IEooc_Methods6_Reading4

Resource tracing with input output (IO) models – an overview

This reading material is the supplement of a review, conceptual work, and empirical analysis on estimating end-use shares for material flows (how many % of total steel production go into vehicles, etc.) with monetary input-output tables.

The link to the paper on this topic, which is also referred to below in the text, will be added as soon as it is published! Lead author of this work is Jan Streeck, and Dominik Wiedenhofer, Hanspeter Wieland, and Stefan Pauliuk contributed to the work.

Resource tracing with input output (IO) models – an overview

by Stefan Pauliuk

Content:

1. The system definition of IO analysis

A note on notation:

Vectors are written as lowercase letters in italic font: *a*, *b*.

The summation vector is denoted by an *e*.

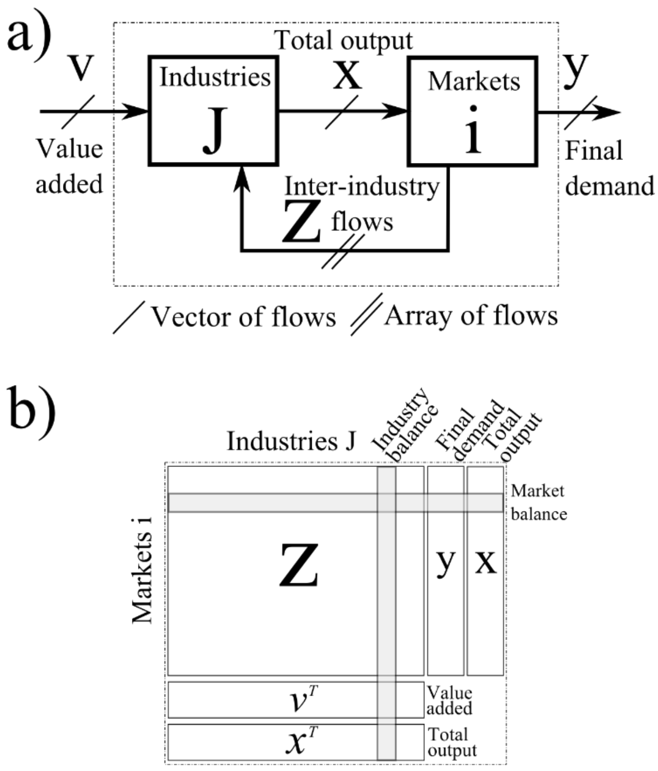
Matrices (tables) are written as uppercase letters in italic font: *Z*, *A*.

To differentiate between products/markets and industries, the former have lowercase letters ($_i$) as index, and the letter uppercase letters ($_J$).

The symbol $(\cdot)^T$ denotes matrix transposition.

Input-output models cover the flows of commodities from industries to markets and from markets to final consumers and industries (Miller and Blair, 2009). We present the system of the industrial metabolism that is at the basis of input-output analysis and assume a 1:1 correspondence between products and industries (Figure 1a). The system contains industries and markets. We introduce the column vectors of industrial output *x*, final demand *y*, and value added *v*. The matrix *Z* contains the flows from markets to industries. The row index *i* of *Z* denotes the market of origin and the column index *J* stands for the destination industry of the flow recorded in z_{iJ}. Figure 1c shows the balancing equations that can be read from the system in Figure 1a, where *e* is an appropriate summation vector, and $(\cdot)^T$ denotes matrix transposition.

The traditional accounting approach (Figure 1b) contains the same system variables as Figure 1a, and it leads to the same balancing equations that be read from the table. From the balancing equations, one can construct the accounting table in Figure 1b by arranging the *v*, *y* and *x* vectors around the Z matrix. One can also construct the system in Figure 1 by assigning an industrial process to each row in the industry balance and a market to each row in the market balance, and assigning x as industry output and market input, $Z^T \cdot e + v$ as industry input, and $Z \cdot e + y$ as market output.



c)

$$x = Z \cdot e + y \quad \text{(Market balance)}$$
$$x = Z^T \cdot e + v \quad \text{(Industry balance)}$$

Figure 1: System definition (a) and the common tabular representation of monetary input-output analysis (b). After Miller and Blair (2009) and Dietzenbacher (1997), see also (Pauliuk et al., 2015). (c): The balancing equations for markets (rows) and industries (columns).

The three representations of the IO system in Figure 1 are therefore equivalent; they contain exactly the same information. Nevertheless can the use of different representations of the system yield new insights into different IO models. If there are *n* industries and commodities, the system contains n^2 inter-industry flows (*Z*) and $3 \cdot n$ flows contained in *v*, *x*, and *y*, respectively. There are *n* balancing equations for industries, and *n* for the markets, which means that $n^2 + n$ independent pieces of information are required to fully quantify the system and to build an IO model on it. We now present the two most common approaches, the Leontief and Ghosh IO models.

2. Leontief and Ghosh models

The system in Fig. 1 is commonly applied to answer two types of research questions:

1) How much of the output of the different industries and their respective value added/resource input is needed to produce a given final demand? (Footprint question)
2) In which products and final demand sectors does a given value added/resource input end up? (Resource allocation question)

For answering both questions, we need to construct the supply chain of different products using a description of markets and industries. The Leontief IO model is commonly used to answer question 1, where the market balance is the Leontief model equation and the industries are modelled with a fixed technical coefficients matrix A.

The second question is commonly answered with the Ghosh IO model, where the industry balance is the model equation and the markets are modelled with a matrix of fixed sales or product allocation coefficients B. Often, however, the matrix B is not directly used but expressed in terms of the matrix A, see the Leontief price model and the WIO-MFA material composition model as examples below. Both are examples of the resource allocation question. In the price model, the per unit value added is propagated into commodity prices using the technical coefficients matrix and the industry balance. In the WIO-MFA material composition model, the per unit material input is propagated into product material composition also using the technical coefficients matrix and the industry balance.

2.1. Introducing model parameters: A and B matrices

The Leontief matrix of technical coefficients *A* (Leontief, 1941) and the Ghosh matrix *B* (Ghosh, 1958) are defined as shown in Equation 3 in Table 1, where ^ denotes the diagonalization operator. Applied to the original data, Equation 3 is a mere reformulation of the *Z* matrix. The transition from accounting to modelling is made when one starts interpreting Equation 3 as independent of the original data. Using the *A*-matrix implies that the use of product *i* in industry *J* is proportional to the industrial output x_J and the proportionality factor is a_{iJ}. It is intuitive to say that the elements of the *A*-matrix characterize the industries, as the inter-industry product requirements are given by the ratio of inflow and outflow from one and the same industry. Using B means that the use of product *i* in industry *J* is proportional to the total supply of the product x_I and the proportionality factor is b_{iJ} (industry I produces product i). It is intuitive to say that the *B*-matrix describe the markets, as the product distribution shares are given by the ratio of outflow to total inflow to one specific market. We can thus say that in the Leontief IO model, all non-trivial process information is attributed to the industries in form of the A matrix, whereas in the Ghosh IO model, all process information is attributed to the markets.

Labelling of industries and products: In practical applications, the important difference between products and industries is often not visible, as due to the 1:1 correspondence between industries and products in the IO table, one label/classification is used for both rows (products/markets) and columns (industries). This underlying meaning of the processes and flows in the IO table is independent of how the IO table was constructed from the original supply-and use table (SUT) for accounting product flow between industries. Trough applying a construct to the SUT (Majeau-bettez et al., 2013), a 1:1 correspondence between industries and products in the IO table it established: each industry produces ‘its’ product and vice versa, each product has its main supplying industry.

The 1:1 product/industry classification it can be either based on the product classification of the SUT ('product-by-product' IO table) or on the industry classification of the SUT ('industry-by-industry'). For product-by-product IO tables, the industry classification is defined after the products classification of the SUT (industry that is the main supplier of product *i*). For industry-by-industry IO tables, the product classification is defined after the industry classification of the SUT (product mix that is the main output of industry *J*).

Equations 4 to 7 show how the industry and market balances (Equations 2 and 3) can be reformulated using *A* and *B* (Table 1). We see that the Leontief and Ghosh quantity models refer to different parts of the system; they represent the balancing equations of markets and industries, respectively (Equations 5 and 6). The Leontief quantity model $x = A \cdot x + y$ (Equation 5) is a special way of writing the balancing equation of the markets, using the technical coefficients attributed to the industries. In the Leontief quantity model, the industries 'own' their input structure, and markets are dummy processes that have no attributes other than being balanced. The Ghosh quantity model $x = B^T \cdot x + v$ (Equation 6) is a special way of writing the balancing equations of the industries, using the allocation coefficients attributed to the markets. Here, the markets 'own' their distribution structure, and industries are dummy processes that have no attributes other than being balanced.

Table 1: Overview of balancing equations for industries and markets in different models for the monetary and physical layer (plain letters vs. letters with ~). Here, *e* is a summation vector.

<table>
<tr><th>Model family</th><th>Industry Balance</th><th>Market Balance</th></tr>
<tr><td>Accounting equations</td><td>$$x = Z^T \cdot e + v \qquad (1)$$ $$\tilde{x} = \tilde{Z}^T \cdot e + \tilde{v}$$</td><td>$$x = Z \cdot e + y \qquad (2)$$ $$\tilde{x} = \tilde{Z} \cdot e + \tilde{y}$$</td></tr>
<tr><td></td><td colspan="2">$$Z = A \cdot \hat{X}, \qquad Z = \hat{X} \cdot B$$ $$\left(z_{iJ} = a_{iJ} \cdot x_J, \quad z_{iJ} = b_{iJ} \cdot x_I \right) \qquad (3)$$ $$\tilde{Z} = \tilde{A} \cdot \hat{\tilde{X}}, \qquad \tilde{Z} = \hat{\tilde{X}} \cdot \tilde{B}$$ $$[A],\ [B] = \$/\$,\ \ [\tilde{A}],\ [\tilde{B}] = kg/kg$$</td></tr>
<tr><td>Model equations with the A matrix</td><td>$$x = \hat{x} \cdot A^T \cdot e + v$$ $$= \left(A^T \cdot e \right)^{\wedge} \cdot x + v \qquad (4)$$ $$\tilde{x} = \hat{\tilde{x}} \cdot \tilde{A}^T \cdot e + \tilde{v}$$</td><td>$$x = A \cdot x + y \qquad (5)$$ $$\tilde{x} = \tilde{A} \cdot \tilde{x} + \tilde{y}$$ Leontief (quantity) model</td></tr>
<tr><td>Model equations with the B matrix</td><td>$$x = B^T \cdot x + v \qquad (6)$$ $$\tilde{x} = \tilde{B}^T \cdot \tilde{x} + \tilde{v}$$ Ghosh (quantity) model</td><td>$$x = \hat{x} \cdot B \cdot e + y$$ $$= \left(B \cdot e \right)^{\wedge} \cdot x + y \qquad (7)$$ $$\tilde{x} = \hat{\tilde{x}} \cdot \tilde{B} \cdot e + \tilde{y}$$</td></tr>
</table>

3. Monetary and physical IO analysis

IO analysis can be performed in monetary and physical units alike (Weisz and Duchin, 2006). There is no a priori preferred unit, and both monetary and physical IO analysis have evolved over time in economics, ecosystem analysis, and industrial ecology (Duchin, 2009; Giljum and Hubacek, 2009; Suh, 2005).

3.1. Basic relations

In Table 1, we write all equations in both monetary and physical units. The tilde ~ indicates the physical layer. The balancing equations and the Leontief and Ghosh IO models hold in both units.

Although the system in Figure 1a looks symmetric, it is not. The reason is that markets and industries are fundamentally different types of processes: industries *transform different products* into new ones, whereas markets *distribute one and the same product* across the industrial system. This has important implications when connecting the monetary and physical layers. We assume that all industry outputs have positive mass $\tilde{x}$ and monetary value *x*. In the simplest case, we can define a homogenous price vector *p* for all commodities, which means that all suppliers and purchasers exchange at the same price per unit of commodity (Weisz and Duchin, 2006). The assumption of *homogenous price* entails a certain relationship between the A, B and $\tilde{A}$, $\tilde{B}$ matrices. As industries transform different quantities of products into new ones, they also mix different prices, and there must be a relationship between price homogeneity, the transformation of the A and B-matrices under conversion from monetary to physical IO, and the industry balance. The following equations hold:

$$\tilde{A} = \hat{p}^{-1} \cdot A \cdot \hat{p}, \quad \tilde{B} = B \qquad (8)$$

$$x = \hat{p} \cdot \tilde{x}, \quad Z = \hat{p} \cdot \tilde{Z} \qquad (9)$$

$$x = \hat{p} \cdot \tilde{x}, \quad Z = \hat{p} \cdot \tilde{Z}, \quad y = \hat{p} \cdot \tilde{y} \qquad (10)$$

(Price homogeneity)

$$p = \tilde{A}^T \cdot p + p_v, \quad p_v = \hat{\tilde{x}}^{-1} \cdot v \qquad (11)$$

(Leontief price model)

First, we show the most important calculation, the derivation of the (Leontief) price model (Equation 11) from the industry balance and equation 10.

Since the factor and resource markets are not included in the system and major factors such as labour and capital do not enter the physical balance of the industry, we cannot introduce a meaningful per-unit factor price. Instead we define the monetary value added per unit of physical output, $p_v = \hat{\tilde{x}}^{-1} \cdot v$. It has the same unit as the prices, namely \$/kg. It is not a price but a ratio of two different system variables in different layers. We combine the industry balance (Equation 1) with the price homogeneity (Equation 10) and the definition of the A-matrix (Equation 3):

$$
\begin{aligned}
& x = Z^T \cdot e + v \\
& \hat{p} \cdot \tilde{x} = \tilde{Z}^T \cdot \hat{p} \cdot e + v, \qquad / \hat{\tilde{x}}^{-1} \\
& p = \hat{\tilde{x}}^{-1} \cdot \tilde{Z}^T \cdot p + p_v \\
& p = \left(\tilde{Z} \cdot \hat{\tilde{x}}^{-1} \right)^T \cdot p + p_v, \qquad \tilde{A} = \tilde{Z} \cdot \hat{\tilde{x}}^{-1} \\
& p = \tilde{A}^T \cdot p + p_v
\end{aligned}
\tag{12}
$$

Here it is important to note that it is the *physical* *A*-matrix that enters the price model.

Equation 8 from equation 9:

$$
\begin{aligned}
& x = \hat{p} \cdot \tilde{x}, \quad Z = \hat{p} \cdot \tilde{Z}, \quad Z = A \cdot \hat{X} = \hat{X} \cdot B \\
& \hat{p} \cdot \tilde{Z} = A \cdot \hat{p} \cdot \hat{\tilde{x}} = \hat{p} \cdot \hat{\tilde{x}} \cdot B \\
& \tilde{Z} = \hat{p}^{-1} \cdot A \cdot \hat{p} \cdot \hat{\tilde{x}} = \hat{p}^{-1} \cdot \hat{p} \cdot \hat{\tilde{x}} \cdot B, \ with\ \tilde{Z} = \tilde{A} \cdot \hat{\tilde{X}} = \hat{\tilde{X}} \cdot \tilde{B} \\
& \Rightarrow \\
& \tilde{A} = \hat{p}^{-1} \cdot A \cdot \hat{p}, \quad \tilde{B} = B
\end{aligned}
\tag{13}
$$

Equation 9 from equation 8:

$$
\begin{aligned}
& \tilde{A} = \hat{p}^{-1} \cdot A \cdot \hat{p}, \quad \tilde{B} = B, \quad Z = A \cdot \hat{X} = \hat{X} \cdot B, \quad \tilde{Z} = \tilde{A} \cdot \hat{\tilde{X}} = \hat{\tilde{X}} \cdot \tilde{B} \\
& B = \hat{X}^{-1} \cdot A \cdot \hat{X}, \quad \tilde{B} = \hat{\tilde{X}}^{-1} \cdot \tilde{A} \cdot \hat{\tilde{X}} \\
& \hat{X}^{-1} \cdot A \cdot \hat{X} = \hat{\tilde{X}}^{-1} \cdot \hat{p}^{-1} \cdot A \cdot \hat{p} \cdot \hat{\tilde{X}} \\
& \hat{X}^{-1} \cdot A \cdot \hat{X} = \left(\hat{p} \cdot \hat{\tilde{X}} \right)^{-1} \cdot A \cdot \left(\hat{p} \cdot \hat{\tilde{X}} \right), \quad \forall x \\
& \Rightarrow \hat{X} = \alpha \cdot \left(\hat{p} \cdot \hat{\tilde{X}} \right), \alpha \in \mathbb{R} \\
& \hat{X}^{-1} \cdot Z = B = \tilde{B} = \hat{\tilde{X}}^{-1} \cdot \tilde{Z} = \frac{1}{\alpha} \cdot \left(\hat{p} \cdot \hat{\tilde{X}} \right)^{-1} \cdot Z \\
& Z = \alpha \cdot \hat{p} \cdot \hat{\tilde{X}} \cdot \hat{\tilde{X}}^{-1} \cdot \tilde{Z} \\
& \Rightarrow x = \alpha \cdot \hat{p} \cdot \tilde{x}, \quad Z = \alpha \cdot \hat{p} \cdot \tilde{Z}
\end{aligned}
\tag{14}
$$

Here, α is a scalar that uniformly applies to all flows in the system. This represents a change in unit, e.g., from kg to ton. Still, prices are homogenous.

Equation 10 from equation 9: Given the market balance in both monetary and physical units,

$$x = Z \cdot e + y \ , \ \tilde{x} = \tilde{Z} \cdot e + \tilde{y} \qquad (15)$$

we assume that two of the terms in the above equations have the same price vector, for example, : $x = \hat{p} \cdot \tilde{x}, \ \ Z = \hat{p} \cdot \tilde{Z}$. Inserting this into the market balance in monetary units and multiplying with $\hat{p}^{-1}$ and comparing with the balancing equation in physical units gives that $\hat{p}^{-1} \cdot y = \tilde{y}$ or $y = \hat{p} \cdot \tilde{y}$. The same approach can be used to prove the two other combinations.

Equation 9 from equation 10: Statement c includes statement b.

Equation 11 from equation 10: See above.

Equation 10 from equation 11: We start from the price model (Equation 11) and combine it with Equation 3:

$$\begin{aligned} \hat{\tilde{x}} \cdot p &= \hat{\tilde{x}} \cdot \tilde{A}^T \cdot p + \hat{\tilde{x}} \cdot p_v \\ \hat{p} \cdot \tilde{x} &= \left(\hat{p} \cdot \tilde{Z} \right)^T \cdot e + v \end{aligned} \qquad (16)$$

We compare Equation 16 with Equation 17 that contains individual prices for both *x* and *Z*, where $\odot$ denotes element-wise multiplication:

$$\hat{p}_x \cdot \tilde{x} = \left(p_z \odot \tilde{Z} \right)^T \cdot e + v \qquad (17)$$

We see by comparing Equations 16 and 17 that $\hat{p}_x = p_z = \hat{p}$. This is equation 10, which is equivalent to equation 11. This completes the proof.

3.2. Validity of the Leontief price model

Above, the Leontief price model was derived from the general industry balancing equation (Equation 1). Here we show that the same price model also follows from the A-matrix industry balance $x = \hat{x} \cdot A^T \cdot e + v$ (Equation 4) and the Ghosh quantity model $x = B^T \cdot x + v$ (Equation 6).

We first formulate the price model in the Leontief case, starting from the industry balance:

$$
\begin{aligned}
& x = \hat{x} \cdot A^T \cdot e + v, \text{ in \$} \\
& \hat{p} \cdot \tilde{x} = \hat{p} \cdot \hat{\tilde{x}} \cdot A^T \cdot e + v \\
& \hat{\tilde{x}} \cdot p = \hat{\tilde{x}} \cdot \hat{p} \cdot A^T \cdot e + v \qquad / \, \hat{\tilde{x}}^{-1} \\
& p = \hat{p} \cdot A^T \cdot e + \hat{\tilde{x}}^{-1} \cdot v \\
& p = \hat{p} \cdot \left(\hat{p} \cdot \tilde{A} \cdot \hat{p}^{-1} \right)^T \cdot e + \hat{\tilde{x}}^{-1} \cdot v, \quad p_v = \hat{\tilde{x}}^{-1} \cdot v \\
& p = \tilde{A}^T \cdot p + p_v, \text{ in \$/kg}
\end{aligned}
\tag{18}
$$

Finally, we formulate the Leontief price model starting from the industry balance with the B-matrix (Equation 6):

$$
\begin{aligned}
& x = B^T \cdot x + v \\
& \hat{p} \cdot \tilde{x} = B^T \cdot \hat{p} \cdot \tilde{x} + v \\
& \hat{\tilde{x}} \cdot p = B^T \cdot \hat{\tilde{x}} \cdot p + v, \qquad / \, \hat{\tilde{x}}^{-1} \\
& p = \hat{\tilde{x}}^{-1} \cdot B^T \cdot \hat{\tilde{x}} \cdot p + \hat{\tilde{x}}^{-1} \cdot v \\
& p = \left(\hat{\tilde{x}} \cdot B \cdot \hat{\tilde{x}}^{-1} \right)^T \cdot p + p_v, \qquad / \, B = \tilde{B} \\
& p = \left(\hat{\tilde{x}} \cdot \tilde{B} \cdot \hat{\tilde{x}}^{-1} \right)^T \cdot p + p_v, \qquad / \, \tilde{A} = \hat{\tilde{x}} \cdot \tilde{B} \cdot \hat{\tilde{x}}^{-1} \\
& p = \tilde{A}^T \cdot p + p_v
\end{aligned}
\tag{19}
$$

4. Price, Ghosh, WIO-MFA (material composition of products), and absorbing Markov chain models

4.1. Ghosh quantity & Leontief price model:

As stated in (Nakamura and Kondo, 2009) the Ghosh quantity model can be transformed into the Leontief price model (and vice versa). The reason for that is that both, the Ghosh quantity and Leontief price model equations are different formulations of the same equation, namely the balance for the industries in the system.

The calculation is shown above in equation 19, and an alternative derivation is presented in equations 20-23: From the industry balance with the B matrix (Equ. 6 in monetary units), we derive the following equation by replacing the left x with price and physical units and multiplying from the left with $\hat{\tilde{x}}^{-1}$:

$$\begin{aligned} &\hat{\tilde{x}}^{-1}\hat{p}\tilde{x} = p = \hat{\tilde{x}}^{-1}B^T x + \hat{\tilde{x}}^{-1}v = \hat{\tilde{x}}^{-1}B^T x + p_v \\ &p = \hat{p}\hat{x}^{-1}B^T x + p_v \end{aligned} \qquad (20)$$

With

$$Z = A\hat{X} = \hat{X}B \rightarrow A = \hat{X}B\hat{X}^{-1} \rightarrow \hat{X}^{-1}B^T\hat{X} \qquad (21)$$

Follows for the above equation:

$$p = \hat{p}A^T e + p_v \qquad (22)$$

Which we expand into

$$\begin{aligned} &p = \hat{p}A^T\hat{p}^{-1}p + p_v = \left(\hat{p}A^T\hat{p}^{-1}\right)p + p_v \\ &p = \tilde{A}^T p + p_v \end{aligned} \qquad (23)$$

In the last step, equation 8 was used. The Leontief price model follows as reformulation of the industry balance equation (with the B matrix).

4.2. Ghosh quantity model & Absorbing Markov Chain (AMC):

From https://en.wikipedia.org/wiki/Absorbing_Markov_chain (Access on Feb 15, 2022): “In the mathematical theory of probability, an absorbing Markov chain is a Markov chain in which every state can reach an absorbing state. An absorbing state is a state that, once entered, cannot be left.”

The Ghosh quantity model can be seen as part of an absorbing Markov chain (AMC): For each input to industrial production (starting state), an output (part of the x vector) is created, which is then partly re-distributed to other industries via the B matrix, whereas the remainder is sent to final demand, which is the absorbing state. Sooner or later, all input to industrial production ends up in the absorbing state.

Duchin and Levine (Duchin and Levine, 2010) formally introduce AMC to IO.

We can write the canonical transition matrix P of the absorbing Markov chain with the help of the elements of the market share matrix B:

$$P = \begin{bmatrix} Q & R \\ 0 & I \end{bmatrix}, \quad Q = B, \quad R = I - diag\left(B \cdot e\right) \qquad (24)$$

To trace a value added input to the end-use sectors, Q is defined as the matrix of transition probabilities from one industry i (via the market for commodity i) to another industry j, which is given by

$$Q_{ij} = \frac{Z_{ij}}{x_i} = B_{ij} \qquad (25)$$

Duchin and Levine (2010) arrive at the same result (in their work, *B* is denoted as $\bar{A}$ and labelled 'Gosh matrix', a term that we do not use here.). Here, we consider the tracing of value added through the industrial network separately from the tracing of natural resource input through the industrial network, which is why the *Q*-matrix here only consists of *B* (or $\bar{A}$) compared to equation 18 in Duchin and Levine (2010).

The equation for R follows from the market balance with the market share matrix (equation 7), which can be solved for y:

$$y = \left(I - diag(B \cdot e)\right) \cdot x \qquad (26)$$

Since the transfer matrix from x to y is a diagonal matrix, the coefficients of this matrix simply indicate the share of x that goes to the absorbing state y or the probability that a given unit of x will go to y. Duchin and Levine (2010) derive R from the same equation as

$$R = \hat{x}^{-1} \cdot \hat{y} \qquad (27)$$

Again, we consider the tracing of value added through the industrial network separately from the tracing of natural resource input through the industrial network, which is why the *R*-matrix here only consists of one compartment compared to equation 17 in Duchin and Levine (2010).

Also, from Duchin and Levine (2010): "Suh (2005) recognized the use of both *A* and *B* matrices in ecological studies and the relationship of the former to AMCs. He also pointed out both the limitations of requiring all variables to be measured in a single unit and that structural path analysis (SPA) has been applied to the Ghosh inverse in ecosystem analysis, although not normalized by that name (Suh, 2005; Suh and Kagawa, 2005)."

5. Leontief price model and WIO-MFA approach

Introduced by Nakamura and colleagues: (Nakamura et al., 2007; Nakamura and Nakajima, 2006, 2005)

The central equation for the material composition of products, C_{mp}, is

$$C_{mp} = \tilde{A}_{mp} \cdot (I - \tilde{A}_{pp})^{-1} \qquad (28)$$

Note: Here, the tilde denotes a yield-corrected version of the A matrices, not the A matrix in physical units!

In this model, the materials m are treated as exogenous inputs to the product-product industry subsystem, which then allows us to propagate the materials through the different products similar to propagating value added through products to determine prices.

This equation can be interpreted as a Leontief IO-model of the product-product industry subsystem that has an exogenous material input coefficients A_{mp}. For a given (fixed) material m, C_{mp} and A_{mp} are both row vectors, and these are denoted with lower case letters as c_{mp} and a_{mp} (with a tilde on A and a). In a first step, we transpose this equation for a fixed material m and separate the terms:

$$\begin{aligned} c_{mp}{}^{T} &= (I - \tilde{A}_{pp}{}^{T})^{-1} \tilde{a}_{mp}{}^{T} \\ c_{mp}{}^{T} &= \tilde{A}_{pp}{}^{T} c_{mp}{}^{T} + \tilde{a}_{mp}{}^{T} \end{aligned} \qquad (29)$$

In the equation above the transposed vectors c and a_tilde are column vectors.

Starting from a different angle with the price model, we now interpret the two layers x and x_tilde not as monetary and physical layers, but as layers of material m and as total mass layers. In this situation, the parameter that was the price before is now the material concentration. The parameter that was the value added before is now the exogenous input of material m, v_m, to the product-product industry subsystem (as defined by Nakamura and Kondo to avoid double-counting).

$$x = \hat{c}_{mp} \cdot \tilde{x}, \quad \mathrm{v} = \mathrm{v}_{\mathrm{m}} \qquad (30)$$

We now take the Leontief price model and replace price and value added with the above re-interpretation *(price->concentration, value added -> exogenous material input)*

$$\begin{aligned}
& p = \tilde{A}^T \cdot p + p_v \\
& here: \\
& {c_{mp}}^T = \tilde{A}^T \cdot {c_{mp}}^T + \hat{\tilde{x}}^{-1} \cdot v_m \\
& with \\
& \tilde{a}_{mp}^T := \hat{\tilde{x}}^{-1} \cdot v_m \qquad (31) \\
& follows: \\
& {c_{mp}}^T = \tilde{A}^T \cdot {c_{mp}}^T + \tilde{a}_{mp}^T
\end{aligned}$$

Note that above, the tilde denotes yield correction and here, it denotes the technical coefficients at the total mass layer (could also be the monetary layer as in Nakamura and Kondo). This calculation shows that with the following reinterpretation of the price model as concentration model:

- Monetary + physical layers → material m layer / total mass layer
- price → concentration of material m in total mass
- value added → exogenous material input of material m per total mass output

the WIO-MFA material composition equation can be understood as a type of price model and is thus a derivative of the industry balance equation in the IO system.

6. Allocation matrix of exogenous input to final demand, case I: value added

IO models are used to answer different research questions. Next to the questions on product environmental footprints (answered with the environmentally extended Leontief IO model) and commodity prices or material composition (answered with Leontief price models), the allocation of resource input to final demand sectors, the so-called *sector split* or, as synonym, *end-use shares*, is an important application.

This type of question is complementary to the footprint question. For footprints, the supply chain of a final demand category is constructed so that different final commodities are linked to multiple upstream resources. For the resource allocation, different resource inputs are traced into multiple downstream commodities.

Resource allocation matrices have been determined by several authors, using Leontief IO (Hashimoto et al., 2007), Ghosh-IO/AMC (Duchin and Levine, 2010), the Leontief price / WIO-MFA model (Nakajima and Nakamura, 2006; Nakamura et al., 2014, 2007; Nakamura and Nakajima, 2005), or ad-hoc calculations that represent a simplified version of the approaches above (Aryapratama and Pauliuk, 2019; Cao et al., 2018).

In this section, we show that the allocation matrix of resources to final products, the so-called end-use shares, sector split or D-matrix, is the same for all three approaches. This finding holds when considering value added as exogenous input to the economy and when working at scale, i.e., performing the calculations for the full inventoried value added and final demand.

In the following chapter, we show that the D-matrix is the same for all three approaches, when considering natural (material) resources as exogenous input to the economy.

Note: *The matrices defined here may differ from those used in the literature and the main paper, simply because there is no universal convention on notation and on which row/column* *definition (transposition) to use. At the end of each subsection below, we convert the result of our calculation into the forms used in the original sources and in the main paper.*

6.1. Background/introduction to the end-use shares / sector split calculation

The column vector *d* shall denote the %-wise split of the final demand of a material *m* into the different consumption categories *p*. This is the simplest case. Nakamura et al. (2014) do not calculate a d vector for a single material but a matrix D for all materials at the same time.

The total flow of material consumption into different final demand categories shall be denoted by the final demand vector $\tilde{y}$. Here, the tilde denotes the physical layer of material m, whereas y (without tilde) denotes the total monetary flow.

From the flows in $\tilde{y}$, the %-allocation can simply be calculated by dividing all elements of $\tilde{y}$ by their sum:

$$d_p = \frac{\tilde{y}_p}{\sum_p \tilde{y}_p} \qquad (32)$$

Or, in matrix notation:

$$d = \left(diag\left(\tilde{y}^T \cdot e\right)\right)^{-1} \cdot \tilde{y} \qquad (33)$$

If now, as in WIO-MFA (Nakamura et al., 2007), the physical layer of the final demand for material m, $\tilde{y}$, is calculated from the monetary layer (*y*) with a material concentration or material composition vector *c* as follows:

$$\tilde{y} = \hat{c} \cdot y = diag(c) \cdot y \qquad (34)$$

The end-use shares / sector split d can be calculated from y and c by combining the two equations above:

$$
\begin{aligned}
d &= \left(diag\left((diag(c)\cdot y)^T \cdot e\right)\right)^{-1} \cdot diag(c)\cdot y \\
d &= \left(diag\left(y^T \cdot diag(c)\cdot e\right)\right)^{-1} \cdot diag(c)\cdot y \\
d &= \left(diag\left(y^T \cdot c\right)\right)^{-1} \cdot diag(c)\cdot y
\end{aligned}
\tag{35}
$$

This equation is also used by Nakamura et al. (2014), though in transposed form.

Below, we do not calculate a d vector for a single material but a matrix D for all materials at the same time, following the same principle. We derive the sector split matrix D for each of the three models independently, starting with the Ghosh/AMC model, and then show that the derived expressions are the same, followed by a discussion.

6.2. End-use shares / Sector split from the Ghosh/AMC model, using the B matrix of market allocation shares

The Ghosh/AMC model follows the flow of resources by first calculating the industrial output x resulting from the value added and then, via the market balance, the final demand. To determine the sector allocation of value added to final demand, *D*, we calculate y from the value added (or resource input) v by first solving for x (industry balance) and then for y (market balance). To keep track of the value added for each industry, we apply the Ghosh IO model to $\hat{v}$ instead of v, to suppress the summing up of the industry dimension. This calculation results first in a table X_I of x vectors for the value added in each industry, and then, via the market balance, in a table Y_I of y vectors for the value added in each industry.

$$
Y_I = \left(I - diag(B\cdot e)\right)\cdot X_I = \left(I - diag(B\cdot e)\right)\cdot\left(I - B^T\right)^{-1}\cdot\hat{v}
\tag{36}
$$

Y_I has the dimension product (row) by industry where the value added was provided (columns), and a single element $(Y_I)_{ab}$ denotes the amount of product a generated from providing the value added (as specified in the IO table) to industry b. The row sum of Y_I is the final demand y, and the column sum is the value added v.

We now define the end-use sector allocation of value added to final products with the Ghosh IO model (D_G) as the table Y_I, normalized to % across all products (rows) for each industry (column):

$$D_G = Y_I \cdot \left(Y_I^{\,T} \cdot e\right)^{\wedge -1} \qquad (37)$$

Where the right matrix is the inverse diagonal of the column sum of Y_I, so that this equation simply described the column-wise normalisation of Y_I so that each column consists of shares that add up to 1 (100%). Inserting the equation for Y_I above yields:

$$\begin{aligned}
\left(Y_I^{\,T} \cdot e\right)^{\wedge -1} &= \left(\hat{v} \cdot \left(I - B\right)^{-1} \cdot \left(I - diag(B \cdot e)\right) \cdot e\right)^{\wedge -1} \\
&= \left(\hat{v} \cdot \left(I - B\right)^{-1} \cdot \left(e - B \cdot e\right)\right)^{\wedge -1} \\
&= \left(\hat{v} \cdot \left(I - B\right)^{-1} \cdot \left(I - B\right) \cdot e\right)^{\wedge -1} \\
&= \left(\hat{v} \cdot e\right)^{\wedge -1} \\
&= \hat{v}^{-1}
\end{aligned} \qquad (38)$$

From which follows:

$$D_G = Y_I \cdot \hat{v}^{-1} = \left(I - diag(B \cdot e)\right) \cdot \left(I - B^T\right)^{-1} \cdot \hat{v} \cdot \hat{v}^{-1} \qquad (39)$$

$$\boxed{D_G = \left(I - diag(B \cdot e)\right) \cdot \left(I - B^T\right)^{-1}} \qquad (40)$$

For a worked example, see columns Z-AJ in the sheet '*Allocate_v_to_y, determine D*' of the accompanying Excel workbook.

Transformation to the equations in the literature and to equation 9 used in the paper: A similar version of this expression was already derived by Duchin and Levine (2010) as their equations 7 and 20. We show this by transposing D_G:

$$
\begin{aligned}
D_G{}^T &= \left(I - B\right)^{-1} \cdot \left(I - diag(B \cdot e)\right) \\
D_G{}^T &= \left(I - \hat{x}^{-1} \cdot Z\right)^{-1} \cdot \hat{x}^{-1} \cdot \hat{y}
\end{aligned} \qquad (41)
$$

In the second line of equation 41, first, equation 3 (definition of B) and then equation 7 (market balance with B) were used. Similar calculations can be found in equations 7, 8, and 9 in the paper. Here, the products of the Z-matrix were compartmentalized into materials and products.

6.3. Leontief IO, Derivation of the "sector split":

The Leontief IO model constructs the supply chains of final commodities. In a first step, we calculate the industry output X_P for each final demand category separately, by supressing the summation over the product dimension of y:

$$
X_P = \left(I - A\right)^{-1} \cdot \hat{y} \qquad (42)
$$

Now, we determine the value added input into each industry for the final demand for each product, by applying the industry balance with the A matrix (equation 4).

$$
\begin{aligned}
V_P &= \left(I - diag(A^T \cdot e)\right) \cdot X_P \\
&= \left(I - diag(A^T \cdot e)\right) \cdot \left(I - A\right)^{-1} \cdot \hat{y}
\end{aligned} \qquad (43)
$$

V_P has the dimension product (column) by industry where the value added was provided (rows), and a single element $(V_P)_{ab}$ denotes the amount of value added inserted into industry a for the production of final demand product b, as specified in the IO table. The columns sum of V_P is the final demand y, and the row sum is the value added v.

As for the Ghosh IO model, we now define the end-use sector allocation of value added to final products with the Leontief IO model (D_L) as the table V_P, normalized to % across all products (columns) for each industry (row). To have an allocation table with the same dimension as for the case of the Ghosh model, we transpose before normalizing and obtain:

$$D_L = V_P{}^T \cdot \left(V_P \cdot e\right)^{\wedge -1} \qquad (44)$$

With the result for V_P, this allocation can be calculated and determined as:

$$\left(V_P \cdot e\right)^{\wedge -1} = \left(I - diag(A^T \cdot e)\right) \cdot \left(I - A\right)^{-1} \cdot y = \hat{v}^{-1} \qquad (45)$$

$$\boxed{D_L = \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \left(I - diag(A^T \cdot e)\right) \cdot \hat{v}^{-1}} \qquad (46)$$

For a worked example, see columns B-L in the sheet '*Allocate_v_to_y, determine D*' of the accompanying Excel workbook.

Transformation to the equations in the literature and to equation 6 used in the paper:

To derive the equation used in the paper, we first transpose equation 46 and use the Leontief quantity model equation:

$$\begin{aligned} D_L{}^T &= \hat{v}^{-1} \cdot \left(I - diag(A^T \cdot e)\right) \cdot \left(I - A\right)^{-1} \cdot \hat{y} \\ D_L{}^T &= \hat{v}^{-1} \cdot \left(I - diag(A^T \cdot e)\right) \cdot L \cdot \hat{y} \end{aligned} \qquad (47)$$

In a second step, we use the industry balance with the *A*-matrix (equation 4) to derive the expression used in the paper:

$$\left(I - diag(A^T \cdot e)\right) \cdot x = v \rightarrow \left(I - diag(A^T \cdot e)\right) \cdot \hat{x} = \hat{v} \rightarrow \hat{v}^{-1} \cdot \left(I - diag(A^T \cdot e)\right) = \hat{x}^{-1}$$
$$D_L{}^T = \hat{x}^{-1} \cdot L \cdot \hat{y} = \left(L \cdot y\right)\wedge^{-1} \cdot L \cdot \hat{y}$$

(48)

6.4. Price model and WIO-MFA approach to the material composition of products,

Derivation of the end-use shares or sector split:

Any industry output consists of monetary flow that were originally added to the system as value added to a certain industry. In a first step, we use the two-layer formulation of the IO table (see Table 1) and define the *base layer* as the layer at which the full monetary value of each flow is quantified (denoted by a tilde, for example, $\tilde{x}$). We also define the *focus layer i* as those monetary flows as part of the total monetary flows that can be attributed to the value added inserted into a given industry *i*, denoted by a subscript i, for example, x_i.

We can then define a *concentration of value added vector* c_i, which translates the total monetary value of a given industrial output into the fraction that is constituted by the value added of industry *i* according to the following equation:

$$x_i = \hat{c}_i \cdot \tilde{x} \qquad (49)$$

In analogy to the price model (equation 12) and the WIO-MFA material concentration model (equation 31), we can use the industry balance to build a concentration model. For the industry balance in terms of flows allocated to value added into industry *i* only, we have

$$x_i = Z_i^T \cdot e + v_i \qquad (50)$$

Where the sub-index i denotes the focus layer i. Combining the two equations above yields, in analogy to equation 12:

$$c_i = \tilde{A}^T \cdot c_i + v_i \cdot \hat{\tilde{x}}^{-1} \qquad (51)$$

This equation holds for all industries i. We can now stack the different c_i next to each other to form a matrix of concentration of value added of industries in products. Stacking the different single-industry value added vectors v_i next to each other simply leads to $\hat{v}$. For the final result, we re-label the full monetary values with the tilde (to be compatible with equation 12) as variables without tilde (to be compatible with the notation of the IO table), and obtain:

$$\begin{aligned} C &= A^T \cdot C + \hat{C}_V, \\ \hat{C}_V &= \hat{v} \cdot \hat{x}^{-1} = \hat{x}^{-1} \cdot \hat{v} \\ C &= \left(I - A^T\right)^{-1} \cdot \hat{C}_V \end{aligned} \qquad (52)$$

The C-matrix denotes the concentrations (in $/$) of value added inserted into industry i (column) in product p (row). The row sum of C is 1 (the unit/summation vector e).

With the help of C, we can break down final demand y into its value-added constituents, Y_P, which was already introduced in equation 42. Since the columns of C denote the industries, we need to transpose C:

$$Y_P = C^T \cdot \hat{y} \qquad (53)$$

We can now normalize Y_P to a unit value added, by multiplying with the inverse of the value added diagonal matrix from the left, to convert all columns to %, summing up to 1. This actually yields, in our notation, the transpose of the D matrix:

$$D_P{}^T = \hat{v}^{-1} \cdot C^T \cdot \hat{y} \tag{54}$$

The direct calculation, directly using equations 43 and 50, yields:

$$\begin{aligned}
D_P &= V_P{}^T \cdot \left(V_P \cdot e\right)^{\wedge-1} \\
&= \hat{y} \cdot C \cdot \left(C^T \cdot y\right)^{\wedge-1} \\
&= \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} \cdot \hat{v} \cdot \left(C^T \cdot y\right)^{\wedge-1} \\
&= \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} \cdot \hat{v} \cdot \left(\hat{v} \cdot \hat{x}^{-1} \cdot \left(I - A\right)^{-1} \cdot y\right)^{\wedge-1} \\
&= \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} \cdot \hat{v} \cdot \left(\hat{v} \cdot \hat{x}^{-1} \cdot x\right)^{\wedge-1} \\
&= \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} \cdot \hat{v} \cdot \left(\hat{v} \cdot e\right)^{\wedge-1} \\
&= \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} \cdot \hat{v} \cdot \hat{v}^{-1}
\end{aligned} \tag{55}$$

$$\boxed{D_P = \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1}} \tag{56}$$

For a worked example, see columns N-X in the sheet '*Allocate_v_to_y, determine D*' of the accompanying Excel workbook.

Transformation to the equations in the literature and to equation 3 used in the paper:

To derive the equation used in the paper, we transpose D_P and use the second line of equation 55:

$$D_P{}^T = \left(C^T \cdot y\right)^{\wedge-1} \cdot C^T \cdot \hat{y} \tag{57}$$

This is identical to equation 3 in the paper if $D_P{}^T$ instead of D_P and C^T instead of C are used.

6.5. Equivalence of the three approaches to determining the sector split D

All three results for D give the same result, as the example in the Excel workbook (sheet '*Allocate_v_to_y, determine D*') shows. Here, we show analytically that all three results are equivalent, even though they used different parameters. We first list the three results and then, in a first step, apply equation 4 to show the equivalence between D_P and D_L.

$$\begin{aligned}
&D_G = \left(I - diag(B \cdot e)\right) \cdot \left(I - B^T\right)^{-1} \\
&D_L = \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \left(I - diag(A^T \cdot e)\right) \cdot \hat{v}^{-1} \\
&D_P = \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} \\
&\quad to \;\; show: \\
&D_G = D_L = D_P
\end{aligned} \tag{58}$$

$$\begin{aligned}
x &= diag(A^T \cdot e) \cdot x + v \\
v &= \left(I - diag(A^T \cdot e)\right) \cdot x \\
\hat{v} &= \left(I - diag(A^T \cdot e)\right) \cdot \hat{x} \\
\hat{x} &= \left(I - diag(A^T \cdot e)\right)^{-1} \cdot \hat{v} \\
\hat{x}^{-1} &= \left(I - diag(A^T \cdot e)\right) \cdot \hat{v}^{-1}
\end{aligned} \tag{59}$$

Adding this result for $\hat{x}^{-1}$ into the equation for D_P directly yields D_L. Thus, $D_P = D_L$.

For showing that $D_G = D_P$, we apply first equation 7 (resolve for $\left(I - diag(B \cdot e)\right)$) and then equation 3 (resolve for $\left(I - B^T\right)^{-1}$):

$$
\begin{aligned}
&x = diag(B \cdot e) \cdot x + y \\
&\left(I - diag(B \cdot e)\right) \cdot x = y \\
&\left(I - diag(B \cdot e)\right) \cdot \hat{x} = \hat{y} \\
&\left(I - diag(B \cdot e)\right) = \hat{y} \cdot \hat{x}^{-1}
\end{aligned}
\tag{60}
$$

The second key to determining the equivalence are the relations between the A and B matrices that can readily be derived from the definition in equation 3:

$$
\begin{aligned}
&Z = A \cdot \hat{x} = \hat{x} \cdot B \\
&\rightarrow \\
&B = \hat{x}^{-1} \cdot A \cdot \hat{x} \\
&B^T = \hat{x} \cdot A^T \cdot \hat{x}^{-1}
\end{aligned}
\tag{61}
$$

And the transformation of the power series expansion for $\left(I - B^T\right)^{-1}$:

$$
\begin{aligned}
&B^T = \hat{x} \cdot A^T \cdot \hat{x}^{-1} \\
&\left(I - B^T\right)^{-1} = I + B^T + B^T \cdot B^T + B^T \cdot B^T \cdot B^T + \ldots \\
&\left(I - B^T\right)^{-1} = \hat{x} \cdot \hat{x}^{-1} + \hat{x} \cdot A^T \cdot \hat{x}^{-1} + \hat{x} \cdot A^T \cdot \hat{x}^{-1} \cdot \hat{x} \cdot A^T \cdot \hat{x}^{-1} + \ldots \\
&\left(I - B^T\right)^{-1} = \hat{x} \cdot \left(I + A^T + A^T \cdot A^T + A^T \cdot A^T \cdot A^T + \ldots\right) \cdot \hat{x}^{-1} \\
&\left(I - B^T\right)^{-1} = \hat{x} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1}
\end{aligned}
$$

(62)

Combining both transformations leads to the desired result:

$$
\begin{aligned}
&D_G = \left(I - diag(B \cdot e)\right) \cdot \left(I - B^T\right)^{-1} \\
&D_G = \left(\hat{y} \cdot \hat{x}^{-1}\right) \cdot \left(x^{-1} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1}\right) \\
&D_G = \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} = D_P \\
&D_P = \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \hat{x}^{-1} \\
&D_P = \hat{y} \cdot \left(I - A^T\right)^{-1} \cdot \left(I - diag(A^T \cdot e)\right) \cdot \hat{v}^{-1} = D_L \\
&\quad thus: \\
&D_G = D_L = D_P
\end{aligned}
\tag{63}
$$

This completes the demonstration of the equivalence of the sector splits derived from the three different models.

6.6. Discussion

Note that the three approaches to determine D, Ghosh/AMC, Leontief-IO, and Leontief-price/WIO-MFA are different models that use different parameters to answer model-specific research questions. But, if these models are applied at scale, i.e., to the flow variables in the IO table, they all yield the same results for the sector split D. This was shown above.

For practical applications, one will not use the value added as exogenous resource but a natural resource, like iron ore. Or one will narrow down the scope of the IO table and consider engineering materials, like steel, as exogenous input to the manufacturing sector subset of economic sectors. This situation is described and discussed in the next section.

7. Allocation matrix of exogenous input to final demand, case II: exogenous resource input

In the previous section, we showed that the allocation matrix of resources to final products, the so-called end-use shares or sector split or D-matrix, is the same for all three approaches, when considering value added as exogenous input to the economy.

In this chapter, we show that the D-matrix is the same for all three approaches, when considering natural (material) resources as exogenous input to the economy.

To start, we include the so-called environmental extensions or satellite accounts F into the picture. F is a table of exogenous resource input the economy (rows) by economic sector where the resource is processed (columns). The stressor matrix S is matrix of the columns of F per industrial output x, and the resource distribution matrix, i.e., the percentage of resources allocated to economic sectors, $\overline{S}$, is the row of F divided by the row sum b of F:

$$S = F \cdot \hat{x}^{-1}, \quad \overline{S} = \hat{b}^{-1} \cdot F, \qquad b = F \cdot e \tag{64}$$

With these coefficient matrices, we now determine how the natural resource input is allocated to final demand categories, provided that the yield of natural resources into industrial output is the same in all sectors. For value added, the ‘yield’ is 100%, as all value added is part of industry economic output.

In general, the end-use shares of value added, D, can be transformed into the corresponding matrix of natural resource allocation, D_{res}, by using the matrix *S_bar*, i.e.:

$$D_{res} = \overline{S} \cdot D^T \tag{65}$$

(see also section 2.2. in the main paper).

7.1. Resource sector split from the Ghosh/AMC model, using the B matrix of market allocation shares

For the Ghosh model /AMC perspective, starting from the input of natural resources into the system, we first allocate resources to industries, using $\bar{S}$, and then allocate resource input to products using D_G. For the required matrix multiplication, the D matrix must be industry (row) by products (columns), which is why it needs to be transposed:

$$\boxed{D_{res\_G} = \bar{S} \cdot D^T}$$

$$D_{res\_G} = \hat{b}^{-1} \cdot S \cdot \hat{x} \cdot D^T \qquad (66)$$

In the latter equation, the definition of $\bar{S}$ (equation 60) was used. It is a special case of the more general equation 65.

7.2. Leontief IO, Derivation of the "resource sector split"

For the consumption-based approach (CBA) via the Leontief model, we can expand the total resource input into the individual final demand items in y, obtaining a product-specific resource use F_P.

$$F_P = SL\hat{y} \qquad (67)$$

Here,

$$L = \left(I - A\right)^{-1} \qquad (68)$$

In the CBA, the Leontief IO model is used to construct the supply chain and the natural resource input for the final demand y. Certain natural resources, like iron ore, are then used as proxy for materials, like steel. We obtain the resource to final demand allocation in the Leontief IO model D_{res_L} by normalizing the rows of F_P as in equation 60.

$$\begin{aligned}
D_{res_L} &= diag(F_P \cdot e)^{-1} \cdot F_P \\
D_{res_L} &= \hat{b}^{-1} \cdot F_P \\
\Aboxed{D_{res_L} &= \hat{b}^{-1} \cdot S \cdot L \cdot \hat{y}}
\end{aligned} \tag{69}$$

Here, we used that F_P contains all resource input, as y is the full final demand, and the row sum of F_P is b.

Each row of D_{res_L} contains the resource allocation coefficients for the resource listed in that row to the different products listed in y.

Relation to equation 5 used in the paper: The first of the three expressions in equation 69 corresponds to Eq. 5 in the main paper (there we use F(s) instead of F(p), s indicates the sectors). Also, we combine the last line of equation 69 with equation 48 (for the right factor on the right side) and 64 (for the left factor on the right side) to arrive at the general expression:

$$\begin{aligned}
D_{res_L} &= \hat{b}^{-1} \cdot S \cdot L \cdot \hat{y} \\
D_{res_L} &= \left(\hat{b}^{-1} \cdot S \cdot \hat{x}\right) \cdot \left(\hat{x}^{-1} \cdot L \cdot \hat{y}\right) \\
D_{res_L} &= \left(\hat{b}^{-1} \cdot F\right) \cdot \left(\left(L \cdot y\right)^{\wedge -1} \cdot L \cdot \hat{y}\right) \\
D_{res_L} &= \overline{S} \cdot D_L^T
\end{aligned} \tag{70}$$

7.3. Price model and WIO-MFA approach to the material composition of products,

Derivation of the “resource sector split”:

For the Leontief price model perspective, starting from the input of natural resources into the system, we first allocate resources to industries, using $\overline{S}$, and then allocate resource input to products using D_P. For the required matrix multiplication, the *meaning* of the indices of the D

matrix must be industry (row) by products (columns), which is why it needs to be transposed, for which we use equation 54:

$$
\begin{aligned}
D_P{}^T &= \hat{v}^{-1} \cdot C^T \cdot \hat{y} \\
\boxed{D_{res\_P} = \bar{S} \cdot \hat{v}^{-1} \cdot C^T \cdot \hat{y}} \\
D_{res\_P} &= \bar{S} \cdot \hat{x}^{-1} \cdot (I - A)^{-1} \cdot \hat{y} \\
D_{res\_P} &= \bar{S} \cdot D_P^T
\end{aligned}
\qquad (71)
$$

In the second to last line of above equation, equation 56 was used. In the last line, equations 48 and 58 were used.

7.4. Equivalence of the three approaches to determining the resource-specific sector split *D_{res}*

We first use the definitions of S and $\bar{S}$ to show the equivalence of the Leontief and Leontief price resource allocation matrices:

$$
\begin{aligned}
D_{res\_P} &= \bar{S} \cdot \hat{x}^{-1} \cdot (I - A)^{-1} \cdot \hat{y} \\
D_{res\_P} &= \hat{b}^{-1} \cdot S \cdot \hat{x} \cdot \hat{x}^{-1} \cdot (I - A)^{-1} \cdot \hat{y} \\
D_{res\_P} &= \hat{b}^{-1} \cdot S \cdot (I - A)^{-1} \cdot \hat{y} \\
D_{res\_P} &= \hat{b}^{-1} \cdot S \cdot L \cdot \hat{y} = D_{res\_L}
\end{aligned}
\qquad (72)
$$

The equivalence of the Ghosh/AMC solution for D_{res} follows from the first line of equation 66, where three actors to the right of $\bar{S}$ can be replaced by D_P^T, which is the same as D_G^T or just D^T (equation 59).

7.5. Discussion

Leontief, Ghosh/AMC, and the Leontief price model represent different models, since they use different parameters and model equations and thus answer different questions. E.g., Leontief IO can calculate b and x from any y, whereas y does not even appear in the Ghosh IO model.

Only when

(1) combined with the balancing equation of the respective other process in the system (e.g., by adding the absorbing state (final demand) via market balance when extending the Ghosh IO model to the AMC),

(2) applied *at scale*, i.e., to the reported flows of the IO table,

(3) given no or the same manipulations to original MIOT data, and

(4) for specific indicators, like the resource allocation matrix *D*,

the three models yield the same result since the underlying system definition is the same.

Not that the above examples include NO data manipulation of original MIOTs to show equivalence of the end-use share calculation. See the discussion section 3.2 in the main paper.

For determining resource allocation and material concentration, several refinements have been proposed, especially for WIO-MFA (Nakamura et al., 2007). To the extent that these refinements (mass filter, yield correction) can also be converted to (implemented into) a complete IO table at scale, also Ghosh and Leontief price models can be constructed, which will then yield the same results, as shown above. For example, one would then construct a modelled IO table from the mass-filtered and yield-corrected *A*-matrix, from which the other (Ghosh, Leontief price) models can be built.

Another typical refinement for resource to products allocation is to narrow down or truncate the system boundary of the IO table. For example, in WIO-MFA, materials like steel, are treated as exogenous input into manufactured goods, rather than as a resource input like iron ore to the entire industry. This is possible by truncating the system boundary of the IO table by yield-correcting the flows (all flows that do not physically enter the products are removed/excluded/subtracted), thereby removing all possible flows of manufactured goods back into material production (capital formation is not part of the inter-industry table but of final demand).

On the output side, the system boundary can be truncated by re-routing flows of intermediate products to final demand. For example, if packaging is to be considered a separate end-use category, or an absorbing state, all input of packaging to other sectors like food production would be removed from the Z matrix and put as final demand of packaging instead. This procedure leaves the total output x and the market balance unchanged but leads to a different IO table and thus different A and B matrices and different material compositions and resource allocations. This is as expected since the final demand now contains a certain share of packaging, whereas the packaging materials are not part of the material composition of the packaged goods anymore. In general, modellers and analysts need to make sure that the end-use categories in the MFA are the same as in the IO table, and that all relevant IO table flows are routed to their respective end-use sectors. This will often require modification of the original IO table. In general, tables with such modifications can be used to calculate more accurate end-use shares but contain modifications that makes them unsuitable for answering other research questions, like footprint-type questions.

7.6. Conclusion

The value added and the resource allocation matrices D and D_{res} can be calculated from three different IO models and the industry and/or market balancing equations of the IO system. If the Ghosh/AMC, Leontief IO, and Leontief price models are applied at scale, i.e., to the reported flows of the IO table, they all yield the exact same result for D and D_{res}.

The value added and the resource allocation matrices D and D_{res} can be refined by modifying the IO table to apply the following corrections:

- Correct for the yield of different material production and manufacturing sectors by subtracting flows that are not physically embedded into final products.
- Truncate the system boundary on the input side to consider engineering materials like steel as resources into products and not natural resource like iron ore.
- Truncate the system boundary on the output side by filtering out non-mass products like services or by re-declaring and re-routing intermediate products as final demand, like packaging.
- Re-route flows to make sure that the end-use categories of the MFA align with the end-use sectors of the IO table

It is crucial to re-balance the IO table and re-calculate the IO model parameters after these modifications, as the modified IO table resulting from these corrections will lead to different IO model parameters and resource allocation matrices. In general, tables with such modifications yield more accurate end-use shares but contain modifications that makes them unsuitable for answering other research questions, like footprint-type questions.

The difference in the value added and the resource allocation matrices is a result of the modification of the underlying IO table and not of the IO model choice.

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