The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA

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ABSTRACT

LCA, even when modeled in the traditional way with linear equations, may show strong non-linear sensitivities. Well-developed tools from matrix perturbation theory may be employed to investigate LCA systems for the presence and location of such extreme sensitivities. This knowledge is useful for stability analysis, error analysis and for detecting and resolving round-off problems in the computations.

INTRODUCTION

It is well known that models that comprise highly non-linear functions may exhibit a large sensitivity with respect to the dependency of output on input. For instance, when a modeled relationship is based on the tangent of a certain input coefficient, say

$$y = \tan x$$

changing the input from $x = 1.5$ to $x = 1.55$ will result in a change of output from $y = 14$ into $y = 48$.

Since the advent of chaos theory in the eighties, a similar phenomenon has been observed for models with weak non-linearities. One famous example is the system of three differential equations

$$\dot{x} = s(y - x)$$
$$\dot{y} = x(r - z) - y$$
$$\dot{z} = xy - bz$$

originally due to Lorenz, which gives rise to what has become known as sensitive dependence on initial conditions. This means that a certain initial state (x_0, y_0, z_0) will develop into a completely different trajectory than a slightly different initial state, say $(x_0+\delta x, y_0, z_0)$.

A discussion of non-linear models and chaos theory is not an obvious thing in the context of LCA. After all, LCA, in its most typical form, deals with simplified linear models, and linear models are not expected to show extreme sensitivities. A simple example will show, however, that sensitive dependence on initial conditions may also show up in a linear LCA model.

This paper addresses such questions as:

- how do sensitivities in LCA arise?
- can we predict from a given LCA-system if it exhibits sensitivities, and at what places?
- can we develop diagnostic measures that warn us for potential sensitivities?

It will be based on theoretical arguments, but extensions to real-world situations are included as well. Most of the features discussed are included in CMLCA [1].

A SIMPLE BUT SENSITIVE LCA SYSTEM

Suppose that the topic of analysis is aimed at the delivery of 1000 kWh of electricity, and that we study a very small product system that consists of only two unit processes: electricity production and fuel production. The process specification is as follows:

- process 1, electricity production, produces 10 kWh electricity with an input of 2 liter of fuel and a CO_2-emission of 1 kg;
- process 2, fuel production, produces 100 liter fuel with an input of 498 kWh electricity and a CO_2-emission of 10 kg.

With an LCA-program that is sufficiently smart to deal with systems with recursive flows, the system-wide CO_2-emission is calculated to be 30.000 kg.

It turns out that this result is highly dependent on the coefficient 498, the amount of kWh of electricity that is needed to produce 100 liter of fuel. If we have mismeasured this coefficient as 499, the resulting CO_2-emission will be 60.000 kg. In other words: a change of one coefficient by 0.2% and keeping the other five coefficients unchanged, induces a change of the variable of interest by 100%! And, note well, in an LCA-setup that is linear.

ANALYSIS OF THE SENSITIVITY

A first question that we may ask is: how can this be? How can a simple linear system exhibit a strong non-linear response to changes in parameters?

An answer starts with the observation that, even though processes are scaled in LCA in a linear way, the final equation that displays how the CO_2-emission depends on the systems' coefficients is non-linear. Straightforward mathematics [2:102] provides an expression for the CO_2-emission of the form

$$CO_2 = \frac{100 \times 1000 \times 1 + 2 \times 1000 \times 10}{-2 \times 498 + 10 \times 100} = 30.000$$

Especially the fraction

$$\frac{1}{-2 \times 498 + 10 \times 100}$$

plays a central role in the extreme sensitivity. In the present form, it is 0.25, but when 498 is changed into 499, it is doubled to 0.5. Thus, even though the formulation of the system is with linear equations, the solution of these equations is non-linear. This is in a certain sense comparable to the example of the chaotic system by Lorenz: even though the equations that describe the system are only weakly non-linear, the solution to these equations is strongly non-linear.

The strong non-linear character of the relationship between a technology coefficient and the system-wide CO_2-emission is shown in Figure 1.

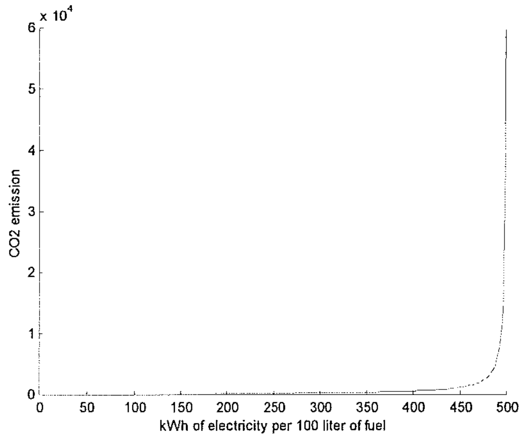

Figure 1. Dependence of the system-wide CO_2-emission as a function of the coefficient that indicates the amount of electricity needed for the production of fuel.

FORMULATION IN MATRIX TERMS

We may formulate the problem of finding the system-wide CO_2-emission in matrix form [2:11]. We introduce a matrix with the coefficients within the technical system:

$$\mathbf{A} = \begin{pmatrix} 10 & -498 \\ -2 & 100 \end{pmatrix}$$

and the matrix of coefficients with exchanges with the environment:

$$\mathbf{B} = \begin{pmatrix} 1 & 10 \end{pmatrix}$$

Notice that rows indicate flows: flows of products and materials in **A** (here electricity and fuel), and elementary flows in **B** (here CO_2), and that columns in both matrices indicate processes. Also notice that some coefficients are negative, to indicate that they represent input flows to a process.

The delivery of 1000 kWh of electricity may be written as a vector

$$\mathbf{f} = \begin{pmatrix} 1000 \\ 0 \end{pmatrix}$$

The variable of interest is a vector of environmental interventions, which is in this case a degenerate vector of only one row:

$$\mathbf{g} = \begin{pmatrix} ? \end{pmatrix}$$

The purpose of LCI is of course to find out which number will be placed at the position of the question mark.

To that aim, the materials balance principle and matrix algebra can be combined to give an explicit formula [2:19]:

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f}$$

where the superscript –1 denotes that matrix **A** is to be inverted. Matrix inversion is a well-defined mathematical operation of which the details go beyond this paper. It can be regarded as a kind of generalization of the ordinary division. And, like dividing by zero produces ill-defined results, inversion of a matrix that has a property called the determinant equal to zero produces ill-defined results as well. Such a matrix is said to be singular, and a matrix that is close to singular is a topic of concern. There exists a large literature on such matrices. It is the purpose of the next section to explore some aspects of this literature.

MATRIX PERTURBATION THEORY

Matrix perturbation theory [3] addresses questions related to the effects of perturbing one or more coefficients of a matrix equation. Applied to the case of LCA, a question to address would be: given the equation

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f}$$

how do the elements of **g** change if one or more of the elements of **A** or **B** change by a specified amount? And in the concrete example given, can we predict from

$$\mathbf{A} = \begin{pmatrix} 10 & -498 \\ -2 & 100 \end{pmatrix}$$

how **g** changes if the number –498 is changed into –499?

To this aim, matrix perturbation theory has developed a number of diagnostic measures. One of the most important of these is the condition number, often indicated as κ. The condition number of a matrix can be regarded as a worst-case indicator of the sensitivity of the result of a matrix inversion to a perturbation of the coefficients of the matrix itself. The condition number of the above matrix is approximately 65,000, hence changing a coefficient by 1% may at most induce a change in result by 65,000%. The change of 498 into 499 results in doubling, so the amplification of the perturbation is approximately 500 times. Not as dramatic as 65,000, but still quite a lot. Anyhow, it shows that a worst-case diagnostic measure may warn us for ill-conditioned systems that require a closer stability study. The condition number warns us also for the intrinsic computational dangers of introducing round-off errors in doing LCA [2:148].

AN ANALYTICAL TREATMENT

We can also conceive more refined diagnostic measures of stability. An important approach starts with the identification of certain local derivatives. In the theory of non-linear dynamics, the Jacobian matrix serves such purposes. The Jacobian is a matrix that contains terms such as

$$\frac{\partial \dot{x}}{\partial y}$$

For the case of the Lorenz system, given in the introduction, we have nine such derivatives, arranged in the Jacbian given by

$$\frac{\partial(\dot{x},\dot{y},\dot{z})}{\partial(x,y,z)} = \begin{pmatrix} -s & s & 0 \\ r-z & -1 & -x \\ y & y & -b \end{pmatrix}$$

When evaluated at a certain point (x, y, z), it provides insight into several stability issues: Lyapunov exponents, dissipating properties, and other characteristics of interest for dynamic systems.

For the linear case of LCA, the derivatives of interest are

$$\frac{\partial g_k}{\partial a_{ij}}$$

and

$$\frac{\partial g_k}{\partial b_{ij}}$$

These derivatives may be arranged into two sets of matrices:

$$\frac{\partial g_k}{\partial \mathbf{A}} = \begin{pmatrix} \frac{\partial g_k}{\partial a_{11}} & \frac{\partial g_k}{\partial a_{21}} & \cdots \\ \frac{\partial g_k}{\partial a_{12}} & \frac{\partial g_k}{\partial a_{22}} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}$$

and a similar matrix for the derivative of the intervention with respect to **B**.

Elementary linear algebra allows the explicit calculation of these quantities, although the expressions obtained may look complicated. For instance [2:135],

$$\frac{\partial g_k}{\partial a_{ij}} = -\sum_{l} b_{kl}\left(\mathbf{A}^{-1}\right)_{li}\sum_{m}\left(\mathbf{A}^{-1}\right)_{jm} f_m$$

and

$$\frac{\partial g_k}{\partial b_{ij}} = \begin{cases} \sum_{m}\left(\mathbf{A}^{-1}\right)_{jm} f_m & \text{if } i = k \\ 0 & \text{otherwise} \end{cases}$$

We can use these equations for every combination of i, j and k, and create a table of sensitivity coefficients. Moreover, we can adjust the formula to derive relative coefficient instead of absolute coefficients, e.g.,

$$\frac{a_{ij}}{g_k}\frac{\partial g_k}{\partial a_{ij}}$$

instead of

$$\frac{\partial g_k}{\partial a_{ij}}$$

Arrangement of the relative coefficients in a table then yields

$$\mathbf{\Gamma}_k(\mathbf{A}) = \begin{pmatrix} \frac{a_{11}}{g_k}\frac{\partial g_k}{\partial a_{11}} & \frac{a_{21}}{g_k}\frac{\partial g_k}{\partial a_{21}} & \cdots \\ \frac{a_{12}}{g_k}\frac{\partial g_k}{\partial a_{12}} & \frac{a_{22}}{g_k}\frac{\partial g_k}{\partial a_{22}} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}$$

and a similar table for the dependency on **B**.

In the example, we find

$$\mathbf{\Gamma}_1(\mathbf{A}) = \begin{pmatrix} -250 & 249 \\ 249 & -249 \end{pmatrix}$$

and

$$\mathbf{\Gamma}_1(\mathbf{B}) = \begin{pmatrix} 0.83 & 0.17 \end{pmatrix}$$

This shows that the sensitivities in the matrix of coefficients within the technical system (**A**) is much larger than that in the matrix of coefficients with exchanges with the environment (**B**). In fact, all coefficients in $\Gamma_1(\mathbf{B})$ are between −1 and 1, which means that they have a moderating influence on pertubations. The tremendous values of order 250 means that small perturbations are amplified with a factor of 250.

NEW SUMMARY MEASURES

The condition number provides a single-number worst-case indicator of the stability of a matrix system. It may well overestimate the instability by many orderd of magnitude. On the other hand, the matrices introduced above provide tableaus of numbers with at least locally exact indicators. But these matrices may in real case studies be so huge that one can never oversee them in full.

There seems to be a need for a compromise: exact numbers but not so many. One obvious candidate for such new measures of stability is a selection of the exact indicators developed above. If we single out the highest one, or the five highest ones, or the percentage of indicators above 1, we may well have found a workable compromise.

Thus, for instance, we could propose to use

$$\gamma_k^{\max} = \max_{i,j}\left(\left|\Gamma_k(a_{ij})\right|, \left|\Gamma_k(b_{ij})\right|\right)$$

or, even more aggregated,

$$\gamma^{\max} = \max_{i,j,k}\left(\left|\Gamma_k(a_{ij})\right|, \left|\Gamma_k(b_{ij})\right|\right)$$

as a sensitivity indicator that is more exact than the condition number, but still single-valued. In the above example, it assumes the value of 250.

UNCERTAINTIES AND THEIR PROPAGATION

Closely related to these stability measures is the topic of uncertainty analysis. The topic of error propagation [4] is well-studied and provides a useful basis for uncertainty analysis in LCA.

If a functional relationship is given as a mathematical relation between two inputs (x and y) and one output (z), say

$$z = f(x, y)$$

the theory of error propagation gives approximation for Δz as a consequence of Δx and Δy. Let us assume that the uncertainty in the data is specified as a standard deviation σ. Then we have, when the uncertainties in x and y are independent

$$\sigma_z^2 = \left(\frac{\partial f}{\partial x}\right)^2 \sigma_x^2 + \left(\frac{\partial f}{\partial y}\right)^2 \sigma_y^2$$

Translating this general result to the case of LCA, we have [2:144]

$$\sigma^2(g_k) = \sum_{i,j}\left[\left(\frac{\partial g_k}{\partial a_{ij}}\right)^2 \sigma(a_{ij})^2 + \left(\frac{\partial g_k}{\partial b_{ij}}\right)^2 \sigma(b_{ij})^2\right]$$

where the expressions for the partial derivatives have been given in a previous section.

It is not surprising that uncertainty and sensitivity are related. If we realize that uncertainties in only one a_{ij} propagate via

$$\sigma(g_k) = \left(\frac{\partial g_k}{\partial a_{ij}}\right)\sigma(a_{ij})$$

and that independent uncertainties as variances, hence as squared standard deviations, we easily make the connection.

ANALYTICAL VERSUS NUMERICAL METHODS

The above expressions for sensitivity and uncertainty analysis are clear example of analytical methods: they are based on explicit algebraic manipulation. An important alternative for analytical methods are numerical methods. We will first illustrate numerical approaches towards sensitivity and uncertainty analysis and finally discuss some advantages and disadvantages.

In the case of the perturbation-theoretic coefficients we approximate the derivative as follows:

$$\frac{\partial g_k}{\partial a_{ij}} \approx \frac{g_k(a_{ij} + \varepsilon) - g_k(a_{ij})}{\varepsilon}$$

with a small value, say 0.001, for ε [2:182]. For the uncertainty analysis, we apply a Monte Carlo method. Here, a number of N realizations of the systems is made, each with a new set of stochastic parameters. For each realization, the interventions are calculated. This yields a series of intervention results,

$$\left\{\mathbf{g}^1, \mathbf{g}^2, \ldots, \mathbf{g}^N\right\}$$

and all sorts of statistical characteristics may be abstracted from this sample: the mean, the standard deviation, the range, and other distributional features [2:182].

So, there are two main ways of achieving sensitivity and uncertainty results: analytical and numerical. The question is which one to use. Numerical approaches are easy to understand and easy to implement. But, especially for large systems, they require much more computer time than analytical solutions. To give an idea: perturbation coefficients of the ETH3-database on the basis of an analytical method takes a few minutes, while a numerical approach requires several hours. A similar argument applies to uncertainty calculations, where the number of Monte Carlo runs may well be 1000.

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