PARAFAC: A POWERFUL STATISTICAL TOOL FOR WATER QUALITY EVALUATION OF FISH RESERVOIRS

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This work proposes the use of a pattern recognition tool for evaluation of physicochemical composition of water samples, based on the use of Parallel Factor Analysis (PARAFAC). The methodology applied is a multivariate analysis technique for high order data of type $\underline{X}(I,J,...N)$, which allows the easy identification of natural similarities and trends in samples, variable correlation, as well as, the outliers detection [1]. The data set consisted of water samples from a fish reservoir located in Monte Alegre do Sul (SP)/Brazil, collected periodically from February 2008 to April 2009 in 4 sampling sites, and characterized according to the levels of 15 variables: pH, conductivity, turbidity, dissolved oxygen (DO), temperature, total dissolved solids (TDS), chlorophyll a, $N(NO_3^-)$, NO_3^-, NO_2^-, $N(NH_3)$, NH_3, NH_4^+, PO_4^{2-}r, PO_4^{2-}t. The data set was organized in a cube structure $\underline{X}(I,J,K)$, in which $I = 26$ samples (from different collection dates), $J = 15$ physicochemical attributes and $K = 4$ sampling sites. PARAFAC was performed with singular value decomposition with scaled data along variable mode using the Nway300 Toolbox [2] for Matlab 7.8 [3].

PARAFAC modeling has identified 4 sample clusters. Factor 1 characterized samples in relation to variables $N(NO_3^-)$, NO_3^-, $N(NH_3)$, NH_3, NH_4^+ and PO_4^{2-}t, which indicates the increasing levels of these variables in the order: II <III <IV <V. Similarly, Factor 2 is responsible for clusters formation in terms of increasing levels of DO, chlorophyll a, NO_2^-, $N(NH_3)$, NH_3 and NH_4^+, which present the order: I <IV <II, III. The modeling also allowed the identification of outlier samples and correlation between variables. The variables conductivity, turbidity, TDS and PO_4^{2-}r did not have any influence on the groupings seen in Figure 1. Temperature and pH were responsible to seasonal effects in grouping of samples (data not shown here). PARAFAC allowed finding a clustering pattern in the samples of the water reservoir with success, and relate them to their physicochemical attributes in order to suggest Best Management Practices (BMPs) for the fish farmers.

References: 1. Bro, R., "Multi-way Analysis in the Food Industry", PhD Thesys, Denmark, 1998; 2. Bro, R., *Chemolab*, 38, 149-171, 1997; 3. MatLab 7.8, The Matworks Inc., USA, 2009.
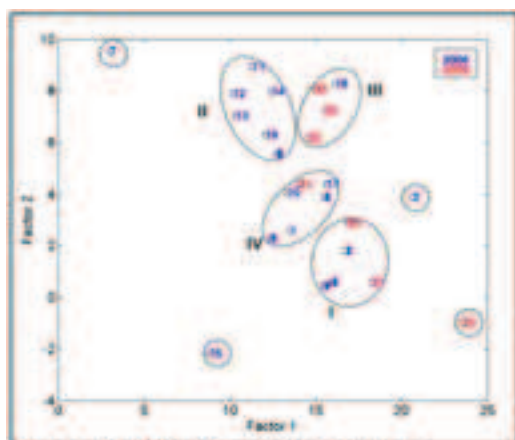
Figure 1: PARAFAC modeling showing cluster formation related to physicochemical composition of samples.

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ABSTRACTS

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