Analogies in Arts and Science: Shape Studies and Artful Molecules

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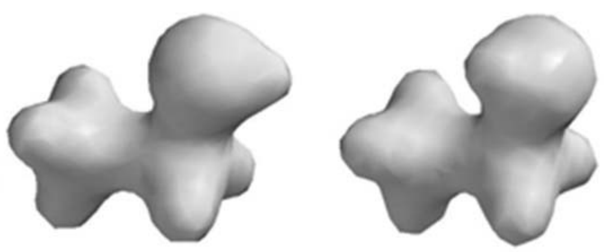
Premise



Are you following me?
Two alcohol molecules falling in love

Two likely shapes of the "bodies" of the electron density clouds of two ethyl alcohol molecules, reminding us to the analogy with a pair of flirting dogs, one following the other.

Abstract

Shape is a universal concept used in most human activities: we deal with shapes in our everyday actions, we use shapes in the process of recognition, in our planning of the future, also in most artistic creations, and in reaching new understanding in the sciences. Shape recognition often connects to the concept of similarities, and on a higher level, when several aspects and several levels and several types of similarities may play roles, then shape recognition may involve entire families of similarities, where a collection of such similarities may be regarded as an analogy.
Analogies, as higher-level or collective similarities, have an interesting mathematical theory, but they can also be visually revealing, often providing useful tools and methods which are transferable between the arts and the sciences. Some of these tools of interpretation, borrowed from arts, can be used with advantage in chemistry, physics, and biology, for example, in the studies of the visually often pleasing shapes of molecules of the "micro-micro-microscopic world".

1. Introduction

Analogies play a very important role in the learning processes: by noticing an analogy of a problem we just try to learn with one we have learned already, the understanding of the new problem becomes simpler: one can, perhaps only cautiously, rely on the already known information to understand and learn the new one. Such analogies of learning appear to work also on a much broader scale, in the developments of both the Sciences and Arts. New scientific advances and inventions, and also new artistic directions and even individual art creations may be regarded as being analogous to learning: the very processes occurring during the inventions of the telegraph, the radio, and the mobile phone, taken as almost random examples, were, indeed, corresponding to learning, not just the learning of some individual human beings, but learning of humanity, a learning process changing human culture on the planet Earth. Similar comparisons can be made, and important analogies can be recognized in artistic achievements, for example, the development and eventual triumph of impressionism has been a learning process for human culture, in some sense analogous to the learning process involved in getting used to and appreciate a new train service to an attractive seaside vacation spot.

The microscopic world of molecules also provides some fascinating analogies, not only to other scientific fields, but also to artistic schools and individual artistic achievements, especially those involving three dimensions, such as sculptures, or dance, or the shape and movements of animals.

One interesting analogy, already pointed out in the Generative Art field, involves the shape concept, where the shapes of molecules have already been studied by methods motivated by artistic sculptures. In fact, the analogy is even more involved, since the original methodology is based on mathematics, due to the works of the famous mathematician, Felix Klein, the initiator of the famous Erlangen Program for the systematization of geometry and related fields. Felix Klein was intrigued by the idea of beauty and tried to use mathematical methods [1], as applied to several well-known sculptures, to find some mathematical regularities employing surface-analysis methods, such as curvature classification on the surfaces of those sculptures. Local convexity, concavity, and saddle like local shapes on those surfaces gave a classification, and the boundary lines of those domains of certain curvature types can be characterized easier. However, he was disappointed, because he was not finding any clear relations between the mathematical characterization he made and the way the beauty of those sculpture could be judged. Nevertheless, his ideas survived and were reported in a book by other mathematicians, and with some modifications, they have become the starting point of a series of methods used in the shape analysis of not some sculptures, but in the study of shapes of molecular electron density clouds [2]. Shape similarity when comparing molecules is an important aspect of the broader concept of molecular similarity, also including molecular symmetry and chirality [3-24], where chirality problems are prime examples for a simple use of analogy: the analogy of left and right hand differences to molecular chirality, with the dominance of “left-handed” amino acids in living creatures on the Earth.

Molecular shape is indeed, the shape of the molecular electron density cloud, underlying the importance of electron density studies [25-28], where some classical concepts, reaching back as far as some traditional art forms, are often appearing, sometimes unexpected ways.

Analogies between objects of nature and their artistic representations are rather obvious examples, some, only partially relevant opinion states this as “Art imitates Nature”. Perhaps one of the most noticeable analogy in the natural sciences is the analogy between two rules (Laws of Nature), seemingly completely unrelated: Newton’s Law of gravity, and Coulomb’s Law of electric charge repulsion (or attraction), are highly analogous: the force produced is proportional to the product of the quantities characterising the two objects, divided by the square of their distance. In the case of Newton’s Law of gravity, the relevant quantities are the two masses, in the case of Coulomb’s Law of electric charge repulsion, the relevant quantities are the electric charges of the two objects. The two equations are fundamentally the same, only the participating quantities are different.

Analogies may be regarded as advanced similarities, and in the molecular field, the various aspects of molecular similarity have been investigated in great detail. In these studies, the relative arrangements of molecular parts are of special importance, and one can always recognize connections to artistic shapes.

In this contribution, some aspects and the main featues of the above and some more general analogies will be discussed, with a focus on the shape of molecules and analogous aspects of some work of arts will be discussed.

However, in the next section, a brief introduction to some of the general aspects of analogies will be given, with a focus on the ideas of using families of similarities in order to simplify the abstract structures of some of the more involved analogies.

2. Some general properties of analogies

In the usual, everyday conversations, the word analogy is used without any strict definition, typically, analogy is regarded as some more elaborate type of similarity. Analogy is often interpreted as some deeper level similarity, or as a similarity with several components. Sometimes one may consider two phenomena, and between them several types of similarities, and the fact that multiple similarities are observed, this appears to justify to call the result of this comparison an analogy.

One may regard analogy as a system of several similarities, alternatively, as a relation where similarities occur on several different levels.

The mathematical tools of a branch of mathematics, Category Theory, appear to be exceptionally suitable to deal with this type of complexity of relations; in particular, the so called functor model [29] appears to be especially useful for characterizing analogies. Systems of similarities can be treated component by component, in a direct way, dealing with each similarity type separately. However, a system of similarities is a richer entity than the mere sum of the component similarities, and a more revealing approach is obtained if the families of similarities are regarded as a higher level entity than the mere individual similarities. If these higher level entities, that is, the families of similarities, are treated collectively, than a better description of the analogy can be achieved. Such a description is provided by Category Theory, specifically, by the so-called functor model, one that carries out comparisons (actually, transformations) on two levels, on the first level, transforming one family of objects into the other family of objects, and also transforming the relations, typically similarity relations in one family to those in the other family. Whereas describing the mathematical details of the functor approach to analogies is not the goal of this contribution, one may find the relevant references in one recent publication [29].

2. Simultaneous treatment of multitudes of similarities, in arts, and sciences

Even if only the terminology of one field is borrowed and used in a different field, this already provides both new ways of seeing the details and this also may trigger new initiatives and methodologies to evaluate the results of comparisons. This is especially true, when the comparisons are extended to several aspects of complex problems with a multitude of similarities, for example, when analogies are actually generating further analogies, where the similarities may occur on several levels.

In such cases, the functor model is an advantageous approach. Such a functor model appears especially useful if one may expect repeated occurrence of meeting with new challenges of comparisons with similar levels and similar types of complexity. One may mention that re-using of approaches and methods originally developed for one set of problems, may often appear useful in a new field, and the functor model can be very beneficial in a different field as well. This is likely to be the case for the development of trans-disciplinary approaches, for example, in those cases where scientific and artistic methodologies are able to learn from each other. In our case, the generation of artistic impression, the message of the artist, in particular, the way the artist sends the message to the observer, is one, that can be also beneficial in the efficient interpretation of the scientific results of molecular shape analysis. If the artistic, efficient impression generation by the artist is translated to the scientific language of molecular shape analysis, this can provide valuable, new scientific understanding. In fact, most of the chemical references listed are containing examples where some of these benefits have played a role, even if in most cases, no systematic, functor-based approach has been used yet.

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