Multiobjective optimization and phase transitions

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Historically, we can fairly attribute the introduction and development of Multi-Objective Optimization (MOO) to economists and engineers. Economic setups usually imply satisfying conflicting interests and thus they pioneered the field quite naturally. Meanwhile, we owe to engineers the development of efficient algorithms to approximate the solutions to complicated MOO problems numerically. Engineering and Economy are relatively peripheral to natural sciences. A side effect of this is that MOO had little impact in areas such as ecology or molecular and systems biology. Only recently we find outstanding applications of MOO to these disciplines which put optimization and natural selection in a different, richer perspective[1,2]. Also physics did not pay much attention to MOO despite that a large literature exists linking Single Objective Optimization (SOO) algorithms–such as the Metropolis-Hastings or Genetic Algorithms–and their dynamics to statistical mechanics.

Contributions from complex systems usually dealt with MOO problems by integrating the many optimization targets into single fitness functions using arbitrary metaparameters[3,4] as in:

$$\Omega = \lambda t_1(x) + (1-\lambda) t_2(x), \tag{1}$$

with Ω the global fitness, λ a bias (the metaparameter) that assigns different and arbitrary importance to $t_1(x)$ and $t_2(x)$. These $t_1(x)$ and $t_2(x)$ are the multiple objectives that we would wish to optimize simultaneously in an ideal scenario. Of course, equation 1 generalizes to any number K of target functions $t_k(x)$. Note that the many targets for optimization can be conflicting and thus impose a trade-off upon the MOO solutions. Systems researched using this SOO methodology usually report interesting features such as phase transitions or the existence of critical regimes[3,4].

In a recent paper[5] we provide an elegant and robust theoretical framework to study systems that involve MOO and their behavior when the different objectives are integrated into SOO problems, such as in equation 1. Our theory relies on the interplay between the Pareto front (a geometric object that encompasses all MOO optimal solutions and that defines the best trade-off possible given the MOO problem) and a hyperplane defined by the global fitness function.

We find out that phase transitions are parsimoniously and precisely explained within our framework–also for thermodynamics. We propose that our theory provides a very robust generalization of the concept of phase transition to any MOO system whose targets are collapsed into SOO by some natural or artificial means. Because the results are valid for any such a system, our generalization of phase transitions does not rely on partition functions and does not require–in principle–that systems are ergodic, although the precise implications of our theory for non-ergodic systems still requires further investigation.

Altogether, the theory allows us to safely talk about phase transitions in a series of systems ranging from biology to social dynamics knowing that a rigorous definition exists. Our framework provides very robust groundings for MOO, which were missing in the literature, and furthers our understanding about solutions to MOO problems. Finally, the novelty of our theory is revealed in that state of the art contributions[1,2] lack any references to our findings.

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