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Quadratic Binary Programming Models in Computational Biology

In this presentation we formulate four problems in computational molecular biology as 0-1 quadratic programs. These problems are all NP-hard, and the current solution methods used in practice consist of heuristic or approximation algorithms tailored to each problem. Using test problems from scientific databases, we address the question, "Can a general-purpose solver obtain good answers in reasonable time?"

In addition, we use the latest heuristics as incumbent solutions to address the question, "Can a general-purpose solver confirm optimality or find an improved solution in reasonable time?" Our computational experiments compare three different reformulation methods: two forms of linearization and one form of quadratic convexification.

Based on joint work with Richard J. Forrester, Dickinson College.