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Euclidean Distance Matrix Completion Problems. Preliminary report.

A Euclidean distance matrix is one in which the (i,j) entry specifies the squared distance between particle i and particle j . Given a partially-specified symmetric matrix A with zero diagonal, the Euclidean distance matrix completion problem (EDMCP) is to determine the unspecified entries to make A a Euclidean distance matrix.

We survey three different approaches to solving the EDMCP. We advocate expressing the EDMCP as a nonconvex optimization problem using the particle positions as variables and solving using a modified Newton or quasi-Newton method. To avoid local minima, we develop a randomized initialization technique that involves a nonlinear version of the classical multidimensional scaling, and a dimensionality relaxation scheme with optional weighting.

Our experiments show that the method easily solves the artificial problems introduced by Moré and Wu. It also solves the 12 much more difficult protein fragment problems introduced by Hendrickson, and the 6 larger protein problems introduced by Grooms, Lewis, and Trosset. (Received January 13, 2011)