CORR 2002-17

Euclidean Distance Matrices and the Molecular Conformation Problem

Abdo Y. Alfakih* & Henry Wolkowicz

Abstract In molecular theory [7] and in multi-dimensional scaling in statistics [17, 6], one is usually interested in the following problem known as the *graph realizability problem* (GRP). Given an edge-weighted undirected incomplete simple graph $G = (V, E, \omega)$ with node set $V = \{v_1, v_2, \ldots, v_n\}$, edge set $E \subset V \times V$, and weights $\omega : E \to \Re^+$, the GRP is the problem of determining whether or not G is realizable in some Euclidean space. A graph $G = (V, E, \omega)$ is said to be realizable in $\Re^r$ if there exist points $p^1, p^2, \ldots, p^n$ in $\Re^r$ such that $||p^i - p^j|| = \omega_{ij}$ for all edges $(v_i, v_j) \in E$, where $||.||$ is the Euclidean norm.

In the context of molecular conformation theory, graph G represents a molecule with V, the set of nodes of G, representing the atoms. It is possible, using nuclear magnetic resonance [24, 22], to determine some of the pair-wise distances of the atoms. If the distance between atoms i and j is known, then edge (v_i, v_j) is created in graph G with weight ω_{ij} equal to the square of this distance. naturally, the missing edges of G correspond to those unknown interatomic distances. Thus the shape of this molecule, which is important in determining its chemical and biological properties, can be found by solving the GRP. Of course in this case we want the graph to be realizable in $\Re^3$.