

The Coherent Multirepresentation Problem in Protein Structure Determination

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The Coherent Multirepresentation Problem (CMP) was recently proposed as a generalization of the well-known and widely studied Distance Geometry Problem (DGP). Given a simple directed graph G , the idea is to associate various types of representations to each arc of the graph, where the source vertices are supposed to play the role of reference for the corresponding destination vertices. Each representation is in charge to transform a given set of internal variables (spherical coordinates, angles, etc) into Cartesian coordinates. In the applications, these internal variables are not precisely known but generally only an approximated value is given, and sometimes bounds on the feasible values are actually available. Since these representations are associated to arcs (and not directly to the vertices) in the CMP, multiple Cartesian coordinates can be computed for every vertex, every time the same vertex appears as a destination vertex for a given arc. Naturally, these Cartesian coordinates obtained for the same vertex may not be compatible with one another. The CMP asks therefore whether a subset of feasible values exists for the internal variables used in the various representations that is able to ensure that all the vertex Cartesian coordinates are identical (or at least close enough to each other). In this situation, we say that the multi-representation associated to the graph G is coherent. In this work, we focus our attention on CMPs arising in the context of protein structure determination, and we explore the possibility to introduce novel representations where several vertices are involved at the same time, for example for modeling the protein secondary structures.

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