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Open Problems

Problem 1. On the Expected Number of Local Optima (Panos M. Pardalos)

Many numerical algorithms for optimization problems are usually tested on randomly generated problems. It is often desired to know an estimate on the average number of local optima of random test problems. This statistical information gives a characterization of the difficulty of the problem when certain algorithms are used.

Consider for example the problem of minimizing a quadratic function $f(x) = x^T Q x$, where Q is a symmetric matrix and $a \leq x \leq b$. Assume that the entries of Q are generated randomly and independently from a probability distribution over the integers symmetric about zero. What is the expected number of local minima of the quadratic problem when the test data is generated using the uniform or the normal distributions? When the variables x are restricted to have 0 or 1 integer values, then this problem has been considered in [5] and [3].

Problem 2. Exact Optima for the Protein-Folding Test Function (Stephen A. Vavasis)

The real-valued function f_n is defined as follows. It is a function of $3n$ variables written as n vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbf{R}^3$. It is defined as:

$$f_n(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} r(||\mathbf{x}_i - \mathbf{x}_j||)$$

where

$$r(s) = s^{-12} - 2s^{-6}.$$

This function f_n is commonly used as a test case for programs seeking to globally minimize energy in molecular dynamics to find the configurations of a protein [1, 2, 3, 6, 7]. The $\mathbf{x}_i$ vectors represent the positions of molecules or atoms embedded in $\mathbf{R}^3$. True energy functions in molecular dynamics have many additional terms, but it is believed that f_n is a good choice for testing algorithms. The function r has a unique minimum but is not convex. The overall function is not convex and has an exponential number of local minima.

1. For $n = 1, 2, 3, 4$ the exact global minimum is easy to construct because it is possible to position up to four of the $\mathbf{x}_i$'s at the vertices of a regular tetrahedron so that each term in the definition of f_n is at its global minimum. For any values $n \geq 5$, however, the exact global minimum is unknown. It would be interesting to have tight bounds on the optimum for small values of n in order to better gauge global optimization algorithms.
2. What is the theoretical complexity of minimizing f_n?

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