16 Estimation of Calculation Time Needed

16.1 Exponentially Growing Space Size

The main aim in optimization is to find the ground state or at least a quasioptimum state of very low energy. A major aspect of reaching this aim is the question of how much time is needed to either achieve the global optimum solution (and in addition to prove that it is really globally optimal) when working with an exact algorithm, or to achieve a solution of at least a certain quality when working with a heuristic algorithm.

With NP-complete problems, one finds that the overall number of configurations in the configuration space explodes exponentially with the system size N, e. g., the number of configurations might be proportional to 2^N or to $N!$, which is roughly given by $N! \approx \exp(N \ln(N) - N)$ according to Stirling's formula. Furthermore, the number of quasioptimum solutions can be exponentially small compared with this overall number of solutions (for a heuristic proof see, e. g., [186]). Therefore, the time it takes to achieve the global optimum increases exponentially for an exact search algorithm, at least in the worst case.

16.2 Polynomial Approach

However, it has been shown already for several problems that one can reduce the calculation time needed if one does not rely on a proof for the global optimality of a solution. Then the calculation time needed is a polynomial function of the system size, with the parameters of the polynomial depending on the probability with which the optimizer wants to get a result of at least a required quality [180].

16.3 Grest Hypothesis

For simulated annealing and the great deluge algorithm there exist proofs that they converge to the ground state if some constraints are met, but only after an infinite amount of time [122]. There is also a construction of a finite nonmonotonic cooling schedule for a specific class of problems, leading to the global optimum with threshold accepting. In practice, however, one performs an optimization run and receives a solution not knowing how good or bad it is if the true optimum is unknown.

Generally, there is no analytic criterion proving that the solution found is the global optimum. However, in simulations of spin glasses, a relation was found between the calculation time used and the mean deviation of the solution to the true optimum [71]. This difference between the mean value $\langle \mathcal{H} \rangle_t$ of energies of final configurations of optimization runs taking a time of t and the energy value of the ground state $\mathcal{H}(\sigma_{\mathrm{opt}})$ depends as follows on the calculation time t:

$$\langle \mathcal{H} \rangle_t - \mathcal{H}(\sigma_{\mathrm{opt}}) \propto \frac{1}{(\ln t)^\zeta} \quad \text{with} \quad \zeta \approx 1\,. \tag{16.1}$$

This Grest hypothesis has not yet been proved generally but has also been shown to be valid for other NP-complete problems (see, e. g., [168, 100]) and can therefore be generally used as an approximation for how much the quality of the results can be increased if all of the available computation time is used and what the true ground state energy is [77].