Real Analysis Exchange
Summer Symposium XXXVIII, 2013, pp. ??–??

Inajara da Silva Freitas, Universidade Federal do Paraná, Brazil. email: MISSING

METHOD OF INTERSECTION OF SPHERES USED TO CALCULATION OF PROTEIN STRUCTURES

In this work, based on a paper by Dong, Qunfeng and Wu, Zhijun, which appeared in J. Global Optim. in 2002, we discuss the problem of determining the structure of a protein when a set of distances between the atoms are known. This problem is also known as molecular geometrical problem away, we will assume that all distances between the atoms are known, which will be addressed two different views. First, we formulate the problem so that it can be solved linearly, using basic techniques of linear algebra. Then we'll talk about the quadratic method in which the problem is formulated using the calculation of the intersection points between spheres. To find the points intersection between spheres in $\mathbb{R}^n$, we will suppose to have a set of n nonlinear equations, where we want to find it's solution by solving a system of quadratic equations. The methods were implemented and tested in MATLAB and then compared using the Root-Mean-Square-Deviation (RMSD), which measures the accumulated error in calculating these structures.

Mathematical Reviews subject classification: Primary: ; Secondary:
Key words: ,