The use of Interior Point Methods for solving the Phase Problem in Crystallogrphy

Leticia Velazquez

Rice University

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Interior Point Methods are a potentially efficient way of solving the Phase Problem that will allow the determination of the molecular structure of Proteins. In a X-ray diffraction experiment intensities I_{hkl} are measured whereas $F_{hkl} = 3D|F_{hkl}|exp(i\Phi_{hkl})$ (scattering function) are necessary to image the electron density function. The density function is actually the one that defines the three dimensional positions of the distribution of the scattering atoms that form the protein.

Now $|F_{hkl}|$ can be calculated straightforward form I_{hkl} but the relative phases Φ_{hkl} are lost in the experiment and cause the so called phase problem. In 1985, Karle and Hauptman redefined the techniques known as Direct Methods which is able to determine the molecular structure for small molecules. But unfortunately, this technique is not useful to solve the phase problem for crystal proteins which consists of more than 1000 atoms.

Our goal will be to try to solve the problem using optimization techniques, essentially using Interior Point Methods. My role will be to posed the problem as a constrained minimizatin problem, find a global solution (if it exists), and write an algorithm that will not stagnate.

Mentors: Amr Elbakry, George Phillips, Richard Tapia.

Address: Rice University, Department of Computational and Applied Mathematics-MS134, 6100 Main Street, Houston, Texas 77005-18 92.