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Analytical Methods

Classification of Iranian bottled waters as indicated by manufacturer's labellings

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ABSTRACT

Water is the most important substance in our daily lives and contains minerals which play an important role in our nutrition. In this study, the chemical composition of Iranian bottled water brands were investigated by correlation analysis, principal component analysis and hierarchical cluster analysis. For this purpose, the chemical composition reported on the label of 73 Iranian bottled waters was used as data set. It was found out that only 26 brands had eight important parameters such as calcium, magnesium, potassium, sodium, chloride, sulphate, bicarbonate and fluoride and 20 brands had acceptable charge balance error. Results showed that Iranian bottled waters can be divided into 11 classes. Most of them were Ca–Mg–HCO_3 type. The relationships among selected variables were also examined by Piper diagram. The best brands were introduced for common customers and kidney stone patients. The chemical content of Iranian bottled water brands was also compared with some world standards. It was observed that only one of the brands had fluoride in excess compare to that of standard values.

1. Introduction

The world market of bottled water has grown quickly and is considered as a global billion dollar business (Güler, 2007a, 2007b; Ikem, Odueyungbo, Egiebor, & Nyavor, 2002; Versari, Parpinello, & Galassi, 2002). In the countries such as the United Arab Emirates, nearly 90% of the population drinks bottled mineral water (Nsanze, Babarinde, & Al Kohaly, 1999).

The dramatic increase in the consumption of bottled water worldwide has been attributed to the consumers' concern over increasing water pollution and their objection to offensive tastes and odours such as chlorine from municipal water supplies and bacterial contamination (Saleh, Ewane, Jones, & Wilson, 2001). Another reason is a common belief that mineral waters have beneficial medicinal and therapeutic effects (Warburton, Dodds, Burke, Johnston, & Laffey, 1992). Apart from the use of bottled water as drinking water, it has found wide usage in infant formula preparation, reconstituting other foods, also for cleaning contact lenses, skin care and filling humidifiers.

The ideal bottled water should be rich in magnesium and calcium and have low sodium content (Garzon & Eisenberg, 1998). Epidemiologic and clinical studies suggest that magnesium may reduce the frequency of sudden death, sodium contributes to the occurrence of hypertension, and calcium may help prevent osteoporosis (Garzon & Eisenberg, 1998). This will help individuals to achieve the recommended daily allowances of these minerals. Because wide variations exist in the mineral contents of commercially available bottled waters, further information on the characterisation of Iranian bottled water is needed to protect the consumers and to draw guidelines for quality control and the regulation of this industry.

Multivariate analysis is widely used for food quality evaluation and differentiation or classification of food samples. Among the different multivariate techniques, cluster analysis (CA) and principal component analysis (PCA) are great potential for classification of problems.

The purpose of this paper is: (1) to investigate the chemical characteristic of domestic brands of bottled water sold in Iran (2) to classify them by utilising parameters reported on their government issued production licenses (3) to compare the chemical composition of water samples with world standards.

2. Materials and methods

2.1. Bottled water database

The chemical compositions reported on the label of 73 bottled waters were used as data set for this study. This data was obtained generally by purchasing the bottled waters from different supermarkets in the Iranian cities and by telephone or electronic mail to manufacturers. The chemical parameter determinations were carried out and certified by official laboratories of analysis and their accuracy and precision were not questioned in this study.

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Distribution of companies is shown in Fig. 1. The majority of water companies are found in western and north parts of Iran. Bottled water dataset is presented as Supplementary material.

Out 73 brands, only 26 brands had eight important parameters (Ca^{2+}, Na^{+}, Mg^{2+}, K^{+}, Cl^{-}, F^{-}, SO_4^{-} and HCO_3^{-}). Routine analysis of mineral water is carried out by each company on a daily basis, whereas a complete analytical control is scheduled, at least, with annual frequency. However, as an independent check on the quality of the chemical analysis in the data set they were tested for charge balance error (CBE) (Freeze & Cherry, 1979):

$$\%\ CBE = \frac{\sum z \cdot m_c - \sum z \cdot m_a}{\sum z \cdot m_c + \sum z \cdot m_a} \times 100 \quad (1)$$

In Eq. (1), z is the absolute value of the ionic valence, m_c the molality of cationic species and m_a the molality of the anionic species. Calculated charge balance errors are less than 10% for 20 samples in the dataset, which is an acceptable error for the purpose of this study. The mean, standard deviation, minimum and maximum of charge balance error were 4.18, 2.14, 0.16 and 8.06, respectively.

2.2. Multivariate analysis

2.2.1. Correlation analysis

Correlation analysis was applied to describe the degree of relation between two water chemistry parameters. In statistics, correlation coefficient indicates the strength and direction of a linear relationship between two variables. The correlation is 1 in the case of an increasing linear relationship, −1 in the case of a decreasing linear relationship, and some value in between in all other cases, indicating the degree of linear dependence between the variables. A correlation coefficient of zero suggests that the two variables are independent of each other. When the coefficient is closer to either −1 or 1, strong correlation occurs between the variables. A number of different coefficients are used for different situations. The best known is the Pearson r correlation coefficient which is obtained by dividing the covariance of the two variables by the product of their standard deviations.

2.2.2. Principal component analysis

PCA is a well-known statistical method for reducing the dimensionality of data sets (Brereton, 2003). PCA is the simplest of the true eigenvector-based multivariate analyses. Often, its operation can be thought of as revealing the internal structure of the data in a way which best explains the variance in the data. If a multivariate data set is visualised as a set of coordinates in a high-dimensional data space (1 axis per variable), PCA supplies the user with a lower-dimensional picture, a "shadow" of this object when viewed from it is (in some sense) most informative viewpoint. PCA involves the calculation of the eigenvalue decomposition of a data covariance matrix or singular value decomposition of a data matrix, usually after mean centering the data for each attribute. The results of a PCA are usually discussed in terms of component scores and loadings.

This approach has been used to extract related variables and infer the processes that control water chemistry (Güler, 2007b; Helena et al., 2000; Versari et al., 2002). A Varimax rotation is carried out in order to ensure that the resulting factors are uncorrelated and to facilitate the interpretation of the results. The number of PCs extracted is chosen by using Kaiser's criterion where only the PCs with eigenvalues greater than unity are retained (Kaiser, 1960).

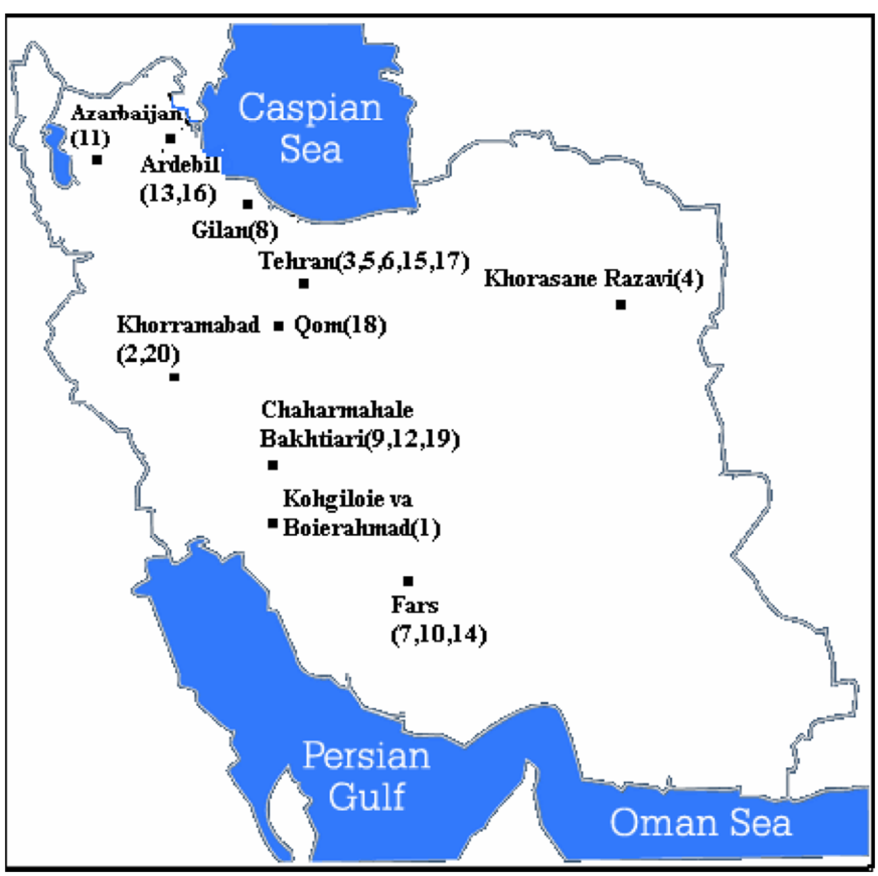

Fig. 1. Distribution of Iranian bottled water companies.