

Die Fakultät für Informatik an der Universität Wien lädt Sie herzlich ein zum

## CS-Colloquium

# Scalable Algorithms for Machine Learning with Graphs

mit Dr. Nils Kriege (TU Dortmund)

**Wann?** 13. März, 11:00  
**Wo?** Seminarraum 6 (SR6), Fakultät für Informatik  
Währinger Straße 29  
1090 Wien

### Abstract

Graphs are ubiquitous in many domains such as computer vision, social network analysis, cheminformatics and bioinformatics, where they are used to represent structured data. In order to learn from the ever-growing amount of data in these areas, new scalable techniques are required.

I give an overview of my work on efficient machine learning and data mining methods for graphs, which can be divided into two areas:

(i) Graph kernels are specific similarity measures for graphs, which enable the application of established machine learning approaches such as support vector machines to graphs. I introduce efficient methods for graphs with continuous attributes. Hashing techniques are used to construct feature vectors such that their dot product equals or approximates known graph kernels. I present a class of kernels based on optimal assignments between substructures. For particular similarity measures between substructures that can be expressed by a hierarchy, the assignment problem is solved exactly in linear time and valid kernels are derived.

(ii) The maximum common subgraph problem asks for a largest substructure that is contained in two given graphs. The problem is of major importance, e.g., in cheminformatics, but NP-hard in general. I present polynomial-time algorithms for trees and tree-like graphs, as well as molecular graphs. These enable the similarity analysis of large data sets with millions of molecules in practice.

Finally, an overview of practical applications of the presented methods and interdisciplinary work is given.