sum_{r=1}^{R} g(x_r). \tag{3}$$

Putting (2) and (3) together, we obtain an approximation to the integral:

$$\int_{a}^{b} g(x)f_{X}(x)dx \approx \frac{1}{R} \sum_{r=1}^{R} g(x_{r}). \tag{4}$$

Also, we have

$$\int_{a}^{b} g(x)f_{X}(x)dx = \lim_{R \to \infty} \frac{1}{R} \sum_{r=1}^{R} g(x_{r}).$$
 (5)

Therefore, the procedure to calculate the following integral

$$I = \int_{a}^{b} g(x) dx \tag{6}$$

is the following

- 1. Select a random variable X such that you can generate realizations of X, and such that the pdf f_X is known;
- 2. Generate R draws x_r , r = 1, ..., R from X;
- 3. Calculate

$$I \approx \frac{1}{R} \sum_{r=1}^{R} \frac{g(x_r)}{f_X(x_r)}.$$
 (7)

In order to obtain an estimate of the approximation error, we must calculate the variance the random variable. The sample variance is an unbiased estimate of the true variance:

$$V_{R} = \frac{1}{R-1} \sum_{r=1}^{R} \left(\frac{g(x_{r})}{f_{X}(x_{r})} - I \right)^{2}.$$
 (8)

Alternatively as

$$\operatorname{Var}[g(X)] = \operatorname{E}[g(X)^2] - \operatorname{E}[g(X)]^2, \tag{9}$$

the variance can be approximated by simulation as well:

$$V_{R} \approx \frac{1}{R} \sum_{r=1}^{R} \frac{g(x_{r})^{2}}{f_{X}(x_{r})} - I^{2}.$$
 (10)

Note that, for the values of R that we are using in this document, dividing by R or by R-1 does not make much difference in practice. The approximation error is then estimated as

$$e_{R} = \sqrt{\frac{V_{r}}{R}}.$$
(11)

We refer the reader to Ross (2012) for a comprehensive introduction to simulation methods.

2 Uniform draws

There are many algorithms to draw from various distributions. All of them require at some point draws from the uniform distribution. There are several techniques that generate such uniform draws. In PythonBiogeme, one of them must be selected by setting the parameter RandomDistribution.

Each programming language provides a routine to draw a random number between 0 and 1. Such routines are deterministic, but the sequences of numbers that they generate share many properties with sequences of random numbers. Therefore, they are often called "pseudo random numbers".

```
BIOGEME_OBJECT.PARAMETERS['RandomDistribution'] = "PSEUDO"
```

Researchers have proposed to use other types of sequences to perform Monte-Carlo integration, called "quasi-random sequences" or "low-discrepancy sequences". PythonBiogeme implements the Halton draws, from Halton (1960). They have been reported to perform well for discrete choice models (Train, 2000, Bhat, 2001, Bhat, 2003, Sándor and Train, 2004).

```
BIOGEME_OBJECT.PARAMETERS['RandomDistribution'] = "HALTON"
```

The third method to generate uniform random numbers implemented in PythonBiogeme is called "Modified Latin Hypercube Sampling", and has been proposed by Hess et al. (2006).

```
BIOGEME_OBJECT.PARAMETERS['RandomDistribution'] = "MHLS"
```

In the following, we are using these three options, and compare the accuracy of the corresponding Monte-Carlo integration.

3 Illustration with PythonBiogeme

We first illustrate the method on a simple integral. Consider

$$I = \int_0^1 e^x dx. \tag{12}$$

In this case, it can be solved analytically:

$$I = e - 1 = 1.7183. (13)$$

In order to use Monte-Carlo integration, we consider the random variable X that is uniformly distributed on [0,1], so that

$$f_X(x) = \begin{cases} 1 & \text{if } x \in [0, 1], \\ 0 & \text{otherwise.} \end{cases}$$
 (14)

Therefore, we can approximate I by generating R draws from X and

$$I = E[e^X] \approx \frac{1}{R} \sum_{r=1}^{R} \frac{e^{x_r}}{f_X(x_r)} = \frac{1}{R} \sum_{r=1}^{R} e^{x_r}.$$
 (15)

Moreover, as

$$Var[e^{X}] = E[e^{2X}] - E[e^{X}]^{2}$$

$$= \int_{0}^{1} e^{2x} dx - (e - 1)^{2}$$

$$= (e^{2} - 1)/2 - (e - 1)^{2}$$

$$= 0.2420356075,$$
(16)

the standard error is 0.0034787613 for R=20000, and 0.0011000809 for R=200000. These theoretical values are estimated also below using Python-Biogeme.

We use PythonBiogeme to calculate (15). Note that PythonBiogeme requires a data file, which is not necessary in this simplistic case. We use the simulation mode of PythonBiogeme. It generates output for each row of the data file. In our case, we just need one output, so that we take any data file, and exclude all rows of the file except the first one, using the following syntax:

```
_rowId__ = Variable('__rowId__')
BIOGEME_OBJECT.EXCLUDE = _rowId__ >= 1
```

For this specific example, the data included in the file are irrelevant. The generation of draws in PythonBiogeme is performed using the command bioDraws('U'), where the argument 'U' provides the name of the random variable associated with the draws. The distribution of the random variable is specified using the following syntax:

```
BIOGEME_OBJECT.DRAWS = { 'U': 'UNIFORM'}
```

Note that the valid keywords are

- UNIFORM, for a uniform distribution on the interval [0, 1],
- UNIFORMSYM, for a uniform distribution on the interval [-1, 1],
- NORMAL, for a standard normal distribution, and
- TRUNCNORMAL, for a truncated standard normal distribution. The truncation is defined by the parameter NormalTruncation:

```
BIOGEME_OBJECT.PARAMETERS['NormalTruncation'] = "1.96"
```

The integrand is defined by the following statement:

```
integrand = exp(bioDraws('U'))
```

and the Monte-Carlo integration is obtained as follows:

```
simulatedI = MonteCarlo(integrand)
```

The number of draws is defined by the parameter NbrOfDraws:

```
BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "20000"
```

We calculate as well the simulated variance, using (10):

```
sampleVariance = \setminus \\ MonteCarlo(integrand*integrand) - simulatedI * simulatedI
```

and the standard error (11):

```
stderr = (sampleVariance / 20000.0)**0.5
```

Also, as we know the true value of the integral

```
trueI = exp(1.0) - 1.0
```

we can calculate the error:

```
error = simulatedI - trueI
```

The calculation is obtained using the following statements:

We obtain the following results:

```
Simulated Integral 1.72007
Analytical Integral 1.71828
Sample variance 0.240135
Std Error 0.00346508
Error 0.00178739
```

Remember that the true variance is 0.2420356075, and the true standard error is 0.0034787613. If we use ten times more draws, that is 200,000 draws, we obtain a more precise value:

Simulated Integral 1.71902 Analytical Integral 1.71828 Sample variance 0.24175 Std Error 0.00109943 Error 0.000739329

Remember that the true variance is 0.2420356075, and the true standard error is 0.0011000809. The complete specification file for PythonBiogeme is available in Appendix A.1.

4 Variance reduction

There are several techniques to reduce the variance of the draws used for the Monte-Carlo integration. Reducing the variance improves the precision of the approximation for the same number of draws. Equivalently, they allow to use less draws to achieve the same precision. We introduce two of them in this document: antithetic draws, and control variates. As the focus of this document is on PythonBiogeme, we urge the reader to read an introduction to variance reduction methods in simulation, for instance in Ross (2012).

4.1 Antithetic draws

Instead of drawing from X, consider two random variables X_1 and X_2 , identically distributed with pdf $f_X = f_{X_1} = f_{X_2}$, and define a new random variable

$$Y = \frac{X_1 + X_2}{2}. (17)$$

Then, as $E[Y] = E[X_1] = E[X_2] = E[X]$, we can rewrite (1) as follows:

$$E[Y] = \frac{1}{2}E[X_1] + \frac{1}{2}E[X_2] = E[X] = \int_a^b x f_X(x) dx.$$
 (18)

The variance of this quantity is

$$Var[Y] = \frac{1}{4}(Var(X_1) + Var(X_2) + 2Cov(X_1, X_2)).$$
 (19)

If X_1 and X_2 are independent, this variance is equal to

$$Var[Y] = \frac{1}{2} Var[X]. \tag{20}$$

Therefore, using Y for Monte-Carlo integration is associated with a variance divided by two, but requires twice more draws (R draws for X_1 and R draws

for X_2). It has no advantage on drawing directly R draws from X. Formally, we can compare the standard errors of the two methods for the same number of draws. Drawing 2R draws from X, we obtain the following standard error:

$$\sqrt{\frac{\operatorname{Var}[X]}{2R}}.$$
 (21)

Drawing R draws from X_1 and R draws from X_2 to generate R draws from Y, we obtain the same standard error

$$\sqrt{\frac{\mathrm{Var}[Y]}{R}} = \sqrt{\frac{\mathrm{Var}[X]}{2R}}.$$
 (22)

However, if the variables X_1 and X_2 happen to be negatively correlated, that is if $Cov(X_1,X_2) < 0$, then Var[Y] < Var[X]/2, and drawing from Y reduces the standard error. For instance, if X_1 is uniformly distributed on [0,1], then $X_2 = 1 - X_1$ is also uniformly distributed on [0,1], and

$$Cov(X_1, X_2) = E[X_1(1 - X_1)] - E[X_1] E[1 - X_1] = -\frac{1}{12} < 0.$$
 (23)

If X_1 has a standard normal distribution, that is such that $\mathrm{E}[X_1]=0$ and $\mathrm{Var}[X_1]=1$, then $X_2=-X_1$ has also a standard normal distribution, and is negatively correlated with X_1 , as

$$Cov(X_1, X_2) = E[-X_1^2] - E[X_1] E[-X_1] = -1 < 0.$$
 (24)

The other advantage of this method is that we can recycle the draws. Once we have generated the draws x_r from X_1 , the draws from X_2 are obtained using $1 - x_r$ and $-x_r$, respectively.

Now, we have to be careful when this technique is used for the general case (2). Indeed, it must be verified first that $g(X_1)$ and $g(X_2)$ are indeed negatively correlated. And it is not guaranteed by the fact that X_1 and X_2 are negatively correlated. Consider two examples.

First, consider $g(X) = (x - \frac{1}{2})^2$. Applying the antithetic method with

$$X_1 = \left(X - \frac{1}{2}\right)^2 \text{ and } X_2 = \left((1 - X) - \frac{1}{2}\right)^2$$
 (25)

does not work, as

$$Cov(X_1, X_2) = \frac{1}{180} > 0.$$
 (26)

Actually, applying the antithetic method would *increase* the variance here, which is not desirable.

Second, consider $g(X) = e^X$, as in the example presented in Section 3. We apply the antithetic method using

$$Y = \frac{e^X + e^{1-X}}{2}. (27)$$

Here, the two transformed random variables are negatively correlated:

$$Cov(e^{X}, e^{1-X}) = E[e^{X}e^{1-X}] - E[e^{X}] E[e^{1-X}]$$

$$= e - (e - 1)^{2}$$

$$= -0.2342106136.$$
(28)

Therefore, the variance of Y given by (19) is 0.0039124969, as opposed to 0.2420356075/2 = 0.1210178037 if the two sets of draws were independent. It means that for 10000 draws from Y, the standard error decreases from 0.0034787613 down to 0.0006254996. Moreover, as we use recycled draws, we need only 10000 draws instead of 20000.

To apply this technique in PythonBiogeme, the integrand is defined as follows:

```
integrand = 0.5 * (\exp(\text{bioDraws}('U')) + \exp(1.0-\text{bioDraws}('U')))
and the number of draws reduced to 10000:
```

```
 \begin{array}{lll} stderr &= (sample Variance \ / \ 10000.0)**0.5 \\ BIOGEME OBJECT.PARAMETERS[ 'NbrOfDraws'] &= "10000" \\ \end{array}
```

We obtain the following results:

Simulated Integral 1.71708

Analytical Integral 1.71828

Sample variance 0.00380337

Std Error 0.000616715

Error -0.00120542

The reader can compare these values with the theoretical derivation presented above. The complete specification file for PythonBiogeme is available in Appendix A.2.

4.2 Control variate

The control variate method reduces the variance by exploiting information from another random variable, correlated with g(X), with a known mean. Consider the random variable Y such that $\mathrm{E}[Y] = \mu$. We define a new random variable Z as follows:

$$Z = g(X) + c(Y - \mu) \tag{29}$$

where $c \in \mathbb{R}$ is a parameter. By construction, E[Z] = E[g(X)] for any c, so that draws from Z can be used instead of draws from g(X) for Monte-Carlo integration. Note that we do not need any assumption on g here. The idea is to identify the value of c that minimizes the variance of Z. We have

$$Var[Z] = Var[g(X) + cY] = Var[g(X)] + c^2 Var[Y] + 2c Cov(g(X), Y),$$
 (30)

which is minimized for

$$c^* = -\frac{\operatorname{Cov}(g(X), Y)}{\operatorname{Var}[Y]}.$$
(31)

Therefore, we use for Monte-Carlo integration the random variable

$$Z^* = g(X) - \frac{\operatorname{Cov}(g(X), Y)}{\operatorname{Var} Y}(Y - \mu), \tag{32}$$

with variance

$$\operatorname{Var}[\mathsf{Z}^*] = \operatorname{Var}[\mathsf{g}(\mathsf{X})] - \frac{\operatorname{Cov}(\mathsf{g}(\mathsf{X}),\mathsf{Y})^2}{\operatorname{Var}\mathsf{Y}} \le \operatorname{Var}[\mathsf{g}(\mathsf{X})]. \tag{33}$$

Note that, as for antithetic draws, this technique exploits the correlation between two random variables. If Y is independent from g(X), no variance reduction is achieved.

In our example, $g(X) = e^X$. If we select Y = X, we know that

$$E[Y] = \frac{1}{2} \text{ and } Var[Y] = \frac{1}{12}.$$
 (34)

Moreover,

$$Cov(g(X), Y) = Cov(e^X, X) = (3 - e)/2 = 0.1408590858.$$
 (35)

Therefore, we obtain

$$c^* = -\frac{\text{Cov}(g(X), Y)}{\text{Var } Y} = -6(3 - e) = -1.6903090292, \tag{36}$$

and the variance of Z^* is 0.0039402229, which is much lower than the variance of x, that is 0.2420356075. It means that, for 20000 draws, the standard error is 0.0004438594, as opposed to 0.0034787613. With this method, only 326 draws are sufficient to achieve the same precision as the Monte-Carlo integration without control variate. Indeed,

$$\sqrt{\frac{0.0039402229}{326}} = 0.003476575. \tag{37}$$

This is a tremendous saving. The control variate method is invoked in PythonBiogeme using the following statement:

simulated I = MonteCarloControlVariate(integrand, bioDraws('U'), 0.5),

where the second argument bioDraws('U') is Y, and the third, 0.5, is μ . Note that, in addition to the output requested by the user, PythonBiogeme also generates a report containing statistics on g(X), Y and Z^* . In particular, it reports both the simulated value of Y and μ to detect any implementation error.

The results of the Monte-Carlo integration are:

Simulated Integral (E[Z^*]) 1.71759 Simulated Integral (E[X]) 1.72007 Analytical Integral 1.71828 Sample variance (Var[X]) 0.239849 Std Error ($\sqrt{\text{Var}[Z^*]/20000}$) 0.000440564 Error -0.00069233

The complete specification file for PythonBiogeme is available in Appendix A.3.

Finally, we present in Table 1 the results of the three methods, using different types of uniform draws as described in Section 2. For each technique, the standard errors for the three types of draws are comparable, with the antithetic draws achieving the best value, followed by the control variate. However, the precision actually achieved is much better for Halton, and even more for MLHS.

Pseudo	Halton	MHLS
1.71902	1.71814	1.71829
0.00109943	0.00109999	0.00110009
0.000739329	-0.000145885	9.38555e-06
1.71708	1.71828	1.71828
0.000616715	0.000625455	0.0006255
-0.00120542	-2.27865e -06	-6.13416e-10
1.71759	1.71828	1.71828
0.000440564	0.000443827	0.000443872
-0.00069233	-2.84647e-06	1.52591e-07
	1.71902 0.00109943 0.000739329 1.71708 0.000616715 -0.00120542 1.71759 0.000440564	1.71902 1.71814 0.00109943 0.00109999 0.000739329 -0.000145885 1.71708 1.71828 0.000616715 0.000625455 -0.00120542 -2.27865e-06 1.71759 1.71828 0.000440564 0.000443827

Table 1: Comparison of variants of Monte-Carlo integration on the simple example

We encourage the reader to perform similar tests for other simple integrals. For instance,

$$\int_0^1 \left(x - \frac{1}{2} \right)^2 dx = \frac{1}{12} \tag{38}$$

or

$$\int_{-2}^{2} \left(e^{-x} + \frac{1}{2 + \varepsilon - x} \right) dx = e^{2} - e^{-2} + \log \frac{4 + \varepsilon}{\varepsilon}, \tag{39}$$

where $\varepsilon > 0$. Note that the domain of integration is not [0, 1].

5 Mixtures of logit

Consider an individual n, a choice set C_n , and an alternative $i \in C_n$. The probability to choose i is given by the choice model:

$$P_{n}(i|x,\theta,\mathcal{C}_{n}), \tag{40}$$

where x is a vector of explanatory variables and θ is a vector of parameters to be estimated from data. In the random utility framework, a utility function is defined for each individual n and each alternative $i \in \mathcal{C}_n$:

$$U_{in}(x,\theta) = V_{in}(x,\theta) + \varepsilon_{in}(\theta), \tag{41}$$

where $V_{in}(x, \theta)$ is deterministic and ε_{in} is a random variable independent from x. The model is then written:

$$P_{n}(i|x,\theta,\mathcal{C}_{n}) = \Pr(U_{in}(x,\theta) > U_{in}(x,\theta), \forall j \in \mathcal{C}_{n}). \tag{42}$$

Specific models are obtained from assumptions about the distribution of ϵ_{in} . Namely, if ϵ_{in} are i.i.d. (across both i and n) extreme value distributed, we obtain the logit model:

$$P_{n}(i|x,\theta,C_{n}) = \frac{e^{V_{in}(x,\theta)}}{\sum_{j\in\mathcal{C}_{n}} e^{V_{jn}(x,\theta)}}.$$
(43)

Mixtures of logit are obtained when some of the parameters θ are distributed instead of being fixed. Denote $\theta = (\theta_f, \theta_d)$, where θ_f is the vector of fixed parameters, while θ_d is the vector of distributed parameters, so that the choice model, conditional on θ_d , is

$$P_{n}(i|x,\theta_{f},\theta_{d},\mathcal{C}_{n}). \tag{44}$$

A distribution is to be assumed for θ_d . We denote the pdf of this distribution by $f_{\theta_d}(\xi;\gamma)$, where γ contains the parameters of the distribution. Parameters γ are sometimes called the *deep parameters* of the model. Therefore, the choice model becomes:

$$P_{n}(i|x,\theta_{f},\gamma,\mathcal{C}_{n}) = \int_{\xi} P_{n}(i|x,\theta_{f},\xi,\mathcal{C}_{n}) f_{\theta_{d}}(\xi) d\xi, \tag{45}$$

where θ_f and γ must be estimated from data. The above integral has no analytical solution, even when the kernel $P_n(i|x,\theta_f,\xi,\mathcal{C}_n)$ is a logit model. Therefore, it must be calculated with numerical integration or Monte-Carlo integration. We do both here to investigate the precision of the variants of Monte-Carlo integration.

5.1 Comparison of integration methods on one integral

We consider the Swissmetro example (Bierlaire et al., 2001). The data file is available from biogeme.epfl.ch. Consider the following specification:

- \bullet Variables x: see variables in the data file and new variables defined in Section A.4.
- Fixed parameters θ_f

```
ASC\_CAR = 0.137

ASC\_TRAIN = -0.402

ASC\_SM = 0

B\_COST = -1.29
```

• Deep parameters γ :

```
B_{\text{-TIME}} = -2.26

B_{\text{-TIME}}S = 1.66
```

• We define the coefficient of travel time to be distributed, using the random variable omega, that is assumed to be normally distributed:

```
B_{-}TIME_{-}RND = B_{-}TIME + B_{-}TIME_{-}S * omega
```

The parameter B_TIME is the mean of B_TIME_RND, and B_TIME_S² is its variance. Note that B_TIME_S is **not** the standard deviation, and can be positive of negative.

• Utility functions V_{in} :

```
V1 = ASC_TRAIN + \
B_TIME_RND * TRAIN_TT_SCALED + \
B_COST * TRAIN_COST_SCALED

V2 = ASC_SM + \
B_TIME_RND * SM_TT_SCALED + \
B_COST * SM_COST_SCALED

V3 = ASC_CAR + \
B_TIME_RND * CAR_TT_SCALED + \
B_COST * CAR_CO_SCALED

V = {1: V1, 2: V2, 3: V3}
```

• Choice set \mathcal{C}_n , characterized by the availability conditions:

As there is only one random parameter, the model (45) can be calculated using numerical integration. It is done in PythonBiogeme using the following procedure:

1. Mention that omega is a random variable:

```
omega = RandomVariable('omega')
```

2. Define its pdf:

```
density = normalpdf(omega).
```

Make sure that the library distributions is loaded in order to use the function normalpdf, using the following statement:

```
from distributions import *
```

3. Define the integrand from the logit model, where the probability of the alternative observed to be chosen is calculated (which is typical when calculating a likelihood function):

```
integrand = bioLogit (V, av, CHOICE)
```

4. Calculate the integral:

```
analyticalI = Integrate(integrand*density, 'omega')
```

The complete specification file for PythonBiogeme is available in Appendix A.4. The value of the choice model for first observation in the data file is

$$I = \int_{\xi} P_n(i|x, \theta_f, \xi, C_n) f_{\theta_d}(\xi) d\xi = 0.637849835578.$$
 (46)

Note that, in order of obtain so many significant digits, we have used the following statement:

BIOGEME_OBJECT.PARAMETERS['decimalPrecisionForSimulation'] = "12"

To calculate the same integral with Monte-Carlo integration, we use the same syntax as described earlier in this document:

```
omega = bioDraws('B_TIME_RND')
BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "20000"
BIOGEME_OBJECT.DRAWS = { 'B_TIME_RND': 'NORMAL' }
B_TIME_RND = B_TIME + B_TIME_S * omega
integrand = bioLogit(V, av, CHOICE)
simulatedI = MonteCarlo(integrand)
```

The complete specification file for PythonBiogeme is available in Appendix A.5. Using the result of the numerical integration as the "true" value of the integral, We obtain the following results:

```
Simulated integral 0.637263

Numerical integration 0.63785

Sample variance 0.0299885

Std Error 0.000387224

Error -0.000586483
```

We now apply the variance reduction methods. The antithetic draws described in Section 4.1 are generated as follows:

1. As we are dealing with draws from the normal distribution, the antithetic draw of x_r is $-x_r$. We create two versions of the parameter, one with the draw, and one with its antithetic:

```
B_TIME_RND = B_TIME + B_TIME_S * bioDraws('B_TIME_RND')
B_TIME_RND_MINUS = B_TIME - B_TIME_S * bioDraws('B_TIME_RND')
```

2. Consistently, we then generate two versions of the model:

```
V1_MINUS = ASC_TRAIN + \
B_TIME_RND_MINUS * TRAIN_TT_SCALED + \
B_COST * TRAIN_COST_SCALED

V2_MINUS = ASC_SM + \
B_TIME_RND_MINUS * SM_TT_SCALED + \
B_COST * SM_COST_SCALED

V3_MINUS = ASC_CAR + \
B_TIME_RND_MINUS * CAR_TT_SCALED + \
B_COST * CAR_CO_SCALED

V_MINUS = {1: V1_MINUS,
2: V2_MINUS,
3: V3_MINUS}
```

3. The integrand is the average of the integrands generated by the two versions of the model:

```
integrand_plus = bioLogit(V, av, CHOICE)
integrand_minus = bioLogit(V_MINUS, av, CHOICE)
integrand = 0.5 * (integrand_plus + integrand_minus)
```

The complete specification file for PythonBiogeme is available in Appendix A.6.

The control variate method, described in Section 4.2, requires an output of the simulation such that the analytical integral is known. We propose here to consider

$$\int_0^1 e^{V_{in}(x,\theta_f,\xi)} d\xi = \frac{e^{V_{in}(x,\theta_f,1)} - e^{V_{in}(x,\theta_f,0)}}{\partial V_{in}(x,\theta_f,\xi)/\partial \xi},$$
(47)

if $\partial V_{\rm in}(x,\theta_f,\xi)/\partial \xi$ does not depend on ξ . This integral is calculated by Monte-Carlo after recycling the uniform draws used to generate the normal draws for the original integration. We follow the following procedure:

1. We recycle the draws:

```
UNIFDRAW = bioRecycleDraws('B_TIME_RND')
```

2. We calculate the control variate integrand:

```
VCV = ASC_TRAIN + \
(B_TIME + B_TIME_S * UNIFDRAW) * TRAIN_TT_SCALED + \
B_COST * TRAIN_COST_SCALED
```

Note that the derivative with respect to UNIFDRAW is

```
B_TIME_S * TRAIN_TT_SCALED$.
```

3. We provide the analytical value of the control variate integral:

```
VCV_ZERO = ASC_TRAIN + \
B_TIME * TRAIN_TT_SCALED + \
B_COST * TRAIN_COST_SCALED

VCV_ONE = ASC_TRAIN + \
(B_TIME + B_TIME_S ) * TRAIN_TT_SCALED + \
B_COST * TRAIN_COST_SCALED

VCV_INTEGRAL = (exp(VCV_ONE) - exp(VCV_ZERO)) / \
(B_TIME_S * TRAIN_TT_SCALED)
```

4. We perform the Monte-Carlo integration:

```
simulatedI = MonteCarloControlVariate(integrand,\
exp(VCV),\
VCV_INTEGRAL)
```

The complete specification file for PythonBiogeme is available in Appendix A.7. Table 2 provides the results of the Monte-Carlo integration using different variance reduction methods (none, antithetic and control variates), different uniform draws (pseudo, Halton and MLHS), and different number of draws. We can observe the following:

- In terms of standard errors of the draws, the Monte-Carlo integration without variance reduction has a standard error about 7.5 times as large as the anthitetic version, and 2 times as large as the control variate.
- In terms of absolute error, when compared to the value provided by the numerical integration, the error of the Monte-Carlo integration without variance reduction is about the same for the pseudo draws, 12 times larger for the Halton draws, and 25 times larger for the MHLS draws, when compared to the antithetic draws. If it between 3 and 4 times larger, when compared to the control variates.
- There is no significant difference in terms of standard errors across the types of draws, irrespectively of the variance reduction method used.
- In terms of actual error, though, the Halton draws improves the precision of the output, and the MHLS even more.
- Using the antithetic draws with 1000 draws achieves a similar precision as no variance reduction with 20000 draws.
- Using the control variates with 2000 draws achieves a similar precision as no variance reduction with 20000 draws.
- Reducing the number of draws to 500 does not deteriorate much the precision for the antithetic draws.

It would be useful to perform the same experiment for some other observations in the data file. Such experiments can give useful insights to for the choice of the most appropriate integration technique. In the following, we compare some of these techniques for the maximum likelihood estimation of the parameters of the model.

5.2 Comparison of integration methods for maximum likelihood estimation

We now estimate the parameters of the model using all observations in the data set associated with work trips. Observations such that the dependent variable CHOICE is 0 are also removed.

```
exclude = (( PURPOSE != 1 ) * ( PURPOSE != 3 ) + \ ( CHOICE == 0 )) > 0 
BIOGEME_OBJECT.EXCLUDE = exclude
```

The estimation using numerical integration is performed using the following statements:

```
integrand = bioLogit(V, av, CHOICE)
prob = Integrate(integrand*density, 'omega')
l = log(prob)
rowIterator('obsIter')
BIOGEME_OBJECT.ESTIMATE = Sum(l, 'obsIter')
```

The complete specification file for PythonBiogeme is available in Appendix A.8. For Monte-Carlo integration, we use the following statements:

```
prob = bioLogit(V, av, CHOICE)
l = mixedloglikelihood(prob)
rowIterator('obsIter')
BIOGEME_OBJECT_ESTIMATE = Sum(l, 'obsIter')
```

where the statement 1 = mixedloglikelihood(prob) is equivalent to

```
integral = MonteCarlo(prob)
l = log(integral)
```

The complete specification file for PythonBiogeme is available in Appendix A.9. The following estimation results are presented:

- Table 4: numerical integration;
- Table 5: Monte-Carlo integration, no variance reduction, 2000 MHLS draws;
- Table 6: antithetic draws, 1000 MHLS draws;
- Table 7: control variates, 2000 MHLS draws;
- Table 8: Monte-Carlo integration, 500 MHLS draws;
- Table 9: antithetic draws, 250 MHLS draws;
- Table 10: control variates, 500 MHLS draws.

The final log likelihood in each case, as well as the estimation time are summarized in Table 3. In this experiment, when looking at the estimates, it seems that the MLHS draws provide relatively good precision, even for a lower number of draws, and with no variance reduction. Clearly, this result cannot be generalized, and should be investigated on a case by case basis. Note however that the default type of draws in PythonBiogeme is MLHS, because it is performing particularly well in this example.

6 Conclusion

This document describes the variants of Monte-Carlo integration, and suggests how to perform some analysis using the SIMULATE operator of Python-Biogeme, that helps investigating the performance of each of them before starting a maximum likelihod estimation, that may take a while to converge. In the example provided in this document, the antithetic draws method, combined with MLHS appeared to be the most precise. This result is not universal. The analysis must be performed on a case by case basis.

	Draws	Pseudo	Halton	MHLS
		20000 draws		
Monte-Carlo	20000	0.637263	0.637923	0.637845
Standard error		0.000387224	0.000390176	0.000390301
Actual error		-0.000586483	7.35443e-05	-5.08236e-06
Antithetic	10000	0.638383	0.637856	0.63785
Standard error		5.13243e-05	5.24484e-05	5.24949e-05
Actual error		0.000533174	6.1286 e- 06	1.96217e-07
Control variate	20000	0.6377	0.637871	0.637848
Standard error		0.000176759	0.000179054	0.00017928
Actual error		-0.000149889	2.127e-05	-1.72413e-06
		2000 draws		
Antithetic	1000	0.638783	0.637965	0.637853
Standard error		5.05914e-05	5.17454e-05	5.24619e-05
Actual error		0.000933592	0.000114998	3.32666e-06
Control variate	2000	0.637876	0.637975	0.637835
Standard error		0.000551831	0.00056032	0.000567009
Actual error		2.66122e-05	0.000125218	-1.50796e-05
		500 draws		
Antithetic	250	0.639205	0.638459	0.637869
Standard error		5.17638e-05	4.97379e-05	5.23141e-05
Actual error		0.00135483	0.000609069	1.87082 e-05
Control variate	500	0.637587	0.638158	0.637798
Standard error		0.00111188	0.00109022	0.00113287
Actual error		-0.000262395	0.000308626	-5.2274e-05

 $\label{thm:comparison} \mbox{Table 2: Comparison of variants of Monte-Carlo integration on the mixture of logit example}$

Method	Draws	Log likelihood	Run time
Numerical	_	-5214.879	02:37
Monte-Carlo	2000	-5214.835	31:11
Antithetic	1000	-5214.899	39:26
Control variate	2000	-5214.835	42:11
Monte-Carlo	500	-5214.940	09:26
Antithetic	250	-5214.897	09:21
Control variate	500	-5214.940	08:59

Table 3: Final log likelihood and run time for each integration method

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	t-stat	p-value
1	ASC_CAR	0.137	0.0517	2.65	0.01
2	ASC_TRAIN	-0.401	0.0656	-6.12	0.00
3	B_COST	-1.29	0.0863	-14.90	0.00
4	$B_{-}TIME$	-2.26	0.117	-19.38	0.00
5	$B_{-}TIME_{-}S$	-1.65	0.125	-13.26	0.00

Number of observations = 6768

Number of excluded observations = 3960

Number of estimated parameters = 5

Number of iterations = 13

Estimation time: 00:02:37

$$\begin{array}{rcl} \mathcal{L}(\beta_0) & = & -7157.671 \\ \mathcal{L}(\hat{\beta}) & = & -5214.879 \\ -2[\mathcal{L}(\beta_0) - \mathcal{L}(\hat{\beta})] & = & 3885.585 \\ \rho^2 & = & 0.271 \\ \bar{\rho}^2 & = & 0.271 \end{array}$$

Table 4: Estimation results with numerical integration

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	t-stat	p-value
1	ASC_CAR	0.137	0.0517	2.65	0.01
2	ASC_TRAIN	-0.402	0.0658	-6.10	0.00
3	$B_{-}COST$	-1.29	0.0864	-14.89	0.00
4	$B_{-}TIME$	-2.26	0.117	-19.31	0.00
5	$B_{-}TIME_{-}S$	1.66	0.132	12.59	0.00

Number of observations = 6768

Number of excluded observations = 3960

Number of estimated parameters = 5

Number of iterations = 9

Estimation time: 00:31:11

$$\begin{array}{rcl} \mathcal{L}(\beta_0) & = & -6964.663 \\ \mathcal{L}(\hat{\beta}) & = & -5214.835 \\ -2[\mathcal{L}(\beta_0) - \mathcal{L}(\hat{\beta})] & = & 3499.656 \\ \rho^2 & = & 0.251 \\ \bar{\rho}^2 & = & 0.251 \end{array}$$

Table 5: Estimation results with Monte-Carlo, no variance reduction, 2000 MHLS draws

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	t-stat	p-value
1	ASC_CAR	0.137	0.0517	2.65	0.01
2	ASC_TRAIN	-0.402	0.0658	-6.10	0.00
3	$B_{-}COST$	-1.29	0.0863	-14.89	0.00
4	$B_{-}TIME$	-2.26	0.117	-19.31	0.00
5	$B_{-}TIME_{-}S$	1.66	0.132	12.59	0.00

Number of observations = 6768

Number of excluded observations = 3960

Number of estimated parameters = 5

Number of iterations = 12

Estimation time: 00:39:26

$$\begin{array}{rcl} \mathcal{L}(\beta_0) & = & -7155.875 \\ \mathcal{L}(\hat{\beta}) & = & -5214.899 \\ -2[\mathcal{L}(\beta_0) - \mathcal{L}(\hat{\beta})] & = & 3881.952 \\ \rho^2 & = & 0.271 \\ \bar{\rho}^2 & = & 0.271 \end{array}$$

Table 6: Estimation results with antithetic draws, 1000 MHLS draws

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	t-stat	p-value
1	ASC_CAR	0.137	0.0517	2.65	0.01
2	ASC_TRAIN	-0.402	0.0658	-6.10	0.00
3	B_COST	-1.29	0.0864	-14.89	0.00
4	$B_{-}TIME$	-2.26	0.117	-19.31	0.00
5	$B_{-}TIME_{-}S$	1.66	0.132	12.59	0.00

Number of observations = 6768

Number of excluded observations = 3960

Number of estimated parameters = 5

Number of iterations = 12

Estimation time: 00:42:11

$$\begin{array}{rcl} \mathcal{L}(\beta_0) & = & -7155.867 \\ \mathcal{L}(\hat{\beta}) & = & -5214.835 \\ -2[\mathcal{L}(\beta_0) - \mathcal{L}(\hat{\beta})] & = & 3882.063 \\ \rho^2 & = & 0.271 \\ \bar{\rho}^2 & = & 0.271 \end{array}$$

Table 7: Estimation results with control variates, 2000 MHLS draws

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	t-stat	p-value
1	ASC_CAR	0.137	0.0517	2.65	0.01
2	ASC_TRAIN	-0.402	0.0658	-6.10	0.00
3	$B_{-}COST$	-1.29	0.0864	-14.88	0.00
4	$B_{-}TIME$	-2.26	0.117	-19.33	0.00
5	$B_{-}TIME_{-}S$	1.66	0.131	12.63	0.00

Number of observations = 6768

Number of excluded observations = 3960

Number of estimated parameters = 5

Number of iterations = 12

Estimation time: 00:09:26

$$\begin{array}{rcl} \mathcal{L}(\beta_0) & = & -7155.962 \\ \mathcal{L}(\hat{\beta}) & = & -5214.940 \\ -2[\mathcal{L}(\beta_0) - \mathcal{L}(\hat{\beta})] & = & 3882.044 \\ \rho^2 & = & 0.271 \\ \bar{\rho}^2 & = & 0.271 \end{array}$$

Table 8: Estimation results with Monte-Carlo integration, no variance reduction, 500 MHLS draws

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	t-stat	p-value
1	ASC_CAR	0.137	0.0517	2.65	0.01
2	ASC_TRAIN	-0.402	0.0658	-6.11	0.00
3	$B_{-}COST$	-1.29	0.0864	-14.88	0.00
4	$B_{-}TIME$	-2.26	0.117	-19.33	0.00
5	$B_{-}TIME_{-}S$	1.66	0.131	12.61	0.00

Number of observations = 6768

Number of excluded observations = 3960

Number of estimated parameters = 5

Number of iterations = 12

Estimation time: 00:09:21

$$\begin{array}{rcl} \mathcal{L}(\beta_0) & = & -7155.877 \\ \mathcal{L}(\hat{\beta}) & = & -5214.897 \\ -2[\mathcal{L}(\beta_0) - \mathcal{L}(\hat{\beta})] & = & 3881.960 \\ \rho^2 & = & 0.271 \\ \bar{\rho}^2 & = & 0.271 \end{array}$$

Table 9: Estimation results with antithetic draws, 250 MHLS draws

			Robust		
Parameter		Coeff.	Asympt.		
number	Description	estimate	std. error	t-stat	p-value
1	ASC_CAR	0.137	0.0517	2.65	0.01
2	ASC_TRAIN	-0.402	0.0658	-6.10	0.00
3	B_COST	-1.29	0.0864	-14.88	0.00
4	$B_{-}TIME$	-2.26	0.117	-19.33	0.00
5	$B_{-}TIME_{-}S$	1.66	0.131	12.63	0.00

Number of observations = 6768

Number of excluded observations = 3960

Number of estimated parameters = 5

Number of iterations = 12

Estimation time: 00:08:59

$$\begin{array}{rcl} \mathcal{L}(\beta_0) & = & -7155.962 \\ \mathcal{L}(\hat{\beta}) & = & -5214.940 \\ -2[\mathcal{L}(\beta_0) - \mathcal{L}(\hat{\beta})] & = & 3882.044 \\ \rho^2 & = & 0.271 \\ \bar{\rho}^2 & = & 0.271 \end{array}$$

Table 10: Estimation results with control variates, 500 MHLS draws

A Complete specification files

A.1 01simpleIntegral.py

```
2
  \# File: 01simpleIntegral.py
3
  # Author: Michel Bierlaire, EPFL
  # Date: Sat Jul 25 11:41:13 2015
5
6
  7
  from biogeme import *
  from headers import *
10
11
  integrand = exp(bioDraws('U'))
  simulatedI = MonteCarlo(integrand)
13
14
  trueI = exp(1.0) - 1.0
15
16
  sampleVariance = \setminus
17
    MonteCarlo(integrand*integrand) - simulatedI * simulatedI
18
  stderr = (sample Variance / 200000.0) **0.5
   error = simulatedI - trueI
20
21
  simulate = {'01 Simulated Integral': simulatedI,
22
23
              '02 Analytical Integral': trueI,
              '03 Sample variance': sample Variance,
24
              '04 Std Error': stderr,
25
              '05 Error': error}
26
27
  rowIterator('obsIter')
28
29
  BIOGEME_OBJECT.SIMULATE = Enumerate(simulate, 'obsIter')
30
BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "5"
32 BIOGEME_OBJECT.PARAMETERS['RandomDistribution'] = "PSEUDO"
  _rowId__ = Variable('__rowId__')
  BIOGEME\_OBJECT.EXCLUDE = \_rowId\_. >= 1
  BIOGEME_OBJECT.DRAWS = { 'U': 'UNIFORM'}
```

A.2 02 antithetic .py

```
7
   from biogeme import *
9
   from headers import *
10
11
   integrand = 0.5 * (exp(bioDraws('U'))) + exp(1.0-bioDraws('U')))
12
   simulatedI = MonteCarlo(integrand)
13
14
   trueI = exp(1.0) - 1.0
15
16
   sampleVariance = \
17
     MonteCarlo(integrand*integrand) - simulatedI * simulatedI
18
   stderr = (sampleVariance / 10000.0)**0.5
19
   error = simulatedI - trueI
20
21
   simulate = {'01_Simulated Integral': simulatedI,
22
               '02_Analytical Integral': trueI,
23
               '03_Sample variance': \operatorname{sampleVariance},
24
25
               '04_Std Error': stderr,
               '05_Error': error}
26
27
   rowIterator('obsIter')
28
29
  BIOGEME_OBJECT.SIMULATE = Enumerate(simulate, 'obsIter')
30
31
  BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "5"
32
   _rowId__ = Variable('__rowId__')
33
  BIOGEME_OBJECT.EXCLUDE = __rowId__ >= 1
  BIOGEME_OBJECT.DRAWS = { 'U': 'UNIFORM'}
```

A.3 03controlVariate.py

```
1
2
  # File: 03controlVariate.py
  # Author: Michel Bierlaire, EPFL
  # Date: Sat Jul 25 12:24:25 2015
5
6
  7
8
9
  from biogeme import *
10
  from headers import *
12
  integrand = exp(bioDraws('U'))
13
  simulatedI = MonteCarloControlVariate(integrand, bioDraws('U'), 0.5)
14
15
  trueI = exp(1.0) - 1.0
16
17
```

```
error = simulatedI - trueI
18
19
   simulate = {'01_Simulated Integral': simulatedI,
20
                '02_Analytical Integral': trueI,
21
                '05_Error': error}
22
23
   rowIterator('obsIter')
25
  BIOGEME_OBJECT.SIMULATE = Enumerate(simulate, 'obsiter')
26
27
  BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "5"
28
   __rowId__ = Variable(',__rowId__')
29
  BIOGEME_OBJECT.EXCLUDE = __rowId__ >= 1
  BIOGEME_OBJECT.DRAWS = { 'U': 'UNIFORM'}
```

A.4 05normalMixtureTrueAnalytical.py

```
1
2
  \# File: 05normalMixtureTrueAnalytical.py
  # Author: Michel Bierlaire, EPFL
  # Date: Sat Jul 25 18:50:11 2015
5
6
7
  8
  from biogeme import *
9
  from headers import *
11
  from distributions import *
  from loglikelihood import *
12
13
  #Parameters
14
  ASC\_CAR = 0.137
15
  ASC_TRAIN = -0.402
16
  ASC\_SM = 0
17
  B_{-}TIME = -2.26
  B_TIME_S = 1.66
  B_{-}COST = -1.29
20
21
  # Define a random parameter, normally distributed,
22
  # designed to be used for integration
23
  omega = RandomVariable('omega')
24
  density = normalpdf(omega)
  B_TIME_RND = B_TIME + B_TIME_S * omega
27
  # Utility functions
28
29
  #If the person has a GA (season ticket) her
  #incremental cost is actually 0
31
  #rather than the cost value gathered from the
```

```
\# network data.
   SM\_COST = SM\_CO
                      * (GA = 0)
   TRAIN\_COST = TRAIN\_CO
                            * ( GA == 0
36
   \# For numerical reasons, it is good practice to scale the data to
37
   # that the values of the parameters are around 1.0.
   \# A previous estimation with the unscaled data has generated
   \# parameters around -0.01 for both cost and time.
40
   # Therefore, time and cost are multipled my 0.01.
41
42
   TRAIN\_TT\_SCALED = \
43
     Define Variable ('TRAIN_TT_SCALED', TRAIN_TT / 100.0)
44
   TRAIN\_COST\_SCALED = \
45
     Define Variable ('TRAIN_COST_SCALED', TRAIN_COST / 100)
46
   SM_TT_SCALED = DefineVariable('SM_TT_SCALED', SM_TT / 100.0)
47
   SM_COST_SCALED = DefineVariable('SM_COST_SCALED', SM_COST / 100)
48
   CAR_TT_SCALED = Define Variable ('CAR_TT_SCALED', CAR_TT / 100)
49
   CAR_CO_SCALED = Define Variable ('CAR_CO_SCALED', CAR_CO / 100)
51
   V1 = ASC\_TRAIN + \setminus
52
        B\_TIME\_RND * TRAIN\_TT\_SCALED + \setminus
53
        B_COST * TRAIN_COST_SCALED
54
   V2 = ASC\_SM + \setminus
55
        B_TIME_RND * SM_TT_SCALED + \
56
        B_COST * SM_COST_SCALED
57
   V3 = ASC\_CAR + \setminus
58
        B_TIME_RND * CAR_TT_SCALED + \
59
        B_COST * CAR_CO_SCALED
60
61
62
   # Associate utility functions with the numbering of alternatives
63
   V = \{1: V1,
64
        2: V2,
65
        3: V3}
66
67
   # Associate the availability conditions with the alternatives
68
69
   CAR_AV_SP = Define Variable ('CAR_AV_SP', CAR_AV * (SP
   TRAIN_AV_SP = Define Variable ('TRAIN_AV_SP', TRAIN_AV * (SP
71
   0)
72
   av = \{1: TRAIN\_AV\_SP,
73
         2: SM_AV,
74
         3: CAR_AV_SP}
75
76
   # The choice model is a logit, with availability conditions
77
   integrand = bioLogit(V, av, CHOICE)
78
```

```
analyticalI = Integrate(integrand*density, 'omega')
simulate = {'Analytical': analyticalI}

rowIterator('obsIter')

BIOGEME.OBJECT.PARAMETERS['decimalPrecisionForSimulation'] = "12"
BIOGEME.OBJECT.SIMULATE = Enumerate(simulate, 'obsIter')

-rowId_ = Variable('__rowId__')
BIOGEME.OBJECT.EXCLUDE = __rowId__ >= 1
```

A.5 06normalMixture.py

```
1
2
  #
  \# File: 06normalMixture.py
3
  # Author: Michel Bierlaire, EPFL
  # Date: Sat Jul 25 18:37:37 2015
6
  7
8
  from biogeme import *
9
  from headers import *
10
  from loglikelihood import *
11
  from statistics import *
12
13
14 #Parameters
ASC\_CAR = 0.137
ASC_TRAIN = -0.402
ASC\_SM = 0
  B_{-}TIME = -2.26
  B_TIME_S = 1.66
19
  B_{-}COST = -1.29
20
21
  # Define a random parameter, normally distributed,
  # designed to be used for integration
  omega = bioDraws('B_TIME_RND')
  B_TIME_RND = B_TIME + B_TIME_S * omega
26
  \# Utility functions
27
28
  #If the person has a GA (season ticket) her
30 #incremental cost is actually 0
  #rather than the cost value gathered from the
31
  \# network data.
32
  SM\_COST = SM\_CO
                   * ( GA == 0
                        * ( GA == 0
  TRAIN\_COST = TRAIN\_CO
34
35
```

```
# For numerical reasons, it is good practice to scale the data to
   # that the values of the parameters are around 1.0.
37
   # A previous estimation with the unscaled data has generated
   \# parameters around -0.01 for both cost and time. Therefore, time and
39
   \# cost are multipled my 0.01.
40
41
   TRAIN\_TT\_SCALED = \setminus
42
     Define Variable ('TRAIN_TT_SCALED', TRAIN_TT / 100.0)
43
   TRAIN\_COST\_SCALED = \setminus
44
     Define Variable ('TRAIN_COST_SCALED', TRAIN_COST / 100)
45
   SM_TT_SCALED = Define Variable ('SM_TT_SCALED', SM_TT / 100.0)
46
   SM_COST_SCALED = DefineVariable('SM_COST_SCALED', SM_COST / 100)
47
   CAR_TT_SCALED = Define Variable ('CAR_TT_SCALED', CAR_TT / 100)
48
   CAR_CO_SCALED = Define Variable ('CAR_CO_SCALED', CAR_CO / 100)
49
50
   V1 = ASC_TRAIN + 
51
        B_TIME_RND * TRAIN_TT_SCALED + \
52
        B_COST * TRAIN_COST_SCALED
53
   V2 = ASC\_SM + \setminus
54
        B_TIME_RND * SM_TT_SCALED + \
55
        B_COST * SM_COST_SCALED
56
   V3 = ASC\_CAR + \setminus
57
        B_TIME_RND * CAR_TT_SCALED + \
58
        B_COST * CAR_CO_SCALED
59
60
   # Associate utility functions with the numbering of alternatives
61
   V = \{1: V1,
62
        2: V2,
63
        3: V3
64
   # Associate the availability conditions with the alternatives
66
67
   CAR_AV_SP = DefineVariable('CAR_AV_SP', CAR_AV * ( SP
   TRAIN_AV_SP = Define Variable ('TRAIN_AV_SP', TRAIN_AV * ( SP
69
   0)
70
   av = \{1: TRAIN\_AV\_SP,
71
          2: SM_AV,
72
         3: CAR_AV_SP}
73
74
   # The choice model is a logit, with availability conditions
75
   integrand = bioLogit (V, av, CHOICE)
76
   simulatedI = MonteCarlo(integrand)
77
78
   trueI = 0.637849835578
79
80
   sampleVariance = \setminus
81
     MonteCarlo(integrand*integrand) - simulatedI * simulatedI
```

```
stderr = (sample Variance / 200000.0)**0.5
83
   error = simulatedI - trueI
84
   simulate = {'01 Simulated Integral': simulatedI,
86
                '02 Analytical Integral': trueI,
87
                '03 Sample variance': sample Variance,
88
                '04 Std Error': stderr,
89
                '05 Error': error}
90
91
   rowIterator('obsIter')
92
93
  BIOGEME_OBJECT.SIMULATE = Enumerate(simulate, 'obsIter')
94
95
   __rowId__ = Variable(',__rowId__')
96
  BIOGEME\_OBJECT.EXCLUDE = \_rowId\_. >= 1
97
98
  BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "5"
99
  BIOGEME_OBJECT.DRAWS = { 'B_TIME_RND': 'NORMAL' }
```

A.6 07normalMixtureAntithetic.py

```
1
2
  \# File: 07normalMixtureAntithetic.py
3
  # Author: Michel Bierlaire, EPFL
  # Date: Sat Jul 25 19:14:42 2015
5
  #
6
  8
  from biogeme import *
9
  from headers import *
10
  from loglikelihood import *
11
  from statistics import *
12
13
14 #Parameters
ASC\_CAR = 0.137
ASC_TRAIN = -0.402
ASC\_SM = 0
18 B_TIME = -2.26
  B_TIME_S = 1.66
  B_{\text{-}COST} = -1.29
20
21
 # Define a random parameter, normally distributed,
# designed to be used for integration,
\# and its antithetic.
25 B_TIME_RND = B_TIME + B_TIME_S * bioDraws('B_TIME_RND')
  B_TIME_RND_MINUS = B_TIME - B_TIME_S * bioDraws('B_TIME_RND')
27
28 # Utility functions
```

```
29
   #If the person has a GA (season ticket) her
30
   #incremental cost is actually 0
   #rather than the cost value gathered from the
32
   \# network data.
33
   SM\_COST = SM\_CO
                       * ( GA == 0
   TRAIN\_COST = TRAIN\_CO
                             * ( GA == 0
36
   \# For numerical reasons, it is good practice to scale the data to
37
   # that the values of the parameters are around 1.0.
   # A previous estimation with the unscaled data has generated
   # parameters around -0.01 for both cost and time.
40
   # Therefore, time and cost are multipled my 0.01.
41
42
   TRAIN\_TT\_SCALED = \setminus
43
     Define Variable ('TRAIN_TT_SCALED', TRAIN_TT / 100.0)
44
   TRAIN\_COST\_SCALED = \setminus
45
     Define Variable ('TRAIN_COST_SCALED', TRAIN_COST / 100)
   SM_TT_SCALED = Define Variable ('SM_TT_SCALED', SM_TT / 100.0)
47
   SM_COST_SCALED = Define Variable ('SM_COST_SCALED', SM_COST / 100)
48
   CAR_TT_SCALED = Define Variable ('CAR_TT_SCALED', CAR_TT / 100)
49
   CAR_CO_SCALED = Define Variable ('CAR_CO_SCALED', CAR_CO / 100)
51
   V1 = ASC\_TRAIN + \setminus
52
        B_TIME_RND * TRAIN_TT_SCALED + \
53
        B_COST * TRAIN_COST_SCALED
54
   V2 = ASC\_SM + \setminus
55
        B_TIME_RND * SM_TT_SCALED + \
56
        B_COST * SM_COST_SCALED
57
   V3 = ASC\_CAR + \setminus
        B_TIME_RND * CAR_TT_SCALED + \
59
        B_COST * CAR_CO_SCALED
60
61
   V1\_MINUS = ASC\_TRAIN + 
62
               B_TIME_RND_MINUS * TRAIN_TT_SCALED + \
63
               B_COST * TRAIN_COST_SCALED
64
   V2\_MINUS = ASC\_SM + \setminus
               B_TIME_RND_MINUS * SM_TT_SCALED + \setminus
66
               B_COST * SM_COST_SCALED
67
   V3_MINUS = ASC_CAR + \
68
               B_TIME_RND_MINUS * CAR_TT_SCALED + \
69
               B_COST * CAR_CO_SCALED
70
71
   # Associate utility functions with the numbering of alternatives
72
   V = \{1: V1,
73
        2: V2,
74
        3: V3}
75
76
   V_{MINUS} = \{1: V1_{MINUS},
```

```
2: V2_MINUS,
78
                3: V3_MINUS}
79
   # Associate the availability conditions with the alternatives
81
82
   CAR_AV_SP = DefineVariable('CAR_AV_SP', CAR_AV * (SP
   TRAIN\_AV\_SP = DefineVariable('TRAIN\_AV\_SP', TRAIN\_AV * (SP')
84
   0)
85
   av = \{1: TRAIN\_AV\_SP,
86
          2: SM_AV,
87
          3: CAR_AV_SP}
88
89
   # The choice model is a logit, with availability conditions
90
   integrand_plus = bioLogit (V, av, CHOICE)
91
   integrand\_minus = bioLogit(V\_MINUS, av, CHOICE)
92
   integrand = 0.5 * (integrand_plus + integrand_minus)
   simulated I = MonteCarlo (integrand)
94
95
   trueI = 0.637849835578
96
97
   sampleVariance = \
98
      MonteCarlo(integrand*integrand) - simulatedI * simulatedI
99
   stderr = (sample Variance / 200000.0) **0.5
100
   error = simulatedI - trueI
101
102
   simulate = { '01 Simulated Integral': simulatedI,
103
                 '02 Analytical Integral': trueI,
104
                 '03 Sample variance': sampleVariance,
105
                 '04 Std Error': stderr,
106
                 '05 Error': error}
107
108
   rowIterator('obsIter')
109
110
   BIOGEME_OBJECT.SIMULATE = Enumerate(simulate, 'obsIter')
111
112
    __rowId__ = Variable('__rowId__')
113
   BIOGEME_OBJECT.EXCLUDE = __rowId__ >= 1
114
115
   BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "5"
116
   BIOGEME_OBJECT.DRAWS = { 'B_TIME_RND': 'NORMAL' }
```

A.7 08normalMixtureControlVariate.py

```
# Date: Sat Jul 25 18:50:11 2015
5
  #
6
   8
   from biogeme import *
9
   from headers import *
   from loglikelihood import *
   from statistics import *
12
13
  \#Parameters
15
  ASC\_CAR = 0.137
  ASC_TRAIN = -0.402
16
  ASC\_SM = 0
17
_{18} B_TIME = -2.26
  B_TIME_S = 1.66
  B_{-}COST = -1.29
20
21
  # Define a random parameter, normally distributed,
22
23
  # designed to be used for Monte-Carlo simulation
  B_TIME_RND = B_TIME + B_TIME_S * bioDraws('B_TIME_RND')
24
25
  # Utility functions
26
27
  #If the person has a GA (season ticket) her
28
  #incremental cost is actually 0
29
  #rather than the cost value gathered from the
  \# network data.
31
  SM\_COST = SM\_CO
                      * ( GA == 0
32
  TRAIN\_COST = TRAIN\_CO
                           * ( GA == 0
  # For numerical reasons, it is good practice to scale the data to
35
  # that the values of the parameters are around 1.0.
36
  # A previous estimation with the unscaled data has generated
   \# parameters around -0.01 for both cost and time.
  # Therefore, time and cost are multipled my 0.01.
39
40
  TRAIN\_TT\_SCALED = \setminus
41
     Define Variable ('TRAIN_TT_SCALED', TRAIN_TT / 100.0)
42
  TRAIN\_COST\_SCALED = \
43
     Define Variable ('TRAIN_COST_SCALED', TRAIN_COST / 100)
44
  SM_TT_SCALED = Define Variable ('SM_TT_SCALED', SM_TT / 100.0)
45
  SM_COST_SCALED = Define Variable ('SM_COST_SCALED', SM_COST / 100)
46
  CAR_TT_SCALED = DefineVariable('CAR_TT_SCALED', CAR_TT / 100)
47
  CAR_CO_SCALED = Define Variable ('CAR_CO_SCALED', CAR_CO / 100)
48
49
  V1 = ASC\_TRAIN + \setminus
50
        B_TIME_RND * TRAIN_TT_SCALED + \
51
        B\_COST \ * \ TRAIN\_COST\_SCALED
52
  V2 = ASC\_SM + \setminus
```

```
B\_TIME\_RND * SM\_TT\_SCALED + \setminus
54
         B_COST * SM_COST_SCALED
55
   V3 = ASC\_CAR + \setminus
         B_TIME_RND * CAR_TT_SCALED + \setminus
57
         B_COST * CAR_CO_SCALED
58
59
   # Associate utility functions with the numbering of alternatives
60
   V = \{1: V1,
61
         2: V2,
62
         3: V3}
63
64
   # Associate the availability conditions with the alternatives
65
66
   CAR_AV_SP = DefineVariable('CAR_AV_SP', CAR_AV * ( SP
                                                                    !=
67
   TRAIN_AV_SP = Define Variable ('TRAIN_AV_SP', TRAIN_AV * ( SP
68
      ))
69
   av = \{1: TRAIN\_AV\_SP,
70
          2: SM_AV,
71
          3: CAR\_AV\_SP
72
73
   # The choice model is a logit, with availability conditions
74
   integrand = bioLogit (V, av, CHOICE)
75
76
   # Control variate
77
78
   # Recycle the uniform draws used to generate the
79
   #normal draws of B_TIME_RND
80
   UNIFDRAW = bioRecycleDraws('B_TIME_RND')
82
   # Utility function with the uniform draws instead of the normal.
83
   VCV = ASC\_TRAIN + \setminus
84
          (B_TIME + B_TIME_S * UNIFDRAW) * TRAIN_TT_SCALED + \
          B_COST * TRAIN_COST_SCALED
86
   \# The analytical integral of exp(VCV) between 0 and 1
87
   # is now calculated
88
   VCV_ZERO = ASC_TRAIN + \
89
                B_TIME * TRAIN_TT_SCALED + \
90
                B_COST * TRAIN_COST_SCALED
91
   VCV\_ONE = ASC\_TRAIN + 
92
               (B\_TIME + B\_TIME\_S) * TRAIN\_TT\_SCALED + \setminus
93
                B_COST * TRAIN_COST_SCALED
94
   VCV\_INTEGRAL = (exp(VCV\_ONE) - exp(VCV\_ZERO)) / 
95
                    (B_TIME_S * TRAIN_TT_SCALED)
96
97
98
   simulatedI = MonteCarloControlVariate(integrand, \
99
                                              \exp(VCV),
100
```

```
VCV_INTEGRAL)
101
102
   trueI = 0.637849835578
103
104
   error = simulatedI - trueI
105
106
   simulate = {'01 Simulated Integral': simulatedI,
107
                 '02 Analytical Integral': trueI,
108
                 '05 Error': error}
109
110
   rowIterator('obsIter')
111
112
   BIOGEME_OBJECT.SIMULATE = Enumerate(simulate, 'obsIter')
113
114
   __rowId__ = Variable(',__rowId__')
   BIOGEME_OBJECT.EXCLUDE = __rowId__ >= 1
116
117
   BIOGEME_OBJECT.PARAMETERS['NbrOfDraws'] = "5"
118
   BIOGEME_OBJECT.DRAWS = { 'B_TIME_RND': 'NORMAL' }
```

A.8 11estimationNumerical.py

```
1
2
  \# File: 11estimationNumerical.py
3
  # Author: Michel Bierlaire, EPFL
  # Date: Thu Jul 30 10:40:49 2015
5
  #
  7
  from biogeme import *
9
  from headers import *
10
  from distributions import *
11
  from loglikelihood import *
  from statistics import *
14
  #Parameters to be estimated
15
  \# Arguments:
16
      1 Name for report. Typically, the same as the variable
17
  #
      2
         Starting value
18
         Lower bound
  #
      3
19
  #
         Upper bound
20
      4
         0: estimate the parameter, 1: keep it fixed
21
22
23 ASC\_CAR = Beta('ASC\_CAR', 0, -10, 10, 0)
ASC_TRAIN = Beta ('ASC_TRAIN', 0, -10, 10, 0)
  ASC\_SM = Beta('ASC\_SM', 0, -10, 10, 1)
_{26} B_TIME = Beta('B_TIME', _{0}, _{-10}, _{10}, _{0})
_{27} B_TIME_S = Beta('B_TIME_S', _{9}, _{-10}, _{10}, _{0})
```

```
B_{-}COST = Beta(, B_{-}COST, 0, -10, 10, 0)
   \# Define a random parameter, normally distributed,
   # designed to be used for simulation
31
   omega = RandomVariable('omega')
32
   density = normalpdf(omega)
   B_TIME_RND = B_TIME + B_TIME_S * omega
35
   # Utility functions
36
37
   #If the person has a GA (season ticket) her
38
   #incremental cost is actually 0
39
   #rather than the cost value gathered from the
   \# network data.
                      * ( GA == 0
   SM\_COST = SM\_CO
   TRAIN\_COST = TRAIN\_CO
                             * ( GA == 0
43
44
   # For numerical reasons, it is good practice to scale the data to
   # that the values of the parameters are around 1.0.
46
   # A previous estimation with the unscaled data has generated
   \# parameters around -0.01 for both cost and time.
   # Therefore, time and cost are multipled my 0.01.
50
51
   TRAIN\_TT\_SCALED = \setminus
52
     Define Variable ('TRAIN_TT_SCALED', TRAIN_TT / 100.0)
53
   TRAIN\_COST\_SCALED = \setminus
54
     Define Variable ('TRAIN_COST_SCALED', TRAIN_COST / 100)
55
   SM_TT_SCALED = Define Variable ('SM_TT_SCALED', SM_TT / 100.0)
   SM_COST_SCALED = Define Variable ('SM_COST_SCALED', SM_COST / 100)
   CAR_TT_SCALED = Define Variable ('CAR_TT_SCALED', CAR_TT / 100)
   CAR_CO_SCALED = DefineVariable('CAR_CO_SCALED', CAR_CO / 100)
59
60
   V1 = ASC\_TRAIN + \setminus
61
        B_TIME_RND * TRAIN_TT_SCALED + \
62
        B_COST * TRAIN_COST_SCALED
63
   V2 = ASC\_SM + \setminus
        B_TIME_RND * SM_TT_SCALED + \
65
        B_COST * SM_COST_SCALED
66
   V3 = ASC\_CAR + \setminus
67
        B_TIME_RND * CAR_TT_SCALED + \setminus
68
        B_COST * CAR_CO_SCALED
69
70
   # Associate utility functions with the numbering of alternatives
71
   V = \{1: V1,
72
        2: V2,
73
        3: V3}
74
75
   # Associate the availability conditions with the alternatives
```

```
77
   CAR_AV_SP = Define Variable ('CAR_AV_SP', CAR_AV * (
   TRAIN\_AV\_SP = DefineVariable('TRAIN\_AV\_SP', TRAIN\_AV * (SP')
   0)
80
   av = \{1: TRAIN\_AV\_SP,
81
          2: SM_AV,
82
          3: CAR_AV_SP}
83
   # The choice model is a logit, with availability conditions
85
   integrand = bioLogit (V, av, CHOICE)
86
   prob = Integrate(integrand*density, 'omega')
87
   1 = \log(\text{prob})
88
89
   # Defines an itertor on the data
90
   rowIterator('obsIter')
91
   # Define the likelihood function for the estimation
93
   BIOGEME_OBJECT.ESTIMATE = Sum(1, 'obsIter')
94
95
   \# All observations verifying the following expression will not be
   # considered for estimation
97
   # The modeler here has developed the model only for work trips.
98
   # Observations such that the dependent variable CHOICE is 0
99
   \# are also removed.
   exclude = ((PURPOSE != 1) * (
                                     PURPOSE
                                               != 3 ) + \
101
               (CHOICE = 0) > 0
102
103
   BIOGEME_OBJECT.EXCLUDE = exclude
104
105
   # Statistics
106
107
   nullLoglikelihood(av,'obsIter')
108
   choiceSet = [1,2,3]
109
   cteLoglikelihood(choiceSet,CHOICE, 'obsIter')
110
   availability Statistics (av, 'obsIter')
111
112
   BIOGEME\_OBJECT.PARAMETERS[\ 'Random Distribution'] \ = \ "MLHS"
113
114
   BIOGEME_OBJECT.PARAMETERS['optimizationAlgorithm'] = "BIO"
115
   BIOGEME_OBJECT.FORMULAS['Train utility'] = V1
   BIOGEME\_OBJECT.FORMULAS['Swissmetro utility'] = V2
```

A.9 12estimationMonteCarlo.py

```
# File: 12estimationMonteCarlo.py
  # Author: Michel Bierlaire, EPFL
  # Date: Thu Jul 30 18:33:34 2015
6
  7
   from biogeme import *
   from headers import *
10
   from loglikelihood import *
11
   from statistics import *
12
13
  #Parameters to be estimated
14
  # Arguments:
15
       1 Name for report. Typically, the same as the variable
  #
16
  #
          Starting\ value
17
       3 Lower bound
  #
18
   #
          Upper bound
       4
19
          0: estimate the parameter, 1: keep it fixed
20
21
  ASC\_CAR = Beta(`ASC\_CAR', 0, -10, 10, 0)
22
  ASC\_TRAIN = Beta('ASC\_TRAIN', 0, -10, 10, 0)
23
  ASC\_SM = Beta(,ASC\_SM,0,-10,10,1)
  B_{\text{TIME}} = \text{Beta}('B_{\text{TIME}}', 0, -10, 10, 0)
  B_{\text{TIME\_S}} = \text{Beta}(,B_{\text{TIME\_S}}, 9, -10, 10, 0)
  B_{-}COST = Beta('B_{-}COST', 0, -10, 10, 0)
27
  # Define a random parameter, normally distirbuted, designed to be used
29
  # for Monte-Carlo simulation
30
  B_TIME_RND = B_TIME + B_TIME_S * bioDraws('B_TIME_RND')
31
  # Utility functions
33
34
  #If the person has a GA (season ticket) her incremental cost is actually 0
35
   #rather than the cost value gathered from the
  \# network data.
37
  SM\_COST = SM\_CO
                      * ( GA == 0
38
                           * ( GA == 0
  TRAIN\_COST = TRAIN\_CO
  # For numerical reasons, it is good practice to scale the data to
41
  # that the values of the parameters are around 1.0.
42
  # A previous estimation with the unscaled data has generated
  \# parameters around -0.01 for both cost and time. Therefore, time and
  # cost are multipled my 0.01.
45
46
  TRAIN_TT_SCALED = DefineVariable('TRAIN_TT_SCALED', TRAIN_TT / 100.0)
  TRAIN_COST_SCALED = DefineVariable ('TRAIN_COST_SCALED', TRAIN_COST / 100)
48
  SM_TT_SCALED = DefineVariable('SM_TT_SCALED', SM_TT / 100.0)
49
  SM_COST_SCALED = Define Variable ('SM_COST_SCALED', SM_COST / 100)
50
  CAR\_TT\_SCALED = DefineVariable(`CAR\_TT\_SCALED', CAR\_TT / 100)
```

```
CAR_CO_SCALED = Define Variable ('CAR_CO_SCALED', CAR_CO / 100)
53
   V1 = ASC\_TRAIN + B\_TIME\_RND * TRAIN\_TT\_SCALED + B\_COST * TRAIN\_COST\_SCALED
   V2 = ASC\_SM + B\_TIME\_RND * SM\_TT\_SCALED + B\_COST * SM\_COST\_SCALED
55
  V3 = ASC\_CAR + B\_TIME\_RND * CAR\_TT\_SCALED + B\_COST * CAR\_CO\_SCALED
56
57
  # Associate utility functions with the numbering of alternatives
58
  V = \{1: V1,
59
        2: V2,
60
        3: V3}
61
62
  # Associate the availability conditions with the alternatives
63
64
  CAR_AV_SP = DefineVariable('CAR_AV_SP', CAR_AV * ( SP
  TRAIN_AV_SP = DefineVariable('TRAIN_AV_SP', TRAIN_AV * ( SP
66
     ))
67
   av = \{1: TRAIN\_AV\_SP,
68
         2: SM_AV,
69
         3: CAR\_AV\_SP
70
71
  # The choice model is a logit, with availability conditions
72
  prob = bioLogit (V, av, CHOICE)
73
   l = mixedloglikelihood(prob)
74
75
   # Defines an itertor on the data
76
   rowIterator('obsIter')
77
78
  # Define the likelihood function for the estimation
79
  BIOGEME_OBJECT.ESTIMATE = Sum(1, 'obsIter')
80
81
   # All observations verifying the following expression will not be
82
   # considered for estimation
   # The modeler here has developed the model only for work trips.
84
   # Observations such that the dependent variable CHOICE is 0 are also removed.
85
   exclude = ((PURPOSE != 1) * (PURPOSE != 3) + (CHOICE == 0)) > 0
87
  BIOGEME_OBJECT.EXCLUDE = exclude
88
89
   # Statistics
90
91
   nullLoglikelihood (av, 'obsIter')
92
   choiceSet = [1,2,3]
93
   cteLoglikelihood (choiceSet,CHOICE, 'obsIter')
   availabilityStatistics(av,'obsIter')
95
96
  BIOGEME_OBJECT.PARAMETERS[', NbrOfDraws', ] = "2000"
97
  BIOGEME_OBJECT.PARAMETERS['RandomDistribution'] = "MLHS"
```

```
BIOGEME_OBJECT.PARAMETERS['optimizationAlgorithm'] = "BIO"
BIOGEME_OBJECT.DRAWS = { 'B_TIME_RND': 'NORMAL' }
BIOGEME_OBJECT.FORMULAS['Train utility'] = V1
BIOGEME_OBJECT.FORMULAS['Swissmetro utility'] = V2
BIOGEME_OBJECT.FORMULAS['Car utility'] = V3
```

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