On Combinatorial Optimization and Self-Avoiding Walks in Hyperhedra: from Minimum Vertex Cover and Maximum Clique to Protein Folding

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Abstract

Self-avoiding walks (SAWs) were first introduced by the chemist Paul Flory in order to model the real-life behavior of chain-like entities such as solvents and polymers, whose physical volume prohibits multiple occupation of the same spatial point [1]. In mathematics, a SAW lives in the n-dimensional lattice $\mathcal{Z}^n$ which consists of the points in $\mathcal{R}^n$ whose components are all integers [2].

In this paper, SAWs are a metaphor for walks across faces *of n-dimensional dice, or more formally, a* hyperhedron *family $\mathcal{H}(\Theta, b, n)$ [3]. Each of the faces is assigned a label $\{\underline{\xi}; \Theta(\underline{\xi})\}$; $\underline{\xi}$ represents a unique n-dimensional coordinate string $\underline{\xi}$, $\Theta(\underline{\xi})$ represents the value of the function Θ for $\underline{\xi}$.*

A large number of combinatorial optimization problems can be mapped onto faces of such hyperhedra; simple examples in [3] illustrate several walking strategies to search for optima in a given problem instance. Combined with experimental results in this paper, we implement an effective walking strategy to search for optima by applying a few simple rules: (0) select a random coordinate as an 'initial pivot'; (1) select the pivot coordinate for the next step by probing all of the adjacent coordinates and selecting the coordinate with the 'best value' that has not been used as a pivot in the walk before; (2) continue the walk until either the 'target value' has been found or the walk is being blocked by adjacent coordinates that are already pivots; (3) if the walk has been blocked, resume the walk from a randomly selected 'new initial pivot'; (4) if needed, manage the memory overflow with a streaming-like buffer of appropriate size.

We have prototyped a number of functions that map well-known NP-hard problems onto appropriate hyperhedra: ranging from the aperiodic low-autocorrelation binary sequences (labs) problem (also known to physicists as the one-dimensional spin system with long-range 4-spin interactions), search for optimal Golomb rulers, instances of hard problems that arise in VLSI design, genomics, and biochemistry, including protein folding. The findings that are supported by the implementation of the current prototypes include: (1) optimum solutions based on a SAW are found consistently before the SAW would be blocked by adjacent pivots, (2) the average length of a SAW that terminates at the known 'target value' is a very small fraction of the upper bound on the SAW length (effectively the length of the Hamiltonian cycle for a specific hyperhedron). In fact, an efficient implementation of a SAW-solver applied to the aperiodic low-autocorrelation binary sequences (labs) problem demonstrates not only the scalability of the approach to large problems but also results that by far exceed the performance of state-of-the-art solvers which rely on latest evolutionary strategies as well as on alternative stochastic search methods [4].

References

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