SUPPORTING INFORMATION FOR:

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Critical Analysis of the Path-Exchange Method for Hybrid Life-Cycle Assessment

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Summary

This document formalizes the mathematical definitions for Input-Output Analysis and Process-based Life-Cycle Assessment (LCA), detailing their integration into Hybrid LCA via concordance and adjacency matrices. It critically examines the path-exchange method, correcting its historical lineage to originating with Bullard and Seeman rather than with Defourny. It also includes an excerpt from the thesis of Seeman, which constitutes the earliest identified description of the path-exchange method. Finally, this supplement distinguishes the specific definitions of *structural path analysis* within economic versus environmental contexts and concludes with the queries used for the systematic literature review of case studies applying the path-exchange algorithm.

Contents

1 Mathematical Definitions and Notation

1.1 Computational Structure of Input-Output Analysis

Leontief developed the framework for economic input-output analysis in the 1930s, for which he received the Nobel Memorial Prize in Economic Science in 1973 [1]. From the 1960s, Leontief and others extended this framework to account for the interaction of the economy and the environment [2, Sec.13.1]. In this notation, we can represent the interaction of a sector of the economy with all other sectors of the economy as a vector in linear space. The bases for these vector spaces are

$$\{\vec{b}_1, \vec{b}_2, \dots, \vec{b}_N\} \tag{SI-1}$$

$$\{\vec{b}_1, \vec{b}_2, \dots, \vec{b}_R\} \tag{SI-2}$$

where

$$\begin{aligned} \vec{b}_i &\dots \text{basis vector of economic sector } i \\ \vec{b}_j &\dots \text{basis vector of environmental burden } j \\ i \in \mathbb{N}, \text{for } (1 \leq i \leq N) &\dots \text{sector of the economy} \\ j \in \mathbb{N}, \text{for } (1 \leq i \leq R) &\dots \text{environmental burden} \end{aligned}$$

Economic flows between sectors are usually compiled for a basis period of one year with flows in economic units (eg. USD) for reasons of convenience. We now assume that inter-industry flows z_{ij} from sector i to j for a given period depend entirely on the total output x_j of sector j for that same time period [2, Sec. 2.2.2]. This is known as the *proportionality assumption.* With this assumption, we can define fixed ratios $a_{ij} = z_{ij}/x_j$, termed *technical coefficients.* These allow us to write for the total output x_i of sector i associated with an arbitrary final demand f_i

$$x_1 = \left(\frac{z_{11}}{x_1}\right)x_1 + \left(\frac{z_{12}}{x_2}\right)x_2 + \dots + \left(\frac{z_{1n}}{x_n}\right)x_n + f_1 \tag{SI-3}$$

$$= a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n + f_1 \tag{SI-4}$$

where

$$\begin{aligned} f_i[\$] &\dots \text{(exogenous) final demand for output of sector } i \\ x_i[\$] &\dots \text{total output of sector } i \\ z_{ij}[\$] &\dots \text{inter-industry sales (sector } i \rightarrow j) \\ a_{ij}[1] = z_{ij}/x_j &\dots \text{technical coefficient} \end{aligned}$$

If we write this as a function of final demand f_i

$$x_1 - a_{11}x_1 - a_{12}x_2 - \dots - a_{1n}x_n = f_1 \tag{SI-5}$$

$$(1 - a_{11})x_1 - a_{12}x_2 - \dots - a_{1n}x_n = f_1 \tag{SI-6}$$

we see that for all sectors, this system of equations can be express in matrix form.

$$(\mathbf{I} - \mathbf{A})\vec{x} = \vec{f} \tag{SI-7}$$

Solving for the output vector as a function of the final demand vector and the matrix of technical coefficients, the equation takes the form usually presented in literature [2, (2.6)-(2.10)]

$$\begin{aligned} \vec{x} = (\mathbf{I} - \mathbf{A})^{-1}\vec{f} := \mathbf{L}\vec{f} \\ [N \times 1] = [N \times N][N \times 1] \end{aligned} \tag{SI-8}$$

where

$$\vec{x} \in M_{N\times 1}(\mathbb{R})[\$] \ldots \text{output vector}$$
$$\vec{f} \in M_{N\times 1}(\mathbb{R})[\$] \ldots \text{final demand vector}$$
$$\mathbf{A} \in M_{N\times N}(\mathbb{R})[1] \ldots \text{technical coefficient matrix}$$
$$\mathbf{L} \in M_{N\times N}(\mathbb{R})[1] \ldots \text{Leontief inverse}$$

The vector of environmental burdens $\vec{g}$ associated with the output vector $\vec{x}$ can be calculated by means of an environmental burden coefficient matrix $\mathbf{B}_c$

$$\begin{aligned} \vec{g} &= \mathbf{B}_c\vec{x} = \mathbf{B}_c\mathbf{L}\vec{f} \\ [R\times 1] &= [R\times N][N\times N][N\times 1] \end{aligned} \quad \text{(SI-9)}$$

where

$$\vec{g} \in M_{R\times 1}(\mathbb{R})[\text{kg}(\text{CO}_2)] \ldots \text{environmental burden vector}$$
$$\mathbf{B}_c \in M_{R\times N}(\mathbb{R})[[\text{kg}(\text{CO}_2)]/\$] \ldots \text{environmental burden coefficient matrix}$$
$$b^c_{ij}[[\text{kg}(\text{CO}_2)]/\$] = \text{amount of environmental burden } i/x_j$$

1.2 Computational Structure of Process-based Life-Cycle Assessment

Heijungs in 1994 developed the mathematical formalism for the matrix-representation of life-cycle assessment [3][4]. In this notation, we can represent the physical flows between an economic process and other processes (the technosphere) and the environment (the biosphere) as a vector p in a linear space. The bases for these vector spaces are

$$\{\vec{b}_1, \vec{b}_2, \ldots, \vec{b}_M\} \tag{SI-10}$$

$$\{\vec{b}_1, \vec{b}_2, \ldots, \vec{b}_R\} \tag{SI-11}$$

where

$$\begin{aligned} i &\in \mathbb{N}, \text{for } (1 \leq i \leq M) \ldots \text{technosphere flow} \\ k &\in \mathbb{N}, \text{for } (1 \leq k \leq R) \ldots \text{biosphere flow} \\ \vec{b}_i &\in M_{M\times 1}(\mathbb{R}) \ldots \text{technosphere basis vector } i \\ \vec{b}_k &\in M_{R\times 1}(\mathbb{R}) \ldots \text{biosphere basis vector } k \end{aligned}$$

Column vectors of economic processes $\vec{p}$ can be arranged to form a process matrix $\mathbf{P} = (\vec{p_1}, \vec{p_2}, \ldots, \vec{p_L})$ where

$$j \in \mathbb{N}, \text{for } (1 \leq j \leq L) \ldots \text{economic process}$$

If each economic process produces only a single output, $L = M$. The case where any economic process is *multifunctional*, thereby producing more than one technosphere flow, is termed the *allocation problem* [4, Sec. 3.2]. The process matrix can now be split according to the basis vectors of Eq. (SI-10) into the technosphere matrix (technology matrix) $\mathbf{A}$ and the biosphere matrix (environmental flow matrix) $\mathbf{B}$.

$$\mathbf{P} = \left(\frac{\mathbf{A}}{\mathbf{B}}\right) \tag{SI-12}$$

where

$$\begin{aligned} \mathbf{A} \in M_{M\times(L=M)}(\mathbb{R})[\text{kg}] &\ldots \text{technosphere matrix} \\ t_{ij}[\text{kg}] &= \frac{\text{technosphere flow } i \ \{\ominus \text{ from}/\oplus \text{ to}\} \text{ unit process } j}{\text{output of unit process } j} \\ \mathbf{B} \in M_{R\times(L=M)}(\mathbb{R})[\text{kg}(\text{CO}_2)] &\ldots \text{biosphere matrix} \\ b_{ij}[\text{kg}(\text{CO}_2)] &= \frac{\text{biosphere flow } i \ \{\ominus \text{ from}/\oplus \text{ to}\} \text{ unit process } j}{\text{output of unit process } j} \end{aligned}$$

Here, [kg] indicates physical units such as kg, l, m^3, etc. while [kg(CO2)] indicates any unit associated with an environmental burden.

Economic processes are interdependent, consuming flows from other processes and producing flows that are consumed by other processes. Determining the total technosphere output for a given vector of arbitrary final demand $\vec{f}$ therefore requires solving a system of linear equations. We introduce a scaling vector $\vec{s}$ such that

$$\begin{aligned} f_i &= t_{i1}s_1 + t_{i2}s_2 + \ldots \\ \vec{f} &= \mathbf{A}\vec{s} \\ \vec{s} &= \mathbf{A}^{-1}\vec{f} \end{aligned} \tag{SI-13}$$

where

$$
\begin{aligned}
\vec{s} &\in M_{M\times 1}(\mathbb{R})[1] \ldots \text{scaling vector} \\
\vec{f} &\in M_{M\times 1}(\mathbb{R})[\text{kg}] \ldots \text{final demand vector} \\
\vec{g} &\in M_{R\times 1}(\mathbb{R})[\text{kg}(\text{CO}_2)] \ldots \text{biosphere flow vector}
\end{aligned}
$$

The scaling vector s determines the amount of technosphere output required by the final demand vector f. The associated vector of total biosphere output b can be calculated from $\vec{s}$ as

$$\vec{g} = \mathbf{B}\vec{s} \tag{SI-14}$$

which can be combined with Eq. (SI-13) to provide the biosphere output b as a function of the final demand f:

$$\vec{g} = \mathbf{B}\mathbf{A}^{-1}\vec{f} \tag{SI-15}$$

$$[R \times 1] = [R \times M][M \times M][M \times 1] \tag{SI-16}$$

1.3 Computational Structure of Hybrid Life-Cycle Assessment

The basic assumption of the method is that production processes consume inputs from other production processes. In addition, they consume inputs from different sectors of the economy. The final demand on the process system $\vec{f}_P$ therefore induces "upstream" output $\vec{u}_S$ of the sectors of the economy, with associated additional environmental burdens $\vec{b}_S$. We can write this assumption as:

$$\vec{e}_H = \vec{e}_P + \vec{e}_S \tag{SI-17}$$

Using the governing equations of process-based life-cycle assessment in monetary units derived in the supplementary information

$$\vec{e}_S = \mathbf{B}_S \vec{x}_S = \mathbf{B}_S (\mathbf{I} - \mathbf{A}_S)^{-1} \vec{u}_S \tag{SI-18}$$

$$\vec{e}_P = \mathbf{B}_P \vec{x}_P = \mathbf{B}_P \mathbf{A}_P^{-1} \vec{f}_P \tag{SI-19}$$

we can write the governing equation of the tiered hybrid method:

$$\vec{e}_{H(tiered)} = \vec{e}_S + \vec{e}_P = \mathbf{B}_S (\mathbf{I} - \mathbf{A}_S)^{-1} \vec{u}_S + \mathbf{B}_P (\mathbf{A}_P^{-1} \vec{f}_P \tag{SI-20}$$

$$\vec{e}_{H(tiered)} = \begin{pmatrix} \mathbf{B}_P & 0 \\ 0 & \mathbf{B}_S \end{pmatrix} \begin{pmatrix} \mathbf{A}_P & 0 \\ 0 & \mathbf{I} - \mathbf{A}_S \end{pmatrix}^{-1} \begin{pmatrix} \vec{f}_P \\ \vec{u}_S \end{pmatrix} \tag{SI-21}$$

Since final demand is assumed to be placed *only* on the process system, the upstream demand on the sectoral system $\vec{f}_S$ is induced by the process system alone. This means that we can introduce a matrix describing the amount of flow from sectors to processes. Using this matrix, the final demand of the sectoral system $\vec{f}_S$ induced by the process system can be expressed as

$$\mathbf{C}_U \vec{x}_P = \vec{u}_S \tag{SI-22}$$

where

$$\mathbf{C}_U[1] \in M_{N \times M}(\mathbb{R}) \ldots \text{upstream cutoff matrix} \tag{SI-23}$$

$$c_{ij}^U = \frac{\text{flow [\$] from sector } i \rightarrow \text{activity } j}{x_j[\$]} \tag{SI-24}$$

With this, the governing equation of the tiered hybrid matrix method takes the form most frequently used in literature:

$$\vec{e}_{H(tiered)} = \begin{pmatrix} \mathbf{B}_P & 0 \\ 0 & \mathbf{B}_S \end{pmatrix} \begin{pmatrix} \mathbf{I} - \mathbf{A}_P & 0 \\ \mathbf{C}_U^{uncorr} & \mathbf{I} - \mathbf{A}_S \end{pmatrix}^{-1} \begin{pmatrix} \vec{f}_P \\ 0 \end{pmatrix} \tag{SI-25}$$

1.4 Concordance Matrices

Definition A concordance matrix contains the information required to assign each process to one or more sectors of the economy. It can be used to convert vectors or matrices from the process-basis into the sector-basis.

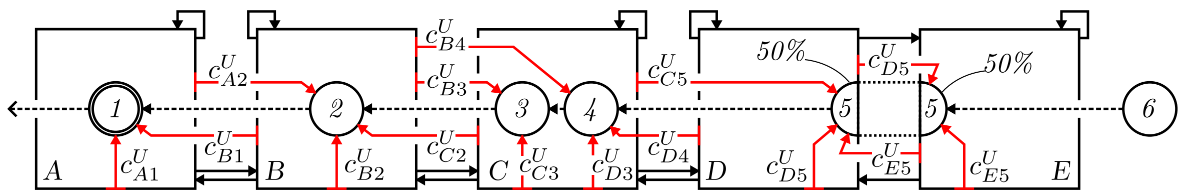


Figure 1: An example system to illustrate the different kinds of process-to-sector correspondences. Upstream flows from sectors to processes are also shown. From left to right: Sectors A and B: one-to-one correspondence, one process per sector; Sector C: one-to-one correspondence, more than one process per sector; Sectors D and E: one-to-many correspondence, 50% fraction of process 5 in Sector D, 50% fraction of process 5 in sector E. It should be noted that the case of one-to-many correspondence was not encountered by Agez et al. in their large-scale hybridization effort [5, Sec. 3.2.1]. For the associated concordance matrix and the resulting hybrid matrix, compare Eq. (SI-29). For a legend of the diagrammatic notation, compare the right panel of Figure 1 in the main text.

$$\mathbf{H} = \begin{array}{c} \\ A \\ B \\ C \\ D \\ E \end{array} \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & 0 \end{bmatrix} \end{array} \tag{SI-26}$$

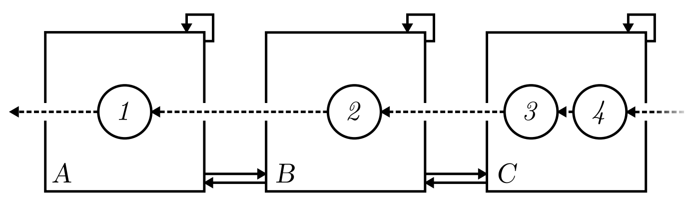


Figure 2: Excerpt of the example system from Fig. 1, showing only the first three sectors with associated processes.

$$\vec{x}_P = \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{bmatrix} x_1^P \\ x_2^P \\ x_3^P \\ x_4^P \end{bmatrix}, \vec{x}_S = \begin{array}{c} A \\ B \\ C \end{array} \begin{bmatrix} x_A^S \\ x_B^S \\ x_C^S \end{bmatrix} \tag{SI-27}$$

$$\vec{x}_{P(S)} = \begin{array}{c} A \\ B \\ C \end{array} \begin{bmatrix} x_1^P \\ x_2^P \\ x_3^P + x_4^P \end{bmatrix} \tag{SI-28}$$

$$
\mathbf{Z}_P[\$] = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} z_{11}^P & 0 & 0 & 0 \\ z_{21}^P & z_{22}^P & 0 & 0 \\ 0 & z_{32}^P & z_{33}^P & 0 \\ 0 & 0 & z_{43}^P & z_{44}^P \end{bmatrix} \end{array}, \mathbf{Z}_S[\$] = \begin{array}{c} \\ A \\ B \\ C \end{array} \begin{array}{c} \begin{array}{ccc} A & B & C \end{array} \\ \begin{bmatrix} z_{AA}^S & 0 & 0 \\ z_{BA}^S & z_{BB}^S & 0 \\ 0 & z_{BC}^S & z_{CC}^S \end{bmatrix} \end{array} \quad \text{(SI-29)}
$$

We can transform the matrices like this:

$$
\mathbf{Z}_{P(S)}[\$] = \begin{array}{c} \\ A \\ B \\ C \end{array} \begin{array}{c} \begin{array}{ccc} A & B & C \end{array} \\ \begin{bmatrix} z_{11}^P & 0 & 0 \\ z_{21}^P & z_{22}^P & 0 \\ 0 & z_{32}^P & z_{33}^P + z_{44}^P + z_{43}^P \end{bmatrix} \end{array} \quad \text{(SI-30)}
$$

$$
\mathbf{H} = \begin{array}{c} \\ A \\ B \\ C \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \end{array} \quad \text{(SI-31)}
$$

let's look only at one coefficient of the matrix:

$$
z_{CC}^{P(S)} = \sum_{k=1}^{M} \sum_{l=1}^{M} h_{Ck} z_{kl}^P h_{lC} \quad \text{(SI-32)}
$$

1.4.1 Derivation

We can derive the structure of the concordance matrix by defining the desired properties of the matrix. We know, for instance, how to convert an output vector $\vec{x}$ from the process basis to the sectoral basis:

$$x_i^S = \sum_j h_{ij} x_j^P \tag{SI-33}$$

$$\vec{x}^S = \mathbf{H}\vec{x}^P \tag{SI-34}$$

$$[N \times 1] = [N \times M][M \times 1] \tag{SI-35}$$

We can see that coefficient h must have the property:

$$\mathbf{H} \rightarrow h_{ij} = \begin{cases} 1, \text{if sector } i \text{ contains process } j \\ 0, \text{else} \end{cases}$$

where

$$\begin{aligned} i \in \mathbb{N}, \text{for } (1 \leq i \leq N) &\ldots \text{sector} \\ k \in \mathbb{N}, \text{for } (1 \leq k \leq M) &\ldots \text{process} \\ \vec{x}^S \in M_{N\times1}(\mathbb{R}) &\ldots \text{output vector} \\ \vec{x}^P \in M_{N\times1}(\mathbb{R}) &\ldots \text{output vector} \\ \mathbf{M} \in M_{N\times M}(\mathbb{R}) &\ldots \text{concordance matrix} \end{aligned}$$

Similarly, we know how to convert the intermediate output matrix $\mathbf{Z}$ from the process basis to the sectoral basis:

$$z_{ij}^S = \sum_{k,l} h_{ik} z_{kl}^P h_{jl} = \sum_{k,l} h_{ik} z_{kl}^P h_{lj}^T \tag{SI-36}$$

$$\mathbf{Z}^S = \mathbf{H}\mathbf{Z}^P\mathbf{H}^T \tag{SI-37}$$

$$[N \times N] = [N \times M][M \times M][M \times N] \tag{SI-38}$$

$$\mathbf{H}^T \rightarrow h_{ij}^T = h_{ji} = \begin{cases} 1, \text{if process } j \text{ in sector } i \\ 0, \text{else} \end{cases}$$

1.5 Adjacency Matrix

Based on the general definition of the adjacency matrix $\mathbf{D}$ of a directed graph [6, Chapter 13], we can define the special case of the adjacency matrix of the hybrid inventory system as

$$d_{ij} = \begin{cases} 1 & a_{ij} \neq 0 \\ 0 & else \end{cases} \tag{SI-39}$$

This adjacency matrix can be used to compute the number of possible paths of length n between nodes in a graph [6, Theorem 13.1(b)]. For the number of possible paths k of order n terminating in node (either process or sector) i, we can write

$$k = \vec{I}^T \mathbf{D}^n \vec{s} \tag{SI-40}$$

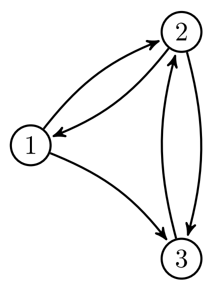
where

$$\begin{aligned} \vec{s}[1 \times N] &\ldots \text{column selector vector} \\ \vec{I}[N \times 1] &\ldots \text{unity vector} \\ \mathbf{D}_H[N \times N] &\ldots \text{adjacency matrix of hybrid system} \end{aligned}$$

and

$$s_j = \begin{cases} 1 & j = 1 \\ 0 & else \end{cases}$$

For a simple example system of three nodes: We can calculate the number k of possible paths of length



$$\mathbf{D} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Figure 3: Example system and adjacency matrix.

$n = 10$ terminating in node 2. First, we compute the matrix exponential of the adjacency matrix $\mathbf{D}$

$$\mathbf{D}^{10} = \begin{bmatrix} 34 & 55 & 55 \\ 33 & 56 & 55 \\ 22 & 33 & 34 \end{bmatrix} \tag{SI-41}$$

Now, we can use Eq. (SI-40)

$$k = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 34 & 55 & 55 \\ 33 & 56 & 55 \\ 22 & 33 & 34 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 55 + 56 + 33 = 144 \tag{SI-42}$$

1.6 Differences in Terminology and Notation

To aid the reader in comparing our equations to those originally used by Lenzen et al. in their 2009 publication [7], we present both conventions and present the concordance of variables in a table below.

In Section 1.1 and the main part of our manuscript, we try to follow the convention and notation used by Miller & Blair [8][9][2]. The environmental burden vector $\vec{b}$ associated with placing an arbitrary final demand $\vec{f}$ onto an economic system described by a matrix of technical coefficients $\mathbf{A}$ is

$$\vec{b} = \mathbf{B_c}(\mathbf{I} - \mathbf{A})^{-1}\vec{f} \tag{SI-43}$$

For the case of a single environmental burden, such as carbon dioxide emission, the environmental burden vector $\vec{b}$ becomes an environmental burden scalar b

$$b = \vec{b_c}(\mathbf{I} - \mathbf{A})^{-1}\vec{f} \tag{SI-44}$$

Lenzen et al. [7, Eqn.(1)-(2)] describe this equation in their notation as

$$Q = \vec{q}(\mathbf{I} - \mathbf{A})^{-1}\vec{y} \tag{SI-45}$$

In addition, Lenzen et al. introduce the concept of the multiplier vector $\vec{m}$ as

$$\vec{m} = \vec{q}(\mathbf{I} - \mathbf{A})^{-1} \tag{SI-46}$$

Table 1: Mathematical notation equivalency table between Lenzen et al. (eg.[7]) and the notation defined in the Supplementary Information.

authors	*variable*	*variable name*	*comment*
Weinold	$\vec{b} \in M_{R\times 1}(\mathbb{R})$	environmental burden vector	
Lenzen	N/A		
Weinold	$b \in \mathbb{R}$	environmental burden	
Lenzen	$Q \in \mathbb{R}$	factor inventory	*"such as energy, resources, pollutants."* [7]
Weinold	$\mathbf{B}_c \in M_{R\times N}(\mathbb{R})$	env.burd. intensity matrix	
Lenzen	$\mathbf{q} \in M_{R\times N}(\mathbb{R})$	intensity matrix	*"factor inputs per unit of gross output"*
Weinold	$\vec{B_c} \in M_{1\times N}(\mathbb{R})$	env.burd. intensity vector	
Lenzen	$\mathbf{q} \in M_{1\times N}(\mathbb{R})$	intensity vector	*"factor inputs per unit of gross output"*

with the index limits

$$N \ldots \text{number of sector of the economy}$$
$$R \ldots \text{number of environmental burdens}$$

1.6.1 Practicability of Recording Data in Matrix Form

One may now ask a second question *"Is such a recording of specific supply chain information in a process matrix not significantly more burdensome than editing nodes in a path?"*.

While this is a valid concern from the practical perspective of the life-cycle assessment practitioner, this is ultimately a question of software development and adequate user interface design. To date, no software implementing the path-exchange hybrid algorithm has been released [10, Sec.2.2]. Any software for hybrid life-cycle assessment can easily be designed to conduct a structural path analysis, allow the user to change nodes and record the relevant information in matrix form.

This second question is therefore beyond the scope of a mathematical discussion, falling instead entirely into the field of software development.

1.6.2 Relation to Data Collection in Tiered Hybrid Approach

The choice of input-output data as the starting point for an assessment suggests that the life-cycle assessment practitioner does not have access to either a self-compiled foreground inventory of metal production or a large-scale generic background database such as Ecoinvent of GaBi.

Under the well-established tiered hybrid approach first described by Bullard et al. [11], the practitioner has detailed information on the first few nodes in the supply chain of a certain product. For instance, he may know the parameters of the metal production process and the parameters of the wind-power electricity production process. However, he may not have such detailed information on the inputs to wind-power electricity production. This could be because he has set the system boundary of his assessment at that point - either for practical reasons, or because he cannot allocate further resources to the collection of his foreground inventory.

2 Notes on the Historical Lineage of the Method

Lenzen in his first formulation of the path-exchange method describes his work [12, Sec.1] as building on an earlier, similar method by Treloar which is described most comprehensively in [13, Sec.4]. He then mentions that *"The general decomposition approach [used in this method] was introduced into economics and regional science in 1984 under the name Structural Path Analysis [by Defourny et al. [14] and Crama et al. [15]]."*. However, Crawford et al. in 2018, state on the origin of the path-exchange method of Lenzen et al. that *"In the mid-1980s, Miller and Blair (2009) reported a mathematical equation that could be used to disaggregate the Leontief inverse formula into a series of stages starting from zero and theoretically going to infinity."* [16, Sec.5.2]. The disaggregation referred to here was first proposed in 1950 by Waugh [17]. Some confusion regarding the provenance of the path-exchange method has therefore made its way into the scientific literature on hybrid life-cycle assessment.

Regrettably, neither of the proposed origins is correct. To our knowledge, the first documented use of a power-series expansion of the Leontief inverse to replace selected coefficients with process-specific data was made as early as 1975 by Bullard et al. [11, (2.10)-(2.11)]. The power-series expansion itself was then still commonly referred to as *vertical analysis*, referring to the tree-like structure of the graph. A 1984 thesis by Seeman [18, P.20] described the same method, this time already as *"classical hybrid analysis"*. This work of Seeman was cited by Treloar [19][13], albeit without acknowledging it as the basis for his method, which improves on both the work of Bullard et al. and Seeman. We describe the nature of the improvement in some detail in this section. The correct mathematical lineage of the path-exchange method therefore goes back from Lenzen [7][12] and Treloar [13] to Waugh [17] and Bullard et al. [11] via Seeman [18], rather than to Defourny and Crama [14] as described by Lenzen [12], or to Miller & Blair as described by [16].

The core methodology of the path-exchange method for hybrid life-cycle assessment was formalized by Lenzen and Crawford under the name *path-exchange hybrid* in 2009 [7]. Additional methodological improvements were made by Crawford et al. in 2017 [10] and Stephan et al. in 2019 [20]. A Python software package, containing the core structural path analysis functionality of the method, was released under the name `pyspa` in 2019 [21][22].

As detailed in the main text, the path-exchange method for hybrid life-cycle assessment can be traced back to Bullard et al. via Seeman. Here, we provide the relevant excerpts from their work and elaborate on the nature of the improvement introduced by Treloar:

Excerpt from Seeman [18, P.8], with mathematical notation adapted such that $\overset{0}{x}_j \rightarrow (\vec{x}_0)_j$

Vertical analysis using the iterative method takes advantage of the identity:

$$(\mathbf{I} - \mathbf{A})^{-1} = \mathbf{I} + \mathbf{A} + \mathbf{A^2} + \mathbf{A^3} + \mathbf{A^4} + \dots$$

For an N sector model it is possible to examine one sector at a time as:

$$(\mathbf{I} - \mathbf{A})^{-1} = \sum_{j=1}^{N} (\vec{x}_0)_j + (\vec{x}_1)_j + (\vec{x}_2)_j + (\vec{x}_3)_j + \dots$$

where

$$\mathbf{A}\vec{x}_0 := \vec{x}_1$$
$$\mathbf{A}\vec{x}_1 := \vec{x}_2$$
$$\mathbf{A}\vec{x}_2 := \vec{x}_3$$

$\vec{x}_0$ is a column vector consisting of $(N-1)$ zero's and a one. The input structure of sector j is analysed by placing the "one" in row j of $\vec{x}_0$, e.g. to look at sector 2:

$$\vec{x}_0 = \begin{pmatrix} 0 \\ 1.0 \\ 0 \end{pmatrix}$$

Excerpt from Seeman [18, P.20], with mathematical notation adapted such that $\overset{0}{x}_j \rightarrow (\vec{x}_0)_j$

Method 3

"Classical" hybrid analysis where the first few stages of the expansion are replaced with problem specific data and the average coefficients from Input-Output analysis used for the remainder, i.e.

$$(\mathbf{I} - \mathbf{A}^*)^{-1} = \sum_{j=1}^{N} \left((\vec{x}_0)_j + \underbrace{(\vec{x}^*_1)_j + (\vec{x}^*_2)_j}_{\text{process specific}} + \underbrace{(\vec{x}_3)_j + (\vec{x}_4)_j + \dots}_{\text{average data}} \right) \tag{SI-47}$$

The relative merits of these three methods have not been tested and cannot be commented upon. It is felt, however, that method 2 would provide a new approach to Input-Output analysis and require less work than method 3.

It should be noted that the equality sign used by Seeman in the "Method 3" equation can be misleading. While the LHS is a matrix of dimension $[N \times N]$, the RHS is a sum of scalars. Using our notation from Eq. (SI-8) in Section 1.1, we can write the second term on the RHS of the "Method 3" equation as:

$$\sum_{j=1}^{N} (\vec{x}_0)_j = \sum_{j=1}^{N} (\mathbf{A}\vec{f})_j = \sum_{j=1}^{N} (a_{ji} f_i)_j \tag{SI-48}$$

If we now, as suggested by Seeman [18, P.8], investigate only a single sector. Our final demand vector $\vec{f}$ in this case could be

$$\vec{f}^T = (1, 0, 0, \dots) \tag{SI-49}$$

in which case, we can write Eq. (SI-48) as

$$\sum_{j=1}^{N}(a_{j1})_j \tag{SI-50}$$

This term in the power series expansion therefore describes the sum of all direct (order $n = 1$) inputs $a_{11}, a_{21}, \ldots$ to sector 1.

This power series expansion used by Seeman in "Method 3" must not be confused with the version used in our main text. There, both sides of the equation are of dimension $[N \times 1]$:

$$m_i = b_i + \sum_{j=1}^{N} b_j a_{ji} + \sum_{j=1}^{N}\sum_{k=1}^{N} b_j a_{jk} a_{ki} + \sum_{k=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N} b_j a_{jk} a_{kl} a_{li} + \ldots \tag{SI-51}$$

therefore If we again investigate only a single sector with the final demand vector defined in Eq. (SI-50), the first sum of the expansion becomes

$$\sum_{j=1}^{N} b_j a_{j1} \tag{SI-52}$$

This term in the power series expansion therefore describes the sum of all direct (order $n = 1$) environmental burdens $b_1 a_{11}, b_2 a_{21}, \ldots$ to sector 1.

We can see that out of the governing equation of environmentally extended input-output analysis Eq. (SI-9)

$$e = \vec{b}_c^T \mathbf{L} \vec{f}$$

Lenzen et al. [7] in their introduction to the path-exchange hybrid method show the power series expansion for the left two terms $\vec{b}_c^T \mathbf{L}$ (the environmental burden *multiplier vector*), while while Seeman [18] shows the power series expansion of the right two terms $\mathbf{L}\vec{f}$.

There is only *one* difference between the formulation proposed as "Method 3" by Seeman in Eq. (SI-47) [18, P.20] to the path-exchange formulation of Lenzen et al. [7]. The formulation of Seeman implicitly assumes that, for instance, data on *all* first order and second order paths into a process of interest is available. Only for higher order paths input-output data is used. Of course, the more general path-exchange method of Lenzen et al. also allows for the case where paths of all orders from both processes and sectors are considered. This case is illustrated in Fig. 4:

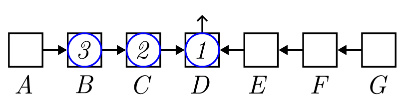


Figure 4: A simple example system with seven economic sectors ($A-G$) and three production processes ($1-3$). Final demand is placed on process 1, which is contained in sector D. The Seeman Eq. (SI-47) does not consider this case, where process data could is not available for *every* $n = 1$ order input into process 1. For a legend of the diagrammatic notation, compare the right panel of Figure 1 in the main text.

3 Notes on the Definition of "Structural Path Analysis"

The authors of the path-exchange method use the term *structural path analysis* to refer to *"(...) the decomposition (...)* [$(\mathbf{I}-\mathbf{A})^{-1} = \mathbf{I} + \mathbf{A} + \mathbf{A^2} + \ldots$, which] *can be unraveled further in order to systematically extract important supply chains, or structural paths."* [23]. However, for the historical lineage of this method, they mention [12][7][20] that *"It was introduced into economics and regional science by Defourny and Thorbecke [14] and Crama et al. [15] (...)"* [23]. Similarly, the *Open Risk Manual* in its entry for *structural path analysis* [24] cites a definition provided by Lenzen [25], and on the same page refers to the work by Lantner [26], on which the publications of Defourny and Thorbecke as well as Crama et al. are based.

However, a different lineage of the path-exchange method is provided in a recent review Crawford: *"In the mid-1980s, Miller and Blair (2009) reported a mathematical equation that could be used to disaggregate the Leontief inverse formula into a series of stages starting from zero and theoretically going to infinity."* [16, Sec.5.2]. The provenance of the decomposition underlying the path-exchange method and its connection to the work of Lantner as well as Defourny & Thorbecke is therefore a little confusing.

It is true that the term *structural path analysis* was introduced in the context of economic analysis by Defourny and Thorbecke in their 1984 publication "Structural Path Analysis and Multiplier Decomposition within a Social Accounting Matrix Framework" [14]. However, the authors simply adapted the seminal work on *economic influence* and the associated *"structural approach" (fr. "approche structurale")* of Lantner in 1972 [27] and *"structural analysis" (fr. "analyse structurale")* by Lantner in 1974 [26] and Gazon in 1976 [28] in the context of Social Accounting Matrices (SAM), on which Thorbecke had been working since at least 1976 [29]. Structural path analysis was at this point defined by the authors as (emphasis ours):

*"(...) Whereas [the solving of the system of linear equations] provides the solution of a model by expressing endogenous variables as functions of exogenous variables, **structural analysis** attempts, in addition, to clarify and explain this solution through the study of the transmission of influence within the network of structural relations starting with changes in exogenous variables to their ultimate effects on endogenous variables."* [14, Sec. III]

The core of the structural analysis method referred to here is the *theorem of influence* developed by Lantner [27][30] under the supervision of Ponsard [31]. It is a theorem of graph theory, which gives an equation to compute the amount of *global influence* I^G between two sectors i, j of the economy. This is defined as measuring *"(...) the total effects on income or output of (...) [sector j] consequent to an injection of one unit of output or income in (...) [sector i]."* [14, Sec.3]:

$$I^T_{(i\to j)}(\mathrm{p}(i \to j)) = a_{jx_1} a_{x_1x_2} \ldots a_{x_{n-1}x_n} \frac{\mathrm{M}_{i,j}(\mathbf{I}-\mathbf{A})}{\det(\mathbf{I}-\mathbf{A})} \tag{SI-53}$$

$$I^G_{(i\to j)} = \sum_{\mathrm{p}(i\to j)} I^T(\mathrm{p}(i \to j)) \tag{SI-54}$$

where

$I^T_{(i\to j)}(\mathrm{p}(i \to j)) \ldots$ total influence of i on j along an elementary path

$I^G_{(i\to j)} \ldots$ global influence of i on j

$\mathrm{M}_{i,j}(\mathbf{X}) \ldots (i, j)-$minor of the matrix $\mathbf{X}$

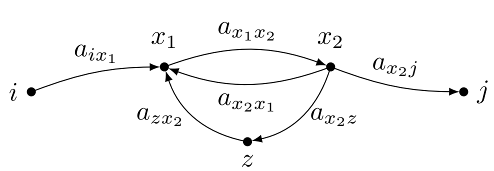
$\det(\mathbf{X}) \ldots$ determinant of the matrix $\mathbf{X}$

Here, an *elementary path is defined as "A path which does not pass more than one time through the same pole [=node of the graph, in this case a sector of the economy] (...)"* [14, Sec.III]. An example system is shown in Fig. 5.

In the years following the publications of Defourny & Thorbecke, the term *structural path analysis* (SPA) continued to be used only in the context of the of the *theorem of influence*:

"Structural path analysis, elaborated by Lantner (1974), Gazon (1976), Crama et al (1984), and others (see Defourny and Thorbecke, 1984) introduces the important concept of economic influence and its transmission within the input-output or social accounting system." [32] and *"SPA is a technique developed by Defourny and Thorbecke (1984) that uses standard matrix algebraic techniques to obtain a detailed map of the web of linkages at various levels in the economy and the economic forces transmitted along them.* [33, Sec.2.2]

It is important to realize that in the case of the economic analysis as undertaken by Lantner et al., it is desirable to compute the global effect that changes in one sector of interest can have on another sector of interest. This does not necessarily mean that knowledge of the changes induced in other sectors along the path between the two sectors of interest is desired. For instance, it may be of interest to compute only the change in economic output in the sector *natural gas production* induced by a change in demand in the sector *automotive manufacturing.*



index	*sector description*
j	automotive manufacturing
x_2	aluminium production
z	mechanical parts production
x_1	electricity production
i	natural gas production

Figure 5: Left: An example system of 5 nodes (=economic sectors), based on [14, Fig.3]. Note that we use the convention of Miller & Blair [2] which defines the notation of a technical coefficient for flow from sector $a \to b$ as a_{ab}, rather than a_{ba}, as was the case in the original rendering of this figure. In *structural path analysis* as the term is used by Defourny & Thorbecke [14], Sonis & Hewings [32] and other, more recent reviews [34], the *global influence* transmitted between two sectors, by means of all elementary paths, is investigated. Right: Table of sector descriptions.

On the other hand, in the case of environmental analysis as undertaken by Lenzen et al., it is desirable to compute the environmental burden produced by *all* sectors connected to the sector of interest, which is the subject of the environmental study. For instance, it may be of interest to compute the environmental ramifications of a specific amount of output of the sector *automotive manufacturing.* More specifically, the *elementary paths* resulting in the highest environmental burdens should be ranked. In this case, knowledge of all *elementary paths* leading to the sector of interest is desirable. This is illustrated in Fig. 6.

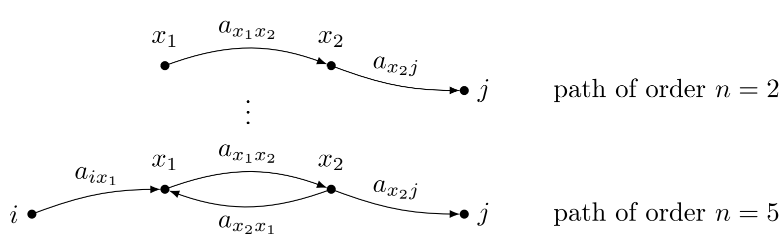


Figure 6: Two *elementary paths* from the system in Fig. 5. The top path is of order 2 and follows (x_1, x_2, j). The bottom path is of order 5 and follows $(i, x_1, x_2, x_1, x_2, j)$. In *structural path analysis* as the term is used by Lenzen [12][23], Peters & Hertwich [35][36] and other authors employing the path-exchange method for hybrid life-cycle assessment [10][20], these *elementary paths* are investigated.

Ultimately, none of the more sophisticated theorems of graph theory developed by Lantner are used as a basis for the method. This was confirmed by Lenzen in 2023 [37].

4 Systematic Literature Review

Table 2: Publications using the path-exchange hybrid method hybrid life-cycle assessment in specific case-studies, based on a systematic literature review described in the Supplementary Information. See also similar tables in recent review publications [16, Appendix A] [38, Appendix A1][39, Table 1].

year	*authors*	*case study*	*reference*
2010	Baloulet et al.	Higher Education	[40]
2011	Acquaye et al.	Biodiesel	[41]
2011	Wiedmann et al.	Wind Power Production	[42]
2014	Zafrilla et al.	Nuclear Energy Production	[43]
2016	Hong et al.	Construction	[44]
2016	Guan et al.	Construction	[45]
2017	Bontinck et al.	Construction	[46]
2018	Bunster et al.	Construction	[47]
2019	Kennelly et al.	Comparative Environmental Assessment	[48]
2020	Jiang et al.	Construction	[49]
2022	Yao et al.	Household Energy Consumption	[50]
2022	Pomponi et al.	Packaging	[51]
2022	Crawford et al.	Construction	[52]
2022	Lausselet et al.	Construction	[53]
2022	Stephan et al.	Construction	[54]

Table 3: *Elsevier Scopus* Advanced Search query used to collect case-studies employing the path-exchange method for hybrid life-cycle assessment.

```
TITLE-ABS-KEY (
   hybrid W/2 (
      "lca"
      OR
      "life-cycle assessment"
      OR
      "life cycle assessment"
      )
   )
AND
(
   REFTITLE ( "The Path Exchange Method for Hybrid LCA" )
   OR
   REFTITLE ( "Towards an Automated Approach for Compiling
   Hybrid Life Cycle Inventories" )
   OR
   REFTITLE ( "A model for streamlining and automating
   path exchange hybrid life cycle assessment" )
)
```

Table 4: *The Lens* Advanced Search query used to collect case-studies employing the path-exchange method for hybrid life-cycle assessment.

```
(
    full_text:(hybrid life cycle)
    OR
    full_text:(hybrid life-cycle)
)
AND
(
    reference.lens_id:(048-667-876-393-732) # "The Path Exchange Method for Hybrid LCA"
    OR
    reference.lens_id:(194-383-338-993-246) # "Towards an Automated Approach (...)"
    OR
    reference.lens_id:(124-212-987-876-036) # "A model for streamlining and automating (...)"
)
```

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