

FREIE UNIVERSITÄT BERLIN Fachbereich Mathematik und Informatik

Promotionsbüro, Arnimallee 14, 14195 Berlin

DISPUTATION

Montag, 15. Dezember 2014, 16.00 Uhr

Ort: Raum 049, Takustr 9, 14195 Berlin

Disputation über die Doktorarbeit von

Herrn Sandro Claudio Andreotti

Thema der Dissertation:

**Linear Programming and Integer Linear Programming
in Bioinformatics**

Thema der Disputation:

**Integer programming methods
for finding the maximum contact map overlap**

Die Arbeit wurde unter der Betreuung von **Prof. Dr. K. Reinert** durchgeführt.

Abstract: One fundamental problem in structural genomics is the comparison of protein structures. A measure to quantify the similarity between three-dimensional protein structures is the maximum contact map overlap.

For a given protein, the contact map is defined as the set of all pairs of amino acid residues whose Euclidean distance in the three-dimensional fold is below a certain threshold. Given two proteins and their respective contact maps, a contact overlap is defined by a matching of a pair residues forming a contact in the first protein to a pair of residues in the second protein also forming a contact.

The maximum contact map overlap problem then asks for a matching of residues of one protein to residues from a second protein with a maximum number of contact overlaps. As the problem of computing a maximal contact map overlap of two proteins is NP-hard, integer linear programming methods have been applied to solve the problem.

In this talk, we will discuss different integer linear programming approaches based on branch and cut and Lagrangian relaxation that also influenced the development of algorithms for related problems like structural RNA-alignment.

Die Disputation besteht aus dem o. g. Vortrag, danach der Vorstellung der Dissertation einschließlich jeweils anschließenden Aussprachen.

Interessierte werden hiermit herzlich eingeladen

Der Vorsitzende der Promotionskommission
Prof. Dr. K. Reinert