THE BEETHOVEN CONNECTION

Symphonies are some of the most complex musical pieces. They involve different instruments, each with their own unique sound, and each instruments section playing their own tunes. Yet, what are symphonies in comparison to the complexity of life? Proteins for example, they are made of a limited number of building blocks, amino acids, but take highly complex shapes and assume a broad range of functions in the body.

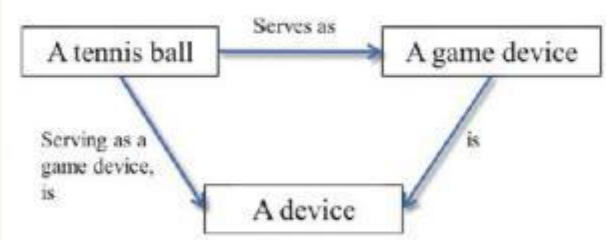
Still, there is a commonality underlying such complex systems, in many cases they are hierarchical, which means they're made of different objects on different scales – instruments playing tunes, amino acids forming proteins and so on. As David Spivak,Markus Buehler and others from MIT have described in a recent paper, a mathematical approach, known as category theory, can be used as a versatile tool that is capable of modelling complex systems by using the underlying rules governing a structure's components. This is a very powerful approach and there is a lot to be gained by using this mechanism in materials science, to describe biomolecules or other hierarchical materials. Moreover, their approach makes it easy to connect different complex system. To put it crudely, understanding a Beethoven symphony may also provide insights into the properties of a protein, because category theory helps us links various complex systems.

Photo by Wayne Dixon via flickr.

To understand how this works, let's take a look at an example provided by Buehler and colleagues – spider webs. These are made of individual fibres, consisting of smaller fibrils. The fibrils are made of a nanocomposite of crystal-like structures connected by flexible links. These structures are in turn made of various amino acids.

The complex structural hierarchy of spider silk (and other systems) is of course well-known. The problem researchers face is, however, that knowing the individual components of a material doesn't necessarily mean that the properties of the full system are known. For example, even though the molecular composition of a protein may be known, predicting its three-dimensional shape
is notoriously difficult. It is the behaviour of structural elements in the context of

their use that can be so difficult to understand. And this is where category theory is useful.



Example of a structure used in category theory. It relates objects such as tennis balls to its properties and uses.

The aim is to reduce complex interactions between different objects to a network of interactions and relations based on certain rules. These are called ontology logs, or *ologs*. Each olog must be mathematically well-defined, expressing a clear relation between properties of a system. “Ologs offer means to reveal the origin of the described system property and connect them to previous results or other topics and fields,” write the authors (ref. 2).

So how does such an olog look in practice? Basically any structure needs to be broken down into various objects that make up a system on different levels, along with arrows describing their relation – as shown in the image here for one such relation concerning tennis balls. Ologs typically consist of *many* such objects linked together. An olog describing spider silk, for example would establish relations between all those objects I mentioned above, and also involve structural characteristics.

It would also make quantitative comparisons, say to look at the amount of crystal-like structures in the silk protein and compare that to the number of flexible links embedded to decide whether the structure is flexible or not. In other words, a computer program would parse an olog in way that’s somewhat related to a complex flowchart, taking decisions at different nodes, which makes these really easy to implement with a computer – especially with object-oriented computer languages. The difficulty is of course to define an olog in the first place, which can quickly take quite complex forms.

Photo by Delexed via flickr.

The strength of ologs is that these could be applied to a different problem. In mathematics, the advantage of category theory is that findings in one area of mathematics can be directly applied to another if these areas are similarly structured. The same could turn out to be very important here as well.

Buehler and colleagues show this by drawing an analogy between spider silk proteins and social networks. The amount of strong social connections (nanocrystals in spider silk) versus more loose ones (flexible links) provides direct clues on the strength of a social network. A computer can parse the different input parameters in the same way, so what is an olog for spider silk could also be seen as an olog for a social network.

While I don’t know about the immediate use of the conclusions that could be drawn by comparing materials with social networks or symphonies, the implications for more related scientific areas are clear – most hierarchically structured material follow similar design rules. By using ologs it might be possible to use structural concepts used in natural compounds and transfer these to artificial materials, to obtain stronger man-made fibres for example.

The problem is of course to come up with appropriate ologs, and this is the hard part. Still, we are only at the beginning to realize what could (or could not) be done with ologs, and it will be really interesting to see how this plays out.

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