sustainability

MDPI

Article

An Introductory Review of Input-Output Analysis in Sustainability Sciences Including Potential Implications of Aggregation

Jonas Bunsen *,† and Matthias Finkbeiner †

Chair of Sustainable Engineering, Technische Universität Berlin, 10623 Berlin, Germany
* Correspondence: jonas.bunsen@tu-berlin.de
† Current address: Fachgebiet für Sustainable Engineering, Technische Universität Berlin, Institut für Technischen Umweltschutz, Sekr. Z 1, Straße des 17. Juni 135, 10623 Berlin, Germany.

Abstract: Input-output analysis has become a widely established method in sustainability sciences. It is primarily used in macroeconomic footprint analyses for allocating an economy's externalities among the agents in that economy based on the agents' input-output interdependencies. However, databases for input-output analyses are commonly compiled by aggregating data. Aggregation of input-output data inevitably leads to a loss of information and in some instances can lead to misinformed decision-making. The goal of this paper is to provide a simple *hands-on* numerical introduction to input-output analysis including the potential implications of data aggregation in an original manner. First, the calculation of production-based and consumption-based inventories is introduced based on a dummy 2 × 2 input-output table. Next, the inventories of the 2 × 2 input-output table are compared with the production-based and consumption-based inventories of a corresponding non-aggregated 4 × 4 input-output table. A comparison of the inventories of both dummy input-output tables allows for an exemplary demonstration of inaccurate allocation as a result of data aggregation and to conclude on potential implications for decision-making. Overall, this work offers a succinct and numerically substantiated introductory review of input-output analysis for practitioners in sustainability sciences including the potential implications of aggregation of input-output data. Its simplistic approach sets this work apart from other publications on aggregation in input-output analysis that are founded in economics or econometrics.

Keywords: input-output analysis; methods for sustainability assessment

Citation: Bunsen, J.; Finkbeiner, M. An Introductory Review of Input-Output Analysis in Sustainability Sciences Including Potential Implications of Aggregation. *Sustainability* **2023**, *15*, 46. https://doi.org/10.3390/su15010046

Academic Editor: Cuihong Yang

Received: 21 November 2022
Revised: 13 December 2022
Accepted: 14 December 2022
Published: 20 December 2022

1. Introduction

Over the last few centuries, humanity's footprint on planet earth has grown dramatically. Particularly since the middle of the 20th century, the world's population and its wealth have increased enormously and accompanied by an escalated anthropogenic appropriation of the earth's resources and exhaustion of the earth's capacity to absorb emissions [1–3]. It is now widely accepted that humanity's current patterns of consumption and production cannot be sustained without causing significant and potentially threatening changes to the earth's biosphere [4–8]. Consequently, individuals, organisations and entire nations have committed to reducing their ecological footprint, as well as the entirety of humanity's ecological footprint. Hence, there is a need for robust methods and tools to examine which agents in the global economy are responsible for the extraction and emission of physical substances.

One such method is input-output analysis. Initially, input-output analysis was founded in macroeconomics by Wassily Leontief for investigating the interdependencies between producers and consumers based on their input-output interdependencies [9–11]. Later, Leontief formulated how "undesirable by-products . . . are linked directly to the network of physical relationships . . . of our economic system" and elaborated on "how such 'externalities' can be incorporated into the [. . .] input-output picture of [an] economy" [10]. In other words, Leontief extended the initially macroeconomic application of input-output analysis with e.g., environmental or social metrics [10]. This expanded the scope of application of input-output analysis to topics commonly understood as sustainability sciences.

Leontief [10] and Kitzes [12] offer concise introductions to environmental input-output analysis. Leontief [10] provides a solid introduction to the basic mathematics of environmentally-extended input-output analysis, including the derivation of the structural matrix of an economy from a set of linear equations. A strength of Kitzes [12] is its straightforward approach and its accessibility for those without a mathematical background. Miller and Blair [11] has become a standard reference for input-output analysis and elaborates extensively on the foundations of input-output analysis, data organisation, input-output multipliers, incorporation of environmental and social metrics into input-output analysis, decomposition analysis and numerous other topics.

Input-output analysis has been applied in countless sustainability-related studies e.g., on cities [13–18], organisations [19,20], economic sectors [21,22], nations [23–30], local impacts of global trade [26,31,32] and other topics. The externalities analysed using input-output analyses are versatile, and include carbon emissions [17,18,33], biodiversity [34], land use [35,36], water consumption [24,37], human exploitation [38] and other indicators.

Building databases for input-output analyses involves the temporal, sectoral and regional aggregation of source data. For instance, several products or small sectors are typically aggregated into one large sector. Aggregation is applied if detailed information is lacking as well as to reduce calculation requirements. The importance of aggregation in input-output analysis has been recognised ever since and is subject to thorough scientific debate [9,10,39–41]. A review of scientific literature on aggregation in input-output analysis was first published by Kymn [42]. Fisher [40], Ara [43] and Neudecker [44] studied the optimisation of aggregation for minimising the loss of information. Lenzen [45] elaborated on *aggregation versus disaggregation* as well as on the disaggregation of environmentally relevant sectors and Wood et al. [46] studied sectoral harmonisation.

However, most of these works are founded in economics or econometrics and target expert practitioners of input-output analysis. However, input-ouput analysis is subject to ever-increasing popularity in sustainability sciences. Often, sustainability scientists have different scientific backgrounds and varying levels of technical knowledge and may not be experts in input-output analysis.

A concise and numerical introduction to input-output analysis including the potential implications of aggregation of input-output data for those without a strong technical background does not exist. Yet, the aggregation of input-output data and implications thereof can potentially undermine the robustness of input-output analysis-based assessments and, in worst-case scenarios, lead to misinformed decision-making.

Therefore, the main aim of this work is to provide an introductory review of input-output analysis including the potential implications of aggregation of input-output data based on numerically substantiated examples. This work aids sustainability scientists and policymakers in betters understanding the potential implications of aggregation of input-output data for their work.

In this work, instead of the frequently used terms *environmentally-extended input-output analysis* [12] and *environmental input-output analysis* [11], the term *input-output analysis* is used. The reason is that the former terms neglect that non-environmental externalities, e.g., social metrics, can as well be incorporated into input-output analyses [38,47–50]. This paper uses the terms *direct* and *total intensities* for monetary requirements and *direct* or *total externalities* for the externalities that are associated with the monetary requirements.

First, a dummy 2×2 input-output table is introduced (Section 2.1), structural path analysis (Section 2.2) and the calculation of production-based and consumption-based inventories (Section 2.3) is explained. Next, a dummy 4×4 input-output table is gradually introduced which serves as the hypothetical non-aggregated counterpart of the lower-resolved 2×2 input-output table (Sections 2.4.1 and 2.4.2). Subsequently, the inventories of both differently-resolved input-output tables are calculated (Section 3.4.2) and subject to discussion (Section 4). This work concludes with a summary of the findings including the potential implications of aggregation in input-output analysis (Section 5).

2. Method

This work expands on Kitzes [12] and the 2 × 2 dummy input-output table published therein. Because this work is considered *introductory*, the fundamentals of input-output analysis are covered in-depth. Equations (1)–(6) are the same as in Kitzes. However, more in-depth explanations are given on structural path analysis, geometric series expansion and the *Leontief Inverse Matrix* including explanatory depictions. Section 3 shows the production-based and consumption-based inventories of the differently resolved dummy input-output tables, which makes possible a discussion of the differences in production-based and consumption-based inventories, as well as the potential implications of aggregation of input-output data.

Readers should note that the input-output table adapted from Kitzes is fictitious. Moreover, all input-output tables in this work are a stark simplification of real input-output tables which are significantly more complex and typically consist of thousands or ten thousands region-sector combinations.

2.1. Input-Output Tables

Input-output tables represent the input-output characteristics of a given economy for a specified period of time, e.g., a particular year. The represented economy could, for example, comprise the economy of a country, the entire world, selected regions or sub-national entities, such as that of states or provinces. Typically, an input-output table consists of the following components (see Figures 1 and A1):

- Transactions (T)
- Final demand (Y)
- Value-added (V)
- Total output (x_{out}) and total input (x_{in})
- Satellite accounts (Q)

The economy in the dummy input-output table in Kitzes [12] comprises two sectors: *Agriculture* and *Manufacturing* (Figure 1). The rows in the transaction matrix (also known as the *Intermediate Demand Matrix*) contain the sectors' output to all other sectors (production). For example, the *Agriculture* sector produces €8 of output for itself (intra-sectoral transaction) and €5 of output for the *Manufacturing* sector (inter-sectoral transaction). In addition, the *Agriculture* sector produces €3 of output to satisfy final demand (e.g., household consumption). The total output of the *Agriculture* sector is €16. Analogously, the columns in the transaction matrix contain the sectors' input from all other sectors (consumption). For example, the *Manufacturing* sector consumes €5 from the *Agriculture* sector and €2 of input from itself. In addition, the *Manufacturing* sector consumes €5 of added value (e.g., capital and labour). The total output of the *Manufacturing* sector is €12.

For sustainability assessments, input-output tables can be extended by the sectors' externalities e.g., resource use (water, land, etc.), emissions (nitrogen, phosphorous, greenhouse gases, etc.), environmental impacts (water scarcity, global warming potential, etc.), social- (working hours, occupational fatalities, etc.) and other metrics. These extensions are also referred to as *satellite accounts* (or *environmental extensions*). The satellite account of the input-output table in Figure 1 contains information on *Water consumption—Total*. It indicates that 8 m^3 and 4 m^3 of *Water consumption—Total* are associated with the sectors' total output of €16 and €12 worth of produce, respectively.

Large input-output databases are typically given in a monetary unit. The reason is that transactions of all sorts of goods (e.g., wheat, cheese, ore, iron, cars, etc.) and services (e.g., insurance, medical care, banking, education, etc.) in an economy can all be converted into transactions in a common monetary unit. This allows the aggregation of thousands of goods and services into a manageable number of aggregated sectors.

			Agriculture Region A €	Manufacturing Region A €	Final demand Region A €	Total output - €
Agriculture	Region A	€	8	5	3	16
Manufacturing	Region A	€	4	2	6	12
Value added	Region A	€	4	5		
Total input	-	€	16	12		
Water consumption - Total		m³	8	4		

Figure 1. Monetary 2 × 2 dummy input-output table based on Kitzes [12]. The sectors' structural paths are shown in Figure 2. The externalities per production layer are shown in Figures 3 and A2. The production-based and consumption-based inventories are given in Section 3.1 and shown in Figure A3. Orange: Intra-sectoral and inter-sectoral transactions (T); Yellow: Value added (V) and final demand (Y); Green: Sectors' total input (x_{in}) and sectors' total output (x_{out}); Blue: Sectors' satellite account(s) (Q).

2.2. Structural Path Analysis

Structural path analysis refers to the systematic tracing of a sector's inputs from all other sectors on an infinite number of production layers based on the transaction matrix [51–53]. A structural path can broadly be understood as a sector's supply chain [33,51]. Before conducting a structural path analysis, the transaction matrix T and the externalities q are normalised by the sectors' total output x_{out}. The normalisation yields the sectors' input requirements from all other sectors to produce one unit of output, also referred to as *Technical Coefficient Matrix A* (Equation (1)), and the sectors' externalities per one unit of output, herein referred to as the sectors' *direct externalities f* (Equation (2)). Consequently, the results of the structural path analysis are given in *externality per one unit of output*.

$$A = T/x_{out} = \begin{bmatrix} 8 & 5 \\ 4 & 2 \end{bmatrix} \; / \; \begin{bmatrix} 16 & 12 \end{bmatrix} = \begin{bmatrix} 8/16 & 5/12 \\ 4/16 & 2/12 \end{bmatrix} = \begin{bmatrix} 0.50 & 0.42 \\ 0.25 & 0.17 \end{bmatrix} \tag{1}$$

$$f = q/x_{out} = \begin{bmatrix} 8 & 4 \end{bmatrix} \; / \; \begin{bmatrix} 16 & 12 \end{bmatrix} = \begin{bmatrix} 8/16 & 4/12 \end{bmatrix} = \begin{bmatrix} 0.50 & 0.33 \end{bmatrix} \tag{2}$$

In the following, an example of a structural path analysis is given. For instance, the *Agriculture* sector requires inputs from itself and the *Manufacturing* sector. Analogously, the *Agriculture* and *Manufacturing* sectors require inputs from sectors further up the supply chain. In theory, this trace can be continued indefinitely. However, for sustainability assessments a purely hierarchical description of the sectors' structural paths is of limited informative value. Mostly, structural paths and the quantity of an externality associated with the respective structural path are of interest. The externalities associated with €1 of output from the *Agriculture* sector are calculated by multiplying the corresponding direct externality $f_{Agriculture}$ by €1, thus yielding 0.5 m^3 × €1 = 0.5 m^3/€. The externalities associated with €1 of output from the *Agriculture* sector on the subsequent production layers (first, second, third, etc.) are calculated by multiplying €1 by the corresponding series of technical coefficients and the direct externalities of the final sector in the structural path. For example, the externalities of the *Manufacturing* sector on the first production layer, the structural path *Agriculture—Manufacturing*, are 0.33 m^3 × €1 × €0.25 = 0.521 m^3/€. The externalities of the *Agriculture* sector on the second production layer, the structural path *Agriculture—Manufacturing—Agriculture*, are 0.5 m^3 × €1 × €0.25 × €0.42 = 0.347 m^3/€ (Figure 2). If this series is continued indefinitely, it becomes possible to determine a sector's total externalities associated with €1 of the sector's output.

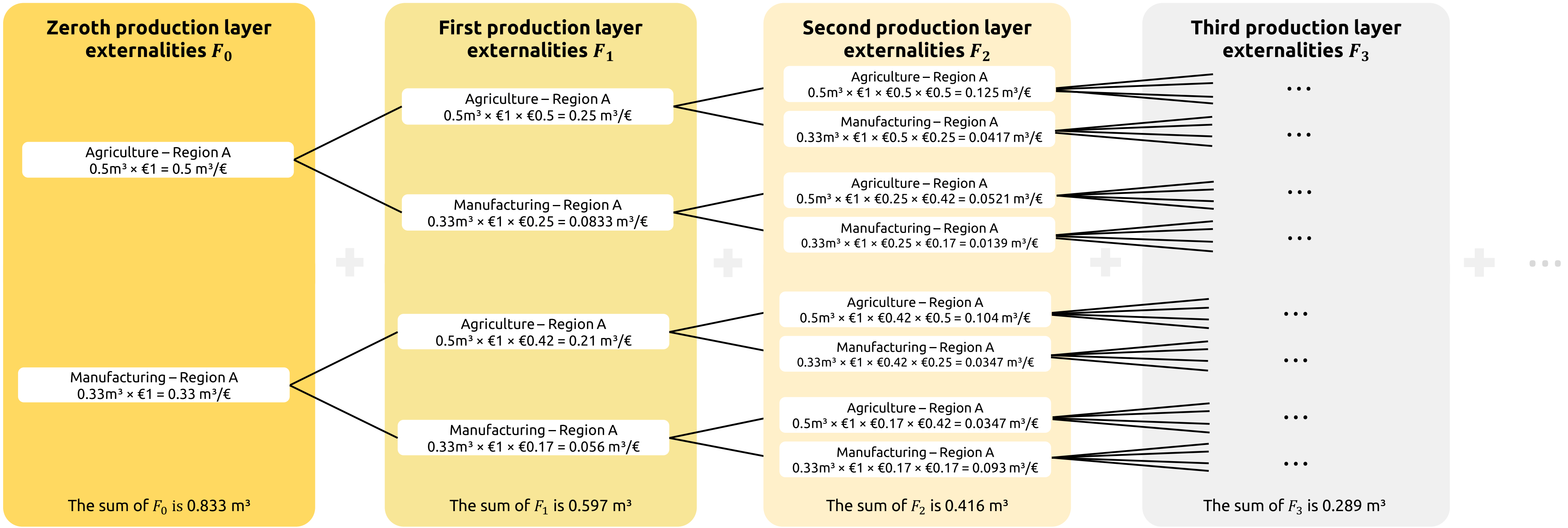

Figure 2. Structural paths and the associated externalities of the *Agriculture* and *Manufacturing* sectors for the first three production layers (per one unit of final demand). The totals of the externalities of a given production layer are shown at the bottom (see also Figures 3 and A2).

For each production layer, the number of branches of a sector's structural path equals the number of sectors in the input-output table to the power of the number of the production layer. In a 2 × 2 input-output table for example: zeroth production layer $2^0 = 1$ branch; first production layer $2^1 = 2$ branches; second production layer $2^2 = 4$ branches; ... tenth production layer $2^{10} = 1024$ branches, etc. Overall, a limited number of production layers contribute the highest proportion of a sector's externalities (Figure A2) [51].

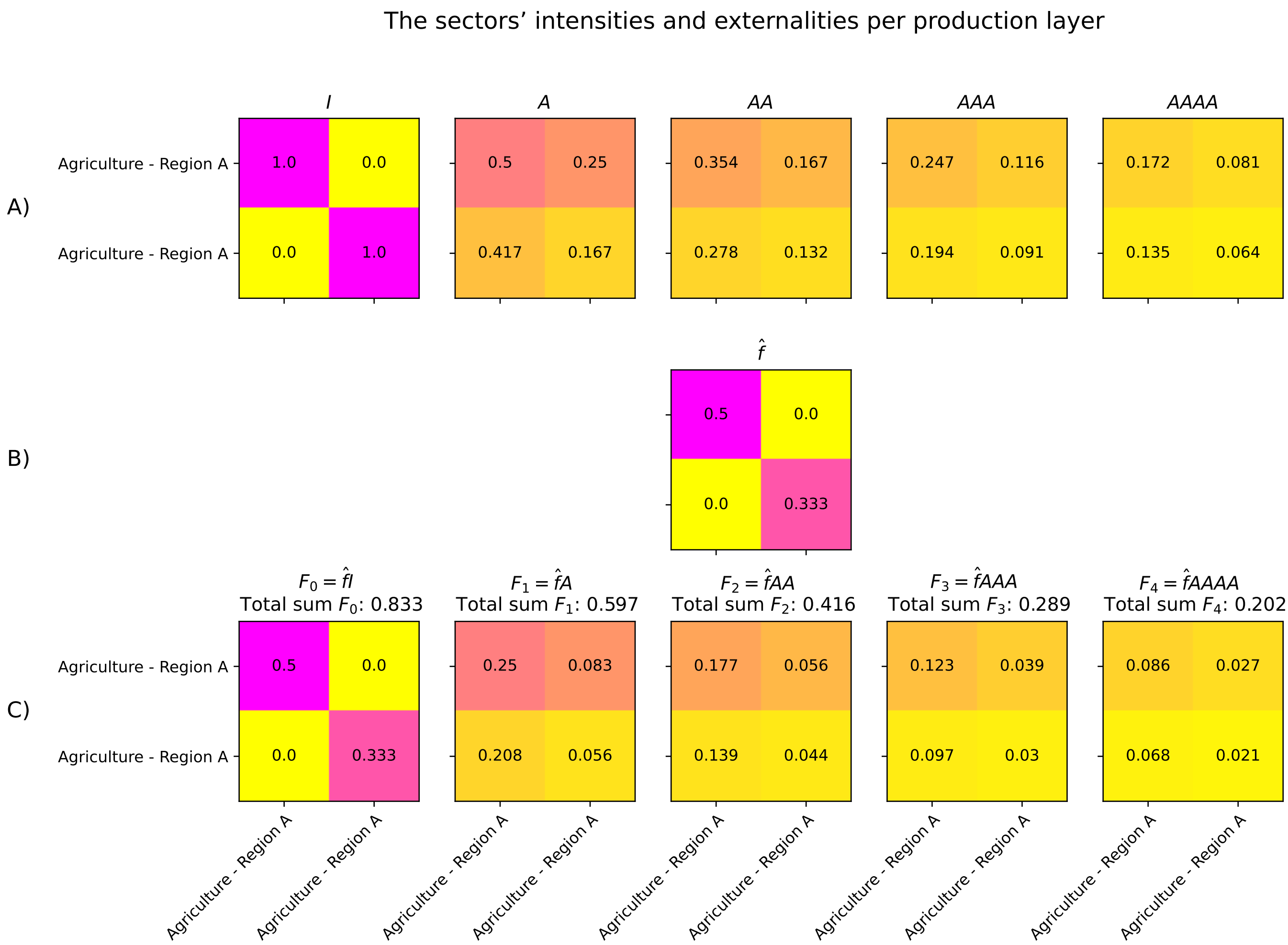

Figure 3. (**A**) Intensities (monetary requirements) associated with a single unit of final demand per production layer in € per €1; (**B**) Diagonalised direct externalities; (**C**) Externalities associated with a single unit of final demand per production layer in m^3 per €1. The total of F_i equals the sum of all externalities of all sectors on a production layer i in the structural path analysis in Figure 2. While the sum of externalities per production layer decreases with each ensuing production layer, the cumulative externalities from the considered production layers increase (Figure A2).

2.3. Production-Based and Consumption-Based Inventories

The calculation of production-based and consumption-based inventories based on matrix multiplication is a simpler approach than structural path analysis. Yet, often it is equally suitable for many research objectives and more straightforward if the goal is to allocate an externality between producers and consumers based on final demand.

If a matrix C is the product of two matrices A and B, each element in C is the result of multiplying each element in A with each corresponding element in B. C is then also referred to as the *dot product* of two matrices. In input-output analysis, the dot product is used to determine all externalities associated with the production of one unit of output on a given production layer. Mathematically, the dot product is the same as determining the structural paths and associated externalities of all sectors. The following paragraphs demonstrate an example of this process.

First, the transaction matrix T and externalities q are again normalised by the sectors' total output x_{out} (Equations (1) and (2)). On the zeroth production layer, the sectors' externalities are equal to the direct externalities f. Mathematically, this is expressed by multiplying the direct externalities f by an identity matrix I (Equation (3) and Figure 4). However, multiplying a vector by a matrix yields a vector, which implies that one of the two dimensions of the input-output table, input (consumption) or output (production), is lost. To preserve both dimensions, the direct externality vector f is diagonalised ($\hat{f}$) before calculating the dot product.

$$F_0 = \hat{f} I = \begin{bmatrix} 0.50 & 0 \\ 0 & 0.33 \end{bmatrix} \times \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.33 \end{bmatrix} \quad (3)$$

The externalities from the subsequent production layers (first, second, third, etc.) are determined by calculating the dot product of $\hat{f}$ and a series of the technical coefficient matrix A (Equation (4)). Eventually, the sum of the externalities from the zeroth (F_0) and the externalities from an infinite number of subsequent production layers yields the sectors' total externalities per unit of output F (Figure 3). Although the sum of externalities per production layer decreases with each ensuing production layer, the cumulative externalities from the considered production layers increase (Figure A2). If an input-output table contains more than one row of satellite accounts, this step can be repeated for each row of the satellite accounts separately.

$$\begin{aligned} F = \hat{f} I + \hat{f} A + \hat{f} A A + \ldots = \begin{bmatrix} 0.50 & 0 \\ 0 & 0.33 \end{bmatrix} \times \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0.50 & 0 \\ 0 & 0.33 \end{bmatrix} \\ \times \begin{bmatrix} 0.50 & 0.42 \\ 0.25 & 0.17 \end{bmatrix} + \begin{bmatrix} 0.5 & 0 \\ 0 & 0.33 \end{bmatrix} \times \begin{bmatrix} 0.50 & 0.42 \\ 0.25 & 0.17 \end{bmatrix} \times \begin{bmatrix} 0.50 & 0.42 \\ 0.25 & 0.17 \end{bmatrix} + \ldots = \begin{bmatrix} 1.33 & 0.67 \\ 0.27 & 0.53 \end{bmatrix} \end{aligned} \quad (4)$$

To account for the total externalities on an infinite sum of production layers, the series expansion in Equation (4) can be rewritten using the Leontief Inverse Matrix L (Equation (5)).

$$F = \hat{f} L = \hat{f}(I - A)^{-1} = \begin{bmatrix} 0.50 & 0 \\ 0 & 0.33 \end{bmatrix} \times \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 0.50 & 0.42 \\ 0.25 & 0.17 \end{bmatrix} \right)^{-1} = \begin{bmatrix} 1.33 & 0.67 \\ 0.27 & 0.53 \end{bmatrix} \quad (5)$$

Finally, the sectors' total externalities per unit of output F can be multiplied by a given region's final demand to determine the total externalities associated with the region's consumption (Equation (6)). The sum of the rows in E (*outputs* or *production*) is the production-based inventory. The sum of the columns in E (*inputs* or *consumption*) is the consumption-based inventory (see Figure 1).

$$E = F \times y = \begin{bmatrix} 1.33 & 0.67 \\ 0.27 & 0.53 \end{bmatrix} \times \begin{bmatrix} 3 & 6 \end{bmatrix} = \begin{bmatrix} 4.00 & 4.00 \\ 0.08 & 3.20 \end{bmatrix} \quad (6)$$

2.4. Disaggregating the Input-Output Table

Real input-output tables consist of significantly more sectors, regions, and satellite accounts than the dummy input-output in Figure 1. Typically, they consist of aggregated data. This leads to the question of potential implications of aggregation in input-output analysis. To address this question, in this section, we disaggregate the satellite accounts (Section 2.4.1) and sectors (Section 2.4.2) of the 2 × 2 dummy input-output in Figure 1 are disaggregated into hypothetical non-aggregated dummy input-output tables.

2.4.1. Disaggregating Satellite Accounts

A common approach to approximate a sector's total externalities is to multiply the production volumes of products produced by the sector with the externalities associated with a single unit of each product's production. If, for example, the *Agriculture* sector produces *Wheat* and *Cotton*, the sector's total water consumption would be the sum of the production volumes of *Wheat* and *Cotton* multiplied by their respective water consumption, e.g., per ton of production. In the input-output table in Figure 4, the externalities of *Water consumption—Total* of the 2 × 2 dummy-input-output table in Figure 1 is disaggregated into the separate externalities of *Water consumption—Cotton*, *Water consumption—Wheat*, *Water consumption—Textiles* and *Water consumption—Agricultural machinery*. The sum of these separate satellite accounts equals the externalities of *Water consumption—Total* in the input-output table in Figure 1.

			Agriculture Region A €	Manufacturing Region A €	Final demand Region A €	Total output - €
Agriculture	**Region A**	**€**	8	5	3	16
Manufacturing	**Region A**	**€**	4	2	6	12
Value added	**Region A**	**€**	4	5		
Total input	**-**	**€**	16	12		
Water consumption - Total		**m³**	8	4		
Water consumption - Cotton		**m³**	2	0		
Water consumption - Wheat		**m³**	6	0		
Water consumption - Textiles		**m³**	0	2.5		
Water consumption - Agricultural machinery		**m³**	0	1.5		

Figure 4. Hypothetical 2 × 2 dummy input-output table. Expanded based on the input-output table in Figure 1. The production-based and consumption-based inventories are shown in Figure 5.

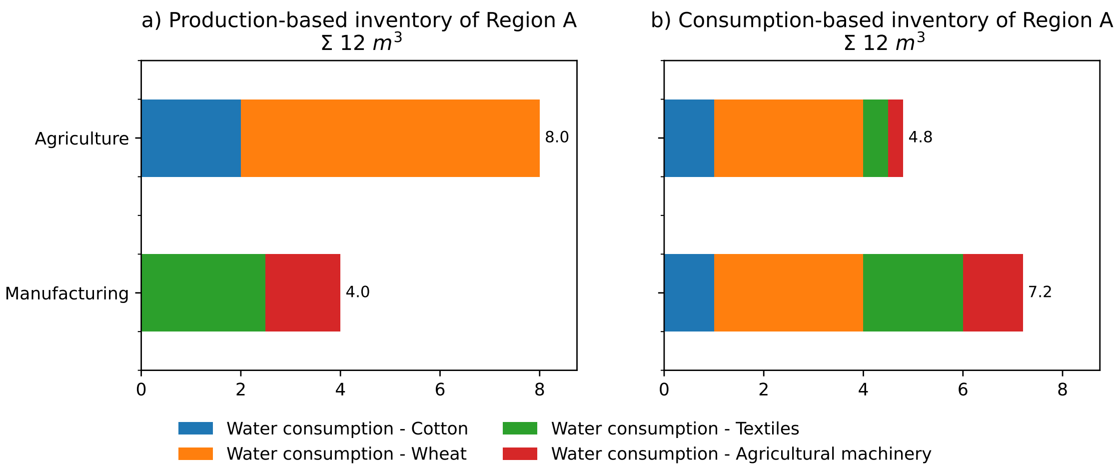

Figure 5. The production-based and consumption-based inventories of the input-output table are given in Figure 4. The numeric contributions of externalities are shown in Figure A5.

2.4.2. Disaggregating the Transaction- and Final Demand Matrix

Large input-output databases with hundreds or thousands of sectors are typically assembled by aggregating data from, e.g., annual macroeconomic databases with a high level of detail. To demonstrate the potential implications of aggregation in input-output analysis, also the sectors in the 2 × 2 dummy input-output in Figure 1 were subject to (hypothetical) disaggregation and a second region was introduced. The resulting 4 × 4 dummy input-output table is given in Figure 6 and can be interpreted as the non-aggregated *correct* or *true* counterpart of the 2 × 2 dummy input-output table in Figure 1.

			Agriculture - Wheat	Agriculture - Cotton	Manufacturing - Textiles	Manufacturing - Agricultural machinery	Final demand	Final demand	Total output
			Region A	Region A	Region B	Region B	Region A	Region B	-
			€	€	€	€	€	€	€
Agriculture - Wheat	**Region A**	**€**	3	0	0.25	0.5	1.5	0.75	6
Agriculture - Cotton	**Region A**	**€**	0	5	3.75	0.5	0.25	0.5	10
Manufacturing - Textiles	**Region B**	**€**	0	0	1.25	0.25	0.5	5.5	7.5
Manufacturing - Agricultural machinery	**Region B**	**€**	1.5	2.5	0	0.5	0	0	4.5
Value added	**Region A**	**€**	1.5	2.5	0	0			
Value added	**Region B**	**€**	0	0	2.25	2.75			
Total input	**-**	**€**	6	10	7.5	4.5			
Water consumption - Total		**m^3**	6	2	2.5	1.5			
Water consumption - Cotton		**m^3**	0	2	0	0			
Water consumption - Wheat		**m^3**	6	0	0	0			
Water consumption - Textiles		**m^3**	0	0	2.5	0			
Water consumption - Agricultural machinery		**m^3**	0	0	0	1.5			

Figure 6. Hypothetical 4 × 4 dummy input-output table. Expanded based on the input-output table in Figure 1. The production-based and consumption-based inventories are shown in Figure 7. See Figure A9 for a hypothetical counterpart of this input-output table with non-monetary values.

It should be noted that the disaggregation did not change the total transaction volume, value-added, total input, final demand, total output, or sum of externalities. For example, the sum of all transactions among the agricultural sectors in the input-output table in Figure 6 is the same as the intra-sectoral transaction of the *Agriculture* sector in the input-output table in Figure 1 (€3 + €5 = €8). The same applies, e.g., to the total input of the manufacturing sectors (€0.25 + €3.75 + €1.25 + €0.5 + €0.5 + €0.25 + €0.5 = €5 + €2), final demand among all regions from the agriculture sectors (€1.5 + €0.25 + €0.75 + €0.5 = €3), the total output from the manufacturing sectors (€7.5 + €4.5 = €12), *Water consumption—Total* from the agricultural sectors (6.5 m^3 + 1.5 m^3 = 8 m^3), etc.

The 4 × 4 dummy input-output table in Figure 6 can be interpreted as a two-sector economy in which *Region A* has a rather agrarian economy, and a rather low final demand and *Region B* has a rather industrial economy and a rather high final demand. The agrarian economy of *Region A* is rather water-intensive. *Region A's* staple crop (wheat) is mainly consumed domestically, while its cash crop (cotton) is mainly consumed abroad. The industrial economy of *Region B* has a rather low water intensity. *Region B's* textile industry imports a lot of cotton from *Region A* and produces mainly for the domestic market. *Region B*'s agricultural machinery is mainly sold to *Region A*'s agricultural sectors.

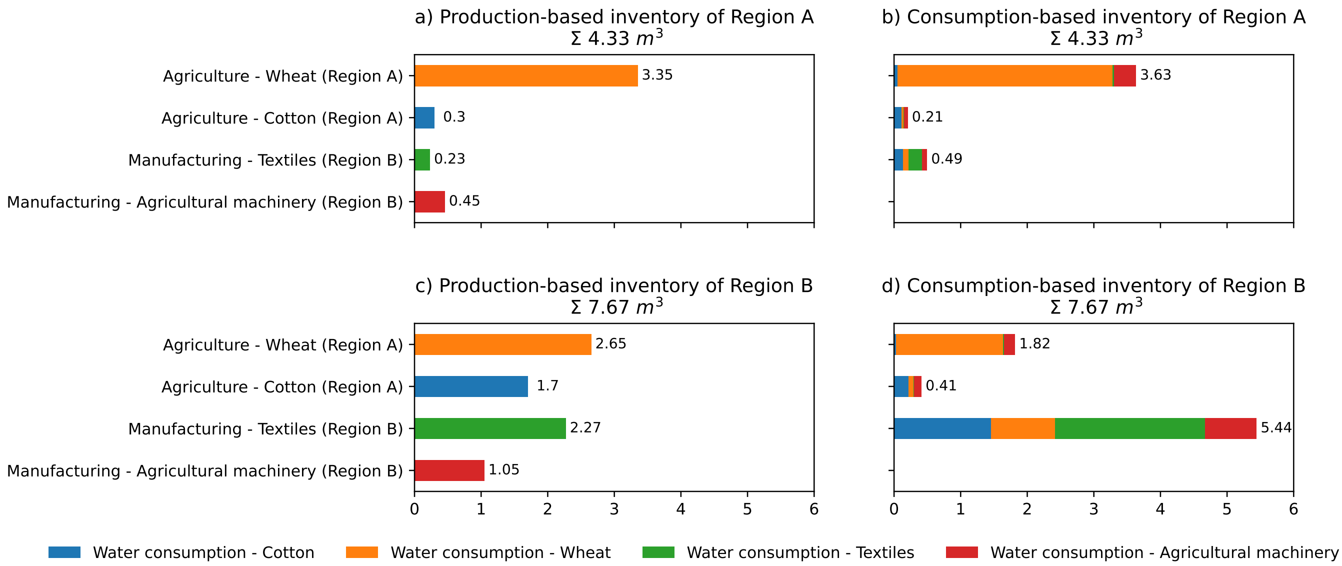

Figure 7. Production-based and consumption-based inventories of *Region A* and *Region B* based on the monetary-based input-output in Figure 6. The exact quantities are given in Figure A6.

2.5. Implementation

All calculations were done in the *Python* programming language [54] using the *Pandas* [55,56] and *Numpy* [57] libraries. The structural path analysis was conducted using *pySPA* [58]. The results plots were created with *Matplotlib* [59]. A most simple implementation of the basic steps of input-output analysis described in Kitzes [12] in Python is available via Zenodo [60].

3. Results

This section shows the production-based and consumption-based inventories of the input-output tables in Figures 1, 4 and 6. It also touches on the differences in the inventories and potential implications for policymaking. Section 4 discusses more general aspects with no specific reference to the calculated inventories. For definitions of production-based and consumption-based inventories, readers are advised to revisit Section 2.3 or refer to Table A1.

3.1. Baseline Input-Output Table

In the production-based inventory of the input-output table in Figure 1, 8 m^3 and 4 m^3 of *Water consumption—Total* induced by the final demand of *Region A* is allocated to the *Agriculture* and *Manufacturing* sectors, respectively (where the externality occurs). In the consumption-based inventory of the input-output table in Figure 1, 4.8 m^3 and 7.2 m^3 of *Water consumption—Total* created by the final demand of Region A is allocated to the *Agriculture* and *Manufacturing* sectors, respectively (which correspond to the final demand/consumption).

The comparison of the production-based and consumption-based inventories shows a shift in the allocation of a major share of *Water consumption—Total* from the *Agriculture* sector in the production-based inventory towards the *Manufacturing* sector in the consumption-based inventory (Figure A1). The reason for this is that a larger proportion of the output of the *Agriculture* sector is an input for the *Manufacturing* sector than for the *Agriculture* sector itself or the final demand of *Region A*. This means that a large proportion of the water consumption associated with the final demand from the *Manufacturing* sector originates from the *Agriculture* sector (Figure 1).

If the inventories are calculated for the entire final demand, the total amount of a satellite account is the same in the production-based and consumption-based inventories, and the production-based inventory is equal to the satellite account q.

3.2. Disaggregated Satellite Accounts

Figure 5 depicts the production-based and consumption-based inventories of the input-output table in Figure 4. The overall results are the same as those shown in the input-output table in Figure 1 (8 m^3 and 4 m^3 and 4.8 m^3 and 7.2 m^3 in the production-based and consumption-based inventories, respectively; see the previous section). However, disaggregating the *Water consumption—Total* satellite account into its (fictitious) subparts allows for a more in-depth analysis of the composition of the inventories. The production-based inventory shows that all water consumption associated with wheat (6 m^3) and cotton (2 m^3) originates from the *Agriculture* sector, and all water consumption associated with textiles (2.5 m^3) and agricultural machinery (1.5 m^3) originates from the *Manufacturing* sector. This is different compared to the consumption-based inventory, which comprises water consumption originating from all sectors. The added level of detail shows of what externalities an inventory consists of. This helps practitioners understanding the implications of aggregation in input-output analysis and potentially misleading inventories as a result (see Section 3.4).

3.3. Disaggregated Transactions and Final Demand—Production-Based Inventory

In the production-based inventory of the 4 × 4 dummy input-output in Figure 6 (Figure 7), 3.63 m^3 of *Water consumption—Wheat* originating from *Region A* is allocated to *Region A*. The remaining 2.87 m^3 are allocated to *Region B*. Although all the 1.5 m^3 of *Water consumption—Cotton* originate from *Region A*, only 0.22 m^3 are allocated to *Region A*, with the remainder allocated to *Region B*. *Water consumption—Textiles* and *Water consumption—Agricultural machinery* solely originate from *Region B*, but most of these externalities are also allocated to *Region B*. Nevertheless, the overall sum of the externalities allocated to agricultural sectors (wheat and cotton) and manufacturing sectors (textiles and agricultural machinery) in both regions are the same as in the inventories of the 2 × 2 dummy input-output tables (8 m^3 and 4 m^3).

3.4. Implications of Aggregation

3.4.1. Sectoral Contributions in the Consumption-Based Inventory

The externalities allocated to the agricultural sectors (*Agriculture—Wheat* and *Agriculture—Cotton*) and the manufacturing sectors (*Manufacturing—Textiles* and *Manufacturing—Agricultural* machinery) in the production-based inventory of the 4 × 4 dummy input-output table in Figure A8 are different compared to the externalities allocated to the agricultural (*Agricul-*

ture) and manufacturing (*Manufacturing*) sectors in the production-based inventory of the 2 × 2 dummy input-output table in Figure A7. Instead of 4.8 m^3 (as in the 2 × 2 dummy input-output table), in the 4 × 4 input-output table 6.06 m^3 of water consumption (3.63 m^3 + 0.21 m^3 + 1.82 m^3 + 0.41 m^3 = 6.06 m^3) is allocated to the agricultural sectors (1.26 m^3 or 26.3% more; see Table 1). Instead of 7.2 m^3 in the 2 × 2 dummy input-output table, in the 4 × 4 input-output table 5.94 m^3 of water consumption (0.49 m^3 + 5.44 m^3 = 5.94 m^3) is allocated to the manufacturing sectors (1.57 m^3 or 17.5% less; see Table 1).

Table 1. A comparison of the sums of externalities allocated to the agricultural sectors (wheat and cotton) and manufacturing sectors (textiles and agricultural machinery) in the inventories of the 4 × 4 dummy input-output table and the externalities allocated to the agriculture and machinery sectors in the 2 × 2 dummy input-output table. See also Figure A7.

Inventory	Sector(s)	2 × 2 IO-Table	4 × 4 IO-Table	Δ (abs.)	Δ (rel.)
Production-based	Agriculture	8 m^3	8 m^3	0	0
Production-based	Manufacturing	4 m^3	4 m^3	0	0
Consumption-based	Agriculture	4.80 m^3	6.06 m^3	+1.26 m^3	+26%
Consumption-based	Manufacturing	7.20 m^3	5.94 m^3	−1.26 m^3	−18%

3.4.2. Composition of the Externalities in the Consumption-Based Inventory

The consumption-based inventory of the 2 × 2 input-output table in Figure 4 suggests that *Region A*'s final demand from both sectors, *Agriculture* and *Manufacturing*, causes most externalities through *Water consumption—Wheat* (Figure 5). In contrast, the consumption-based inventory of the 4 × 4 input-output table in Figure 6 suggests that both regions' manufacturing sectors together cause the most externalities, through *Water consumption—Textiles* followed by *Water consumption—Cotton* (Figure 7). If it is assumed that the 4 × 4 input-output table provides a more accurate representation of the fictitious economy, the less detailed aggregated 2 × 2 input-output table would misinform any decision-making process. Table 2 summarises the differences in the allocation of the externalities in the consumption-based inventories of the 2 × 2 and 4 × 4 dummy input-output tables. The values can be interpreted as the changes in the inventories because of aggregation. Table 2 shows that the aggregation led to:

- An increase in the allocation of *Water consumption—Cotton* from the agricultural sectors (*Agriculture—Wheat* and *Agriculture—Cotton*) to the *Agriculture* sector by +141.5%
- An increase in the allocation of *Water consumption—Wheat* from the manufacturing sectors (*Manufacturing—Textiles* and *Manufacturing—Agricultural machinery*) to the *Manufacturing* sector by +185%
- An increase in the allocation of *Water consumption—Textiles* from the agricultural sectors (*Agriculture—Wheat* and *Agriculture—Cotton*) to the *Agriculture* sector by +1040%
- An increase in the allocation of *Water consumption—Agricultural machinery* from the manufacturing sectors (*Manufacturing—Textiles* and *Manufacturing—Agricultural machinery*) to the *Manufacturing* sector by 42.5%
- . . . as well as corresponding decreases in the allocation of water consumption to the other sectors.

Table 2. Comparison of the allocation of externalities in the consumption-based inventories of the 2 × 2 and 4 × 4 dummy input-output tables in Figure 4 and Figure 6, respectively. The *Agriculture* rows in the 2 × 2 input-output table column contain the values of the *Agriculture (Region A)* sector. The *Agriculture* rows in the 4 × 4 input-output table column contain the sum of the values of the *Agriculture—Wheat (Region A)* and *Agriculture—Cotton (Region A)* sectors. The *Manufacturing* rows in the 2 × 2 input-output table column contain the values of the *Manufacturing (Region A)* sector. The *Manufacturing* rows in the 4 × 4 input-output table column contain the sum of the values of the *Manufacturing—Textiles (Region B)* and *Manufacturing—Agricultural machinery (Region B)* sectors. The changes in the "Δ (abs.)" and "Δ (abs.)" columns consider the 4 × 4 dummy input-output table as a baseline scenario (Figure A8). The results in the resolution of the input-output table in Figure 4 are shown in Figure A4.

Externality	Sector(s)	2 × 2 IO-Table	4 × 4 IO-Table	Δ (abs.)	Δ (rel.)
Water consumption—Wheat	Agriculture	3.00 m^3	4.95 m^3	−1.95 m^3	−39.4%
Water consumption—Wheat	Manufacturing	3.00 m^3	1.05 m^3	+1.95 m^3	+185%
Water consumption—Cotton	Agriculture	1.00 m^3	0.41 m^3	+0.59 m^3	+141.5%
Water consumption—Cotton	Manufacturing	1.00 m^3	1.59 m^3	−0.59 m^3	−36.9%
Water consumption—Textiles	Agriculture	0.50 m^3	0.04 m^3	+0.46 m^3	+1040%
Water consumption—Textiles	Manufacturing	2.00 m^3	2.46 m^3	−0.46 m^3	−18.6%
Water consumption—Agricultural machinery	Agriculture	0.30 m^3	0.66 m^3	−0.36 m^3	−54.4%
Water consumption—Agricultural machinery	Manufacturing	1.20 m^3	0.84 m^3	+0.36 m^3	+42.5%

4. Discussion

This section reflects on the implications of aggregation in input-output analysis (Section 4.1) and lists some of the most established input-output databases (Section 4.2). It concludes with a summary of the study's limitations (Section 4.3).

4.1. Aggregation

In input-output analysis, the input mixes of all sectors consuming from another sector are proportional to the producing sector's output mix. Leontief formulated this as "the distribution [. . .] among the different consumers is made [. . .] on a strictly proportional basis. For each kind of use, each source of supply is drawn upon in proportion to its total output" [9]. In most cases, this is unlikely to be the case in any real economic scenario. Consequently, aggregation of economic data in input-output tables inevitably leads to loss of information and distorted inventories (Section 3.2). The comparison of the inventories of differently-resolved input-output tables (Figures 1, 4 and 6) has shown the potential implications e.g., in a worst case, misinformed decision-making. In the given examples, the difference in allocation between the differently resolved input-output tables diverges by more than 1000% for one specific sector and by more than 100% for two other sectors (Table 2). Other studies on aggregation in input-output analysis corroborate these observations. Bouwmeester and Oosterhaven [61] analysed regional and sectoral aggregation errors of carbon dioxide emissions and water use. Steen-Olsen et al. [62] investigated the required level of detail of input-output data to mitigate the effects of sectoral aggregation. De Koning et al. [63] applied a scenario-based approach to investigate the effects of sectoral aggregation, satellite account aggregation and regional aggregation. Schulte et al. [64] quantified the aggregation-induced uncertainty in the Exiobase database and found particularly high coefficients of variations for small economies with a high share of trade.

To improve the robustness of input-output analyses, scholars have repeatedly advocated the development of input-output databases with a high resolution [9,65–67]. This endeavour was also formulated by Wassily Leontief [9] who suggested that "a distribution of all [. . .] transactions among some smaller, more homogeneous, quasi-independent accounting units appears to be highly desirable" and, despite major advancements, continues. Yet, for the near future, even the most comprehensive input-output tables for sustainability assessments will always be subject to aggregation. Therefore, practitioners' awareness of and clear communication of potential aggregation-induced distortions of inventories is crucial. Particular attention should be paid to those sectors, products or product groups that are of high relevance concerning a study's objective or the externality under study. For instance, concerning agricultural primary production. According to best practice, some input-output tables feature dedicated sectors for the most prevalent staple crops such as rice or wheat [68,69].

Alternatively, practitioners can develop custom satellite accounts to best meet the requirements of their research objective. However, eventually, the resolution of any satellite account must match the input-output data's given level of aggregation. Even if this implies aggregating data concerning an externality with a resolution higher than the resolution of the input-output data. Nonetheless, providing separate satellite accounts for the aggregated externalities can still introduce transparency regarding the composition of inventories (Section 3.2). This can help practitioners better understand the impacts of aggregation on their research results—and the implications this has for decision-making. An approach superior to working with separate satellite accounts is to disaggregate input-output data through hybridisation with other data sources offering a higher resolution [45]. A challenge in hybridisation that remains is that even if a sector has been disaggregated, it is often unknown for which sectors the disaggregated outputs serve as an input [66].

4.2. Input-Output Databases

A recent overview of input-output databases for sustainability assessments was published by Pfister and Kulionis [70]. It covers the Eora [71,72], Exiobase [69,73], WIOD [74], GTAP [75] and OECD ICIO [76] databases. More recently published input-output databases for sustainability assessments include RMRIO [77,78], FABIO [79] and GLORIA [68]. RMRIO is a merge of the Eora and Exiobase databases. FABIO is a food and agriculture biomass input-output model. At the time of writing, GLORIA is the most comprehensive global generic input-output database in terms of regional and sectoral coverage.

4.3. Limitations

Both, the 2×2 dummy input-output table in Figure 1 by Kitzes [12] as well as the hypothetically non-aggregated 4×4 dummy input-output tables in Figures 4 and 6 are fictitious. The input-output tables were devised to facilitate an accessible yet comprehensive introduction to input-output analysis and the implications aggregation has for decision-making. None of the given tables represents the full complexity of real input-output databases. It should also be noted that aggregation can as well be performed in an optimised manner to minimise the effects of aggregation.

It is worth taking note that production-based and consumption-based allocation schemes are the two opposite extremes along a more nuanced range of avaialble allocation schemes. Other allocation schemes include extraction-based, income-based, and value-based [80] as well as combinations thereof such as shared producer and consumer responsibility [81].

This study did not cover the derivation of an input-output table from a set of linear equations. Readers interested in this matter are referred to Leontief [10]. To better understand how input-output analysis is founded in the field of economics, readers are advised to resort to the literature referenced in the introduction e.g., Miller and Blair [11] who published the most exhaustive overview of input-output analysis.

5. Conclusions

Albeit having been found in economics, input-output analyses have become an established tool in sustainability sciences for allocating the externalities of a given economy to agents in that economy based on the agents' input-output interdependencies.

This work aimed to provide a hands-on introduction to input-output analysis with a particular focus on the potential effects of the aggregation of input-output data. For this, a set of differently resolved fictitious dummy input-output tables was presented. The production-based and consumption-based inventories of the presented tables were compared which allowed for demonstrating the potential effects of aggregation. This work's numerical and hands-on approach communicates the topic of aggregation in input-output analysis in an original manner and targets non-technical practitioners of input-output analysis from the field of sustainability sciences to whom this work aims to offer new perspectives. It supplements other works on aggregation in input-output analysis, some of which are summarised in Section 1.

This work has demonstrated that aggregation of input-output data, which is rather the rule than the exception, can distort the allocation of externalities in consumption-based inventories. In worst-case scenarios, this can lead to misinformed decision-making. Consequently, it is crucial to always consider the potential implications of aggregation in input-output analysis-based assessments and in the decision-making processes that involve input-output analysis-based assessments. In many input-output analysis-based studies, however, aggregation is not considered or receives negligible attention.

Assessments based on input-output analysis can offer valuable insights for exploring many sustainability-related macroeconomic research questions. Consequently, input-output analysis is an essential method in sustainability sciences, and the endeavour to develop ever more comprehensive and detailed input-output databases, possibly with specific foci, continues and keeps improving input-output analysis-based assessments. In the meantime, practitioners should carefully consider the potential implications of aggregation in input-output analysis-based assessments and communicate findings transparently and with consideration of the potential effects of the aggregation of input-output data.

Author Contributions: Conceptualization, J.B.; methodology, J.B.; formal analysis, J.B.; data curation, J.B.; writing—original draft preparation, J.B.; writing—review and editing, J.B. and M.F.; visualization, J.B.; supervision, M.F. All authors have read and agreed to the published version of the manuscript.

Funding: We acknowledge support by the German Research Foundation and the Open Access Publication Fund of TU Berlin.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Supplementary Information on Input-Output Analysis

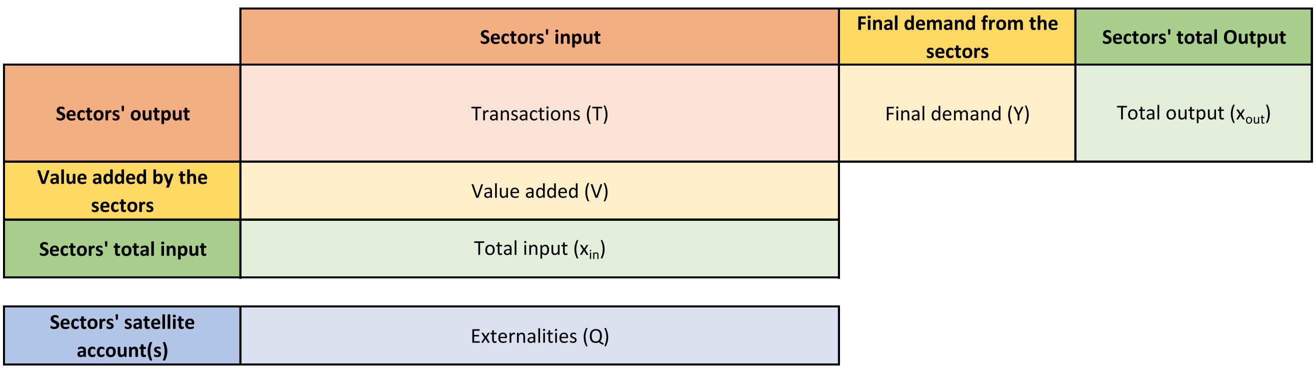

Figure A1. Schematic illustration of the typical structure of an input-output table. See Figure 1 (2 × 2), Figure 4 (4 × 4) and Figure 6 (4 × 4) for numeric dummy input-output tables with different dimensions.

Table A1. Definitions of the terms "production-based inventory" and "consumption-based inventory". See Section 3.2 in the manuscript for additional allocation schemes.

Inventory	Peters [82]	Wood et al. [73]	Arnold et al. [80]
Production-based	"Domestic production including exports"	"The production-based indicators account for the value added as well as the substances emitted within the geographical bounds of a region or country."	"emissions generated during production. Responsibility is fully allocated to producers of goods and services where they occur in the value chain."
Consumption-based	"Domestic consumption ([excluding] exports but includ[ing] imports)"	"On the other hand, consumption-based indicators (footprints) represent the direct and indirect value added/emitted substances caused by the final demand in a specific country or region."	"emissions generated for satisfying consumption. Responsibility of life cycle emissions is fully allocated to final consumers of goods and services."

Appendix B. Supplementary Information on the Results

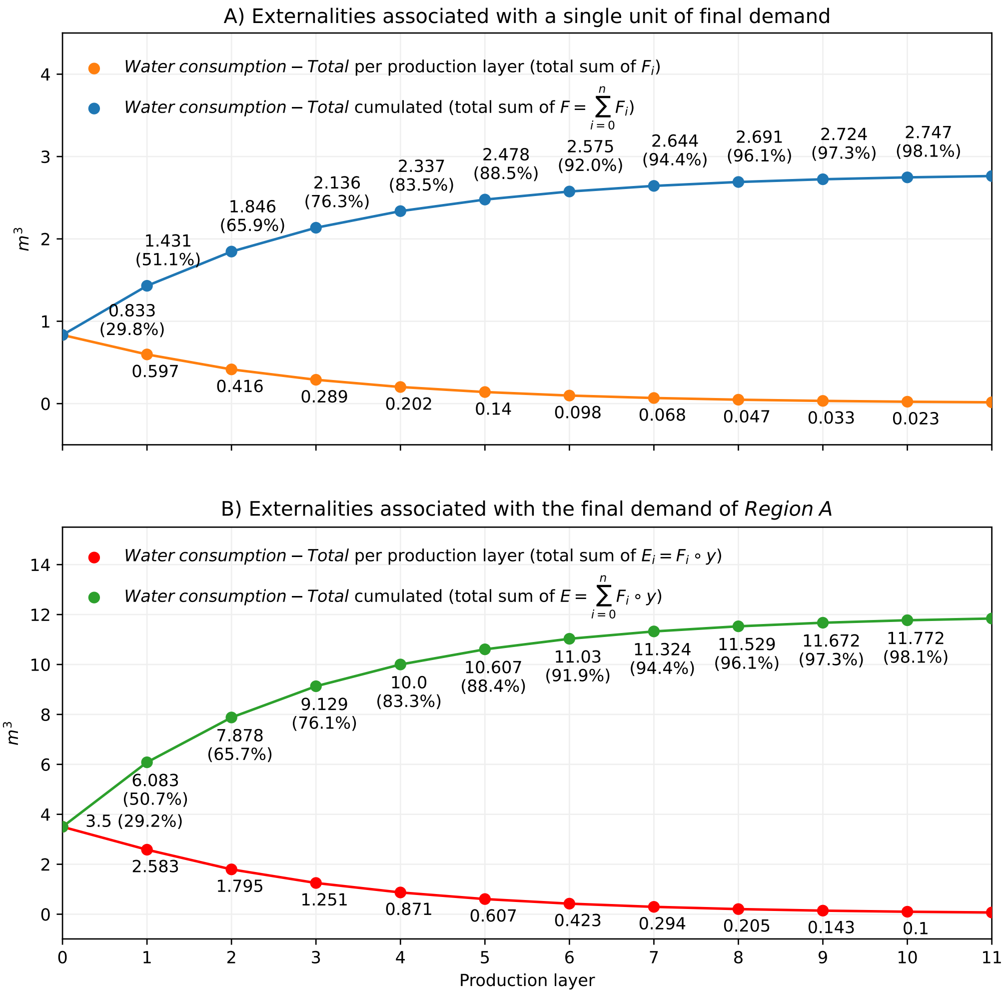

Figure A2. (**A**) The externalities associated with a single unit of final demand; (**B**) The externalities associated with the total final demand of *Region A*; Both are given per production layer (absolute) and cumulative. Calculated based on the 2 × 2 dummy input-output table in Figure 1. More than 95% of all externalities accrue on the first nine production layers. The figures were determined using series expansion (see Equation (4) and Figure 3) and can also be determined using structural path analysis (see Figure 2).

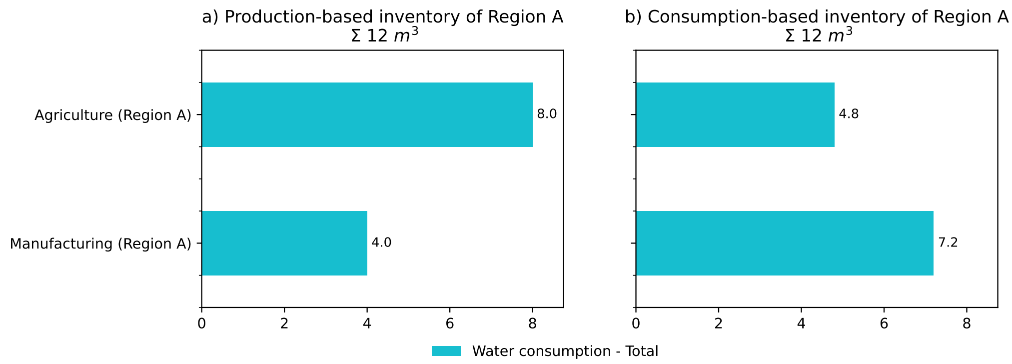

Figure A3. The production-based and consumption-based inventories of the input-output in Figure 1.

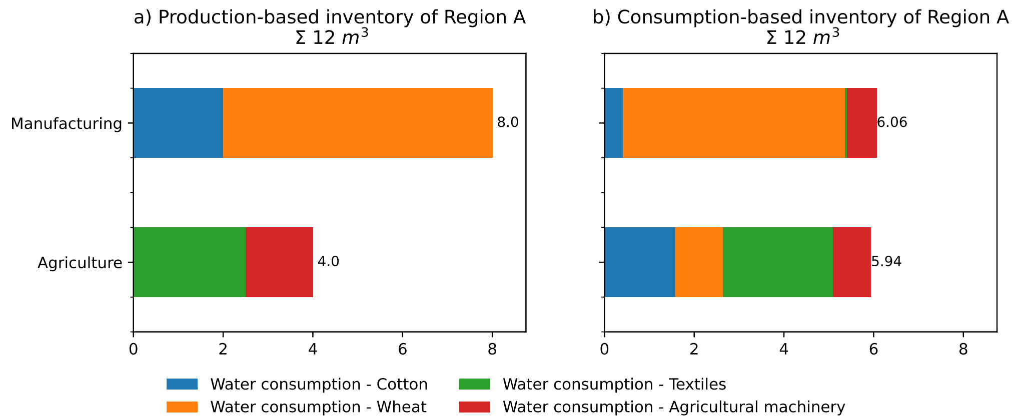

Figure A4. (Re-)Aggregated production-based and consumption-based inventories from Figure 7. The figure allows a comparison of the production-based inventories of the input-output table in Figure 5 (2 × 2) shown in Figure 4 with the production-based and consumption-based inventory of the input-output table in Figure 6 (4 × 4) shown in Figure 7.

Heat Maps

a) Production-based invenetory of Region A Σ 12 m³	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	
Agriculture (Region A)	2.00	6.00	0	0	8.00
Manufacturing (Region A)	0	0	2.50	1.50	4.00
	2.00	6.00	2.50	1.50	12.00

b) Consumption-based inventory of Region A Σ 12 m³	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	
Agriculture (Region A)	1.00	3.00	0.50	0.30	4.80
Manufacturing (Region A)	1.00	3.00	2.00	1.20	7.20
	2.00	6.00	2.50	1.50	12.00

Figure A5. The production-based and consumption-based inventories of the monetary input-output table in Figure 4. See Figure 5 for the corresponding bar charts.

a) Production-based invenetory of Region A
Σ 4.33 m³

	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	
Agriculture - Wheat (Region A)	0	3.35	0	0	3.35
Agriculture - Cotton (Region A)	0.30	0	0	0	0.30
Manufacturing - Textiles (Region B)	0	0	0.23	0.0	0.23
Manufacturing - Agricultural machinery (Region B)	0	0	0	0.45	0.45
	0.30	3.35	0.23	0.45	4.33

b) Consumption-based inventory of Region A
Σ 4.33 m³

	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	
Agriculture - Wheat (Region A)	0.06	3.22	0.02	0.33	3.63
Agriculture - Cotton (Region A)	0.11	0.04	0.00	0.05	0.21
Manufacturing - Textiles (Region B)	0.13	0.09	0.20	0.07	0.49
Manufacturing - Agricultural machinery (Region B)	0.0	0.0	0.0	0.0	0.00
	0.30	3.35	0.23	0.45	4.33

c) Production-based inventory of Region B
Σ 7.67 m³

	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	
Agriculture - Wheat (Region A)	0	2.65	0	0	2.65
Agriculture - Cotton (Region A)	1.70	0	0	0	1.70
Manufacturing - Textiles (Region B)	0	0	2.27	0	2.27
Manufacturing - Agricultural machinery (Region B)	0	0	0	1.05	1.05
	1.70	2.65	2.27	1.05	7.67

d) Consumption-based inventory of Region B
Σ 7.67 m³

	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	
Agriculture - Wheat (Region A)	0.03	1.61	0.01	0.16	1.82
Agriculture - Cotton (Region A)	0.22	0.07	0.01	0.11	0.41
Manufacturing - Textiles (Region B)	1.45	0.96	2.25	0.77	5.44
Manufacturing - Agricultural machinery (Region B)	0	0	0	0	0.00
	1.70	2.65	2.27	1.05	7.67

Production-based inventory of Region A & Region B

2.00	6.00	2.50	1.50	12.00

Consumption-based inventory of Region A & Region B

5.45	0.62	5.94	0.00	12.00

Figure A6. The production-based and consumption-based inventories of the monetary input-output table in Figure 6. See Figure 7 for the corresponding bar chart.

Appendix C. Supplementary Information on the Implications of Aggregation

A)

	a) Production-based inventory of Region A Σ 12 m³				b) Consumption-based inventory of Region A Σ 12 m³			
	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery
Agriculture (Region A)	2.00	6.00	0	0	1.00	3.00	0.50	0.30
Manufacturing (Region A)	0	0	2.50	1.50	1.00	3.00	2.00	1.20

B.1)

	a) Production-based inventory of Region A Σ 4.33 m³				b) Consumption-based inventory of Region A Σ 4.33 m³			
	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery
Agriculture - Wheat (Region A)	0	3.35	0	0	0.06	3.22	0.02	0.33
Agriculture - Cotton (Region A)	0.30	0	0	0	0.11	0.04	0.00	0.05
Manufacturing - Textiles (Region B)	0	0	0.23	0.0	0.13	0.09	0.20	0.07
Manufacturing - Agricultural machinery (Region B)	0	0	0	0.45	0.0	0.0	0.0	0.0

B.2)

	c) Production-based inventory of Region B Σ 7.67 m³				d) Consumption-based inventory of Region B Σ 7.67 m³			
	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery
Agriculture - Wheat (Region A)	0	2.65	0	0	0.03	1.61	0.01	0.16
Agriculture - Cotton (Region A)	1.70	0	0	0	0.22	0.07	0.01	0.11
Manufacturing - Textiles (Region B)	0	0	2.27	0	1.45	0.96	2.25	0.77
Manufacturing - Agricultural machinery (Region B)	0	0	0	1.05	0	0	0	0

C)

		m³	m³	Δ (abs.)	Δ (rel.)
Production-based inventory	Σ Agriculture 2x2	8	8	0	0
	Σ Manufacturing 2x2	4	4	0	0
Consumption-based inventory	Σ Agriculture 4x4	4.80	6.06	+1.26	+26%
	Σ Manufacturing 4x4	7.20	5.94	−1.26	−18%

Figure A7. (**A**) Production-based and consumption-based inventories of the input-output in Figure 4; (**B.1**) Production-based and consumption-based inventories associated with the final demand of *Region A* in the input-output in Figure 6; (**B.2**) Production-based and consumption-based inventories associated with the final demand of *Region B* in the input-output table in Figure 6; (**C**) A comparison of the sums of the contributions by the agricultural sectors (wheat and cotton) and manufacturing sectors (textiles and agricultural machinery) in the inventories of the 4 × 4 dummy input-output table (**A**) and the contributions of the agriculture and machinery sectors in the 2 × 2 dummy input-output table (**B.1**,**B.2**). The background colours of the cells indicate which cells were used to calculate the respective sums (see Section 3.4).

A)

	Consumption-based inventory of Region A Σ 12 m³			
	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery
Agriculture (Region A)	1.00	3.00	0.50	0.30
Manufacturing (Region A)	1.00	3.00	2.00	1.20

B)

	Consumption-based inventory of Region B Σ 7.67 m³				Consumption-based inventory of Region A Σ 4.33 m³			
	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery	Water consumption - Cotton	Water consumption - Wheat	Water consumption - Textiles	Water consumption - Agricultural machinery
Agriculture - Wheat (Region A)	0.03	1.61	0.01	0.16	0.06	3.22	0.02	0.33
Agriculture - Cotton (Region A)	0.22	0.07	0.01	0.11	0.11	0.04	0.00	0.05
Manufacturing - Textiles (Region B)	1.45	0.96	2.25	0.77	0.13	0.09	0.20	0.07
Manufacturing - Agricultural machinery (Region B)	0	0	0	0	0.0	0.0	0.0	0.0

C)

	Sector(s)	2x2	4x4	Δ (abs.)
Water consumption - Wheat	Agriculture	3.00	4.95	-1.95
	Manufacturing	3.00	1.05	1.95
Water consumption - Cotton	Agriculture	1.00	0.41	0.59
	Manufacturing	1.00	1.59	-0.59
Water consumption - Textiles	Agriculture	0.50	0.04	0.46
	Manufacturing	2.00	2.46	-0.46
Water consumption - Agricultural machinery	Agriculture	0.30	0.66	-0.36
	Manufacturing	1.20	0.84	0.36

Figure A8. (**A**) Comparison of the allocation of externalities from the consumption-based inventory of the input-output table in Figure 4; (**B**) Consumption-based inventories associated with the final demand of *Region A* and *Region B* in the input-output table in Figure 6; (**C**) A sectoral comparison of the consumption-based inventories of the 2 × 2 and 4 × 4 input-output tables in Figures 4 and 6, respectively. The background colours of the cells indicate which cells were used to calculate the respective sums (see Section 3.4.2).

Appendix D. Non-Monetary Input-Output Table

In theory, monetary input-output tables can be derived from non-monetary input-output tables based on the value of transferred goods and services. An example is given in Figure A9, which is the non-monetary counterpart of the monetary input-output table in Figure 6. The production-based and consumption-based inventories of the input-output table in Figure A9 are the same as those of the input-output in Figure A6 (Figure A8). A major advantage of non-monetary input-output tables is that they are not affected by currency conversions, subsidies or taxation schemes [83]. However, large input-output databases are the result of complex aggregation processes, and usually each sector covers a heterogeneous range of products and services [84].

			Agriculture - Wheat	Agriculture - Cotton	Manufacturing - Textiles	Manufacturing - Agricultural machinery	Final demand	Final demand	Total output
			Region A	Region A	Region B	Region B	Region A	Region B	-
			kg	kg	noi	noi	-	-	-
Agriculture - Wheat	**Region A**	**kg**	3	0	0.25	0.500	1.5	0.75	6.000
Agriculture - Cotton	**Region A**	**kg**	0	2.5	1.875	0.250	0.125	0.25	5.000
Manufacturing - Textiles	**Region B**	**noi**	0	0	0.125	0.025	0.05	0.55	0.750
Manufacturing - Agricultural machinery	**Region B**	**noi**	0.1	0.167	0	0.033	0	0	0.300
~~**Value added**~~	~~**Region A**~~	-							
~~**Value added**~~	~~**Region B**~~	-							
~~**Total input**~~	-	-							

		Agriculture - Wheat	Agriculture - Cotton	Manufacturing - Textiles	Manufacturing - Agricultural machinery
Water consumption - Total	**m³**	6.5	1.5	2.5	1.5
Water consumption - Cotton	**m³**	0	1.5	0	0
Water consumption - Wheat	**m³**	6.5	0	0	0
Water consumption - Textiles	**m³**	0	0	2.5	0
Water consumption - Agricultural machinery	**m³**	0	0	0	1.5

Wheat (Region A) €/kg:	1
Cotton (Region A) €/kg:	2
Textiles (Region B) €/noi (number of items):	10
Agricultural machinery (Region B) €/noi (numer of items):	15

Figure A9. A hypothetical non-monetary input-output table based on Figure 6 in the manuscript. The conversion factors for turning the monetary values in the input-output in Figure 6 into non-monetary values are given in the bottom-right corner. The production-based and consumption-based inventories are shown in Figure 7 in the manuscript.

References

1. McNeill, J.R. *The Great Acceleration: An Environmental History of the Anthropocene since 1945*; Harvard University Press: Cambridge, MA, USA, 2014. [CrossRef]
2. Steffen, W.; Sanderson, R.A.; Tyson, P.D.; Jäger, J.; Matson, P.A.; Moore, B., III; Oldfield, F.; Richardson, K.; Schellnhuber, H.J.; Turner, B.L.; et al. *Global Change and the Earth System: A Planet Under Pressure*; Global Change—The IGBP Series; Springer: Berlin/Heidelberg, Germany, 2004. [CrossRef]
3. Steffen, W.; Richardson, K.; Rockstrom, J.; Cornell, S.E.; Fetzer, I.; Bennett, E.M.; Biggs, R.; Carpenter, S.R.; de Vries, W.; de Wit, C.A.; et al. Planetary boundaries: Guiding human development on a changing planet. *Science* **2015**, *347*, 1259855. [CrossRef] [PubMed]
4. Meadows, D.H.; Meadows, D.L.; Randers, J.; Behrens, W.W. *The Limits to Growth: A Report for the Club of Rome's Project on the Predicament of Mankind*, 2nd ed.; Universe Books: New York, NY, USA, 1972.
5. Rockström, J.; Steffen, W.; Noone, K.; Persson, A.; Chapin, F.S.; Lambin, E.F.; Lenton, T.M.; Scheffer, M.; Folke, C.; Schellnhuber, H.J.; et al. A safe operating space for humanity. *Nature* **2009**, *461*, 472–475. [CrossRef] [PubMed]
6. Rockström, J.; Steffen, W.; Noone, K.; Persson, A.; Chapin, F.S.I.; Lambin, E.; Lenton, T.M.; Scheffer, M.; Folke, C.; Schellnhuber, H.J.; et al. Planetary Boundaries: Exploring the Safe Operating Space for Humanity. *Ecol. Soc.* **2009**, *14*, art32. [CrossRef]
7. Masson-Delmotte, V.; Zhai, P.; Pirani, A.; Connors, S.L.; Péan, C.; Berger, S.; Caud, N.; Chen, Y.; Goldfarb, L.; Gomis, M.I.; et al. (Eds.) *Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*; Cambridge University Press: Cambridge, UK, 2021.
8. WCED. *Our Common Future*; Oxford Paperbacks; Oxford University Press: Oxford, UK; New York, NY, USA, 1987.
9. Leontief, W. Quantitative input and output relations in the economic systems of the United States. *Rev. Econ. Stat.* **1936**, *18*, 105–125. [CrossRef]
10. Leontief, W. Environmental Repercussions and the Economic Structure: An Input-Output Approach. *Rev. Econ. Stat.* **1970**, *52*, 262–271. [CrossRef]
11. Miller, R.E.; Blair, P.D. *Input–Output Analysis: Foundations and Extensions*, 2nd ed.; Cambridge University Press: Cambridge, UK, 2009; p. 784.
12. Kitzes, J. An Introduction to Environmentally-Extended Input-Output Analysis. *Resources* **2013**, *2*, 489–503. [CrossRef]
13. Chen, B.; Han, M.; Peng, K.; Zhou, S.; Shao, L.; Wu, X.; Wei, W.; Liu, S.; Li, Z.; Li, J.; et al. Global land-water nexus: Agricultural land and freshwater use embodied in worldwide supply chains. *Sci. Total Environ.* **2018**, *613–614*, 931–943. [CrossRef]
14. Hung, C.C.W.; Hsu, S.C.; Cheng, K.L. Quantifying city-scale carbon emissions of the construction sector based on multi-regional input-output analysis. *Resour. Conserv. Recycl.* **2019**, *149*, 75–85. [CrossRef]
15. Lenk, C.; Arendt, R.; Bach, V.; Finkbeiner, M. Territorial-Based vs. Consumption-Based Carbon Footprint of an Urban District—A Case Study of Berlin-Wedding. *Sustainability* **2021**, *13*, 7262. [CrossRef]
16. Long, Y.; Yoshida, Y. Quantifying city-scale emission responsibility based on input-output analysis—Insight from Tokyo, Japan. *Appl. Energy* **2018**, *218*, 349–360. [CrossRef]
17. Moran, D.; Kanemoto, K.; Jiborn, M.; Wood, R.; Többen, J.; Seto, K.C. Carbon footprints of 13.000 cities. *Environ. Res. Lett.* **2018**, *13*, 064041. [CrossRef]
18. Wiedmann, T.; Chen, G.; Owen, A.; Lenzen, M.; Doust, M.; Barrett, J.; Steele, K. Three-scope carbon emission inventories of global cities. *J. Ind. Ecol.* **2021**, *25*, 735–750. [CrossRef]
19. Martinez, S.; Marchamalo, M.; Alvarez, S. Organization environmental footprint applying a multi-regional input-output analysis: A case study of a wood parquet company in Spain. *Sci. Total Environ.* **2018**, *618*, 7–14. [CrossRef]
20. Martinez, S.; Delgado, M.d.M.; Martinez Marin, R.; Alvarez, S. Organization Environmental Footprint through Input-Output Analysis: A Case Study in the Construction Sector. *J. Ind. Ecol.* **2019**, *23*, 879–892. [CrossRef]
21. Acquaye, A.A.; Duffy, A.P. Input–output analysis of Irish construction sector greenhouse gas emissions. *Build. Environ.* **2010**, *45*, 784–791. [CrossRef]
22. Martínez-Blanco, J.; Forin, S.; Finkbeiner, M. Challenges of organizational LCA: Lessons learned from road testing the guidance on organizational life cycle assessment. *Int. J. Life Cycle Assess.* **2020**, *25*, 311–331. [CrossRef]
23. Lenzen, M. An input–output analysis of Australian water usage. *Water Policy* **2001**, *3*, 321–340. [CrossRef]
24. Zhang, C.; Anadon, L.D. A multi-regional input–output analysis of domestic virtual water trade and provincial water footprint in China. *Ecol. Econ.* **2014**, *100*, 159–172. [CrossRef]
25. Dawkins, E.; Moran, D.; Palm, V.; Wood, R.; Björk, I. The Swedish footprint: A multi-model comparison. *J. Clean. Prod.* **2019**, *209*, 1578–1592. [CrossRef]
26. Bunsen, J.; Berger, M.; Finkbeiner, M. Planetary boundaries for water—A review. *Ecol. Indic.* **2021**, *121*. [CrossRef]
27. Wiedmann, T.O.; Schandl, H.; Lenzen, M.; Moran, D.; Suh, S.; West, J.; Kanemoto, K. The material footprint of nations. *Proc. Natl. Acad. Sci. USA* **2015**, *112*, 6271–6276. [CrossRef] [PubMed]
28. Wiedmann, T.; Wood, R.; Minx, J.C.; Lenzen, M.; Guan, D.; Harris, R. A Carbon Footprint Time Series of the Uk—Results from a Multi-Region Input–Output Model. *Econ. Syst. Res.* **2010**, *22*, 19–42. [CrossRef]
29. Tukker, A.; Bulavskaya, T.; Giljum, S.; Koning, A.d.; Lutter, S.; Simas, M.; Stadler, K.; Wood, R. *The Global Resource Footprint of Nations. Carbon, Water, Land and Materials Embodied in Trade and Final Consumption, Calculated with EXIOBASE 2.1*; TNO: The Hague, The Netherlands, 2014.

30. Ivanova, D.; Stadler, K.; Steen-Olsen, K.; Wood, R.; Vita, G.; Tukker, A.; Hertwich, E.G. Environmental Impact Assessment of Household Consumption. *J. Ind. Ecol.* **2016**, *20*, 526–536. [CrossRef]
31. Lenzen, M.; Moran, D.; Bhaduri, A.; Kanemoto, K.; Bekchanov, M.; Geschke, A.; Foran, B. International trade of scarce water. *Ecol. Econ.* **2013**, *94*, 78–85. [CrossRef]
32. Moran, D.; Kanemoto, K. Tracing global supply chains to air pollution hotspots. *Environ. Res. Lett.* **2016**, *11*, 094017. [CrossRef]
33. Davis, S.J.; Peters, G.P.; Caldeira, K. The supply chain of CO_2 emissions. *Proc. Natl. Acad. Sci. USA* **2011**, *108*, 18554–18559. [CrossRef]
34. Lenzen, M.; Moran, D.; Kanemoto, K.; Foran, B.; Lobefaro, L.; Geschke, A. International trade drives biodiversity threats in developing nations. *Nature* **2012**, *486*, 109–112. [CrossRef]
35. Bjelle, E.L.; Többen, J.; Stadler, K.; Kastner, T.; Theurl, M.C.; Erb, K.H.; Olsen, K.S.; Wiebe, K.S.; Wood, R. Adding country resolution to EXIOBASE: Impacts on land use embodied in trade. *J. Econ. Struct.* **2020**, *9*, 14. [CrossRef]
36. Bjelle, E.L.; Kuipers, K.; Verones, F.; Wood, R. Trends in national biodiversity footprints of land use. *Ecol. Econ.* **2021**, *185*, 107059. [CrossRef]
37. Bunsen, J.; Berger, M.; Ward, H.; Finkbeiner, M. Germany's global water consumption under consideration of the local safe operating spaces of watersheds worldwide. *Clean. Responsible Consum.* **2021**, *3*, 100034. [CrossRef]
38. Shilling, H.J.; Wiedmann, T.; Malik, A. Modern slavery footprints in global supply chains. *J. Ind. Ecol.* **2021**, *25*, 1518–1528. [CrossRef]
39. Theil, H. Linear Aggregation in Input-Output Analysis. *Econometrica* **1957**, *25*, 111–122. [CrossRef]
40. Fisher, W.D. Criteria for Aggregation in Input-Output Analysis. *Rev. Econ. Stat.* **1958**, *40*, 250–260. [CrossRef]
41. Miller, R.E.; Blair, P. Spatial aggregation in interregional input-output models. *Pap. Reg. Sci. Assoc.* **1981**, *48*, 149–164. [CrossRef]
42. Kymn, K.O. Aggregation in Input–Output Models: A Comprehensive Review, 1946–71. *Econ. Syst. Res.* **1990**, *2*, 65–93. [CrossRef]
43. Ara, K. The Aggregation Problem in Input-Output Analysis. *Econometrica* **1959**, *27*, 257–262. [CrossRef]
44. Neudecker, H. Aggregation in Input-Output Analysis: An Extension of Fisher's Method. *Econometrica* **1970**, *38*, 921–926. [CrossRef]
45. Lenzen, M. Aggregation Versus Disaggregation in Input–Output Analysis of the Environment. *Econ. Syst. Res.* **2011**, *23*, 73–89. [CrossRef]
46. Wood, R.; Hawkins, T.R.; Hertwich, E.G.; Tukker, A. Harmonising National Input—Output Tables for Consumption-Based Accounting—Experiences from Exiopol. *Econ. Syst. Res.* **2014**, *26*, 387–409. [CrossRef]
47. Papong, S.; Itsubo, N.; Malakul, P.; Shukuya, M. Development of the Social Inventory Database in Thailand Using Input–Output Analysis. *Sustainability* **2015**, *7*, 7684–7713. [CrossRef]
48. Costa, D.; Quinteiro, P.; Pereira, V.; Dias, A.C. Social life cycle assessment based on input-output analysis of the Portuguese pulp and paper sector. *J. Clean. Prod.* **2022**, *330*, 129851. [CrossRef]
49. Benoît Norris, C.; Norris, G. Chapter 8: The Social Hotspots Database Context of the SHDB. In *The Sustainability Practitioner's Guide to Social Analysis and Assessment*; McBain, D., Murray, J., Wiedmann, T., Eds.; Common Ground Research Networks: Champaign, IL, USA, 2015.
50. Ciroth, A.; Eisfeldt, F. A new, comprehensive database for social LCA: PSILCA. In Proceedings of the ILCM 2015, New Delhi, India, 14–15 September 2015.
51. Lenzen, M. Structural path analysis of ecosystem networks. *Ecol. Model.* **2007**, *200*, 334–342. [CrossRef]
52. Defourny, J.; Thorbecke, E. Structural Path Analysis and Multiplier Decomposition within a Social Accounting Matrix Framework. *Econ. J.* **1984**, *94*, 111–136. [CrossRef]
53. Crama, Y.; Defourny, J.; Gazon, J. Structural decomposition of multipliers in input-output or social accounting matrix analysis. *Économie Appliquée* **1984**, *37*, 215–222.
54. Van Rossum, G.; Drake, F.L., Jr. *Python Tutorial*; Centrum voor Wiskunde en Informatica: Amsterdam, The Netherlands, 1995.
55. Reback, J.; Jbrockmendel; McKinney, W.; Van Den Bossche, J.; Augspurger, T.; Cloud, P.; Hawkins, S.; Gfyoung; Roeschke, M.; Sinhrks; et al. Pandas-dev/pandas: Pandas 1.3.4. *Zenodo* **2021**. [CrossRef]
56. McKinney, W. Data Structures for Statistical Computing in Python. In Proceedings of the 9th Python in Science Conference, Austin, TX, USA, 28 June–3 July 2010; pp. 51–56.
57. Harris, C.R.; Millman, K.J.; van der Walt, S.J.; Gommers, R.; Virtanen, P.; Cournapeau, D.; Wieser, E.; Taylor, J.; Berg, S.; Smith, N.J.; et al. Array programming with NumPy. *Nature* **2020**, *585*, 357–362. [CrossRef]
58. Stephan, A.; Bontinck, P.A. *pyspa—An Object-Oriented Python Package for Structural Path Analysis*; GitHub: San Francisco, CA, USA, 2019. [CrossRef]
59. Hunter, J.D. Matplotlib: A 2D graphics environment. *Comput. Sci. Eng.* **2007**, *9*, 90–95. [CrossRef]
60. Bunsen, J. A most simple implementation of Kitzes (2013) in Python. *Zenodo* **2022**. [CrossRef]
61. Bouwmeester, M.C.; Oosterhaven, J. Specification and Aggregation Errors in Environmentally Extended Input–Output Models. *Environ. Resour. Econ.* **2013**, *56*, 307–335. [CrossRef]
62. Steen-Olsen, K.; Owen, A.; Hertwich, E.G.; Lenzen, M. Effects of Sector Aggregation on Co2 Multipliers in Multiregional Input–Output Analyses. *Econ. Syst. Res.* **2014**, *26*, 284–302. [CrossRef]
63. de Koning, A.; Bruckner, M.; Lutter, S.; Wood, R.; Stadler, K.; Tukker, A. Effect of aggregation and disaggregation on embodied material use of products in input–output analysis. *Ecol. Econ.* **2015**, *116*, 289–299. [CrossRef]

64. Schulte, S.; Jakobs, A.; Pauliuk, S. Relaxing the import proportionality assumption in multi-regional input–output modelling. *J. Econ. Struct.* **2021**, *10*, 20. [CrossRef] [PubMed]
65. Tukker, A.; Dietzenbacher, E. Global Multiregional Input-Output Frameworks: An Introduction and Outlook. *Econ. Syst. Res.* **2013**, *25*, 1–19. [CrossRef]
66. Wiedmann, T.O.; Suh, S.; Feng, K.; Lenzen, M.; Acquaye, A.; Scott, K.; Barrett, J.R. Application of Hybrid Life Cycle Approaches to Emerging Energy Technologies—The Case of Wind Power in the UK. *Environ. Sci. Technol.* **2011**, *45*, 5900–5907. [CrossRef] [PubMed]
67. Kitzes, J.; Galli, A.; Bagliani, M.; Barrett, J.; Dige, G.; Ede, S.; Erb, K.; Giljum, S.; Haberl, H.; Hails, C.; et al. A research agenda for improving national Ecological Footprint accounts. *Ecol. Econ.* **2009**, *68*, 1991–2007. [CrossRef]
68. Lenzen, M.; Geschke, A.; Abd Rahman, M.D.; Xiao, Y.; Fry, J.; Reyes, R.; Dietzenbacher, E.; Inomata, S.; Kanemoto, K.; Los, B.; et al. The Global MRIO Lab—Charting the world economy. *Econ. Syst. Res.* **2017**, *29*, 158–186. [CrossRef]
69. Stadler, K.; Wood, R.; Bulavskaya, T.; Södersten, C.J.; Simas, M.; Schmidt, S.; Usubiaga, A.; Acosta-Fernández, J.; Kuenen, J.; Bruckner, M.; et al. EXIOBASE 3: Developing a Time Series of Detailed Environmentally Extended Multi-Regional Input-Output Tables: EXIOBASE 3. *J. Ind. Ecol.* **2018**, *22*, 502–515. [CrossRef]
70. Pfister, S.; Kulionis, V. *Feasibility Study on Strengthening the Environmental Footprints and Planetary Boundaries Concepts within the Green Economy Progress Measurement Framework*; UN Environment Document Repository Home; UNEP: Nairobi, Kenya, 2020.
71. Lenzen, M.; Kanemoto, K.; Moran, D.; Geschke, A. Mapping the Structure of the World Economy. *Environ. Sci. Technol.* **2012**, *46*, 8374–8381. [CrossRef]
72. Lenzen, M.; Moran, D.; Kanemoto, K.; Geschke, A. Building Eora: A global multi-region input-output database at high country and sector resolution. *Econ. Syst. Res.* **2013**, *25*, 20–49. [CrossRef]
73. Wood, R.; Stadler, K.; Bulavskaya, T.; Lutter, S.; Giljum, S.; de Koning, A.; Kuenen, J.; Schütz, H.; Acosta-Fernández, J.; Usubiaga, A.; et al. Global Sustainability Accounting - Developing EXIOBASE for Multi-Regional Footprint Analysis. *Sustainability* **2015**, *7*, 138–163. [CrossRef]
74. Timmer, M.P.; Dietzenbacher, E.; Los, B.; Stehrer, R.; de Vries, G.J. An Illustrated User Guide to the World Input-Output Database: The Case of Global Automotive Production: User Guide to World Input-Output Database. *Rev. Int. Econ.* **2015**, *23*, 575–605. [CrossRef]
75. Aguiar, A.; Chepeliev, M.; Corong, E.L.; McDougall, R.; Mensbrugghe, D.v.d. The GTAP Data Base: Version 10. *J. Glob. Econ. Anal.* **2019**, *4*, 1–27. [CrossRef]
76. OECD. *OECD Inter-Country Input-Output Database*; OECD: Paris, France, 2021.
77. Cabernard, L.; Pfister, S. A highly resolved MRIO database for analyzing environmental footprints and Green Economy Progress. *Sci. Total Environ.* **2021**, *755*, 142587. [CrossRef]
78. Cabernard, L.; Pfister, S. A highly resolved MRIO database for analyzing environmental footprints and Green Economy Progress—A. Code and data from 2006–2015. *Zenodo* **2020**. [CrossRef]
79. Bruckner, M.; Wood, R.; Moran, D.; Kuschnig, N.; Wieland, H.; Maus, V.; Börner, J. FABIO—The Construction of the Food and Agriculture Biomass Input–Output Model. *Environ. Sci. Technol.* **2019**, *53*, 11302–11312. [CrossRef] [PubMed]
80. Tukker, A.; Pollitt, H.; Henkemans, M. Consumption-based carbon accounting: Sense and sensibility. *Clim. Policy* **2020**, *20*, S1–S13. [CrossRef]
81. Lenzen, M.; Murray, J.; Sack, F.; Wiedmann, T. Shared producer and consumer responsibility—Theory and practice. *Ecol. Econ.* **2007**, *61*, 27–42. [CrossRef]
82. Peters, G. From production-based to consumption-based national emission inventories. *Ecol. Econ.* **2008**, *65*, 13–23. [CrossRef]
83. Suh, S. A note on the calculus for physical input–output analysis and its application to land appropriation of international trade activities. *Ecol. Econ.* **2004**, *48*, 9–17. [CrossRef]
84. Hubacek, K.; Giljum, S. Applying physical input–output analysis to estimate land appropriation (ecological footprints) of international trade activities. *Ecol. Econ.* **2003**, *44*, 137–151. [CrossRef]