Applied Mathematical Sciences, Vol. 12, 2018, no. 9, 421 - 430
HIKARI Ltd, www.m-hikari.com
https://doi.org/10.12988/ams.2018.8237

Approximation to the Study of Water Quality

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Abstract

The main objective of this study is to propose a discrete approach to water quality study, applied to freshwater ecosystems, through the fluctuations in the populations of benthic macroinvertebrates and their tolerance to pollution.

Mathematics Subject Classification: 68R10, 05C85, 05C22

Keywords: Bioindicators, BMWP Score, Graphs, Quality Water, Topological Index

1 Introduction

The amount of freshwater around the world is decreasing every day; global warming stresses the ecosystems, especially the water, an essential resource for life in our planet. The presence -or absence- of external factors could disrupt the natural balance of flora and fauna population dynamics. Understanding the biotic and abiotic factors that play a role in such populations is a matter of main importance to assess the ecosystem's health. Water quality monitoring and assessing is vital in order to identify alterations and take decisions to restore and preserve freshwater ecosystems.

Living organisms are indicators of the ecosystem's health and it is very important to know their qualities and needs. The use of biological indices to assess the water quality in lotic ecosystems dates from 1908 [7].

There are several studies of water quality, associated with freshwater ecosystems using bioindicators. As an example, it is worth mentioning the Biological Monitoring Working Party (BMWP) [5], developed to assess the disturbance level of lotic ecosystems, through the study of aquatic macroinvertebrates. Likewise, in the research studies from [14],[15] and [9] abundance and diversity indices were developed with mathematical theoretical support, based on the populations or communities of organisms.

The BMWP index proposed by Hellawell in 1978 for the evaluation of water quality in English rivers, proposes tolerance values to organic pollution associated with certain families of benthic macroinvertebrates. It establishes the water quality according to the presence or absence of taxonomic groups, through the sum of their tolerance values, without taking into account the abundance of each taxon ([6] and [5]), see Table 1.

The BMWP index is used for water quality evaluation together with other parameters: physicochemical, biological and environmental. Among the most commonly used, Dissolved Oxygen, Temperature and pH stand out. Throughout its 38 years of history, it has been applied and adapted in countries such as The United Kingdom and Spain on the initial phase, followed by Central Europe, South America and Africa. In recent years Central America, Asia and some Eastern Europe countries have adapted it. In addition, it has been used to a large extent in studies of water quality in lotic ecosystems, but in lentic ecosystems since 2013, which implies that its practice is still valid nowadays.

The development of new technology, such as the Geographic Information Systems, grants the integration of other descriptors such as: water quality

Taxa Families ex. Oligochaeta	Score
Siphlonuridae, Heptageniidae, Leptophlebiidae, Ephemerellidae, Potamanthidae, Ephemeridae, Taeniopterygidae, Leuctridae, Capniidae, Perlodidae, Perlidae, Chloroperlidae, Aphelocheiridae, Phryganeidae, Molannidae, Beraeidae, Odontoceridae, Leptoceridae, Goeridae, Lepidostomatidae, Brachycentridae, Sericostomatidae	10
Astacidae, Lestidae, Agriidae, Gomphidae, Cordulegasteridae, Aeshnidae, Corduliidae, Libellulidae, Psychomyiidae, Philopotamidae	8
Caenidae, Nemouridae, Rhyacophilidae, Polycentropodidae, Limnephilidae	7
Neritidae, Viviparidae, Ancylidae, Hydroptilidae, Unionidae, Corophiidae, Gammaridae, Platycnemididae, Coenagriidae	6
Mesovelidae, Hydrometridae, Gerridae, Nepidae, Naucoridae, Notonectidae, Pleidae, Corixidae Haliplidae, Hygrobiidae, Dytiscidae, Gyrinidae, Hydrophilidae, Clambidae, Helodidae, Dryopidae Elminthidae, Chrysomelidae, Curculionidae, Hydropsychidae, Tipulidae, Simuliidae, Planariidae, Dendrocoelidae	5
Baetidae, Sialidae, Piscicolidae	4
Valvatidae, Hydrobiidae, Lymnaeidae, Physidae, Planorbidae, Sphaeriidae, Glossiphoniidae, Hirudidae, Erpobdellidae Asellidae	3
Chironomidae	2
Oligochaeta	1

Table 1: Original Biological Monitoring Working Party Score System, Hawkes (1998).

regionalization maps, as a tool that facilitates the location of problematic spots in the aquatic ecosystems, satellite images which allow a thorough ecosystem assessment and models that allow a spatial and temporal description of the characteristics of water bodies.

The study of the fluctuations in aquatic fauna communities and its interrelations with the environment allows the integration of biotic, physical, chemical and multimetric indices in water quality assessments, which has granted the BMWP index affinity, at a greater or lesser extent, with more than 100 metrics. The most applied metrics are: BMWP, BMWP', ASPT, Shannon-Weaver, Margalef, EPT, WQI and Simpson.

Discrete Mathematics is applied to different fields of knowledge: Social Sciences [13], Ecology [2] and Chemistry [17], among others. In the present work it will be necessary to embrace the concept of graph and its properties, to adapt as a mechanism to describe the phenomena associated to water quality and its quantification. For that reason, the aim of this article is to propose a discrete approach for the study of water quality, applied to freshwater ecosystems, through the fluctuations of populations of benthic macroinvertebrates and their tolerance to contamination.

2 Discrete formulation of the BMWP Index

A graph $G(V, E)$ is an ordered pair of disjoint sets of vertices and edges. Each vertex is represented by a point and the edges by lines connecting two vertices. Vertex degree v, denotaded by $\delta(v)$ is the number of edges $e = [v, v_i]$ incidents on it. In this case v and v_i are called adjacent or neighbors.

A graph G is connected if given two vertices are joined for a path (succession of adjacent vertices), otherwise it is disconnected. If there is a partition of V into nonempty subsets $V_1, V_2, \ldots V_r$ such that two vertices u and v are connected if, and only if both u and v belong to the same set V_i, then the subgraphs $G(V_1), \ldots, G(V_r)$ are called the connected components of G. A bipartite graph is one whose vertex set can be partitioned into two subsets X and Y, in such a way that each edge has a vertex in X and one vertex in Y. Particularly, a bipartite graph is complete if every vertex in X is associated with every vertex in Y.

A Topological Index is a numerical value that allows obtain information of a determined discrete structure associated with the invariants of a graph. The topological indices based on the degrees of vertices and edges have been used for more than 40 years. Among them, it is known that several are useful in the field of chemistry research. Probably, the best-known descriptor is the Randic connectivity index (R) [10]. There are several research works on this molecular descriptor (see, for example, [4], [8], [11], [12] and their references). For many years, scientists tried to enhance the predictive power of the Randic Index. This led to the introduction of a large number of topological descriptors correlated with the original Randic Index.

Two of the best-known successors are the first and second Zagreb indices, denoted by M_1 y M_2, and defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) = \sum_{u \in V(G)} d_u^2, \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where uv denotes the edge of the graph G, connecting the vertices u and v, and du is the degree of vertex u. These indices have attracted increasing interest [3]. In the same direction, in [1] the indices are generalized for every real number, in the following way:

$$M_1^\alpha(G) = \sum_{u \in V(G)} d_u^\alpha, \qquad M_2^\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,$$

respectively. The correlation capabilities of 20 topological indices were tested for the case of standard heat formation and normal boiling points of the octane isomers. It is remarkable that the second generalized Zagreb index M_2^α with the exponent $\alpha = -1$ (and at a lesser extent with the exponent $\alpha = -2$) has a significantly better performance than the Randic' index ($R = M_2^{-1/2}$). The second Zagreb variable index is used in the modeling of boiling points of benzenoid hydrocarbon structure. Many properties and relationships of these indices are discussed in several documents ([16]).

The associated graph with the BMWP Index Methodology described in [5], is defined by the correlated between the presence -or absence- of macroinvertebrate families and their value of tolerance to organic pollution. The relationships shown in Fig. 1 represent the macroinvertebrate families and their respective tolerance values, analyzed with the BMWP-CR methodology.

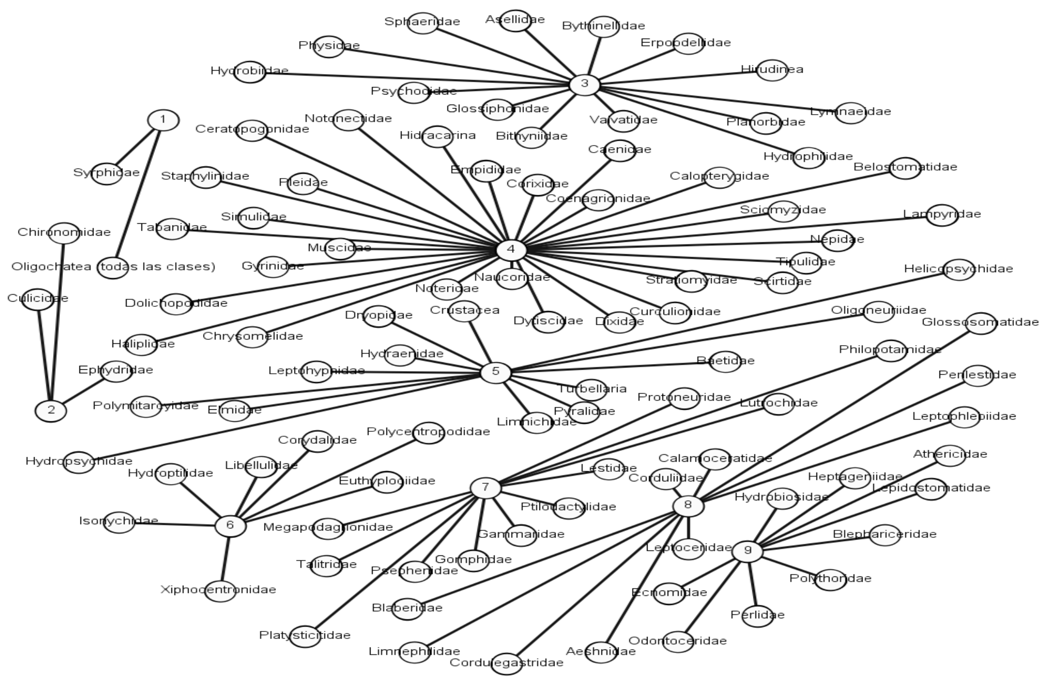

Figure 1: The graph describe the BMWP-CR index methodology.

Let $G_{BMWP}(V, E)$ be a bipartite graph with vertex set $V = \{\beta_i, A_j\}$ where $\beta_i = 1, 2, \ldots, N_1$ are tolerance values to pollution, and A_j with $j = 1, 2, \ldots, N_2$ are the macroinvertebrate families and edge set $E = \{\beta_i \sim A_j\}$ represent the correlation between macroinvertebrate families and their tolerance values to pollution. Vertex degree β_i, denoted by $\delta(\beta_i)$, represent the macroinvertebrate families current with tolerance value to pollution β_i.

Let G_{BMWP} be a graph, then the $BMWP(G_{BMWP})$ index is defined as follows

$$BMWP(G_{BMWP}) = \sum_{i=1}^{N_1} \beta_i * \delta(\beta_i).$$

The next result gives bounds for the $BMWP(G_{BMWP})$ index, where $\lambda = N_1(N_1 + 1)/2$, $\varepsilon = \max\{\delta(\beta_i)\}$ and $\gamma = \min\{\delta(\beta_i)\}$.

Theorem 2.1. *Let G_{BMWP} be a graph, then*

$$\lambda * \gamma \leq BMWP(G_{BMWP}) \leq \lambda * \varepsilon.$$

Proof. Given that $\delta(\beta_i) \leq \varepsilon$, we have that

$$\sum_{i=1}^{N_1} \beta_i * \delta(\beta_i) \leq \sum_{i=1}^{N_1} \beta_i * \varepsilon = \varepsilon * \sum_{i=1}^{N_1} \beta_i = \varepsilon * \lambda.$$

Therefore, $BMWP(G_{BMWP}) \leq \lambda * \varepsilon$. By similar argument we obtain the another inequality. □

If the $BMWP \geq 120$ score means unpolluted waters or non-altered in a sensitive way, then, how many families of benthic macroinvertebrates are needed to reach that value? By Theorem 2.1 shows that $120 \leq \lambda * \gamma$, so then for 9 tolerance values ($N_1 = 9$) we obtain that $2.6 \leq \gamma$, which means that at least 3 families associated with each tolerance value to pollution are needed to reach that value. The next proposition allows the quantification of macroinvertebrate families present.

Proposition 2.2. *If $f(G_{BMWP})$ is the number of macroinvertebrate families, then*

$$\frac{BMWP(G_{BMWP})}{18} \leq f(G_{BMWP}) \leq \frac{BMWP(G_{BMWP})}{2}.$$

3 Index JP Methodology

Let $G_{wp}(V, E)$ be a bipartite graph with weight α_{ji}, vertex set $V = \{\beta_i, A_j\}$ where $\beta_i = 1, 2, \ldots, N_1$ are tolerance values to pollution, and A_j with $j = 1, 2, \ldots, N_2$ are the macroinvertebrate families grouped at order level, and $N_1 \leq N_2$. The number of individuals in each macroinvertebrate family (weight of the edge) is determined by α_{ji}, for example, α_{37} represents the number of individuals in the A_3 macroinvertebrate family with a tolerance value of 7.

The index for water quality assessment is defined as

$$JP(G_{wp}) := \sum_{i=1}^{N_1} \beta_i \sum_{\beta_i \sim A_j} \log_2(\alpha_{ji})^{1/\delta(\beta_i)}.$$

By definition we have that, if the graph G_{wp} has r connected components, $G_1, \ldots, G_r$, then

$$JP(G_{wp}) = JP(G_1) + JP(G_2) + \cdots + JP(G_r).$$

From the previous result and from the experimental analysis, we have that when the resulting graph has less connected components, it implies that there is more diversity of families, i.e., waters are not contaminated or sensitively altered, and vice versa. Therefore, we have the next result.

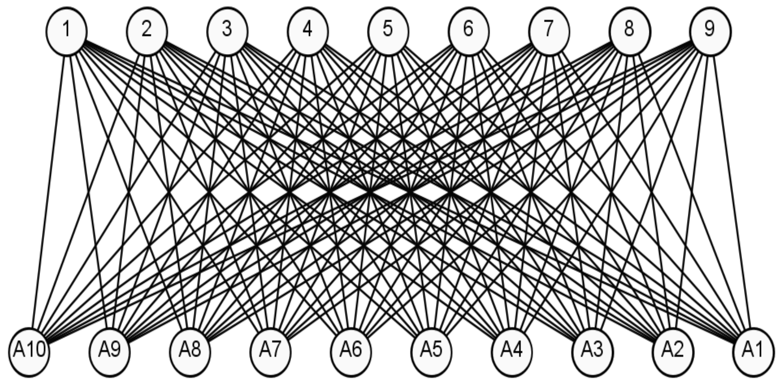

Figure 2: The graph describe a JP score methodology

Proposition 3.1. *If G_{wp} has r connected components, then there is an inverse correlation between the water quality and the number of connected components.*

Theorem 3.2. $JP(G_{wp}) = BMWP(G_{BMWP})$ *if, and only if,* $\alpha_{ji} = 2^{\delta(\beta_i)}$.

Proof. Observe that

$$\begin{array}{rcll} JP(G_{wp}) & = & BMWP(G_{BMWP}) & \Leftrightarrow \\ \sum_{i=1}^{N_1} \beta_i \sum_{\beta_i \sim A_j} \log_2(\alpha_{ji})^{1/\delta(\beta_i)} & = & \sum_{i=1}^{N_1} \beta_i * \delta(\beta_i) & \Leftrightarrow \\ \sum_{\beta_i \sim A_j} \log_2(\alpha_{ji})^{1/\delta(\beta_i)} & = & \delta(\beta_i) & \Leftrightarrow \\ \log_2(\alpha_{ji})^{1/\delta(\beta_i)} & = & 1 & \Leftrightarrow \\ \log_2(\alpha_{ji}) & = & \delta(\beta_i) & \Leftrightarrow \\ 2^{\delta(\beta_i)} & = & \alpha_{ji}. & \end{array}$$

□

The next theorem gives bounds to determine intervals that allow the classification of water quality.

Theorem 3.3. *Let G_{wp} be a graph, then* $\lambda * \tilde{k}_1 \leq JP(G_{wp}) \leq \lambda * \tilde{k}_n$, *where* $\tilde{k}_n = \log_2(k_n)$ *and* $\tilde{k}_1 = \log_2(k_1)$.

Proof. Since that α_{ji} is a natural number , then there are $k_1, k_n \in \mathbb{N}$ such that $0 < k_1 \leq \alpha_{ji} \leq k_n$, moreover $\log_2(x)$ it is a strictly increasing function for all $x > 0$, in particular for $k_1 \leq \alpha_{ji} \leq k_n$, we have that $\log_2(k_1) \leq \log_2(\alpha_{ji}) \leq \log_2(k_n)$ for all α_{ji}. Since that $\tilde{k}_n = \log_2(k_n)$, then

$$\begin{aligned}\sum_{i=1}^{N_1}\beta_i\sum_{\beta_i\sim A_j}\tfrac{1}{\delta(\beta_i)}\log_2(\alpha_{ji}) &\leq \sum_{i=1}^{N_1}\beta_i\sum_{\beta_i\sim A_j}\tfrac{1}{\delta(\beta_i)}*\tilde{k}_n\\ &= \sum_{i=1}^{N_1}\beta_i*\tfrac{\delta(\beta_i)}{\delta(\beta_i)}*\tilde{k}_n\\ &= \sum_{i=1}^{N_1}\beta_i*\tilde{k}_n\\ &= \lambda*\tilde{k}_n.\end{aligned}$$

By similar argument we obtain the another inequality, taking $\tilde{k}_1 = \log_2(k_1)$. □

Note that the bounds found are based on tolerance values to pollution and abundance of each family.

Corollary 3.4. *Let G_{wp} be a graph, then*

$$0 \leq JP(G_{wp}) \leq \tilde{k}_n * \lambda.$$

Corollary 3.5. *Let G_{wp} be a graph and $k \neq 1$ constant, then*

i) $JP(G_{wp}) = 0$ *if, and only if,* $\alpha_{ji} = 1$.

ii) $JP(G_{wp}) = \tilde{k}_n * \lambda$ *if, and only if,* $\alpha_{ji} = k$.

As consequence of the previous results we have to a qualitative approximation for water quality assessment.

Proposition 3.6. *Define* $\sigma = \frac{2JP(G_{wp})}{N_1(N_1+1)*\tilde{k}_n}$, *then*

i) if $\sigma \to 0$ *it implies heavily polluted waters, and*

ii) if $\sigma \to 1$ *it implies very clean waters.*

Acknowledgements. We would like to thank the Universidad Autónoma de Guerrero for the economic support that made this research possible, as well as CONACYT for the scholarship awarded to the first author to study his doctoral program.

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Received: March 5, 2018; Published: March 28, 2018