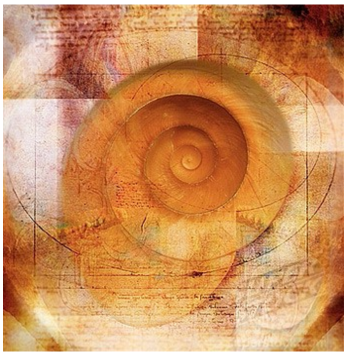
FACULTAD DE CIENCIAS EXACTAS Y NATURALES



Discusiones Informales entre Biólogos y Matemáticos

Morten Nielsen

Introduction to Blosum matrices and MHC peptide binding predictions

In my talk, I will give an introduction to two central topics of bioinformatics prediction method development. First, I will introduce the Blosum matrices, and next describe some of the critical pitfalls of developing and estimating the performance accuracy of bioinformatics prediction methods.

Blosum matrices form an integrated part of most bioinformatics applications including sequence alignment, homology modeling, local structure prediction and receptor-ligands binding prediction. Here, I will describe, using a simple toy-model system, how these matrices are derived, and illustrate how they can be applied to infer biological information in sequence data. At the heart of bioinformatics lies the development of methods for prediction of the behavior of biological systems. One such example is the prediction of peptide binding to the MHC molecule. I will give an overview of some of the methods we have developed in our research to characterize this binding event, and illustrate how serious caution must be taken in general when developing predictions methods and in particular when assessing their predictive performance due to potential redundancy in the data use to train and evaluating the methods. I will demonstrate how one can significantly overestimate performance by not dealing with this issue in a proper manner, and describe how, according to me, proper method development and evaluation should be performed. Finally, I will relate these observations to the work on MHC peptide binding described by Quan-Wu Xiao.

Ignacio Sanchez

Could you be more specific, please?

Most cell functions depend on the establishment of a certain set of protein-protein interactions among the mony possible sets. We are tackling this specificity problem with the help of information theory.

Martes 27 de Marzo de 2012 - 14:30 hs

Aula 2 - Pabellón I

Más información: http://cms.dm.uba.ar/actividades/biomat

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