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Analysis of indirect effects within ecosystem models using pathway-based methodology

Q. Ma[a,*], C. Kazanci[b]

[a] Department of Biological and Agricultural Engineering, University of Georgia, Athens, GA 30602, USA
[b] Faculty of Engineering and Department of Mathematics, University of Georgia, Athens, GA 30602, USA

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ABSTRACT

The role of indirect relations within an ecosystem is crucial to its function. Emergent properties such as adaptability, plasticity, and robustness are hard to explain without understanding the system-wide effects of direct and indirect interactions. In this paper, we take advantage of a different representation of ecosystem models to provide a better understanding of indirect effects. We focus on pathways of individual particles that flow through systems. Particles represent small units of flow material, such as a single carbon atom, 1 g of biomass, or 1 cal of energy. The view of an entire system from an individual particle perspective provides a more practical and intuitive basis to study indirect relations than earlier input–output based algebraic methods. Our findings show that the current two algebraic formulations for indirect and direct effect ratio (I/D) do not exactly compute their intended meaning. We come up with a new throughflow based I/D ratio, which revises the current definition, and accurately compares direct and indirect flows. The two different perspectives (algebraic and pathway-based) enable an insightful analysis and conceptual clarification as to what exactly each formulation measures. We compare all three measures on twenty real-life ecosystem models. Finally, we rescale the I/D ratio to $I/(I+D)$ and define the later one as indirect effect index (IEI), which is better suited to compare indirect effects among different models.

1. Introduction

Network Environ Analysis (NEA) (Patten, 1978; Fath and Patten, 1999b) is a method to study the structure and function of the ecological systems. It applies the idea of economic input–output analysis (Leontief, 1951, 1966) to study environmental systems. NEA methodology formulates various measures to describe the relationships among components in the system and the environment. For example, cycling index (Finn, 1978) quantifies how much of the energy or biomass is recycled; throughflow analysis (Matamba et al., 2009) measures how the environmental inputs contribute to throughflow of each compartment, etc. Computation of most of these properties relies on the data including environmental input and output flows, inter-compartmental flows and compartmental storages. Fath and Borrett (2006) introduces a Matlab function to compute the primary NEA properties. A cloud-based simulation software EcoNet (Kazanci, 2007; Schramski et al., 2011) offers a convenient way to access these properties.

Indirect effect, one important subject of NEA, is crucial to our understanding of how natural systems function, self-organize and can be managed or controlled. For example, Wootton (2002) states that indirect effects are fundamental to the biocomplexity of ecological systems and challenge the prediction of impacts of environmental change; Krivtsov (2004, 2009) believes the understanding of complex interactions is indispensable for sustainable development of humankind, and systematic elucidation of indirect effects is, arguably, becoming central for ecology and environmental science. According to Patten and Higashi (Patten and Higashi, 1984; Higashi and Patten, 1989), effects of indirect interactions among compartments including feedback cycles often exceed the effects of direct connections, producing unexpected behavior such as a predator having a significant positive effect upon its prey (Bondavalli and Ulanowicz, 1999; Patten, 1991). Borrett et al. (2010) shows that indirect flows rapidly exceed direct flows in the extended path network of ecosystem. Chen and Chen (2011) develop a new concept indirect uncertainty (IU) to represent the variability among with the indirect process of information propagation within the system.

Indirect effects have such many applications to study ecosystem functioning. However, how the indirect effect is defined and measured might affect the results of analysis. Patten (1978) defines the ratio of indirect to direct flow (I/D) as a measure to quantify the effect of indirect relations among compartments relative to direct connections. The mathematical definition of I/D ratio (Patten, 1985)

* Corresponding author. Tel.: +1 919 599 8023; fax: +1 706 542 8806.
E-mail addresses: maqian12@uga.edu (Q. Ma), caner@uga.edu (C. Kazanci).

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is based on the flow matrix F, which represents the flow rate of a currency (energy, biomass, nutrients, carbon, etc.) among compartments. Alternative definitions (Borrett and Freeze, 2010) for I/D ratio have been formulated to reflect various aspects of indirect relations, also based on the flow matrix F. One issue with I/D, as well as other similar measures, is verification of how well the mathematical formulations reflect the actual intended meaning. The issue here is mainly due to the complexity of the algebraic formulations, which include a series of linear algebraic operations such as matrix power sums or matrix inverses. Following the meaning of such measures through the equations becomes intractable at some point.

Then why do we not come up with simpler definitions? Well, the complexity in these mathematical formulations is mainly due to the way we choose to represent our systems. We use the flow matrix to represent the flow rate among compartments. The flow matrix only contains direct connections. The process of deriving indirect relations from a matrix of direct connections causes the complexity in the formulations. Therefore, one way to reduce the complexity of formulations is to change the way we represent ecosystem models. This requires new mathematical and computational approaches, and is possible thanks to recent advances in modern computer technology and efficient numerical algorithms.

Network Particle Tracking (NPT) (Kazanci et al., 2009; Tollner et al., 2009) is an individual-based stochastic simulation algorithm that enables us to represent a compartmental model as pathways traveled by particles (energy-matter quantum). Each particle represents very small unit of flow material, such as a single carbon atom, 1g of biomass, or 1cal of energy. A pathway is an ordered list of compartments visited by a particle. The results of an NPT simulation include a list of pathways, and how frequently each pathway is utilized by particles. Note that for ecosystem models with cycling, the list of all possible pathways is infinite. Therefore, NPT results in this case will be approximate. Longer simulations provide more pathways which can satisfy arbitrarily accurate computation.

We have previously used the pathway-based methodology provided by NPT simulations to study how well Finn's cycling index reflects its intended meaning (Kazanci et al., 2009), which is the fraction of flows that occurs due to cycling (Finn, 1976, 1978). We found that the pathway-based NPT formulation agrees with the algebraic NEA formulation, verifying both approaches. Compared with the original definition in algebraic formulation, pathway-based method serves as an easier way for beginners to understand what FCI represents. We obtained the same results for throughflow analysis as well (Matamba et al., 2009).

In this paper, we repeat the pathway-based approach to analyze indirect effects. We show that the conventional I/D formulation differs from its intended meaning, which is supposed to compare direct and indirect flows. We investigate this issue in detail by constructing both algebraic and pathway-based formulations for different indirect to direct effects ratio definitions. Our results emphasize the significance of this new approach in helping us understand the complex and intricate mechanisms that are inherent in even the simplest compartment models.

2. Network Environ Analysis: indirect effect

Fig. 1 is a hypothetical three-compartment ecosystem model. Three compartments are connected by four inter-compartmental flows. Only one compartment (*Producers*) has environmental input, whereas all compartments have environmental outputs because they all are dissipative and lose substance to the environment. The

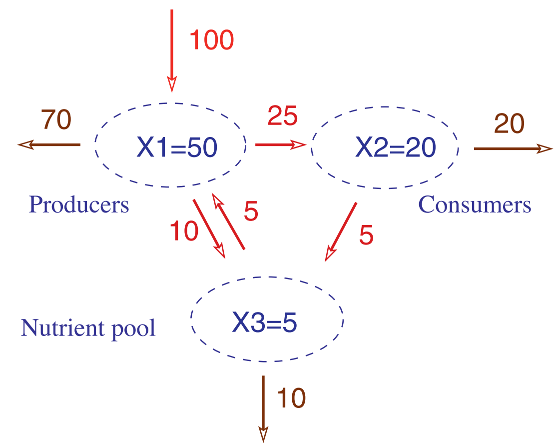

Fig. 1. A hypothetical three-compartment ecosystem model with flow and stock information. This model consists of *Producers*, *Consumers*, and *Nutrient Pool* with stocks $X1 = 50$, $X2 = 20$ and $X3 = 5$ units, respectively.

environmental inputs ($\mathbf{z}$), outputs ($\mathbf{y}$), storage values ($\mathbf{x}$) and flow matrix (F) are defined as follows:

$$\mathbf{z} = \begin{bmatrix} 100 \\ 0 \\ 0 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 70 \\ 20 \\ 10 \end{bmatrix} \quad \mathbf{x} = \begin{bmatrix} 50 \\ 20 \\ 5 \end{bmatrix} \quad F = \begin{bmatrix} 0 & 0 & 5 \\ 25 & 0 & 0 \\ 10 & 5 & 0 \end{bmatrix}$$

z_i : rate of environmental input to compartment i

y_i : rate of environmental output from compartment i

x_i : storage value of compartment i

f_{ij} : rate of direct flow from compartment j (columns of F) to compartment i (rows of F)

Throughflow T_i is the rate of material (or energy) moving through compartment i. It is defined as the sum of flow rates to compartment i from other compartments and the environment. For a system at steady state, it equals the sum of flow rates from compartment i to other compartments and the environment:

$$T_i = \sum_{j=1}^{n} f_{ij} + z_i = \sum_{j=1}^{n} f_{ji} + y_i$$

For the Fig. 1 model,

$$T = \begin{bmatrix} 105 \\ 25 \\ 15 \end{bmatrix}$$

$\mathbf{z}$, F and T are used to define direct and indirect effects. The flow intensity matrix G is obtained by normalizing the flow matrix F by the throughflow T:

$$g_{ij} = \frac{f_{ij}}{T_j}$$

G is actually a one-step probability transition matrix, where g_{ij} represents the probability of transitioning from state j to state i directly. For compartmental systems, g_{ij} is the fraction of the flow material originating from j moving to i directly ($j \to i$). Similarly, $[G^2]_{ij}$ is the fraction of the flow moving from j to i in two steps. In general, $[G^m]_{ij}$ represents the fraction of the flow material from j to i in exactly m steps ($j \to \cdots \to i$). The sum of all powers of the G matrix defines the N matrix:

$$N = \underbrace{I}_{\text{Boundary}} + \underbrace{G}_{\text{Direct}} + \underbrace{G^2 + G^3 + \cdots}_{\text{Indirect}} = (I - G)^{-1} \tag{1}$$

where I is the identity matrix, not to be confused with I used later to denote indirect effects. Direct effects are contributed by direct flows among compartments, while indirect effects are generated by flows that take multiple steps. As shown in Eq. (1), direct effects in the system are given by G only. The indirect effects are denoted by $G^2+G^3+\cdots$, which can be calculated as $N-I-G$. Since both G and $N-I-G$ are matrices, the straight-forward way to compare them is by summing up all elements in each matrix and taking the ratio (Higashi and Patten, 1986). So, for a system with n compartments, the ratio of indirect to direct effects (I/D) is a scalar value defined as follows:

$$\left(\frac{I}{D}\right)_{\text{unit}} = \frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(G^2+G^3+\cdots)}{\sum_{i=1}^{n}\sum_{j=1}^{n}G} = \frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(N-I-G)}{\sum_{i=1}^{n}\sum_{j=1}^{n}G} = \frac{\sum_{i=1}^{n}\left[(N-I-G)\vec{1}\right]}{\sum_{i=1}^{n}(G\vec{1})} \quad (2)$$

Scalars I and D are used to denote indirect and direct effects, respectively. The sum of all elements of G can also be written as $\sum_{i=1}^{n}(G\vec{1})$, where $\vec{1}$ is a vector of ones, with size n by 1. Borrett (Borrett and Freeze, 2010; Borrett et al., 2011) calls this definition "*unit* indirect to direct effects ratio", and points out that it only quantifies the indirect to direct effects ratio when there is a unit input at each compartment, but does not reflect the effects generated by actual environmental inputs (**z**). He defines "realized indirect to direct effects ratio", where the matrices are weighted and dimensionalized with environmental inputs (**z**) before computing the summation:

$$\left(\frac{I}{D}\right)_{\text{realized}} = \frac{\sum_{i=1}^{n}\left[(G^2+G^3+\cdots)\mathbf{z}\right]}{\sum_{i=1}^{n}(G\mathbf{z})} = \frac{\sum_{i=1}^{n}\left[(N-I-G)\mathbf{z}\right]}{\sum_{i=1}^{n}(G\mathbf{z})} \quad (3)$$

3. Pathway-based definition for *I*/*D* ratio

3.1. From flows to pathways

As shown in the previous section, the two conventional definitions for I/D are computed using matrix algebra. Both definitions are similar in that the denominator quantifies one-step relations (direct effects D), and the numerator computes multiple-step relations (indirect effects I). The difference lies in how they derive scalar quantities to represent direct and indirect effects. The original definition simply adds the matrix entries, whereas the realized definition uses inputs (**z**) as weighting terms. This brings out the question of an optimal weighting term to quantify indirect to direct effects ratio. How can we figure out the optimal mathematical formulations for I and D that quantify the indirect and direct flow interactions? This is not an easy question, simply because the algebraic formulations are rather unintuitive. It is difficult to grasp what Eqs. (2) and (3) actually represent. However, we have no other choice, given that the ecological models are represented with flow rates (F), inputs (**z**) and outputs (**y**).

To pursue a solution, we temporarily discard the conventional representation of ecological models, and try to find a more natural way to study this measure. The system is generally considered as continuous flows of energy or matter. From another angle, these continuous flows can be regarded as numerous discrete energy-matter quanta passing through the system. We call such small unit of discrete flow material **particle**. Particle pathways within a system are similar to food chains. In each pathway, a direct flow from one compartment to another constitutes a direct effect. If the flow material from one compartment reaches another through other compartments in multiple steps, this constitutes an indirect effect. Both direct and indirect effects depend on the relationships within the system. Therefore, any environmental inputs and outputs are not involved in this regard.

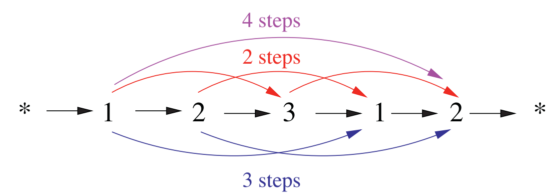

Fig. 2. Counting direct and indirect relations in a pathway of a single atom from the three-compartment model shown in Fig. 1. The numbers 1, 2 and 3 correspond to the compartments *Producers*, *Consumers*, and *Nutrient Pool*. Arrows at both ends are environmental input and output.

Fig. 2 is the pathway of a single particle (energy-matter quantum) in the Fig. 1 system. This particle goes through compartments 1, 2, 3 and then cycles back to 1, and leaves the system at 2. The black arrows represent the direct relations: 1 on 2, 2 on 3, 3 on 1, and 1 on 2. The number of direct relations is four. Colored arrows show multiple-step relations. There exist three two-step relations (1 on 3, 2 on 1, and 3 on 2), two three-step relations (1 on 1 and 2 on 2) and one four-step relation (1 on 2), all of which are counted as indirect relations. Therefore, the number of indirect effects is six.

Fig. 2 only shows one possible pathway a particle can travel. There are infinitely many different pathways even for this simple model. So, to accurately count indirect and direct effects for an entire ecosystem, we need to find out all possible pathways, and how frequently each pathway is utilized. The difficulty is how to derive this set of chains, which are **equivalent** to the whole system.

Network Particle Tracking (NPT) (Kazanci et al., 2009; Tollner et al., 2009) is an individual based simulation method, where discrete quanta (particles) of material or energy are numbered and tracked in time as they flow through the model compartments. NPT starts with breaking input flows into discrete packets which we call particles. For example, for a Nitrogen flow model, a particle could represent a Nitrogen atom. Next, based on flow rates, NPT determines which flow is likely to occur and when. A particle is then chosen randomly from the donor compartment and introduced to the recipient compartment. Ecosystem models are open systems and therefore new particles enter the system continuously. So if the chosen flow is an environment input, a new particle is labeled and introduced to the recipient compartment. NPT keeps the record of pathway history of all particles, including when and where each particle movement occurs. This data is dumped into a text file after the simulation ends.

NPT is particularly useful because unlike similar individual based algorithms, it deduces all the rules on how an individual particle will move directly from the flow, input and output rates of the model. Therefore no additional information is needed to run an NPT simulation. NPT is a stochastic method that is compatible with the differential equation representation. In other words, for the same model, the average of many NPT simulations agrees with the differential equation solution.

3.2. A pathway-based formulation

Fig. 3 shows a partial NPT simulation output for the three-compartment system in Fig. 1. Pathways visited by eight particles are listed. We randomly choose these eight pathways to show the computation of indirect (I) and direct (D) effects. There is no special reason we select such eight pathways. The same method can be applied to any other set of pathways. In Table 1, we compute the direct and indirect relations for each pathway. Then I/D is computed as the sum of all indirect relations divided by

Particle 1 * → 1 → 2 → 3 → *
Particle 2 * → 1 → *
Particle 3 * → 1 → 2 → *
Particle 4 * → 1 → 2 → 3 → 1 → *
Particle 5 * → 1 → 3 → *
Particle 6 * → 1 → 3 → 1 → *
Particle 7 * → 1 → 2 → 3 → 1 → 3 → *
Particle 8 * → 1 → 2 → 3 → 1 → 2 → *

Fig. 3. Partial NPT output for three-compartment system in Fig. 1. The numbers 1, 2 and 3 in all pathways correspond to the compartments *Producers*, *Consumers*, and *Nutrient Pool*.

Table 1
Computation of direct and indirect effects based on the pathways in Fig. 3.

Particle #s	1	2	3	4	5	6	7	8	Sum
Direct relations	2	0	1	3	1	2	4	4	17
Indirect relations	1	0	0	3	0	1	6	6	17

Table 2
Number of direct and indirect flows among compartments based on the pathways in Fig. 3.

	Comp 1	Comp 2	Comp 3
Direct flows			
Comp 1	0	0	4
Comp 2	6	0	0
Comp 3	3	4	0
Indirect flows			
Comp 1	4	3	0
Comp 2	1	1	1
Comp 3	5	1	1

the sum of all direct relations. So the indirect to direct effects ratio is

$$\frac{I}{D} = \frac{17}{17} = 1$$

The same information presented in Table 1 can also be represented in the form of two matrices (direct flow and indirect flow), as shown in Table 2. Each entry represents the number of direct and indirect relations among compartment pairs. Column compartments are donors, and row compartments are recipients. For example, 6 in column "Comp 1" and row "Comp 2" represents the six direct flows from compartment 1 to compartment 2. The sum of all entries in each matrix is both 17 and therefore the I/D is one.

Information in Tables 1 and 2 is equivalent in computing the overall I/D ratio. However, compared to Table 1, Table 2 has an advantage of comparing direct and indirect effects between any two compartments. For example, from this partial output, the number of direct and indirect flow from "Comp 1" to "Comp 3" are 3 and 5. For these two compartments, indirect effects are dominant. Such information can be utilized to study relations between compartments. For example, the compartment with dominant indirect effects on others may indicate key species. In addition, the dominance of indirect effects is validated, it will be interesting to study if the dominance of indirect effects still exists for any two compartments.

For this partial pathway output, indirect effects are the same as the direct effects. In this computation, we use only eight pathways, therefore the accuracy is limited. Since there are infinitely many possible pathways, it is impossible to get an exact result using the pathway-based definition. Still, the probability of the occurrence of a pathway decreases to zero as the length of the pathway increases. Therefore, arbitrary accuracy can be obtained by using more pathways. We use the method described here to compute the I/D ratio for the well-known Oyster Reef ecosystem model (Dame and Patten, 1981). The flow currency is energy, and is measured in kcal/m^2. The units for the flow rates are kcal/m^2/day. Fig. 4 shows its network diagram created by EcoNet (Kazanci, 2007, 2009). Note that we just randomly choose this model. It can be replaced by any ecosystem model. We first use NPT simulations to generate pathways, then utilize these pathways to compute the I/D ratio. Longer NPT simulations provide a larger number of pathways, enabling more accurate computation of I/D. Since NPT is a stochastic simulation method, the results of each simulation are different. Fig. 4 shows that the pathway-based computation of I/D converges to 1.46 as more pathways are used. This value remains the same for three different simulations. Note that with this model, around 1×10^6 particle pathways are required for an accurate computation. Nevertheless, it takes less than a second to simulate this many pathways on a modern dual-core 3 GHz computer. Therefore, high accuracy can be achieved by increasing the number of particles being used, without consuming too much simulation time. We

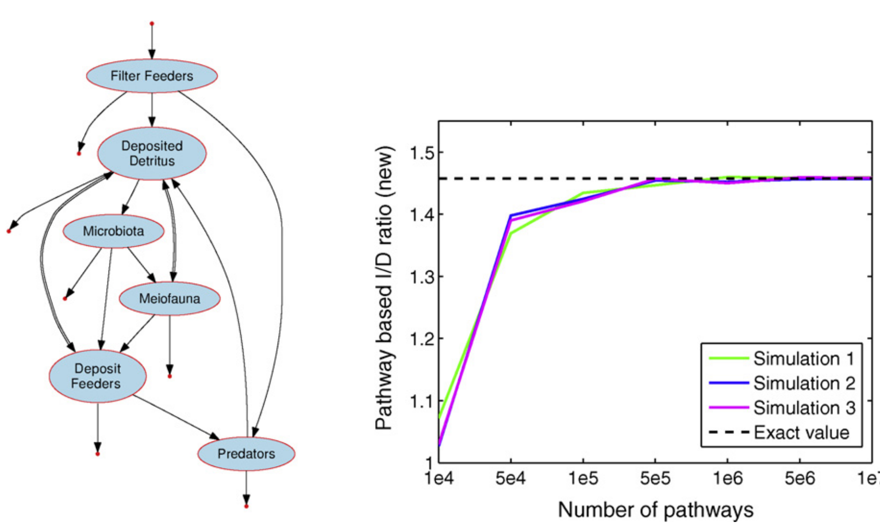

Fig. 4. Network diagram created by EcoNet (Kazanci, 2007, 2009) is shown for the Oyster Reef ecosystem model. The figure shows the pathway-based computation of the I/D ratio using varying numbers of pathways. The value of I/D converges to 1.46 as the number of pathways increases. To make the X-axis tick labels concise, we use "5e4" to represent 5×10^4.

expect that this value would match the value obtained by one of the two conventional definitions (Eqs. (2) and (3)). However, this value is different from both the unit I/D (1.53) and the realized I/D (1.58) ratios. This difference indicates that the pathway-based definition introduced in this section computes a different version of I/D ratio than the two currently available. An algebraic definition, instead of a pathway-based definition, is highly desirable for this new I/D measure, so that we can compare it to the currently available I/D ratios.

Actually, there does exist an algebraic definition that corresponds to the pathway-based computation introduced previously. Eq. (4) shows the algebraic definitions for this new pathway-based I/D ratios. Compared with Eqs. (2) and (3), the only difference among these three definitions are the weighting terms (T, $\vec{1}$, $\mathbf{z}$) used to obtain a scalar value out of the matrices in the denominators and numerators that represent direct and indirect flows.

$$\left(\frac{I}{D}\right)_{\text{new}} = \frac{\sum_{i=1}^{n}\left[(G^2 + G^3 + \cdots)T\right]}{\sum_{i=1}^{n}(GT)} \tag{4}$$

The pathway-based definition we formulated uses throughflows (T) as the weighting term. The direct effects for the new I/D ratio is computed as:

$$\sum_{i=1}^{n}(GT) = \sum_{i=1}^{n}\left(\begin{bmatrix} \frac{f_{11}}{T_1} & \frac{f_{12}}{T_2} & \cdots & \frac{f_{1n}}{T_n} \\ \frac{f_{21}}{T_1} & \frac{f_{22}}{T_2} & \cdots & \frac{f_{2n}}{T_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{f_{n1}}{T_1} & \frac{f_{n2}}{T_2} & \cdots & \frac{f_{nn}}{T_n} \end{bmatrix}\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_n \end{bmatrix}\right) = \sum_{i=1}^{n}\sum_{j=1}^{n} f_{ij}$$

The product of G and T is exactly the sum of all direct flows (per unit time) in the system. Thinking about G as a probability matrix, it becomes clear that G^2 represents the probability that two consecutive flows occur. Then the product $[G^2]_{ij}T_j$ represents the amount of indirect flow from j to i over two steps. Considering all powers of G, the product of $([G^2]_{ij}+[G^3]_{ij}+\cdots)$ and T_j equals the total indirect flows from j to i per unit time. So, the indirect effects in the entire system are:

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left[([G^2]_{ij} + [G^3]_{ij} + \cdots)T_j\right] = \sum_{i=1}^{n}\left[(G^2 + G^3 + \cdots)T\right]$$

We showed that this new formulation captures the ratio of direct to indirect flows, and therefore reflects the intended meaning of I/D ratio more accurately. Then, the similar yet different two definitions using $\vec{1}$ and z as their weighting term compute something different. Unfortunately, the complexity of the algebraic formulations in Eqs. (2), (3) and (4) provides little insight as to how these three I/D measures differ in reality. On the other hand, pathway-based definitions are simple, intuitive, insightful and informative. In the next section, we construct pathway-based definitions for the two conventional I/D measures, which clearly reveal what actually is being computed from a particle or quantum point of view.

4. Pathway-based formulations for conventional *I/D* measures

4.1. Pathway-based formulation for the conventional (unit) I/D ratio

The new I/D ratio (Eq. (4)) uses throughflow values (T) as weighting terms to compute the direct and indirect effects. However, the unit definition (Eq. (2)) lacks this weighting term, and directly adds up all the entries in the G matrix. Recall that each entry of $[G^n]_{ij}$ represents the fraction of flow from j to i over n steps. Therefore, to compute the unit I/D ratio using pathways, we can use the same counting algorithm we used in the previous section. However, we will need to reverse the throughflow weighting term by normalizing all the counts by the throughflow. In order to construct a pure pathway-based definition, we need to compute throughflows using the pathways as well.

Table 3
Normalization of direct and indirect flow counts by throughflow, where throughflow T = [12, 6, 7].

	Comp 1	Comp 2	Comp 3
Normalized direct flows			
Comp 1	0	0	4/7
Comp 2	6/12	0	0
Comp 3	3/12	4/6	0
Normalized indirect flows			
Comp 1	4/12	3/6	0
Comp 2	1/12	1/6	1/7
Comp 3	5/12	1/6	1/7

Using the same partial pathway output in Fig. 3, three compartments appear 12, 6, and 7 times, respectively. This means 12 times particles going through compartment 1, 6 times for compartment 2, and 7 times for compartment 3. So in this data set, the sum of throughflow at three compartments are 12, 6, and 7, respectively. To get the unit definition, we need to normalize the counts of direct and indirect relations in Table 2 by throughflow T. Each entry in Table 2 is divided by throughflow at the column compartment, which is the donor in the relation. For example, the direct flow from compartment 1 to compartment 2 is 6 particles. The throughflow at compartment 1 is 12 particles. So 6/12 = 50% of T_1 goes to compartment 2.

The normalized direct and indirect flows are the direct and indirect flows generated by per unit throughflow at the donor compartment. This corresponds to the meaning of matrix G and $G^2 + G^3 + \cdots$. Then direct effects D is the sum of all entries in normalized direct flows in the Table 3, and indirect effects I is the summation of all entries in the normalized indirect flows in the Table 3. Indirect effect ratio I/D is the ratio of these two quantities.

While it seems natural to add up all the entries in the G matrix to compute the direct effects, we learn from the pathway-based formulation that the throughflow weighting term is indeed needed to compare the actual direct and indirect flows. Therefore this new formulation presented in this paper is more correct in assessing flows (F), rather than flow intensities (G).

4.2. Pathway-based formulation for the input-driven (realized) I/D ratio

The realized definition in Eq. (3) is weighted by environmental input $\mathbf{z}$. In this definition, if one entry $z_i = 0$, all entries g_{ji} ($j = 1, \ldots, n$) are not counted in computing direct effects, and all entries $[G^2 + G^3 + \cdots]_{ji}$ ($j = 1, \ldots, n$) are also eliminated from indirect effects. This definition only counts the relations starting with environmental input. All the other relations are ignored. As shown in Fig. 5, the environmental input happens at 1. There is only one direct relation: 1 on 2. Three indirect relations are 1 on 3, 1 on 1, and 1 on 2 with lengths 2, 3, and 4, respectively. All the other relations are not considered in this situation. Compared with Fig. 2, three indirect relations (2 on 1, 2 on 2, and 3 on 2) and three direct relations (2 on 3, 3 on 1, and 1 and 2) are neglected.

Using the partial output in Fig. 3, the accounting of direct and indirect relations is shown in Table 4. This is very different from that in Table 1. Both the numbers of direct and indirect relations

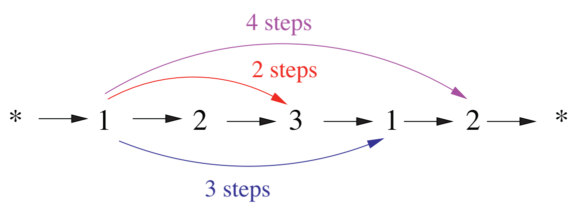

Fig. 5. Counting direct and indirect relations in one pathway for the three-compartment model in Fig. 1. The numbers 1, 2 and 3 correspond to compartments *Producers*, *Consumers*, and *Nutrient Pool*.

Table 4
Computation of direct and indirect relations starting at compartment 1 only.

Particle #s	1	2	3	4	5	6	7	8	Sum
Direct relations	1	0	1	1	1	1	1	1	7
Indirect relations	1	0	0	2	0	1	3	3	10

decrease. Then $(I/D)_{realized} = 10/7$ is different from $(I/D)_{new} = 17/17$. Based on the insight gained from this pathway-based analysis, we will refer to the realized I/D ratio as input-driven I/D ratio.

4.3. Accuracy and convergence of pathway-based formulations for two conventional I/D measures

To check whether our explanations are correct, we calculate two conventional definitions with NPT pathways for the twenty models in Table 5. We observe that pathway-based definitions do match with their algebraic versions (Eqs. (2) and (3)). For demonstration purposes, we use the Oyster Reef ecosystem model (Dame and Patten, 1981) to show the convergence and accuracy properties of the pathway-based definitions for the two conventional measures. Using the regular method, unit I/D is 1.53 and input-driven I/D is 1.58. As we increase the number of pathways used for computations, both the unit I/D and input-driven I/D converge to the results from conventional methods, shown in Fig. 6.

This verifies that our explanations for these two definitions using pathways are indeed correct. The conventional definitions have a clear meaning from a pathway point of view. Borrett et al. (2011) states "the unit method assumes that each node receives a single unit of input". Pathway-based analysis indicates that perhaps a more specific and accurate meaning for "unit" here is "unit throughflow", including both environmental inputs and intercompartment inputs (inflows).

5. Normalization and comparison of the three *I/D* formulations

In this paper, we cover three different I/D ratio formulations. One common issue to all three formulations is the range of these indices. I/D ratio can take any value from zero to infinity. Larger I/D ratio means stronger indirect effects. Zero means no indirect effects. Direct effects are dominant if I/D is less than one. Otherwise, if I/D is larger than one, indirect effects are dominant. Higashi and Patten (1989) and Salas and Borrett (2011) show that indirect effects in ecological networks are significantly dominant. However, arbitrarily large I/D ratios make comparison among models difficult. Therefore we suggest a rescaling of the current measure, representing the fraction of the indirect effects compared to the total of direct and indirect effects:

$$IEI = \frac{I}{I+D} = \frac{(I/D)}{1+(I/D)} \tag{5}$$

We call this new ratio, **indirect effects index** (IEI). Similar to Finn's cycling index, the new measure ranges between 0 and 1. Actually, similar to I/D ratio, the initial definition of cycling index (Finn, 1976) ranged from zero to infinity. This original definition was later revised by Finn (1980) in the exact way that we propose to rescale the I/D ratio. For example, the new I/D ratios for the Aggregated Baltic Ecosystem and Temperate Forest ecosystem model (Table 5) are 1.772 and 27.133, respectively. For the same models, indirect effects indices $(I/(I+D))$ are 0.639 and 0.965. Comparison between models become easier and more accessible using IEI since it reflects percentages. To show how the three formulations of I/D ratios and the associated indirect effect indices $I/(I+D)$ compare, we compute them for twenty ecosystem models (Table 5). All twenty ecosystem models are at steady state.

Fig. 7 show all three IEIs and FCI together for twenty models. We observe that for models with high FCI, the values of the three formulations are not significantly different. We believe this is due to the homogenization property (Fath and Patten, 1999a) of well connected networks with high cycling indices, where the differences between individual compartmental throughflows are less pronounced.

The difference is larger for models with low cycling indices, such as the North Sea and the Silver Springs models shown in Table 5. Furthermore, we observe that the relation between the conventional and the new (revised) indirect effect index is not uniform across models. In other words, for a given model, it is not at all certain which index will be higher than the other. For example, let's consider Generic Freshwater Stream Ecosystem and Cypress Wet Season Ecosystem models (the third and fourth models in Fig. 7). Using the unit definition IEI(I), Cypress Wet Season Ecosystem has

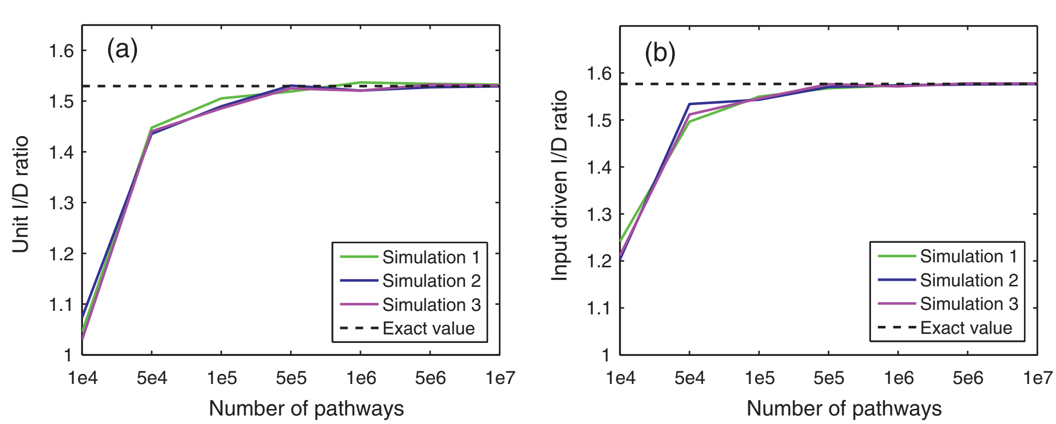

Fig. 6. Accuracy plots for two conventional definitions. As the number of pathways increases, unit I/D converges to 1.53 and input-driven (realized) I/D converges to 1.58.

Table 5
The three formulations for the I/D ratio, the associated indirect effect indices (IEI), and the Finn Cycling Index (FCI) shown for twenty ecosystem models.

Model	Flow currency	Flow unit	I/D			$IEI = I/(I+D)$			FCI
			Unit	Input driven	New	Unit	Input driven	New	
North Sea (Steele, 1974)	Energy	kcal/m^2/year	0.371	0.754	0.616	0.271	0.430	0.382	0
Silver Springs (Odum, 1957)	Energy	kcal/m^2/year	0.084	0.204	0.178	0.077	0.170	0.151	0
Generic Freshwater Stream Ecosystem (Webster et al., 1975)	Mineral	kg/Ha/year	0.587	1.357	0.782	0.370	0.576	0.439	0.001
Cypress Wet Season (Ulanowicz, 1997)	Carbon	g/m^2/year	1.709	0.623	0.710	0.631	0.384	0.415	0.044
Eveglades Graminoid Dry Season (Ulanowicz, 1999)	Carbon	g/m^2/year	1.001	1.408	0.898	0.500	0.585	0.473	0.046
Northern Benguela Upwelling (Heymans and Baird, 2000)	Carbon	mg/m^2/day	0.403	1.043	0.878	0.291	0.514	0.468	0.047
Crystal Creek (Ulanowicz, 1986)	Carbon	mg/m^2/day	0.617	0.672	0.643	0.382	0.402	0.391	0.066
Florida Bay Trophic Exchange Matrix (Ulanowicz, 1998)	Carbon	mg/m^2/year	1.456	1.289	1.197	0.593	0.563	0.545	0.084
Crystal River Creek (Ulanowicz, 1986)	Carbon	mg/m^2/day	0.689	0.709	0.755	0.408	0.415	0.430	0.090
Cone Spring (Tilly, 1968)	Energy	kcal/m^2/year	0.913	1.023	0.859	0.477	0.506	0.462	0.092
Neuse Estuary Network Model	Carbon	mg/m^2/day	2.443	1.482	1.661	0.710	0.597	0.624	0.116
Aggregated Baltic Ecosystem (Wulff and Ulanowicz, 1989)	Carbon	mg/m^2/day	1.530	1.902	1.772	0.605	0.655	0.639	0.129
Somme Estuary (Rybarczyk and Nowakowski, 2003)	Carbon	g/m^2/year	0.674	0.736	0.853	0.403	0.424	0.460	0.139
Florida Bay Wet Season (Ulanowicz, 1998)	Carbon	g/m^2/year	1.904	1.733	1.632	0.656	0.634	0.620	0.144
Ythan Estuary (Baird and Milne, 1981)	Carbon	g/m^2/year	2.143	1.884	1.950	0.682	0.653	0.661	0.225
Lake Wingra (Richey et al., 1978)	Carbon	g/m^2/year	1.903	1.799	1.927	0.656	0.643	0.659	0.396
Tropical Rain Forest (Edmisten, 1970)	Nitrogen	g/m^2/day	6.184	6.140	6.073	0.861	0.859	0.859	0.479
Puerto Rican Rain Forest (Jordan et al., 1972)	Calcium	kg/Ha/year	6.394	7.741	6.610	0.865	0.886	0.869	0.569
Generic Tundra Ecosystem (Webster et al., 1975)	Mineral	kg/Ha/year	23.601	25.553	23.916	0.959	0.962	0.959	0.816
Temperate Forest (Webster et al., 1975)	Mineral	kg/Ha/year	26.881	28.539	27.133	0.964	0.966	0.965	0.833

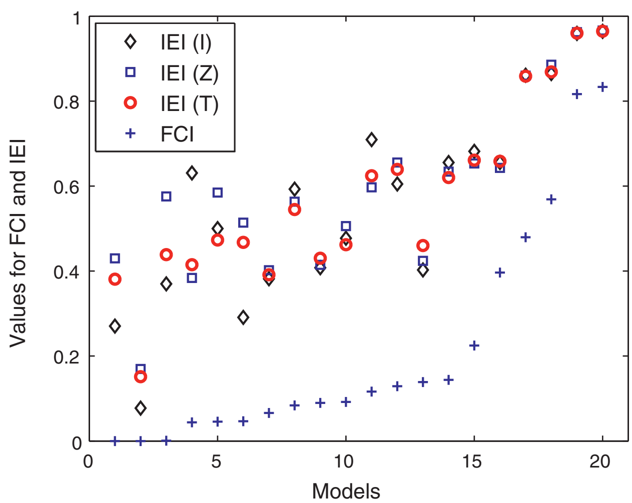

Fig. 7. Comparison of the three indirect effects indices (IEIs) and the cycling index (FCI) for the twenty ecosystem models presented in Table 5.

almost twice the $I/(I+D)$ value of the Generic Freshwater Stream Ecosystem. However, applying our new IEI(T), Generic Freshwater Stream Ecosystem has a slightly higher value. Therefore, if a study comparing these two ecosystems used the old index IEI(I), the conclusion that one of the models has almost twice the indirect effects of the other one would be wrong. One of the main uses of ENA measures is to compare ecosystems (Ray, 2008), and this work has significant impact on past and future studies using indirect effects ratio as a measure for comparison purposes. EcoNet© (http://eco.engr.uga.edu) computes the new revised IEI definition presented here as well as the older definitions.

Pathway-based analysis of three different I/D ratios gives better understanding of this measure. The unit definition quantifies indirect and direct flows generated by per unit throughflow but not the actual flows. So the unit I/D could be called as indirect and direct flow intensities. Input-based definition quantifies indirect and direct flows generated by environmental inputs. This method omits any indirect and direct flows not initiated by environmental input but exist among compartments. The new throughflow-weighted definition is the most natural and intuitive one, which is also the only one computing the actual indirect and direct flow ratio accurately. Hence, our study revises earlier formulations while retaining the original conception of I/D ratios as a way of comparing direct and indirect effects.

6. Conclusion

Since its inception the conceptualization of indirect effects has been based on pathways, but its formulation required rather complicated algebraic input–output formulations. Thanks to recent advances in computational resources, and efficient numerical algorithms (NPT), we are now able to compute direct and indirect effects literally as conceptualized. The methodology provides computational accuracy and conceptual clarity.

The same approach has been successfully applied to Finn's cycling index (Kazanci et al., 2009), throughflow analysis (Matamba et al., 2009) and storage analysis (Kazanci and Ma, 2012). In all three cases, the results of the pathway-based definition matched the algebraic formulation, verifying the accuracy of both methods. Pathway-based definitions are more intuitive, straightforward and simple. Therefore, the agreement of both results also shows that the rather complicated algebraic formulations do indeed reflect their intended meaning. However, in the case of I/D ratio, there was a discrepancy between both methodologies. Our investigation has led to a revised algebraic formulation (Eq. (4)) which accurately reflects the intended meaning of I/D ratio.

To investigate the issue in detail, we constructed pathway-based definitions for the two current I/D ratio formulations. These formulations inform us as to how these algebraic formulations represent I/D from a pathway perspective, clarifying conceptually what exactly is being computed. From the analysis of twenty ecosystem models, the three formulations are numerically close, especially when a significant amount of cycling exists. The mathematical reason for this similarity might be due to the fact that all three definitions are based on powers of the G matrix, but with different weighting terms. However, three definitions are vastly different for low cycling models. Our new definition could possibly reverse some previous conclusions based on original ones.

This study is complete in the sense that all three pathway-based NPT formulations have corresponding algebraic NEA counterparts. However, further studies can focus on indirect effects between compartments. As we referred in Section 3.2, the I/D ratio between any two compartments is available without further computation. It might have many interesting applications, such as identifying the key species in the ecosystem. If one species has very high indirect effects on other species, this indicates it is possibly the key species in the system.

While our focus here has been indirect effects, this work also demonstrates just how useful pathway-based methodologies can be. In this current and our past studies, we noticed that the pathway-based formulations are often easier, simpler, and more intuitive than their algebraic counterparts. It has been our experience that the pathway-based methodology provides a more flexible and potentially useful framework for ecological network analysis compared to using aggregated values (flow matrix, environmental inputs and outputs). The pathway-based methodology has proved to be a powerful tool, not replacing, but complementing the algebraic framework developed over the years. The pathway-based methodology is made possible largely by the NPT algorithm. Generating the pathway data out of the flow, input and output values is a necessity, which can be a tedious task. However, less computation-intensive alternatives to NPT algorithm exists, and our future work will focus on such methods. A significant advantage of NPT algorithm is its ability to extend the applicability of steady-state network measures to dynamic and non-linear models. Many essential and interesting issues involve change, such as environmental impacts, climate change and regime shifts. It is possible to utilize network metrics like the cycling index, throughflow analysis, storage analysis, and now the indirect effects index to tackle such issues.

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