Complexity-Theoretic Explanations of Natural Phenomena

Some motivation for these thoughts on complexity theory in the context of nature is the observation that (natural) systems „want“ to minimize their total (free) energy. In particular, increasing the reciprocal structure of molecules will usually lead to decreasing free energy. An example of this is crystallization, which could thus be viewed as a dynamic optimization problem — minimizing energy by coming up with a good structure — with many parameters. Such a problem is made significantly more difficult with high temperatures (energy) and impurities (other molecules, like salt in water).

A perhaps more straightforward but still interesting avenue of approach is magnetism. We consider a number of particles arranged in a lattice, each with a magnetic field simplified to $\uparrow$ or $\downarrow$ (spin). Neighbouring particles interact with each other based on their spin. The properties of the material (in other words, the kind of particles we are dealing with) determine the sign and magnitude of the energy that is „produced“ by neighbours — for example ferromagnetic materials „like“ having exclusively $\uparrow$s or $\downarrow$s and this will be a configuration that minimizes energy for them.

Minimizing the energy in a system is the object of the ground state problem, where the ground state of a system is its stationary state of lowest energy. This is trivial for ferromagnetic materials which have two such states, all molecules $\uparrow$ or all molecules $\downarrow$. But as mentioned, with added factors this becomes much harder.

Formally, the ground state problem can be stated in the context of a graph with n vertices (atoms) and m edges (couplings). As established, a vertex can have two values, either $\uparrow$ or $\downarrow$. Edges are weighted by their energy,

$$C(x_i, x_j) = J_{i,j}\phi(x_i, x_j) \qquad \phi(x_i, x_j) = 1 \text{ if } x_i \text{ is equal to } x_j\text{, 0 otherwise}$$

where $J_{i,j}$ depends on the material. It would be > 0 for ferromagnetic materials, for example. The total energy of the system is the sum of the energies of all couplings, this is usually negated to fit with the model of decreasing energy.

We can formulate this problem in way that is in 3-SAT, as in

$$f(x_0, \ldots, x_{n-1}) = C_1(x_{1_1}, x_{2_1}, x_{3_1}) \wedge \cdots$$

but this isn't particularly great because we need pairings of three spin locations but we originally restricted ourself to looking at pairs only. Nevertheless, an important conclusion is that the ground state problem with couplings among 3 particles is NP-hard.

Another approach is to limit ourselves to anti-ferromagnetism. We thus consider likewise vertices to be „bad“, so our energy function is the number of vertices which are equal in spin. The goal is to minimize this. In particular, this is equivalent to finding the maximum cut of our graph of particles, that is, a partition of the vertices into sets such that the number of edges between them is as large as possible. Since Max-Cut is NP-complete, the anti-ferromagnic ground state problem on general graphs is NP-hard, but the decision version is NP-complete.