Stadler, P. F.; **Tinhofer, G.**

Equitable partitions, coherent algebras and random walks: Applications to the correlation structure of landscapes. (English) Zbl 1029.05128

Match 40, 215-261 (1999).

Summary: A landcape is a pair (G, f) of a configuration graph G and a fitness function $f : V \to \mathbb{R}$ defined on the vertex set V of G. It is a mathematical model for studying functions on a discrete set V where the neighborhood relation on the graph defines how one is able to move within this set and how one gets access to the values of f. There are many situations where such a model is of high interest, in chemistry and elsewhere. Configuration spaces in molecular biology, spin glass models in physics, QSAR models in chemistry or pharmacology are landscapes in our sense, as well as the solution spaces of combinatorial optimization problems together with a solution heuristic like simulated annealing or some version of a genetic algorithm.

MSC:

05C70 Edge subsets with special properties (factorization, matching, partitioning, covering and packing, etc.)
05C50 Graphs and linear algebra (matrices, eigenvalues, etc.)

Software:

nauty