Advanced LCA PhD course

Aalborg 2022

Module 2 - Stochastic LCA

Learning objectives

Knowledge

At the end of the course you will know about: python data structures, python scientific environment, Brightway2 data structures, Brightway2 functions, key concepts of statistical analysis for LCA (error propagation, statistical testing, variance-based sensitivity indicators).

Skills

At the end of the course you will be able to: program in python at a basic level, use Brightway2 at a level comparable to other commercial LCA software, including importing foreground and background data into Brightway2, running calculations from a simple LCA to more complex simulations and comparative analyses, perform statistical analysis of LCA results, perform local and global sensitivity analysis of LCA results.

Competences

At the end of the course you will be in a position to: apply LCA modelling in Brightway2 to your research questions, by choosing the appropriate data, code, and workflow organisation that solve the case-specific challenges.

Day one

Lecture: Why do we need LCA software? Brush up on computational structure of LCA and a simple LCA in Brightway2.

Brightway2 resources

- Brightway2 official website https://2.docs.brightway.dev/ contains info about installation and key features, and example jupyter notebooks
- On Stackoverflow one can ask questions, give answers, and find answers about Brightway2 using the tag `brightway`
- Brigtway2 source code to understand in detail all Brightway2 functions and contribute to the software development.

A product system from scratch (Notebook 0 and Notebook 1)

First of all we brush up the basic computational structure of LCA using matrix algebra, and we use python to do the calculations so that you get familiar with the bumpy package. The notebook **0-LCI-matrix.ipynb** contains an example reproducing the product system described in Heijungs and Suh (2002).

Heijungs, R., & Suh, S. (2002). The basic model for inventory analysis. In A. Tukker (Ed.), The computational structure of Life Cycle Assessment (pp. 11–28). London: Kluver Academic Publisher.

Then we reproduce the same example in Brightway2 to understand how the Brightway2 syntax works. The most important data structures are represented here and described here. Look at the figure and try to make the parallel with what you know already (e.g. Simapro). I recommend that later you read carefully this documentation page. This is also the terminology to use when working with Brightway2.

The notebook **1-Simple-LCA.ipynb** contains the code for creating manually a Brightway2 database and run calculations, we will read it together and understand how such database is structured and written, as well as alternative ways to obtaining the same result but with different database structures. This means that we will also touch on python-specific data structures (list, tuple, dictionary) and objects (variable, function, class).

A note on co-products

There are at least two ways do model co-products with the substitution method. Besides the exchange types `'technosphere'`, `'biosphere'`, and `'production'` there is a fourth type called `'substitution'`. You can use that (use **plus** sign!). See the docs about exchanges. Alternatively, you can simply create an exchange of the `'technosphere'` type but using the **minus** sign. I.e. a negative input of some product. This is similar to e.g. SimaPro where there are two options: either use the predefined line for co-products or insert a negative input from technosphere.

The signs issue is explained very clearly in the introduction docs under “Getting the signs right”. Note that this is perfectly consistent with the Hejiungs and Suh (2002) book chapter. Diagonal values in the A matrix are positive, off-diagonal inputs are negative. Intervention matrix signs depend on the convention (you decide the sign or you have to follow the convention used of the database, e.g. the database may assume that +10 kg CO2 means the emission of CO2 and +10 kg crude oil means the extraction of oil).

To use the **partitioning method** one needs to calculate the allocated values (by mass/energy/revenue etc)

for each exchange before importing the data into Brightway2 (or write a code that does that automatically), just like in e.g. SimaPro.

Managing Brightway2 Projects

The notebook **Project create and locate.ipynb** (courtesy of Romain Sacchi) is for self-study and helps you setting a project and finding where brightway saves data on your computer.

Lecture: Getting around in Brightway2. Navigating product systems. Importing background and foreground data.

Navigate safely the Brightway2 labyrinth (Notebook 2)

When doing an LCA one needs to access the various activities and look at them to understand what are their inputs and outputs and how they are linked to other activities. The script **2-Navigate.ipynb** includes code to do this in different ways.

Get ecoinvent (Notebook 3)

Now that you know how to work with the foreground system, it's time to learn how to work with the background system. In particular it is useful to import and play around with two databases: *biosphere3* that contains all the exchanges and impact assessment methods, and *ecoinvent*. The notebook **3-Ecoinvent.ipynb** shows how to import biosphere3 and ecoinvent.

A key difference compared to the previous lecture is that in ecoinvent each activity and exchange is defined by a **code** which is a unique identifier. So when navigating ecoinvent it is important to learn how to find both activity code and name and how to match them *(Actually we used the codes also in the previous lectures but they were identical to the activity names for simplicity)*.

Some preparation to make the notebook work:

1. Open the ecoinvent website and login with the username and password you got via mail.
2. You should read somewhere: *To download LCI and LCIA cumulative matrices click here*. Click there.
3. Select *ecoinvent 3.6*
4. Download the file `ecoinvent 3.4_consequential_ecoSpold02.7z` in a folder of yours. Make sure you remember the full path to this directory. E.g. I have downloaded the file in: */Users/massimo/Documents/Databases/ecoinvent v3.6*
5. The file you have downloaded is a compressed archive of many files (like with winzip or winrar). Extract the files from the .7z archive, e.g. by double clicking it. If it does not work, install a software that can do that. E.g. for mac users you can either download theunarchiver or, if you are using brew, just

open terminal and do `brew install p7zip` and then from terminal find the folder and do `7z x 'ecoinvent 3.6_consequential_ecoSpold02.7z'` (here the p7zip instructions in case).

6. Now you can run the script **3-Ecoinvent.ipynb**. Make sure you change the path line and replace it with the one where you have extracted the files. For example, I have extracted the files in a folder called "datasets". The path to this folder is: */Users/massimo/Documents/Databases/ecoinvent v3.6/datasets/* You will see this same line in the script and you need to change it with your directory.

Importing data from Excel (Notebook 4)

Brightway2 has a series of options for data import and export that you are invited to read about and try, they are on the official website and notebook.

However, you can also developed your own importer, that fits with your workflow. For example, the file `lci_to_bw2.py` includes a code to convert a properly formatted csv file into a Brightway2 database dict. You need to install the Python Data Analysis Library pandas to make it work (within your virtual environment, run `conda install pandas` or `pip install pandas` if you are not using conda).

How does this importer work?

1. Prepare your inventory in MS Excel using the template. See the example file *test_db_excel_w_ecoinvent.xlsx*
2. Save the relevant MS Excel sheet as .csv file, see the example file *test_db_excel_w_ecoinvent.csv*
3. Import the module in your script with the command `from lci_to_bw2 import *`
4. Import the .csv file as a dataframe with the pandas function `.read_csv()`. Clean it up for unnecessary columns.
5. Convert the dataframe into a dict using the function `lci_to_bw2()`
6. Save the dict as a Brightway2 database in the usual way i.e. using Brightway's `Database()` and `.write()` functions.

See an example in the Notebook **4-Excel-import.ipynb**.

NOTE: this importer contains no automated tests so you need to make sure manually that the excel and csv files are in good order.

Exercise: Building an example product system in Brightway2.

Take the product system provided in the **Heat-production-exercise.pdf** and convert it into a Brightway database writing by hand the dict structure. Run the calculations on that to calculate the total life-cycle emissions of Carbon dioxide for a demand of 10000 MJ heat from the market for heat. Notebook and data will be provided on the lecture day.

Day two

Lecture: Uncertainty analysis with Monte Carlo Simulation in Brightway2. Comparative uncertainty analysis and statistical testing of the results.

Uncertainties and Monte Carlo simulation (Notebook 5 and Notebook 6)

Now we are ready to start doing more intense simulations. In particular Brightway2 is great to perform fast error propagation with Monte Carlo simulation.

The Notebook **5-Monte-Carlo.ipynb** shows how to add uncertainties to your home-made product system and run a Monte Carlo simulation. To better understand this script, I recommend reading read the paper by Limpert et al. (2001), that is a 'classic' and explains the log-normal distribution.

Limpert, E., Stahel, W. A., & Abbt, M. (2001). Log-normal distributions across the sciences: Keys and clues. Bioscience, 51(5), 341-352. https://doi.org/10.1641/0006-3568(2001)051[0341:lndats]2.0.co;2

The Notebook **6-Comparative-Monte-Carlo.ipynb** shows how to perform a more advanced comparative Monte Carlo simulation. This script shows how to perform a more advanced comparative Monte Carlo simulation. This is the kind of simulation to be used in comparative LCAs, i.e. in analyses where different alternatives to provide the same Functional Unit are compared.

In this comparative case it is important to randomly sample a common technology matrix **A** for all alternatives at each iteration, instead of having a different technology matrix per each alternative at each iteration. This allows for a smaller variance and shorter computational times, but is not possible with e.g. SimaPro. Moreover, this allows to optimally perform the statistical testing of the results with paired tests, to see if the two alternatives are significantly different from each other or not.

To better understand this script, I recommend reading read the paper by Henriksson et al. (2015) which is probably the best example of an LCA with comparative Monte Carlo simulation followed by statistical testing for significant differences between alternatives.

Henriksson, P. J. G., Rico, A., Zhang, W., Ahmad-Al-Nahid, S., Newton, R., Phan, L. T., … Guinée, J. B. (2015). Comparison of Asian Aquaculture Products by Use of Statistically Supported Life Cycle Assessment. Environmental Science and Technology, 49(24), 14176-14183. https://doi.org/10.1021/acs.est.5b04634

Lecture: Sensitivity analysis in Brightway2. Local (OAT)

sensitivity analysis and Global sensitivity analysis.

Using Brightway2 for sensitivity analysis (Notebook 7 and Notebook 8)

The simplest case of sensitivity analysis is the One At the Time (OAT) Sensitivity analysis. Also called a *local* Sensitivity analysis. One parameter is changed by keeping all the other constant and the difference in results is compared to the change. This allows to investigate how much results are affected by the specific change in the parameter.

The notebook **7-OAT-sensitivity-analysis.ipynb** shows various examples of local sensitivity analysis. The notebook also introduces to the use of Brightway2 parameters. Check also this good tutorial about the use of parameters in Brightway2, as well as some theory on what type of parameters (activity-, database-, or project-parameters) one can define in Brightway2. The notebook contains just a simple example of use of parameters but operational in the context of sensitivity analysis.

OAT is good for some types of analysis, but has some problems. The main issue is that the effect of a change in the parameter might be different when other parameters assume different values...so OAT can be misleading! This problem can only be solved with a global sensitivity analysis.

Global sensitivity analysis is a more complex case. Involves varying multiple parameters together and understanding which of these parameter has the largest influence on the results of the model. This involves a large simulation testing the various combinations of values for the different parameters. One could use brute force and test all possible combinations of all parameters, and then run a regression on the results where the dependent variable is the impact value and the independent variables are the parameters. However, calculating a result for every possible combination might end up taking too much computation time, especially if the number of tested variables is high.

Therefore, in the notebook **8-Global-sensitivity-analysis.ipynb** we use the python library SALib which is made for global sensitivity analysis and allows to calculate sensitivity indices to quantify the sensitivity of model results to different parameters. Also in this case the analysis is implemented in Brightway2 using a simple example of a parametrised Brightway2 database. In particular we use Saltelli and Borgonovo indices to explain model variance and total model output respectively.

For further understanding on how the Saltelli sampling method works, and how to correctly interpret the Sobol indices, refer to Chapter 4: *Variance based methods* in Saltelli (2008). Otherwise check the wikipedia page on variance-based sensitivity analysis which contains a reasonably good summary on Sobol indices and the Saltelli sampling method.

You can read more about the Delta index in Borgonovo (2007) as well as about how it is implemented in Salib as *Delta Moment-Independent Measure* and you can see an application in GSA for LCA models in Blanco et al. (2020).

Blanco, C.F., Cucurachi, S., Guinée, J.B., Vijver, M.G., Peijnenburg, W.J.G.M., Trattnig, R., Heijungs, R.,

2020. Assessing the sustainability of emerging technologies: A probabilistic LCA method applied to advanced photovoltaics. J. Clean. Prod. 259, 120968. doi:10.1016/j.jclepro.2020.120968

Borgonovo, E., 2007. A new uncertainty importance measure. Reliab. Eng. Syst. Saf. 92, 771–784. doi:10.1016/j.ress.2006.04.015

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., Tarantola, S., 2008. Global Sensitivity Analysis. The Primer, Global Sensitivity Analysis. The Primer. doi:10.1002/9780470725184

Exercise: Exercise on modifying background database for sensitivity

In this exercise we make OAT sensitivity analysis on the background database by modifying this directly. A notebook example will be provided on the lecture day.

Day three

Includes group-exercises to be done in class.

Exercise: A reproducible and working version of the case study in Brightway2.

Prepare your own product system in excel, linked to biosphere3 and ecoinvent, and import it. Run calculations to see if it works as expected. Send all the code and data to another group and see if they can reproduce your results, in that case, the exercise will be a success. Get feedback from other group on your code and what difficulties they had in reading and running it.

Exercise: comparative uncertainty analysis on the case study.

Run the comparative Monte Carlo simulation on your case study product system and investigate if two alternatives give significantly different results. If you don't have data for multiple alternatives, you can create two versions of your product system changing one background product flow (e.g. using a different electricity mix).

Exercise: sensitivity analysis on the case studies.

Reflect about possible source of variance for your case study. Which activities are you unsure about? Are you in doubt about the type of activity used, or about the value used? Which activities do you expect to affect the results? Formulate some hypotheses based on your expectations and your understanding of your product system case. Then select the relevant parameters that could help you test these hypotheses and identify how sensitive are the results of your case study to these. Finally quantify this influence and rank the parameters based on their influence on the results.

Additional notes on this module

Brightway2 workflow

Working with Brightway2 allows to automate and speed up stuff, but there is still a lot of manual work when doing LCA. Also, LCA is really iterative as often you find a small mistake and you need to correct the data and re-do the calculations, or you want to add a scenario, or repeat the analysis with different data, etc. This means that you have several **iterations** before you get the final results. It also means that you may want to speed up each iteration, and be able to reproduce everything after some months (e.g. if you have submitted a paper) so the stuff should be well-organised.

The ideal workflow depends on your needs and your current skills, but you should expect to use different tools. For example, in a current project of mine I have this workflow:

1. I organise the foreground system in MS Excel. I prepare one or more MS Excel spreadsheets with multiple calculation sheets that ultimately allow building the foreground inventory in the right format for later use in Brightway2 (see chapter about import from Excel). Every time I modify something, I export a new .csv file with the inventory.

2. I use Brightway2 for the LCA calculation and MC simulation. I import the inventory in .csv, run a python script with the calculations, and export the results the results in a tabular format, e.g as another .csv file with the LCIA results. At each iteration I simply run the script again, or modify it if necessary.

3. I use R for the statistical analysis and plots. For example I import the .csv file with the LCIA data, run the R script, and export either some new tables in .csv (e.g. p-values from the statistical tests) or the plots as .pdf files. Also in this case I can simply run the script again at each iteration, or modify it if necessary.

This works for me, might not work for you though. It's something you need to try out.

Resources to understand LCA statistics

When applying a statistical approach to LCA, there are some key concepts that is important to understand in detail: distribution types, error propagation, statistical testing. If you are new to statistics, a first step is reading the wikipedia pages explaining Monte Carlo method, general statistical hypothesis testing, parametric and nonparametric statistics, normality tests, t-test, Wilcoxon signed-rank test. When

implementing this in Brightway2, it is then useful to read the corresponding python documentation for statistical functions of the stats package. For example the following functions were used in the Notebook **6-Comparative-Monte-Carlo.ipynb**: Shapiro-Wilk test, paired t-test, and Wilcoxon signed-rank test.

If you want to learn more, buy a good introductory statistics book. Ideally one which has a good balance between mathematical expressions and pedagogic explanations. There are also many open source or free ones, I can recommend e.g. Statistics which explains testing in general and it's written in a way which is easy to understand, The Elements of Data Analytic Style which introduces to data analysis in general, and Statistical inference for data science which is is very practical and especially useful if you also know R.

In general I would encourage to learn R too if you plan to work with stats - I prefer it to python for doing statistical analysis and also for plots (just personal taste).

Beyond this course, the Brightway2 potential

Sometimes we don't do things because we don't even know that it is possible to do these things, or that they exist. Similarly, there is really a lot of unexplored potential in Brightway2. I will mention just a few things:

- There are many ore import **strategies** to automate the import of data into Brightway2. I am not very good at using them but these can potentially simplify the workflow and reduce the manual work substantially.
- It is possible to work with geographies and time-specific inventories. Thus allowing for **spatially and temporally** differentiated LCA results, building maps, etc.
- In general one can combine all the python possibilities with Brightway2, e.g. the fact that one can take real-time data directly from the web and use them in a LCA to do real-time measurements.

You are welcome to try these things out.

Acknowledgements

I hope you enjoyed this course module.

Thanks to Romain Sacchi and Chris Mutel for helping me solving my Brightway2 problems so far. Some pieces of the code they wrote in response to my questions and queries ended up within the scripts provided in this course, so indirectly they are contributors. Romain also checked the scripts and wrote specific ones.