Elements of computational intelligence and their applications in bio(techno)logy

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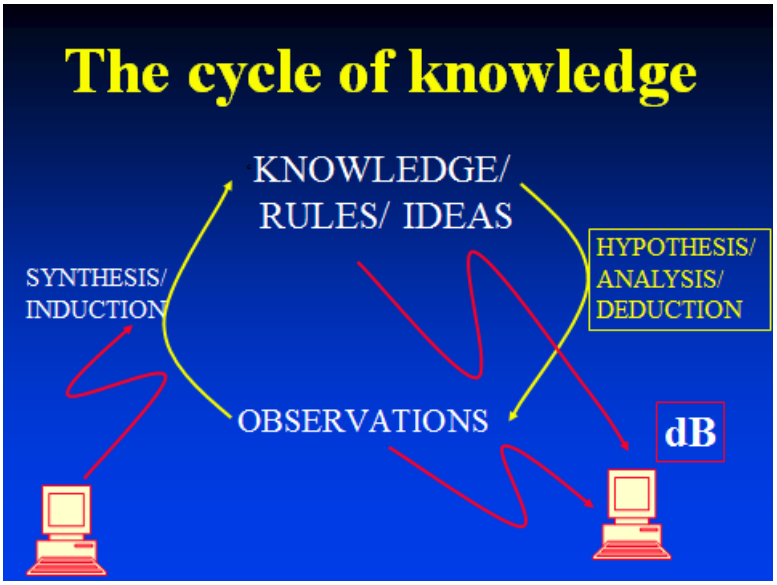
It is reasonable to recognise that most scientific problems are best considered in terms of an (iterative) search between the worlds of ideas (hypotheses, abstract thoughts) and of observations ('data') [1] (and Figure at right). We recognise that in general terms this search occurs on a rugged (but not pathological) landscape, in which 'good' solutions (in terms of either the 'best' experiment to do next, hence of improving one's understanding) are a tiny fraction of the possible ones to test [2; 3]. However, the state of the art of machine intelligence as applied to consumer goods (mostly based on 'deep' neural methods of various kinds (e.g. [4-6])) far exceeds that typically being applied to scientific problems; this provides many opportunities.



Following this, the background (and foreground) knowledge of most scientific problems can be structured as tables of examples and properties (objects and variables), and decomposed, depending on the availability of the objective function(s), into supervised (learning/optimisation [7]), unsupervised (clustering/ similarity [8]), or semi-supervised problems. Supervised methods have a trade-off between potency and intelligibility; our experience is that evolutionary computing (GA and GP) [9-11], random forests [12], and both shallow [13; 14] and deep [6; 15-17] neural systems cover the space adequately. Given the usual availability of many more 'unsupervised' (domain) examples than those with output data, we anticipate considerable growth in the use of variants of semi-supervised learning (much as has been beneficial in object recognition [18]). Feature extraction lies at the heart of computational intelligence [19]. Thus, the biggest issue for computational intelligence remains the representation of ideas and physical objects; thus the various means of representing chemical structures as 'fingerprints' can give very different results, even in simple clustering analyses (e.g. [20-23]).

We recognise that a useful trend is towards the entire ('closed loop') automation of scientific discovery [9; 24]. Synbio-based directed protein evolution [25] coupled to deep learning is a realistic short-term goal, *en route* to a more general intelligence that might help human beings to solve most biological (and other) problems much more efficiently.

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