On science and computation

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Various views of science have been in favor at one time or another, over the many centuries since its inception, in ancient Greece. It started out as the study of the natural world ("physis" in ancient Greek), that is, of the world as independent of the human being. Later, as the deductive method was formalized by Euclid, and various thinkers started to be aware of its power, it came to be seen as almost synonymous to science. After the industrial revolution, as science blossomed and gained enormous prestige, and as other disciplines wanted to wear the scientific "mantle", demarcation became a problem: what distinguishes science from other intellectual human endeavors? Much has been written on the subject. In the scientific community itself (though not necessarily in the philosophical community), the approach of Karl Popper, emphasizing falsifiability, has become popular over the second half of the 20th century.

The strength and the weakness of Popper's approach, however, is its operational emphasis. It delves into too much detail, imposing constraints on what scientists are or are not allowed to do or think. Moreover, in many cases it is difficult to establish clearly whether a theory is falsifiable or not. The difficulty lies in the "-iable", because it refers to experiments which have not yet been done, but which are "doable" in some sense. Making doability precise is a problem. Moreover, it is well known that Bismarck's famous adage about laws being like sausages - it is better not to see how they are made – applies to *scientific* laws as well. In order to arrive at a scientific end, many of the intermediate steps are highly *non*-scientific. Thus, strict observance of falsifiability may actually hinder scientific progress.

A more holistic (less "interventionist" as it were) approach to defining science may be appropriate. This is provided by the approach which concentrates on its empirical feature: *science is composed of theories capable of predicting outcomes of experiments*. A somewhat more qualified version is to say that *a theory is scientific to the extent that it is capable of predicting outcomes of experiments*. This refers to experiments that have already been done, or that can be done right now, of course.

It is very important at this point to distinguish carefully between scientific theories, and the "scientific method". The former may be identified via the data centered empirical definition given above. The latter, however, is only a pair of words with no real meaning. No "method" exists for discovering new theories. If it did exist, then we would have long ago programmed a computer to do it for us. A lot (if not most) of what scientists do is far from scientific, and there is no way around it. Super-string theory is an excellent example, and the controversy around it is due to the fact that it is difficult to argue conclusively either for or against engaging in this kind of activity. Shortly put, it is a necessary evil, it is up to each scientist to decide when enough "evil" is enough.

Note however, that within all *scientific* theories, there is a ranking. Some are superior to others: the simpler ones and the more accurate ones.

A theory which requires fewer principles and rules is preferable to one requiring more, in order to make the same prediction. Indeed, there are theories which make indistinguishable predictions regarding some experiments, but which have different complexity: Newtonian mechanics and general relativity are canonical examples. When sending a rocket to Mars, either can be used, but in practice, the Newtonian theory is the one actually used to engineer the rockets.

Also, a theory which is accurate to 10 significant digits (as quantum theory is in some situations) is preferable to one which is accurate to within a factor of 2 (as classical theory is in some situations). The ability to make *quantitative* predictions is therefore essential, bringing *computation* to the center of the whole scientific enterprise.

In fact, if we take a closer look, computation has always been the engine behind scientific progress.

In the beginning there was arithmetic and geometry. Greek geometry gained prominence, at least initially, as a collection of techniques for measuring distances (to offshore ships, to tops of trees, buildings, pyramids, etc.). Thus, nature, as known to the Greeks, functioned according to integer laws (Pythagoras) and geometrical concepts such as straight lines (light) and circles (Moon, Sun). The Greeks' understanding of the world around them, their ***reality***, was shaped by the computational tools available to them.

Galileo extolled mathematics as the language in which is written the book of nature. Evidently, he considered computation as almost synonymous to science itself. Later, it is no accident that the figure that became, without a doubt, the most influential scientist ever, owes his fame at least as much to his computational insights (the calculus, the approximation technique known as Newton's method) as to his physical insights (mechanics, gravity, optics). Physics laws are empty without a computational prescription. As calculus (and pen and paper of course) became the computational tools of choice, nature was seen to obey sets of differential or integral equations. These (and their generalization, exterior differential systems on manifolds) became our notion of ***reality*** to the present day, being elevated to that status by their ability to *predict accurately*. To us, the world is *made of* solutions to differential equations.

However, in the modern world, a new computational tool has once again emerged, the computer. Where Newton had pen, paper, the derivative and the integral, today we have Opteron, Itanium, and numerical methods, implemented in packages and languages such as Fortran, Matlab, Lapack, Maple, Ansys, Comsol, Python and myriad other scientific computation packages and methods covering all subjects from classical electromagnetism, to macromolecule folding, to cellular dynamics in systems biology, to neural networks of organisms ranging from lowly nematode worms, to humans.

Yet the transition to the new, computational language is slow. Old habits die hard. Science is still being taught mostly in the old differential language, as if it was in some sense more "real" than the new language of numerical methods. Numerical methods are still widely seen as *approximations* to the "true" laws, most often expressed in the language of the differential calculus. An analytical solution is often seen as *a priori* superior, more trustworthy, and in some sense closer to the fundamental "truth" than a numerical solution.

Part of the problem has been that for a long time numerical methods have been quite amateurish. This is because scientists were trained not to take them seriously. It is a self-fulfilling prophecy. Even today most scientists think of numerical methods as a way to "approach", "approximate" or "discretize" some differential equation or system. However, the objective in science, as highlighted in the second paragraph of this text, is to "approach" or "approximate" ***experience***, not equations, which are purely human creations. It is therefore fitting that we refer to the laws of mechanics as "Newton's laws" and not "God's laws". God may have created matter and light as He saw fit (and we have yet to elucidate), but ***equations*** are our invention, for our own ***use***, and no more.

In fact, in many (if not most) cases, the numerical approach can be more faithful to experimental fact than the old analytical approach. Numerical methods are known to exhibit phenomena analogous to experimental realities such as dissipation, dispersion or noise. An excellent example in the context of classical electromagnetic theory is pointed out by David Bohm, Basil Hiley and Allan

Stuart:

"*The laws of electrodynamics were first expressed in terms of integrals of fields over cycles of varying dimensionality, e.g. Ampere's law, Faraday's law, Gauss's law, etc. It is only from the extrapolation of these integral laws to infinitely small cycles that one obtains Maxwell's equations. Thus these equations go considerably beyond what can be inferred from observations alone. The relative ease of the mathematical application of the differential form of Maxwell's equations has made this approach attractive. However, the infinities which arise in the indefinite extension of this form, both classically and quantum mechanically, imply that it may be appropriate to go back to the integral form in spite of the possibility of greater mathematical difficulty. The appropriate mathematics for doing this is just the theory of complexes of chains and cochains that we have described earlier.*"

The theory they refer to in the last sentence is exactly the theory underlying the Finite Element Method, one of the most common numerical methods for studying electromagnetic systems. More generally, notions such as perfect smoothness or derivability are convenient fictions with no experimental support, created solely in order to allow the calculus based toolbox to function. Numerical methods are burdened with no such inventions (though they *may* be burdened with others, see below).

The computational approach to science is truly the most fitting one for our day and age.

In this view, the whole of science fits neatly within the pattern extraction paradigm. In this view the goal of science is to detect patterns in experimental data in order to make predictions. This is appropriate since it integrates science in a natural way into the ongoing trend known as the "information age". It places *data* at the center of the scientific endeavor (as it always has been of course), but this time in a more explicit and direct way than ever before. Moreover, it makes observation (which is just a form of interaction) the crucial event at the heart of our understanding of the universe. It leads naturally to a *relational* view of the universe. This is appropriate because the two competing scientific theories of our day, relativity and quantum theory, are incompatible in every way except one: their emphasis not on substance, but on interaction, on relationships. In the case of relativity this is evident from its very name, while in the case of quantum theory, this is a direct implication of the notoriously (if controversially) participatory role played by the *observer* in the description of any experiment. Both theories are interaction-, or process-centered theories, in contrast to the older, Newtonian and Greek versions, which were essentially substance-centered.

A computational view of science, emphasizing the ability to extract patterns from data in order to predict accurately is therefore clearly the most appropriate for the "information age" which we are now only entering.

Today it seems to us naïve that the Greeks thought their world to be made of circles and lines. Their usefulness for computation, however, made these concepts the right ones for their time. It is time to see the naïveté in our current belief that the world is made of (perfectly and ideally smooth!) solutions to differential equations. Their time has passed. Perhaps several centuries onward, the computational, relational view advocated here will also come to be seen as naïve. But for today, it is clearly the right way to move forward.

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