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In Silico Drug Design

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Drug design is paramount needed and expensive: resistance to antibiotics is always a problem, cancer therapy is often not yet fully satisfactory, several disease could still benefit of therapies characterized by increased efficacy and/or decreased toxicity, not to mention rare diseases less stimulating research because of economical trade off.

Besides traditional intelligent trial and error, previous simulation in silico is more and more used. Modeling of domain interactions in molecules (Sacco, *et al.* Biotechnology Advances 2012) is growing together machine learning inference of desired properties, like hydrophily versus hydrophobic behavior.

An even more ambitious idea is to even design a full molecule atom by atom, or modify it just substituting one or a few atoms in order to hopefully improve effect. In this sense, a growing community involving scientists in both academy and pharma companies is developing for instance under CECAM, the Center for Computation of Atoms and Molecules hosted in EPFL Lausanne. Ab initio simulation of molecular properties is then computed via number crunching algorithms on supercomputers implementing the known chemical and physical knowledge.

Computational burden and propagating errors due to necessary approximations or just alternative possible configuration still make hard to obtain desired results when the number of atoms in the desired molecule increases. A hoped help is the present trial of integrating such modeling with the reminded machine learning algorithms rooted in artificial intelligence. In particular, a couple of approaches, consolidated in other disciplines, do appear keen to possible contribute also in this task.

First of all Logical Networks (Muselli and Liberati, IEEE Trans KDE 2002) enjoys with respect to traditional artificial neural networks at least 3 interesting properties:

- to prune the not salient variables
- to fast learn in polynomial time with respect to binary operations
- to express their knowledge in human ununderstandable way, being their canonical output as OR of ANDs immediately readable in the propositional form IF .. AND … OR … THEN

Moreover, when time data samples are available about the dynamic behavior, a piece-wise affine identification (Ferrari-Trecate, *et al.* Automatica 2003) is able to optimally identify the approximating hyperplanes and their commutation time, giving the best piece-wise linear approximation of the complex nonlinear behavior of the underlying process

Both approaches, proved quite successful in a variety of contexts (Paoli *et al,* Medical and Biological Engineering and Computing 2001) (LIberati, Nonlinear Analysis Hybrid Systems 2008 and 2009), (Liberati, Annals of Biomedical Engineering, 2009) are thus keen to contribute also to in silico drug design, enjoying the possibility to integrate knowledge thus inferred by experimental data with traditional deductive knowledge inherited by traditional modeling.