Faculty of Computer Science 2006-2007 Seminar Series

Stable and unstable foldings of proteins in the H-P model

By

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The "H-P" model of protein folding considers only two classes of monomers (amino acids), namely hydrophobic (H) or hydrophilic (P). In this model hydrophobic monomers tend to cluster together to avoid water, but hydrophilic monomers are considered neutral. A folding in the H-P model consists of a self-avoiding embedding of the chain of monomers in a lattice. The "goodness" of an embedding is measured by how many pairs of H monomers are adjacent (i.e. at unit distance) in the lattice.

Despite the obvious shortcomings of this model in terms of realism, it has several attractive features. Its simple nature means that we have some chance of developing a theory predicting the folding of certain proteins (in the H-P model), rather than just waiting for the outcome of a simulation. Furthermore, it has the potential to provide insight into e.g. symmetry of optimal foldings.

In this talk I will discuss work studying how well the H-P model captures the phenomenon of stability in protein folding, i.e. the fact that proteins almost always fold to a unique configuration. An optimal (or "minimum energy") embedding is one that maximizes the number of bonds.

The talk will be mostly expository, starting with a discussion of the strengths and weaknesses of the model, followed by a menagerie of (infinite families of) examples demonstrating stability in a globular (i.e. like real proteins) or non-globular form. We will also have a look at some examples that are extremely unstable, even though they contain a linear fraction of H nodes.

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STUDENTS ARE ENCOURAGED TO ATTEND

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