On Walk Entropies in Graphs. Response to Dehmer and Mowshowitz

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Abstract

We provide here irrefutable facts that prove the falsehood of the claims published in [1] by Dehmer and Mowshowitz (DM) against our paper published in [2]. We first prove that Dehmer's definition of node probability [3] is flawed. In addition, we show that it was not Dehmer in [3] who proposed this definition for the first time. We continue by proving how the use of Dehmer's definition does not reveal all the physico-mathematical richness of the walk entropy of graphs. Finally, we show a few facts about the failure of DM themselves to cite properly the relevant literature in their field. We also show here how the Editors of *Complexity* have failed to manage the publication of [1] in an appropriate way according to the accepted guidelines given in the *Code of Conduct and Best Practice Guidelines for Journal Editors*, published by the *Committee on Publication Ethics (COPE)*.

1. Introduction

In the "Essay & Commentaries" published in *Complexity* with the title "*A case study of cracks in the scientific enterprise: reinvention of information-theoretic measures for graphs*" [1], Dehmer and Mowshowitz (DM) claim that a group of authors, including the writers of this Note, are examples of "*lack of professionalism*" and "*poor scholarship*". In our case, the reason for such accusations is that in our paper [3] "*Walk entropies for graphs*", we have “slighted” their paper [3]. These claims are “*rethorically extravagant*” using the words of Polkinghorne [4]. In our paper [2] we have cited the paper [3] and an additional review by DM [5] (see refs. [3] and [4] in our paper [2]). We included the comment, which we maintain and develop here in more detail, that those definitions “have been introduced in *ad hoc* ways”. DM based their claim on the use of the following definition given in [3].

Definition 1 (See Definition 2.8 in [3]): *Let* $G=(V,E)$ *be a finite, undirected and connected graph with arbitrary vertex labels. For a vertex* $v_i \in V$ *:*

$$p(v_j)=\frac{f(v_j)}{\sum_j f(v_j)}, \qquad (1)$$

where $f:S\rightarrow\mathbb{R}^+$ *represents an arbitrary information functional ,* S *is an abstract set.*

The so-called information functional is assumed by Dehmer to be “monotonous” (see text below Eq. (3) in [3]). The values of $p(v_j)$ are then interpreted in [3] as vertex probabilities.

We start by remarking that there is no other way of defining such a vertex probability. It would be enough to say that $p(v_j)$ is a probability assigned to the vertex v_j. We can then think in the bizarre situation in which an author claims that her papers have not been properly cited because she has defined previously the arithmetic mean. We assume that there is only one way of defining so and it is common knowledge. Thus we used it without any citation. Here we provide a few facts about the mathematical incorrectness of the Definition 1 in the way it was defined in [3]. We also provide clear evidence of exactly the same definition in previous reports published in the literature. Subsequently we show how the use of this ad hoc way of thinking does not provide a good scientific approach to study the structure of graphs at least from the basis of the walk entropy. We remark how the authors of [1], Dehmer and Mowshowitz, have failed “*willfully or inadvertently*” to cite other major contributions in their area of research, not only in their research papers but more importantly in their reviews of the field. We finally call the attention of the reader about the way in which we discovered the publication [1]. Just by accidental navigation in GoogleScholar®. This means that the Editors of *Complexity* never alerted us to this paper, clearly against the ethical norms for dealing with such kind of accusatory papers.

2. About Dehmer's definition of vertex probability

2.1. The Definition 1 is not well motivated and not properly related to any graph concept. MathSciNet is a source strongly recommended by DM in [1]. In the review of the paper [3] published in MathSciNet, Dr. Chernov has written about the "*information functionals*" [6]:

"***No clear motivation for the choice of the functionals is given, and no relation of the entropies to any other known characteristics of graphs is shown***."

2.2. The Definition 1 as stated in [3] is mathematically incorrect mainly because

i) First, $f : S \to \mathbb{R}^+$ cannot be monotonic if defined over an abstract set. For f to be monotonic, Definition 1 should include the fact that S should have an ordering relation. Then, the set S should be an ordered or partially order set.

ii) There is no proper definition of what "information functional" means. It is just an abstract function on an abstract set (see again the definition 1). Thus, to call such a generic function "*the information functional of* G" makes no sense whatsoever. The graph G is not even a part of the definition, only of the examples given later in the paper, but examples do not make a proper mathematical definition.

2.3. The Definition 1 does not necessarily contain information about the structure of the graph. Although Dehmer claims that "*the abstract set* S *defines a certain set of associated objects of a graph* G*,"* it is possible to build non-structural invariants for graphs using both Definition 1 and his advice. Let us consider a graph $G = (V, E)$ which is finite, undirected and connected as required by Definition 1. Generate a set S of random positive numbers. Let the cardinality $|S| = |V| = n$. Assign each probability to a node in a one-to-one basis. Use the formula (1) to compute $p(v_j)$ for each node. Plug these probabilities into the Shannon information content formula. Because $f(v_j)$ are randomly generated numbers from a homogeneous distribution it is easy to prove that $S = \ln n$. Thus, all the graphs with the same number of nodes have the same entropy. No structural effect is reflected in such definition of probability.

2.4. The Definition 1 was not introduced by the first time by Dehmer in [3]. We have not made an exhaustive search for this definition in the literature, but find a single counterexample will be enough to disprove the conjecture that this definition was introduced by Dehmer in [3]. In the *Handbook of Chemoinformatics* (Ed. J. Gasteiger, Wiley, 2003), chapter "*Topological Indices*" [7], Dr. Ivanciuc defines (we are writing it in the form of a mathematical definition for the sake of simplicity):

Definition 2: *Let $G = (V, E)$ be a graph with n nodes. Let $f(v_j)$ be the modulus of a vertex structural descriptor (VSD) that assigns a numerical invariant to every node of G. Let*

$$SAVSD = \sum_j \left| f(v_j) \right|. \tag{2}$$

The mean information content of the vertex structural descriptor is given by

$$MIC = \frac{\left| f(v_j) \right|}{SAVSD} \log_2 \frac{\left| f(v_j) \right|}{SAVSD} = \frac{\left| f(v_j) \right|}{\sum_j \left| f(v_j) \right|} \log_2 \frac{f(v_j)}{\sum_j \left| f(v_j) \right|} \tag{3}$$

Remark 2.1. Dehmer's definition is just the particular case of Ivanciuc's one in which $f(v_j)$ is limited to be positive.

Remark 2.2. Differently from Definition 1, Definition 2 is correct because Ivanciuc previously defined what a VSD is. Thus, his definition accounts for proper information content on the graph.

Remark 2.3. The book Chapter [7] was published in 2003, incidentally also by Wiley, five years before Dehmer's paper [3]. Who has "*reinvented this information-theoretic measure for graphs"* to paraphrase the title of the DM's "Essay and Comments"?

3. About the walk entropy of graphs

The walk probability is defined by Estrada, de la Peña, and Hatano [2] as

$$p_i^W = \frac{\left[\exp(\beta A)\right]_{ii}}{Z}, \tag{4}$$

where $Z = Tr\exp(\beta A)$ is the canonical partition function of the graph, $\beta = (k_B T)^{-1}$ (k_B is the Boltzmann constant and T is the temperature), A is the adjacency matrix and $\exp(\beta A)$ is defined using the following Taylor series (see [8] for matrix function definitions):

$$\exp(\beta A) = \sum_{k=0}^{\infty} \frac{(\beta A)^k}{k!}. \tag{5}$$

The walk entropy is then expressed in a condensed form by using the Shannon formula

$$S^V = -\sum_{i=1}^{n} \frac{\left[\exp(\beta A)\right]_{ii}}{Z} \log \frac{\left[\exp(\beta A)\right]_{ii}}{Z}. \tag{6}$$

The walk probability can be of course defined in a plug-and-play way using (1) (if it were correct). It is trivial to see that $\left[\exp(\beta A)\right]_{ii}$ is non-negative and that $Tr\exp(\beta A) = \sum_i \left[\exp(\beta A)\right]_{ii}$.

However, we will show that the plug-and-play definition of this entropy does not reflect all of its structural (mathematical) and physical richness, which have been exploited for instance in [9]. In order to do so, we first need the following previous results. Let us consider a system which can be represented by the Hamiltonian $H = -A$, where A is the symmetric adjacency matrix of a non-directional network with n nodes. The system can be a tight-binding model of a quantum particle on the network in question or a set of oscillators connected to each other (see for instance [10, 11]). If the system is immersed in a heat bath of the inverse temperature β [10, 11], the partition function is given by

$$Z = \mathrm{Tr}\, e^{-\beta \hat{\mathcal{H}}} = \sum_{i=1}^{n} \left(e^{\beta A} \right)_{ii} . \tag{7}$$

By introducing real eigenvalues λ_ν and real eigenvectors $\vec{\varphi}_\nu$ as in

$$A\vec{\varphi}_\nu = \lambda_\nu \vec{\varphi}_\nu \text{, or } \sum_j A_{ij} \varphi_\nu(j) = \lambda_\nu \varphi_\nu(i) , \tag{8}$$

where $\varphi_\nu(i)$ is the i th component of $\vec{\varphi}_\nu$, we can diagonalize the matrix A and transform the partition function in the form

$$Z = \sum_{i=1}^{n} \sum_{\nu=1}^{n} \varphi_\nu(i)^2 e^{\beta\lambda_\nu} = \sum_{\nu=1}^{n} e^{\beta\lambda_\nu} . \tag{9}$$

The probability that we find the network in a microstate with energy $E_\nu = -\lambda_\nu$ is given by the Boltzmann weight that we have used in a previous paper [8] in the form

$$p_\nu = \frac{e^{\beta\lambda_\nu}}{Z} . \tag{10}$$

We obviously have $\sum_{\nu=1}^{n} p_\nu = 1$. The entropy [10]

$$S = \sum_{\nu=1}^{n} \frac{e^{\beta\lambda_\nu}}{Z} \log \frac{e^{\beta\lambda_\nu}}{Z} , \tag{11}$$

is not centred at all on the nodes or any other local structure of the graph, but on microstates of the graph structurally defined by the graph as a whole.

On the other hand, the quantum probability that we find a particle on the node i when the network is in the microstate ν is $\varphi_\nu(i)^2$. We have now the following.

3.1. The walk probability is the product of two probabilities, one centred on the nodes of the graph and the other related to the graph as a whole. That is

$$p_i = \sum_{\nu=1}^{n} p_\nu \varphi_\nu(i)^2 = \sum_{\nu=1}^{n} \frac{\varphi_\nu(i)^2 e^{\beta\lambda_\nu}}{Z} = \frac{\left(e^{\beta A}\right)_{ii}}{Z}. \tag{12}$$

Notice that $Tr\exp(\beta A) = \frac{1}{Z}\sum_{i=1}^{n}\sum_{j=1}^{n}\varphi_j^2(i)\exp(\beta\lambda_j) = \frac{1}{Z}\sum_{j=1}^{n}\exp(\beta\lambda_j)$. Thus the two partition functions used for (4) and (10) are the same. In short, the walk probability has the following physical (structural) meaning: it is the product of two independent probabilities, the quantum probability of finding a particle on the node i when the network is in the microstate ν, which is $\varphi_\nu(i)^2$, and the probability p_ν of finding the graph in a microstate with energy $E_\nu = -\lambda_\nu$.

3.2. The use of $\beta = (k_B T)^{-1}$ is only physically justified in the context used in [10, 11] on the basis of the canonical ensemble of statistical mechanics. If you consider that a graph is submerged into a thermal bath or reservoir (the canonical ensemble) after equilibration every edge of the graph is weighted by β. The plug-and-play formula fails in including the effect of the temperature on the structure of the graph. For instance, if you consider the weighted degree w_i of a node, then $f(v_j) = w_i = \beta k_i$ and $\sum_j f(v_j) = \sum_j w_i = \beta\sum_j k_i$, where k_i is just the degree of the node. Then, $p_i = w_i / \sum_j w_i = k_i / 2m$ and the effect of the temperature cancels out. This is true for any non-walk based entropy using the plug-and-play method.

3.3. The walk entropy is not limited to finite graphs. Let G be an infinite graph with finite maximum degree of a node. Then, the adjacency matrix A has a finite number of nonzero entries per row, and $\exp(A)$ is well-defined. Thus, we can define the walk entropy (5) for an infinite graph. Notice that the Definition 1 is limited to finite graphs only.

3.4. The entropy (11) can be defined from first principles as follows. Let $F = -\beta^{-1} \ln Z$ be the Gibbs free energy of the system The entropy is then defined by $S = -\left(\frac{\partial F}{\partial T}\right)_V$, where V is the volume of the system (reservoir plus graph). Then

$$\begin{aligned}
S &= k_B \ln Z + k_B T\left(-\frac{1}{k_B T^2}\right)\frac{\partial}{\partial\beta}\ln Z \\
&= k_B\left[\ln Z - \frac{\beta}{Z}\sum_{\nu}(-E_\nu)\exp(-\beta E_\nu)\right] \\
&= k_B\left[\ln Z\sum_{\nu} p_\nu - \frac{\beta}{Z}\sum_{\nu}(-E_\nu)\exp(-\beta E_\nu)\right] \\
&= k_B\sum_{\nu} p_\nu\left(\ln Z + \beta E_\nu\right) \\
&= -k_B\sum_{\nu} p_\nu \ln p_\nu,
\end{aligned} \tag{13}$$

where $p_\nu = \frac{e^{\beta\lambda_\nu}}{Z}$.

4. About scholarship and ethic of publication

We have to stress here that authors of [3] were never informed, neither by the authors nor by the Editors of *Complexity*, about the existence of the paper [1]. One of the authors of this Note (EE) found [1] by surfing GoogleScholar®.

4.1. In the *Code of Conduct and Best Practice Guidelines for Journal Editors*, published by the *Committee on Publication Ethics (COPE)*, which is signed among others by Wiley, it is written in the Article 14.2 [12]:

"Authors of criticised material should be given the opportunity to respond".

We have been given such possibility only because we have fight for it, but not because we were invited by the Editor of *Complexit*y to do so when the paper [1] was submitted to this journal.

4.2. The review paper [5] "*A history of graph entropy measures*" authored by both Dehmer and Mowshowitz, which as a review paper must consider exhaustively the literature about a specific field, does not cite "*willfully or inadvertently*" (using the rhetorical words of DM in [1]) the papers:

i. "Estrada, E.; Hatano, N., Statistical-mechanical approach to subgraph centrality in complex networks. *Chemical Physics Letters* 439, **2007**, 247-251" [10], which describes a "graph entropy measure".
ii. The papers of Dr. Ivanciuc on graph probabilities and graph entropies. These results can be traced back to 2001 with the paper published in *Revue Roumaine de Chimie* **2001**, 46, 243-253 [13].
iii. The *Handbook of Chemoinformatics* (Ed. J. Gasteiger, Wiley, 2003), chapter "Topological Indices" [7], by Dr. Ovidiu Ivanciuc, which clearly deals with a few indices of information content on graphs.

It could be thought that there are others papers not cited by DM, but we have not considered an exhaustive bibliographic revision of the topic here. Based on the three examples provided in **4.2**, as well as the non-citation of Ivanciuc's book Chapter [7] by Dehmer in his 2008 paper [3], it could be possible to accuse DM of "*lack of professionalism*" and "*poor scholarship*" using their own criteria. We, however, are not accusing them of such misbehaviours. The reason is simply that the authors of this Note are scientists, not inquisitors.

5. Conclusions

These facts should be enough for the reader to have a clear idea of the falsehood of the claims stated in [1] about our paper published in [3]. It should also be clear that the Editorial system of *Complexity* has failed in managing properly [1]. We are completely aware of the fact that *errāre hūmānum est*. But, we have not received any apology, neither from the authors nor from the Editors of *Complexity*. It is not a damaging act to pursue an increase in the visibility of our scientific results. However, the way of doing it by using accusations like the ones stated in [1] is neither ethical nor effective. It is much better simply to publish good papers.

References

1. Dehmer, M.; Mowshowitz, A. A case study of cracks in the scientific enterprise: reinvention of information-theoretic measures for graphs, Complexity, in press.
2. Estrada, E.; de la Peña, J.A.; Hatano, N. Walk entropies for graphs, Lin Algebra Appl 2014, 443, 235-244.
3. Dehmer, M. Information processing in complex networks: Graph entropy and information functionals. Appl Math Comput 2008, 201, 82–94.
4. Polkinghorne, J. *Reason and Reality*, SPCK Classics, London, 1991.
5. Dehmer, M.; Mowshowitz, A. A history of graph entropy measures. Inf Sci 2011, 1, 57–78.
6. MathSciNet MR2432584 (2009k:94064).
7. Ivanciuc, O. Topological Indices, Topological Indices. In: *Handbook of Chemoinformatics*, Ed.: J. Gasteiger, Wiley–VCH, 2003, pp. 981–1003.
8. Higham, N. *Theory of Matrices. Theory and Computations*. SIAM, 2008.
9. Benzi, M. A note on walk entropies in graphs. Lin Algebra Appl 2014, 445, 395-399.
10. Estrada, E.; Hatano, N., Statistical-mechanical approach to subgraph centrality in complex networks. Chem Phys Lett 2007, 439, 247-251.
11. Estrada, E., Hatano, N., Benzi, M. The physics of communicability in complex networks. Phys Rep 2012, 514, 89-119.
12. http://publicationethics.org/about.
13. Ivanciuc, O. Design of topological indices. Part 19: Computation of vertex and molecular graph structural descriptors with operators. Rev Roum Chim 2001, 46, 243-253.