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## Design of a smart biomarker for bioremediation: A machine learning approach

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### ABSTRACT

Many trace elements (TE) occur naturally in marine environments and accomplish decisive functions in humans to maintain good health. *Mytilus galloprovincialis* (MG) is a rich source of TE, but since it is grown near industrial outfalls, they become polluted with elevated levels of TE concentration and serve as biomarkers of pollution. As bioremediation is increasingly reliant on machine learning data processing techniques, we propose the information theoretic concept of using MG for bioremediation. The in situ bioremediation in MG is accomplished by reduction in concentration of TE by the technique of determinant inequalities and the maximization of Mutual Information (MI) without adding any chemical element externally. We bring out the superiority of our technique of MI over that of Principal Component Analysis (PCA) in predicting lower concentration for bioremediation of Cd and Pb in MG.

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### 1. Introduction

Marine pollution has become a global concern because of bioaccumulation of residues from various types of pollutants such as persistent organic pollutants, heavy metals, polynuclear aromatic hydrocarbons and radionuclides in tissues of various species of marine organism leading to serious threat to human health [1]. In view of the continuous increase in pollution levels in the marine environment the use of molecular biomarkers has drawn worldwide attention for pollution monitoring and bioremediation [2]. Biomarker can be defined as the measurements of body fluids, cells or tissues that indicate in biochemical or cellular terms the presence of contaminants or the magnitude of the host response [3]. The goal of the biomarker is to detect these biochemical changes in order to predict the onset of adverse health effects so that evaluation of these early changes can be used to prevent long term effects at the population and the

community level [4]. There are molecular, cellular, animal biomarkers and living organisms like *Mytilus galloprovincialis* (MG) have been used as inexpensive biomarkers [3–6].

Bioremediation is the use of living organisms, primarily microorganisms, to degrade the environmental contaminants into less toxic forms. It uses naturally occurring bacteria and fungi or plants to degrade or detoxify substances hazardous to human health and the environment. As such, it uses relatively low-cost, low-technology techniques, which generally have a high public acceptance and can often be carried out on site [7]. Even though bioremediation is confined to microorganism or plants, the use of filter-feeder invertebrates like MG for bioremediation of heavy metals in aquatic environment has invited recent attention [8–11].

Many trace elements (TE) like Mn, Fe, Cu and Zn, occur naturally in marine environments and these TE accomplish decisive functions in humans to maintain good health. MG is a rich source of TE, but as they are grown extensively near the industrial water outfalls, they become polluted. As there is a mutual interaction among the TE in MG there is correlation among the TE. These correlations lead to a dynamic balance and in situ bioremediation of a specific TE involves complex and uncertain relationship among other contaminants and it is difficult to understand their interactions [12]. Multivariate Principal Component Analysis (PCA) used for statistical comparison of TE concentration in MG creates independence in concentrations by linear transformation [13,14]. PCA even though work in

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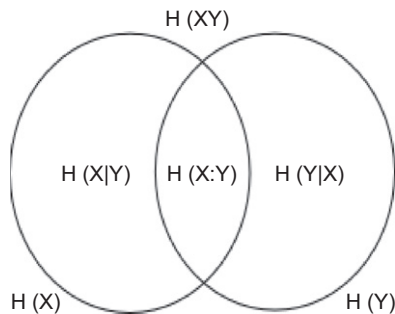
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**Fig. 1.** Mutual Information. In the above figure the uncertainty of  $X$  is measured by its entropy  $H(X)$ . The uncertainty of  $X$  given the knowledge of  $Y$  is measured by the conditional entropy  $H(X|Y)$ . The uncertainty of the pair  $X, Y$  is measured by the entropy  $H(X,Y)$ . Mutual Information,  $I(X; Y)$  is defined as the reduction of the uncertainty of  $X$  due to knowledge of  $Y$  [27].

multivariate environment, target only bivariate and linear feature dependencies and hence are not sufficient to eliminate all dependencies for bioremediation in the data [15,16]. Real-world data like essential concentration versus toxicity in human edibles often contains non-linear structures which PCA is unable to resolve [17,18]. Hence the development of novel bioremediation process is increasingly reliant on machine learning data processing techniques to consider non-linear complex interacting structures [19,20]. In machine learning, the hidden rules that control complex systems are discovered and are incorporated in the design of biomarker.

To our knowledge information theory has not been used so far as supervised machine learning tool to annul the toxicity of a specific TE from among the in situ available elements primarily due to computational complexity [21]. Information theory provides benchmarks for the design of information processing systems as it encompasses a multitude of powerful theorems for computing ideal bounds [22]. As the limit of toxicity reduction varies for each TE and since these TE form a dynamic balance, credible bounds required for bioremediation can be provided by information theory as compared to any other machine learning approaches as information theory alone leads to redundancy reduction [23].

Mutual Information (MI) is a generalized form of correlation analogous to linear correlation but is sensitive to non-linear dependencies between the variables (Fig. 1). In particular, a vanishing MI does imply that the TE are independent, but not so with vanishing Pearson coefficient [24]. Thus MI provides a general measure of association that is applicable regardless of the shape of the underlying distribution. Further, MI unlike linear or rank order correlation is insensitive to non-monotonic dependence between the TE variables [25]. In this paper, we develop an algorithm based on maximizing the Mutual Information (MI) for bioremediation of TE toxicity in the biomarker MG. The technique of determinant inequalities developed by us [26] enables us to estimate the bounds for each of the correlated TE. The lower bounds for the correlated information give a high value of MI as compared to the existing information and hence minimize the toxic concentrations. We demonstrate the superiority our algorithm over the PCA in mitigating the trace element toxicity in MG.

## 2. Machine learning methodology

### 2.1. Preliminaries of information theory

As MG grows in marine environment, we study the interaction between the TE concentrations due to correlation.

Let  $C_i$  ( $i=1,N$ ) be the concentration of trace  $N$  elements and let  $T_i$  be respective toxicity, then according to information theory [27], MI can be written as

$$MI(C,T) = \text{Constant} \log G_p \tag{1}$$

where  $G_p$  is the determinant of the correlation matrix  $\rho$  having elements  $\rho_{ij}$  where correlation coefficient  $\rho_{ij}$  is defined as

$$\rho_{ij} = [\text{Cov}(C_i,C_j) / \{\text{Var.}(C_i)\}^{0.5} \{\text{Var.}(C_j)\}^{0.5}] \tag{2}$$

$\rho_{ij}$  varies between  $+1$  and  $-1$ , is a measure of linear association between the concentrations of the TE and this linear association vanishes when  $\rho_{ij}=0$ .

MI is a measure of statistical correlation in concentration between the TE, and its value depends on the value of the determinant of the correlation matrix  $\rho$ . In order to maximize MI,  $G_p$  has to be maximized.

As an illustration, let us consider a simple case of just two TE, having concentration  $C_1$ , and  $C_2$ , then

$$\rho = \begin{pmatrix} 1 & \rho_{12} \\ \rho_{21} & 1 \end{pmatrix}$$

where  $\rho_{12}$  is the correlation coefficient between  $C_1$  and  $C_2$ .

$$G_p = \det \rho = (1 - \rho_{12}^2)$$

As  $\rho_{12}$  varies between  $+1$  and  $-1$ , the maximum value,  $\det \rho$  is 1 only when  $\rho_{12}=0$ .

$G_p$  can be maximized to unity by finding the upper and lower bounds of  $\rho_{12}$ . Thus, by maximizing  $G_p$  by the knowledge of the bounds for the correlated elements of  $\rho$ , the correlated information between the concentrations of TE is minimized. Minimization of the correlated information leads to lowering of  $\rho$  and the corresponding concentrations of the TE as per Eq. (2). As the concentration is reduced from the initial value, the corresponding toxicity of each of the TE is also reduced. Hence an index of minimization of toxicity in TE for effective bioremediation is the maximization of the MI, by the estimation of upper and lower bounds for the correlated elements of the correlation matrix  $\rho$ . The algorithm developed by us to determine the upper and lower bounds for the correlated elements of  $\rho$  by the technique of determinant inequalities is described below.

### 2.2. Estimation of bounds for correlated concentration by technique of determinant inequalities

We develop the technique of determinant inequalities to estimate the upper and lower bounds for the correlated elements of the correlation matrix. Consider a quantity  $q$ , which is unknown or is difficult to estimate. A rigorous estimate of it, is provided by the upper and lower bounds, say  $U$  and  $L$ , respectively, such that  $U \geq q \geq L$ . The unknown quantity  $q$  in our case is the constant concentration of TE in the sea, which causes correlation or bias. This constant bias appears in one or several elements of the determinant  $G$ . Let us suppose the sign of the determinant  $G$  can be determined. Then  $G$  can be considered as a polynomial in  $q$  i.e.  $G=G(q)$  and the roots of the determinant function  $G(q)=0$  enable us to estimate the permissible values of  $q$  and hence the upper and lower bounds can be determined. Thus to determine the bounds on  $\rho$

- (a) The sign of the determinant  $G$  has to be known.
- (b) The roots of the polynomial  $G(q)=0$  should be determined.

The determinant  $G$  is positive when  $\rho_{ij}=0$ . In this case, only the uncorrelated diagonal elements of  $\rho$  exist. Similarly the determinant  $G$  is zero when  $\rho_{ij}$  is either  $+1$  or  $-1$ . Such a determinant is called

a Gram determinant or Gramian and its positivity is expressed as an inequality

$$G \geq 0 \tag{3}$$

The upper and lower bounds are determined by solving the polynomial equation  $G(q)=0$ .

For the purpose of illustration, let us consider a  $(3 \times 3)$  correlation matrix with elements of  $\rho$  as follows:

$$\begin{pmatrix} 1 & \rho_{12} & \rho_{13} \\ \rho_{21} & 1 & \rho_{23} \\ \rho_{31} & \rho_{32} & 1 \end{pmatrix}$$

Then  $G = \det \rho \geq 0$  requires that

$$1 - \rho_{23}^2 - \rho_{12}^2 + 2\rho_{12}\rho_{13}\rho_{23} - \rho_{13}^2 \geq 0$$

From the above equation, it is clear that  $\rho_{12}$  must lie between two roots of the quadratic equation, which constitute the upper, and lower bounds of  $\rho_{12}$ .

The upper bound is

$$\rho_{13}\rho_{23} + [(1 - \rho_{13}^2)(1 - \rho_{23}^2)]^{0.5}$$

And the lower bound is

$$\rho_{13}\rho_{23} - [(1 - \rho_{13}^2)(1 - \rho_{23}^2)]^{0.5}$$

### 2.3. Robustness of the algorithm

Let us designate the determinant as  $G_i$  with  $i$ th row and column deleted,  $G_{ij}$  with  $i$ th and  $j$ th row and column deleted, (note that when  $G$  has only two rows and columns then  $G_{12}=1$ )

$g_{ii}$  with  $\rho_{ii}=0$ ,

$g_{ij}$  with  $\rho_{ij}=0$ , and row  $j$  and column  $i$  deleted.

According to Eq. (3)  $G \geq 0$  and hence  $G_i$  and  $G_{ij}$  are also Gram determinants of lower order. Thus  $G \geq 0$ ,  $G_i > 0$ ,  $G_{ij} > 0$  and we can establish the following inequalities:

$$\rho_{ij} + (g_{ii}/G_i) \geq 0$$

$$(g_+ - \rho_{ij})(\rho_{ij} - g_-) \geq 0$$

where  $g_{\pm} = \{(-1)^{i+j}g_{ij} \pm (G_i G_j)^{0.5}\}/G_{ij}$ . Thus for the uncorrelated component, the lower bound is  $\rho_{ii} \geq -g_{ii}/G_i$ .

While, for correlated component the upper and lower bounds are

$$g_+ \geq \rho_{ij} \geq g_- \tag{4}$$

According to Hadamard's inequality

$$G = \det \rho = \leq \prod \rho_{ij}$$

The equality is achieved if and only if  $\rho_{ij}=0$ . The maximum value of the determinant is the product of the diagonal elements and the least positive value is zero, when  $\rho_{ij}$  is either  $+1$  or  $-1$ . Since, the MI cannot be negative, the value of either the upper or the lower bounds of  $\rho_{ij}$  which maximizes the determinant  $G$  is the robust value which maximizes the MI.

### 3. Results

The concentration correlation matrix for ten trace elements in MG is depicted in Table 1. The pollution by lead and cadmium in mussel growth near the shore appears to be ubiquitous and characteristic of industrialized coastal areas. The lower bounds for the concentration of nine elements which has correlation with Cd and Pb are obtained using Eq. (4). The lower bound of each of these

**Table 1**

Correlation matrix of the concentrations of trace elements in the biomarker MG.

Al	1	0.85	0.88	0.87	0.30	0.19	-0.21	0.74	0.78	0.75
Cr		1	0.80	0.83	0.31	0.28	-0.08	0.73	0.87	0.72
Mn			1	0.81	0.26	0.25	-0.14	0.71	0.80	0.65
Fe				1	0.45	0.25	-0.17	0.57	0.76	0.62
Co					1	0.44	0.29	0.03	0.23	0.26
Ni						1	0.61	0.11	0.15	0.12
Cu							1	-0.21	-0.10	0.03
Zn								1	0.82	0.71
Cd									1	0.81
Pb										1

**Table 2**

Comparison of  $\rho$  for Cd obtained by maximizing Mutual Information (MI) and the Principal Component Analysis (PCA) in the biomarker MG.

No.	Element	Existing value of $\rho$ of Cd with other TE as in Table 1	Lower bound values of $\rho$ by MI	PCA values
1.	Al	0.78	0.72	0.94
2.	Cr	0.87	0.64	0.93
3.	Mn	0.80	0.59	0.91
4.	Fe	0.76	0.58	0.89
5.	Co	0.23	0.01	0.36
6.	Ni	0.15	-0.003	0.28
7.	Cu	-0.10	-0.29	-0.11
8.	Zn	0.82	0.53	0.82
9.	Pb	0.81	0.53	0.83

**Table 3**

Comparison of  $\rho$  for Pb obtained by maximizing Mutual Information (MI) and the Principal Component Analysis (PCA) in the biomarker MG.

No.	Element	Existing value of $\rho$ of Pb with other TE as in Table 1	Lower bound values of $\rho$ by MI	PCA values
1.	Al	0.75	0.48	0.94
2.	Cr	0.72	0.56	0.93
3.	Mn	0.65	0.50	0.91
4.	Fe	0.62	0.48	0.89
5.	Co	0.26	-0.13	0.36
6.	Ni	0.12	-0.11	0.28
7.	Cu	0.03	-0.40	-0.11
8.	Zn	0.71	0.49	0.82
9.	Cd	0.81	0.53	0.92

elements which maximizes the MI according to Eq. (1) is depicted in Tables 2 and 3, respectively. The corresponding values obtained by the PCA are also tabulated for comparison with that of MI.

### 4. Discussion

In recent years, active research is pursued to develop an inexpensive technique to attenuate the toxicity of TE in the marine mussels before being consumed by the public. Natural attenuation is the preferred methodology for the bioremediation of contaminant concentration as it involves toxicity reduction without adding any chemical externally [28,29].

In this paper, using the concept of maximization of MI as a machine learning tool, bioremediation of the toxicity of a specific TE like, Cd and Pb in the biomarker MG was performed by decreasing the existing concentration of elements as depicted in Table 1, with the lower bound values as depicted in Tables 2 and 3, respectively. As these lower bound values of concentration are much lower than that of the existing values, no external addition

of chemical is required for bioremediation. Consequently, the lower bound values as predicted by the MI technique are ideally suited for natural attenuation in the biomarker MG.

In contrast all the values predicted by PCA both in Tables 2 and 3 are higher than the lower bound values predicted by MI, necessitating external addition of chemicals. As no chemical should be added for bioremediation by natural attenuation, PCA values are not suited as a machine learning tool for bioremediation of MG.

Even though in this paper, we have selectively mitigated the toxicity of Cd and Pb, our MI technique can be extended for the bioremediation of the toxicity of other elements in Table 1 using Eq. (4). But in the case of PCA only large variances have important structure and the potentially toxic TE having lesser variance is not considered. Thus selective bioremediation of TE having lower variance is not all feasible by PCA.

### Conflict of interest statement

No conflict of interest.

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