APPLICATIONS OF RANDOM WALKS: FROM NETWORK EXPLORATION TO CELLULOSE HYDROLYSIS

Abstract

by

Andrea Asztalos

In the first part of the thesis we investigate network exploration by random walks defined via stationary and adaptive transition probabilities on large, but finite graphs. An exact formula for the number of visited nodes and edges as function of time is presented, that is valid for arbitrary graphs and arbitrary walks defined by stationary transition probabilities (STP). We show that for STP walks site and edge exploration obey the same scaling $\sim n^{\nu}$ as function of time n, and therefore edge exploration on graphs with many loops is always lagging compared to site exploration. We then introduce the Edge Explorer Model, presenting a novel class of adaptive walks, that performs faithful network discovery even on dense networks.

In the second part of the thesis we present a random walk-based computational model of enzymatic degradation of cellulose. The coarse-grained dynamical model accounts for the mobility and action of a single enzyme as well as for the synergy of multiple enzymes on a homogeneous cellulose surface. The quantitative description of cellulose degradation is calculated on a spatial model by including free and bound states of all enzymes with explicit reactive surface terms (e.g., hydrogen bond reformation) and corresponding

reaction rates. The dynamical evolution of the system is based on physical interactions between enzymes and cellulose. We show how the model provides insight into enzyme loading and coverage for the degradation process.