Algorithmic Determination of Molecule Flexibility via Resultants

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May 7, 2011

R. H. Lewis uses the Dixon Resultant to solve systems of polynomial equations that arise in chemistry [1] [4], in order to understand how molecules fold. This is a very important topic in biochemistry [8], [6], [5].

The method first computes the resultant of a system of multivariate polynomial equations. Then it analyses the resultant to produce *tables* of relations that yield flexibility. One particular system of polynomial equations that Lewis solved arose from the cyclo-hexane molecule. Initially, the second part of the analysis, Lewis's *Solve* algorithm, ran for seventy hours before producing a set of over three thousand solutions that geometrically describe the molecule when it is flexible.

In order to use this algorithm on larger molecules or geometric structures, we explored ways to improve the overall runtime of the *Solve* algorithm, as well as to analyze the solutions.

We determined that the algorithm could be improved in two ways: first, the final set of solutions (called *tables*) contained many equivalent tables. The equivalence is often masked by subtle differences in arrangement. We will be presenting the algorithm we developed which arranges each table into a canonical form in order to search through the entire set for duplicates. The tables are sets of algebraic substitutions which represent the geometric conditions under which the molecule is flexible. Once a set of substitutions has arisen to reduce the multivariate resultant, the variables in the tables can be rearranged into a "canonical form" by solving for the substitutions in terms of the "highest" variable. Secondly, we found ways to eliminate duplicates as they arise by following a simlar procedure on the fly.

References

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