Solving Complex Polynomials and Molecular Models

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Abstract:

Conformation is known to play an important role in protein function, and chemically identical molecules are able to take on multiple different conformations. I will show a common method of modeling molecular conformation. Solving for possible conformations under geometric constraints can then be converted into solving polynomial systems. While various methods for solving these polynomials have been suggested, problems with efficiency and feasibility of a complete solution still remain. A known method for solving for roots of a polynomial in one variable and ideas on generalizing this will conclude the presentation.