Selected Topics on Combinatorial Optimization

Professor Dr. Petra Mutzel

Lehrstuhl für Algorithm Engineering

Fakultät für Informatik

TU Dortmund

PART 1: Introduction, Motivation, Basics

Vienna Graduate School on Computational Optimization

November 5, 2018

Modern Topics in Combinatorial Optimization on Graphs and Networks (My Personal View)

- Big Data
- Data Mining, Graph Mining
- Data Science
- Machine Learning, Deep Learning
- Computational Analytics
- Algorithms

Modern Topics in Combinatorial Optimization on Graphs and Networks (My Personal View)

- Big Data: Data streaming algorithms, parallel/distributed algorithms, external memory algorithms and data structures, approximation, fixed-parameter algorithms, randomization
- Graph mining: Graph similarity
- Data science: Algorithm engineering, uncertainty, dynamic networks
- Machine learning, deep learning: analyzing methods
- Computational analytics: ILP-models
- Algorithms

Plan (possible topics) for this Lecture Series

- Data streaming algorithms, e.g., for the matching problem in graphs
- Temporal graphs, e.g., for quickest path problems or multicriteria path problems
- Dynamic graph algorithms, e.g., shortest path problems
- Weisfeiler-Lehman algorithms for graph classification
- Graph similarity: maximum common subgraphs
- Parallel/distributed graph algorithms
- Graph clustering (clustering of a set of graphs and clustering of vertices of a graph)
- Graph and network visualization
- Crossing minimization in graphs
- Fixed-parameter algorithms, e.g., for max-cut on 1-planar graphs
- External memory algorithms and data structures
- Anything else you are interested in: max-cut problem for quantum computing, ILP-models for graph coloring, network design problems

Outline

Personal Introduction

- Study at Univ. Augsburg (WiMa/Math), 1983–1990
- Researcher at Rice University, Houston (TX), 1990
- Researcher at FU Berlin, 1990/91
- Researcher an Univ. Köln, 1991–1994
- Ph.D. at Univ. Köln (Informatik), 1994
- PostDoc at Max-Planck-Institut für Informatik, Saarbrücken, 1994–1999
- Habilitation at Max-Planck-Institut für Informatik, Saarbrücken, 1999
- Deputy Professorship (C3) at Univ. Heidelberg, 1999
- Chair for Algorithmen und Datenstrukturen, TU Wien, 1999–2004
- Chair for Algorithm Engineering, LS11, TU Dortmund, since 2004

Research Interests

Algorithm Engineering: Design, theoretical analysis, implementation and experimental evaluation of algorithms and data structures

Graph algorithms and combinatorial optimization

Current research projects, e.g.

- network design and -optimization, e.g., Steiner tree problems, matching problems, shortest paths, multicriteria optimization
- Cheminformatics: graph similarity, graph analysis, graph clustering, visualization
- graph mining, machine learning, geometric deep learning
- graph drawing, crossing minimization
- adiabatic quantum computing: max-cut Problem

Application-oriented

Organizational Questions and Answers

Dates	exact times/breaks to be announced
Monday	05.11. at 10:00 – 12:00
Tuesday	06.11. at 11:30 – 13:00
Wednesday	07.11. at 10:00 – 12:00
Thursday	08.11. at 10:00 – 12:00
Friday	09.11. at 10:00 – 12:00
Monday	12.11. at 10:00 – 12:00
Tuesday	13.11. at 11:30 – 13:00
Wednesday	14.11. at 10:00 – 12:00
Thursday	15.11. at 10:00 – 12:00
Friday	16.11. at 10:00 – 12:00

Prerequisites for Participants

Familiarity with graphs and algorithms would be helpful, e.g.,

- course on basic algorithms and their analysis (e.g., sorting algorithms, O-notation)
- data structures for graphs (static, dynamic)
- graph traversals (BFS, DFS)
- shortest paths
- bipartite matching in graphs

Organizational Questions and Answers

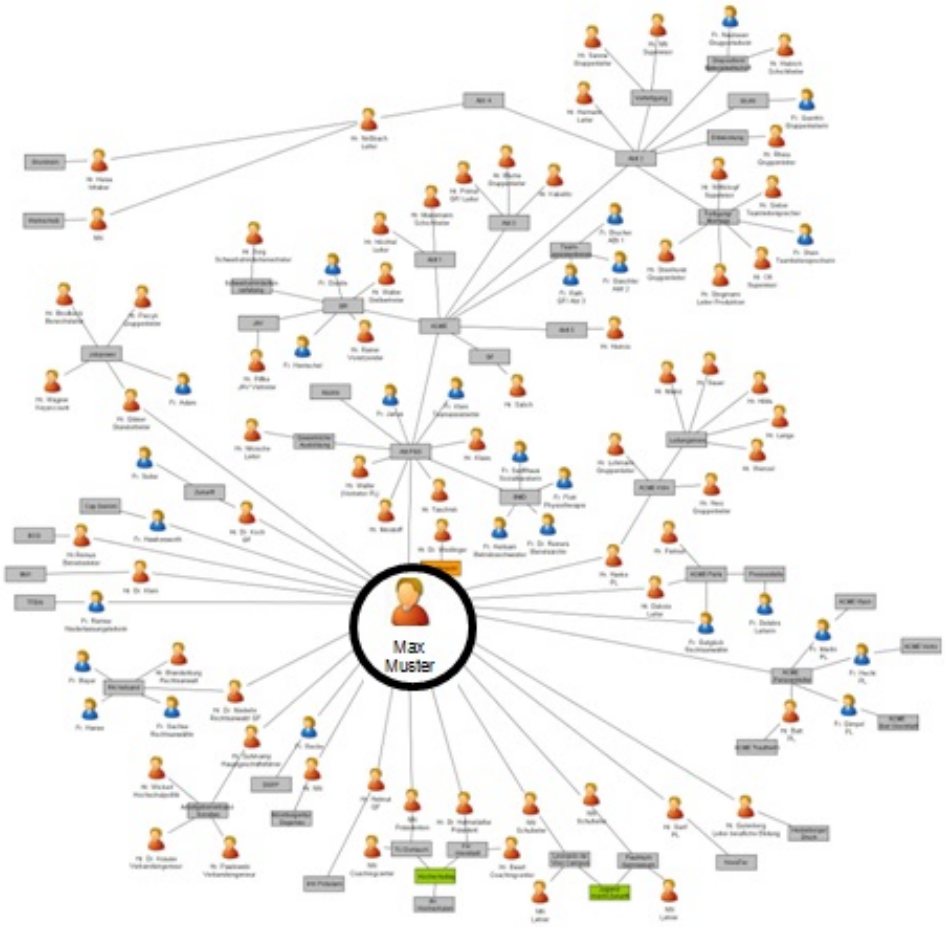
Examinations: to be announced, could be, e.g.,

- a small programming project
- exercises
- quizz

Literature:

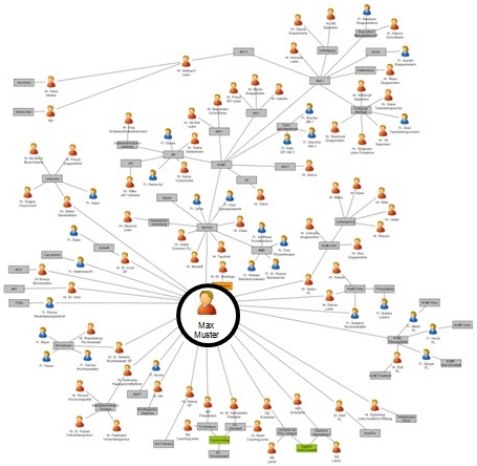
- will be provided in the slides for each topic

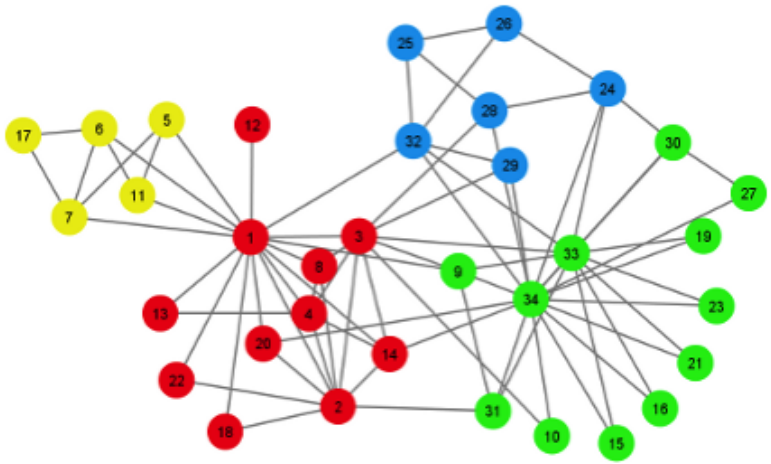
Motivation: Social Network Analysis



Social network with actors (nodes) and relations (edges of the graph)
[Image: `http://wiki.cogneon.de`]

Motivation: Social Network Analysis



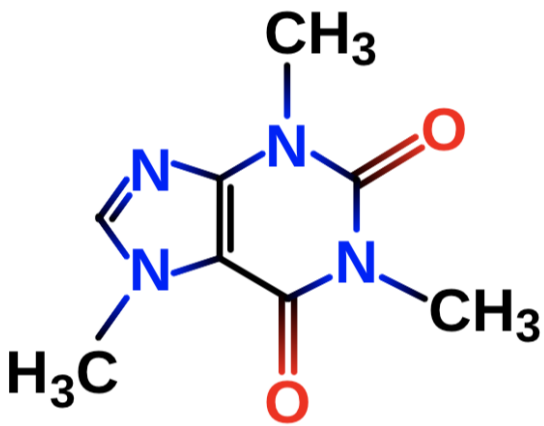


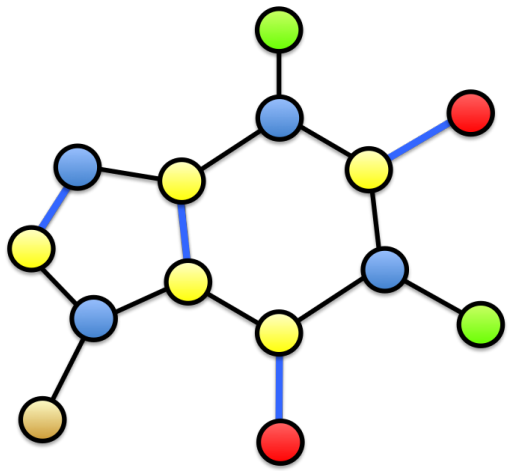
- Which actors are the central/important/most active/most prominent ones? Closeness centrality, betweenness centrality ← Shortest paths
- Which actors can influence/control the network? Matching in graphs
- Which groups exist in the social network (community detection)? Clustering of a graph
- Which networks are similar? Clustering of sets of graphs
- Prediction of dynamics in networks Dynamic/temporal graph classification

[Images: `http://wiki.cogneon.de` und `https://markhneedham.com`]

Motivation: Rational Drug Design

- Which molecules are active against disease X?
- Which molecules have a similar function/effect? (Reduction of side effects)
- Which molecules may have an increased effectiveness?
- High-throughput screening for promising candidates





- Molecules can be modelled as graphs with attributes
- Direct relationship between structure and effects

$\rightarrow$ Graph similarity

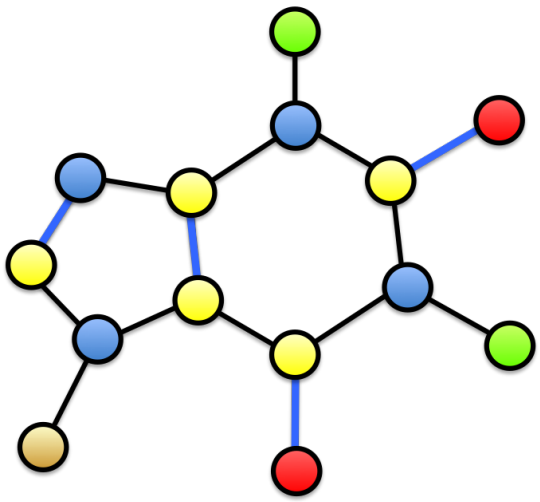
Basics: Graphs

Definition (Graph)

A graph $G = (V_G, E_G) = (V, E)$ consists of a finite set of vertices (also called nodes) V and a multiset of edges E corresponding to pairs of nodes. The vertices and edges may have attributes or labels.

Definition (Directed Graph)

If the vertex pairs are ordered, we call it directed graph. Then we also call the directed relations arcs.



Basics: Graphs

Definition (Graph)

A graph $G = (V_G, E_G) = (V, E)$ consists of a finite set of vertices (also called nodes) V and a multiset of edges E corresponding to pairs of nodes. The vertices and edges may have attributes or labels.

Definition (Simple Graph)

An edge of the form (v, v) is called self-loop. If there exist at least two edges (u, v) with the same end vertices $u, v \in E$ in a graph $G = (V, E)$, then G contains multi-edges. A graph wihtout multi-edges and without self-loops is called a simple graph.

Definition (Degree of a vertex)

The degree $d(v)$ of a vertex $v \in V$ is the number of incident edges to v. Self-loops $(v, v)$are counted twice.

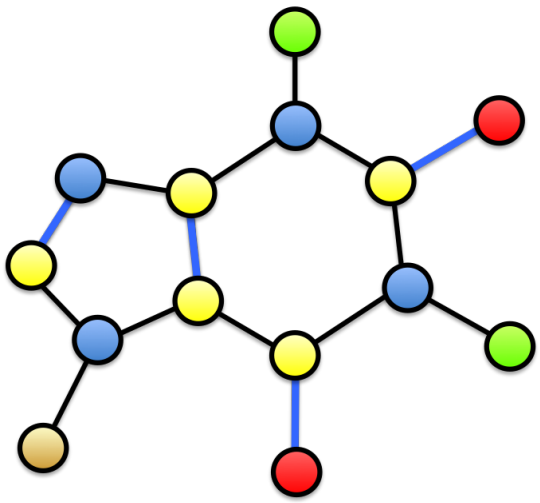
Basics: Graphs

Definition (Graph)

A graph $G = (V_G, E_G) = (V, E)$ consists of a finite set of vertices (also called nodes) V and a multiset of edges E corresponding to pairs of nodes. The vertices and edges may have attributes or labels.

Definition (Induced Subgraph)

Let $R \subseteq V$ be a subset of vertices of $G = (V, E)$. The induced subgraph $G[R]$ consists of R and all edges from E having both end vertices in R.

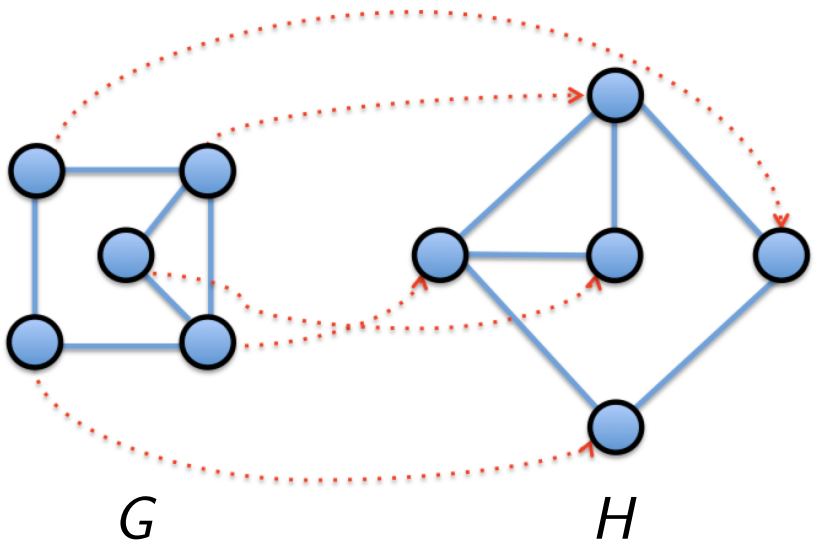


Basics: Graph Similarity

Definition (Graph Isomorphism)

Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be simple graphs. A bijective mapping $\pi : V_G \to V_H$ is called graph isomorphism if the following holds:

$$\forall\, v, w \in V_G : (v, w) \in E_G \iff (\pi(v), \pi(w)) \in E_H$$

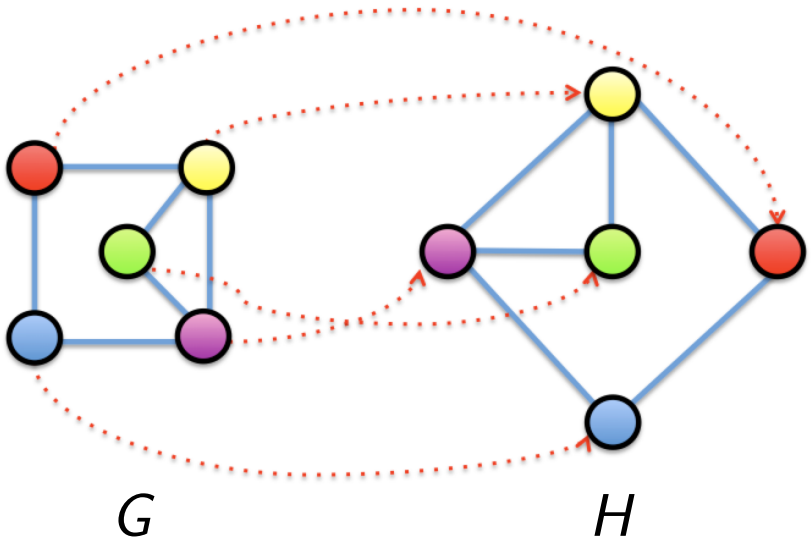


Basics: Graph Similarity

Definition (Graph Isomorphism)

Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be simple graphs. A bijective mapping $\pi : V_G \to V_H$ is called graph isomorphism if the following holds:

$$\forall\, v, w \in V_G : (v, w) \in E_G \iff (\pi(v), \pi(w)) \in E_H$$



Two graphs are called isomorph ($G_1 \simeq G_2$), if a graph isomorphism exists.

Graph Isomorphism Problem

Definition (Graph Isomorphism Problem)

Given: simple graphs G and H
Find: Is G isomorph to H, i.e., $G \simeq H$?

Remarks:

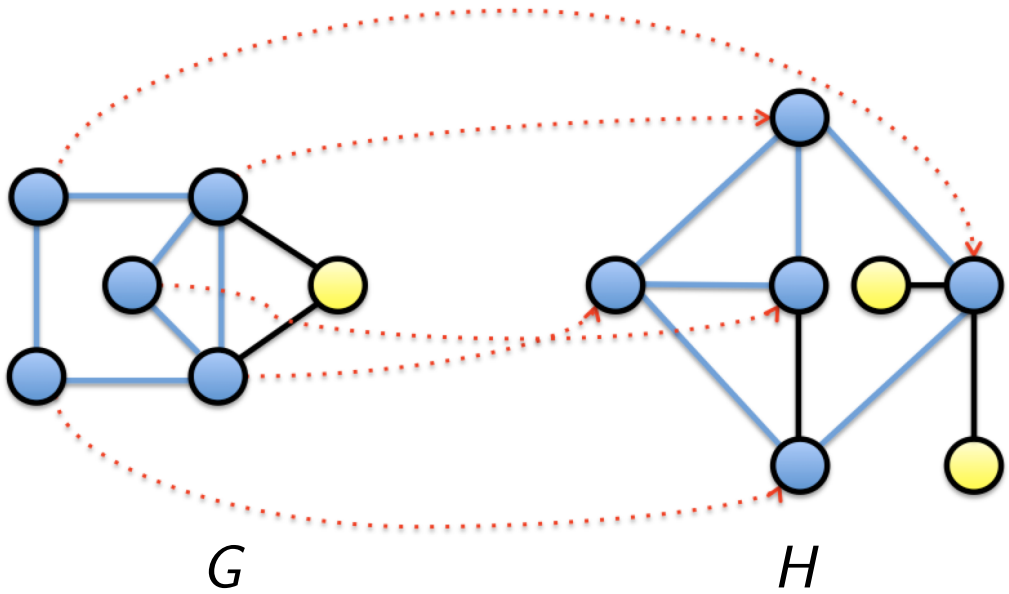
- Complexity: OPEN
- Quasipolynomial algorithm: $n^{(\log n)^{O(1)}}$ [Babai 2015/17]
- Practice: mostly solvable very fast

$\rightarrow$ Weisfeiler-Lehman vertex classification algorithm

Maximum Common Subgraph Problem

Definition (MCS)

Given: $G = (V_G, E_G)$ und $H = (V_H, E_H)$
Find: Largest vertex sets $R \subseteq V_G$ and $S \subseteq V_H$, such that the induced subgraphs $G[R]$ and $H[S]$ are isomorph to each other.



Complexity: Decision problem is NP-complete

Techniques for Big Data

- Utilization of the structure of the input instances
- Analysis of the given problem from practice
- Problem decomposition
- Approximation
- Randomization
- Parallelisation
- Fixed-Parameter Algorithms
- ILP-Modelling

Kriege, Kurpicz, Mutzel 2018, Gutwenger, Mutzel 2000, Kriege, Mutzel 2014