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DIDACTIC

Graphical representation of chemical periodicity of main elements through boxplot

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Abstract Graphics play an important role in data analysis. Boxplots are powerful graphical representation of data that gives an overview and a numerical summary of a data set. In this paper boxplots are used to analyze the periodic trends of main elements. The properties considered are atomic radius, first ionization energy, electron affinity and electronegativity. Boxplots are constructed and metals, nonmetals and metalloids are compared. The results are presented in a manner not explored in chemistry textbooks, pointing out key chemical features visualized through median, quartiles, possible outliers and shape of the distribution. These pictorial representations can show similarities, differences, trends and irregularities among elements, groups and periods, which help better understand their characteristics.

PALAVRAS-CHAVE
Periodicidade química;
Elementos representativos;
Análise exploratória de dados;
Boxplot

Representação gráfica da periodicidade química dos elementos principais usando *boxplot*

Resumo Os gráficos desempenham um papel importante na análise de dados. Os *boxplots* são poderosas representações gráficas dos dados que fornecem uma visão geral e um resumo numérico do conjunto de dados. Neste artigo, os *boxplots* são usados para analisar as tendências periódicas dos elementos principais. As propriedades consideradas são o raio atômico, a primeira energia de ionização, a afinidade eletrônica e a eletronegatividade. Os *boxplots* são construídos e metais, não-metais e metalóides são comparados. Os resultados são apresentados

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de forma não explorada em livros de química, destacando características chaves visualizadas por meio de mediana, quartis, possíveis *outliers* e a forma da distribuição. Estas representações gráficas podem mostrar similaridades, diferenças, tendências e irregularidades entre elementos, grupos e períodos, que ajudam a entender melhor suas características.

Introduction

Graphics are very useful tools when we want to visualize a set of data and extract information from it. Nowadays it is much easier to deal with spreadsheets, graphs and, mainly, calculations (Hibbert, 2006) than in some decades ago when it would be difficult or even impossible to perform some tasks due to limitations related to data processing. In fact, our ability to statistically analyze data has grown significantly with the maturing of computer hardware and software (Schlotter, 2013).

Data analysis should always start by (literally) looking at the data. An efficient way to do this is to use box and whiskers plot (Fig. 1) which, for short, are called box plots (Massart, Smeyers-Verbeke, Capron, & Schlesier, 2005). They were first proposed by the eminent statistician John Tukey (1977) and are powerful graphical representations of data that give an overview and a numerical summary of a data set. The graphic shows a rectangle (the box) with two lines (the whiskers) extending from opposite edges of the box and a further line in the box, crossing it parallel to the same edges. The range of the date is represented by the ends of the whiskers while the upper and lower quartiles are indicated by the edges of the box. Crossing the box there is a line marking the median of the date.

According to Larsen (1985) the construction and interpretation of these graphical formats provides considerable motivation for the ''explanations'' that we traditionally give for chemical and physical trends. According to him, tables of data that appear in introductory textbooks, especially alphabetically arranged data, seems rather uninformative and uninteresting, and should be accompanied by a boxplot showing the content of the table of data. He continuous emphasizing that simply seeking highs and lows and particular groupings in a table does not produce the same results and give the clues that numerical detective work of exploratory data analysis achieves and states ''box-and-whiskers plots are able to be rapidly constructed and thus provide a means for quickly assessing relative data values in a large (or small) data set consisting of chemical and physical properties''.

In this work boxplots are used to analyze the periodic trends of the representative elements of the periodic table. The properties considered are atomic radius (size), first ionization energy (the energy required to remove an electron from a gaseous atom), electron affinity (the energy change involved in adding an electron to a gaseous atom) and electronegativity (a measure of the tendency of an atom to attract electron in a chemical bond). These atomic properties generally vary regularly as we move across a period or up to down in a group. The knowledge of periodicity is important to understand chemical and physical properties of the elements and their compounds. Glasser (2011) believes that the importance of the periodic table of the chemical elements is that it is the principal feature related to the organization of Chemistry.

The representative elements, which are also called main-group elements, comprise both metals and nonmetals. They are found, in the long-form periodic table, in groups numbered 1, 2 and 13 through 18. The disposition of these columns is into two blocks of columns separated by the transition metals. One common aspect about the representative elements is that every element in the group has the same valence electron configuration and shows distinct and fairly regular variations in their properties with changes in atomic number. For the transition elements, the variations are not so regular because electrons are being added to an inner shell. In this discussion the noble gases were not included because they are generally not listed in electron affinity/electronegativity tables. They have no affinity for electrons since they have eight electrons in their outermost shells (except for He, which has two), as a consequence any additional electron must be added to the next higher electron shell.

The main pedagogical objective of this paper is to show how boxplots can be used in exploratory data analysis in Chemistry, particularly in making comparisons, as it is described in this example with the representative elements. The results are presented in a manner not explored in chemistry textbooks. So this work is a guide to the use of boxplots intended to teachers and advanced college students. Authors believe that this technique is important to anyone who deals with chemical information especially when analyzing data.

Methodology

Most people only think of Statistics when faced with a lot of quantitative information to process (Bruns, Scarminio, & Barrros Neto, 2006). In fact, it is not an easy task to extract information by looking so many values. A typical example where statistics is necessary is the analysis of periodic properties of chemical elements. Table 1 is a data matrix with 38 lines for chemical elements, 4 columns for their periodic properties and one column for the corresponding group