Lecture 1: ILP Formulations for the Graph Coloring Problem

Part 1.1: Introduction of Lecturer

Professor Dr. Petra Mutzel

Computational Analytics

Computer Science

University of Bonn

Hausdorff School: Computational Combinatorial Optimization, September 12-16, 2022

Overview

- CV and Research
- Current Projects

Brief CV: Petra Mutzel

- Study at Univ. Augsburg (WiMa/Math), 1983–1990
- Researcher at FU Berlin, 1990/91
- Researcher an Univ. Köln, 1991–1994
- Ph.D. at Univ. Köln (Informatik), 1994

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- Chair for Computational Analytics (Abt. I), Univ. Bonn, since 2019

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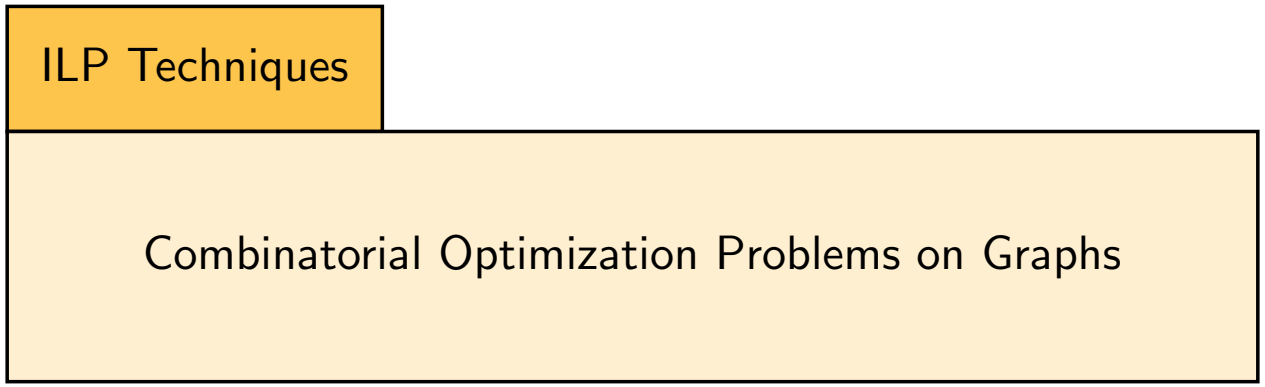
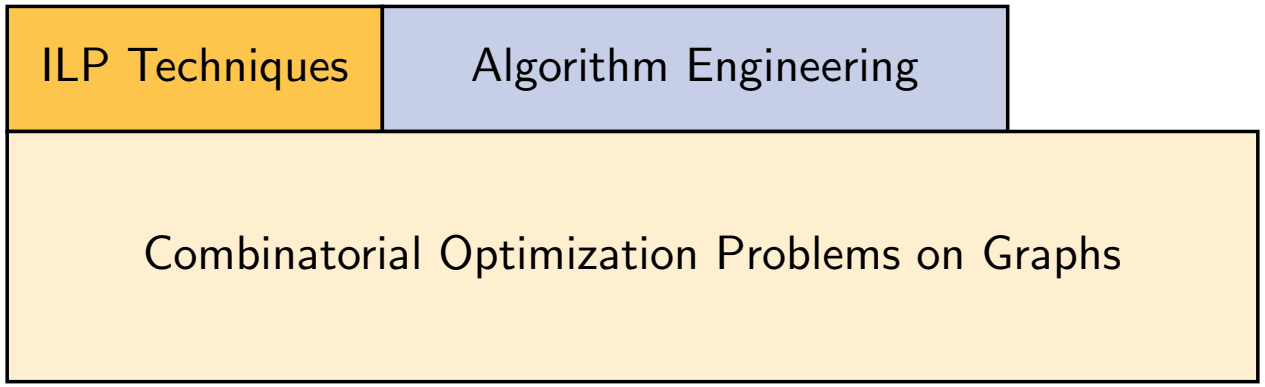
Computational Analytics

Combinatorial Optimization Problems on Graphs

Computational Analytics



Computational Analytics



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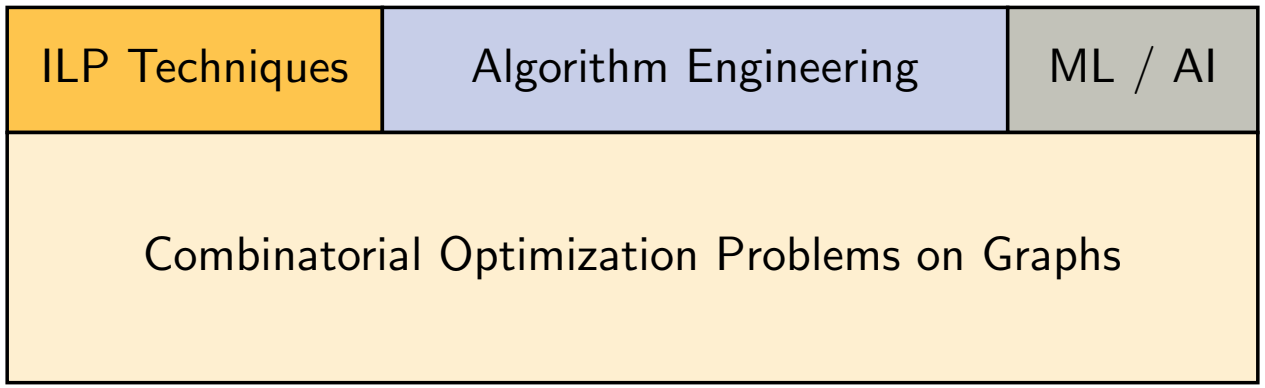
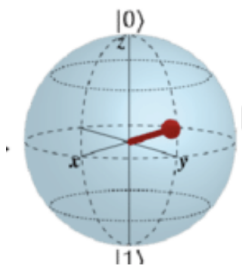
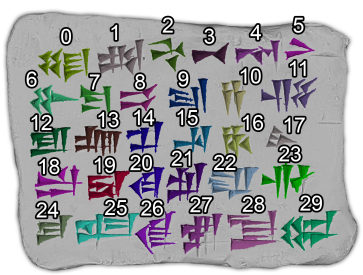


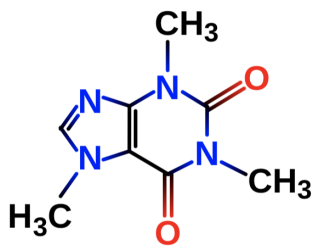
Computational Analytics

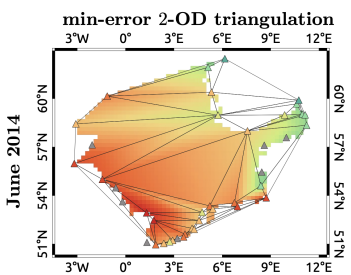
ILP Techniques	Algorithm Engineering	ML / AI
Combinatorial Optimization Problems on Graphs		

Application oriented, e.g.,
Physics, Archeology, Chemistry, Bioinformatics, Geodesy









Computational Analytics: Development of data analysis methods based on Algorithm Engineering, ILP, and ML/AI for graph structured data

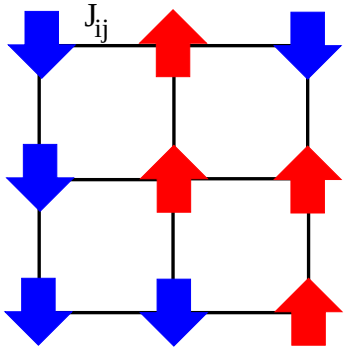
Overview

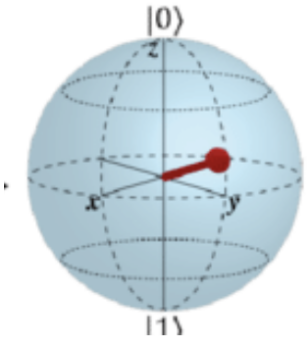
- CV and Research
- Current Projects

Maximum Cut Problems

jointly with Jünger, Reinelt, Rinaldi (since 1990) and Charfreitag, Jünger, Mallach (since 2021)

- Ising spin glass instances in statistical Physics
- Adiabatic Quantum Computing (ILP vs. D-Wave)
- McSparse Webserver for solving Maximum Cut and Quadratic Unconstrained Binary Optimization Problems (`mcsparse.uni-bonn.de`)





→ Integer Linear Programming, Algorithm Engineering

Algorithmic Toolbox

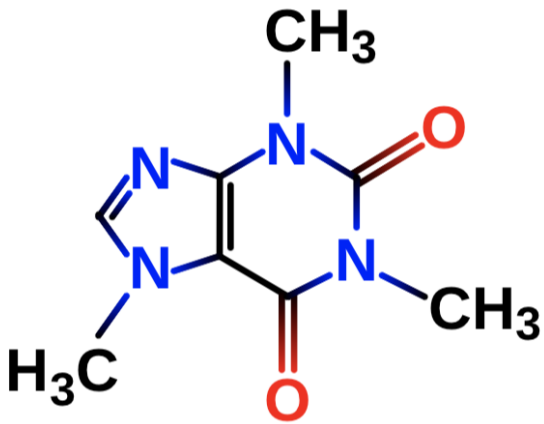
Algorithmic Toolbox for Complex Problems

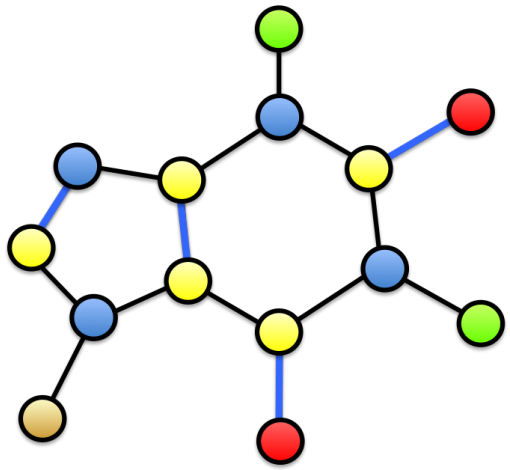
- Analysis of the given practical problem / maybe tweaking it
- Exploitation of the structure of the input instances
- Decomposition
- Approximation
- Randomisation
- Fixed-Parameter Algorithms
- Integer Linear Programming
- Adjust the algorithm to the hardware
- Parallelisation

in red: used for at least one of our max cut codes

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



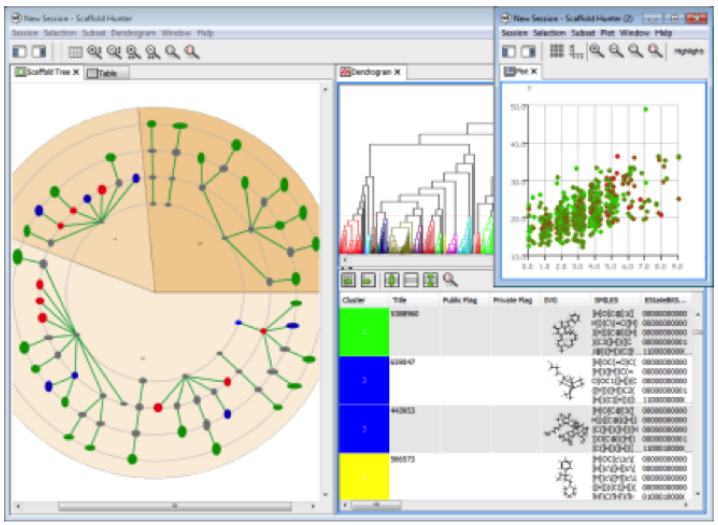


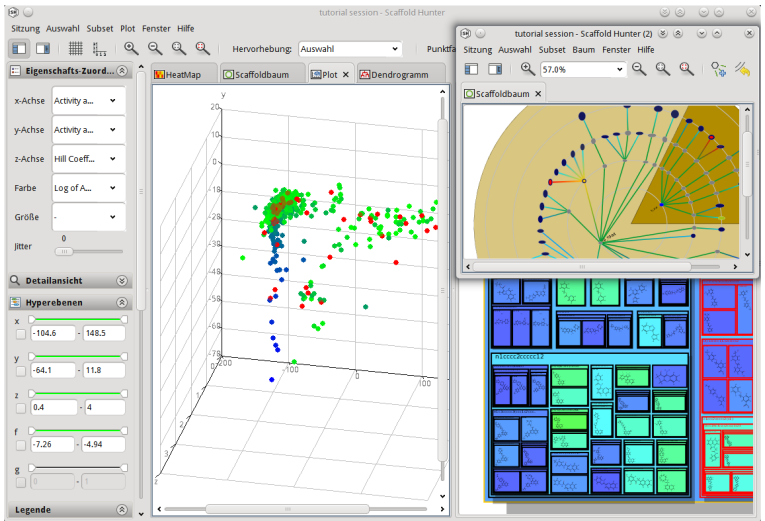
- Molecules can be modelled as graphs with attributes
- Direct relationship between structure and effects

$\rightarrow$ Graph similarity, graph algorithms, ML

Rational Drug Design: GraBaDrug

Project within DFG SPP Algorithms for Big Data





- explorative analysis of molecule data bases ← Scaffold Hunter
- search for similar molecule structures ← graph similarity, clustering
- creation of virtual molecule data bases for drug design
  ← CHIPMUNK: 95 mio. molecules with $\leq$ 700 atoms, 90 attributes

Wetzel, Klein, Renner, Rauh, Oprea, Mutzel, Waldmann: Nature Chem. Biol. 2009, Humbeck, Weigang, Schäfer, Mutzel, Koch: ChemMedChem 2018 + Cover Feature, ...

Algorithmic Toolbox

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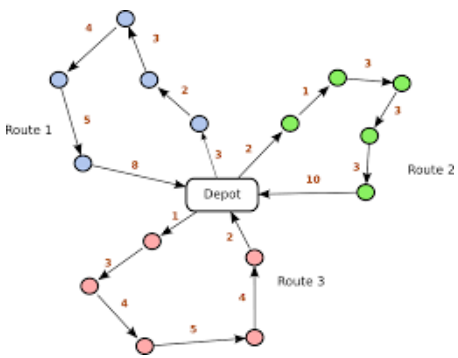
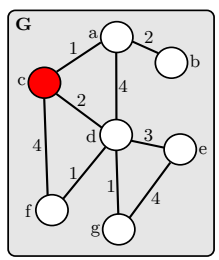
in red: used for our drug design project

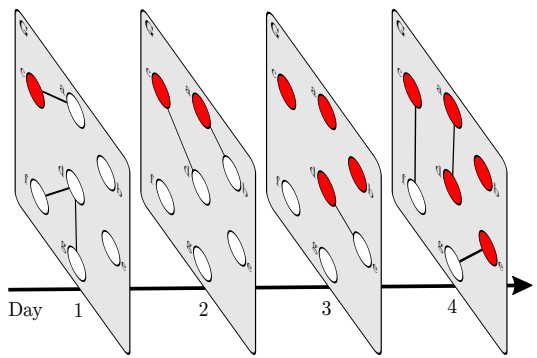
Routing and Path Problems

BMBF project LEOPLAN jointly with Schürmann, Stiller, Kirches, and companies BASF, Logiball GmbH, 4Flow GmbH (since 2020) and temporal graphs with Lutz Oettershagen (since 2020)

- ILP models for vehicle routing problems with heterogeneous time windows
- hybrid methods combining machine learning and ILP solution methods
- shortest path problems with constraints and/or multi-objectives
- efficient algorithms for centrality measures for temporal graphs

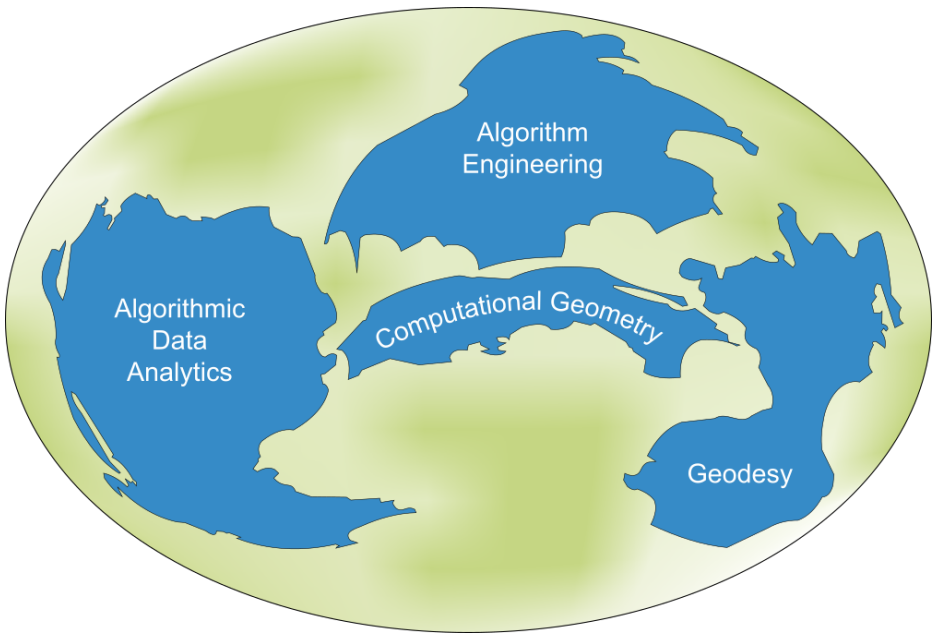






→ Integer Linear Programming, ML, Algorithm Engineering

Algorithmic Data Analytics for Geodesy (new DFG project)

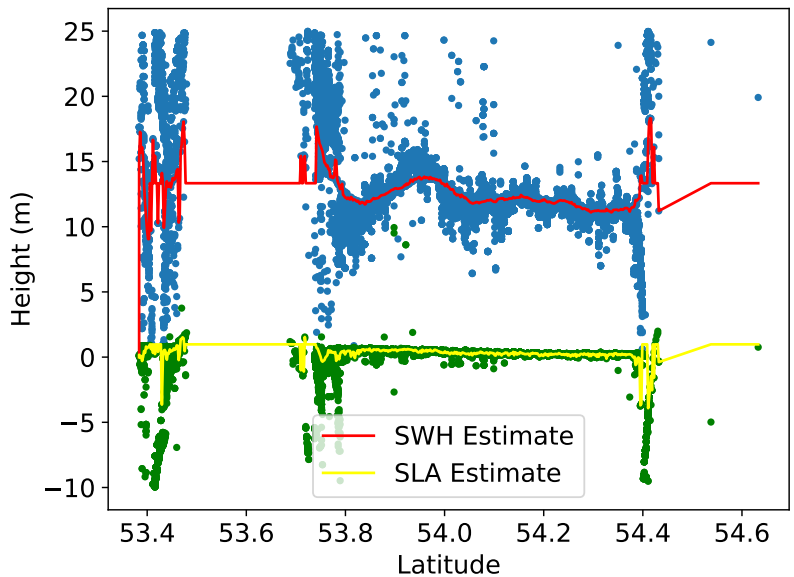


Ongoing work

jointly with Anne Driemel, Jan-Henrik Haunert, Christian Sohler, Jürgen Kusche, Heiko Röglin, Melanie Schmidt

Motivation: Geodesy

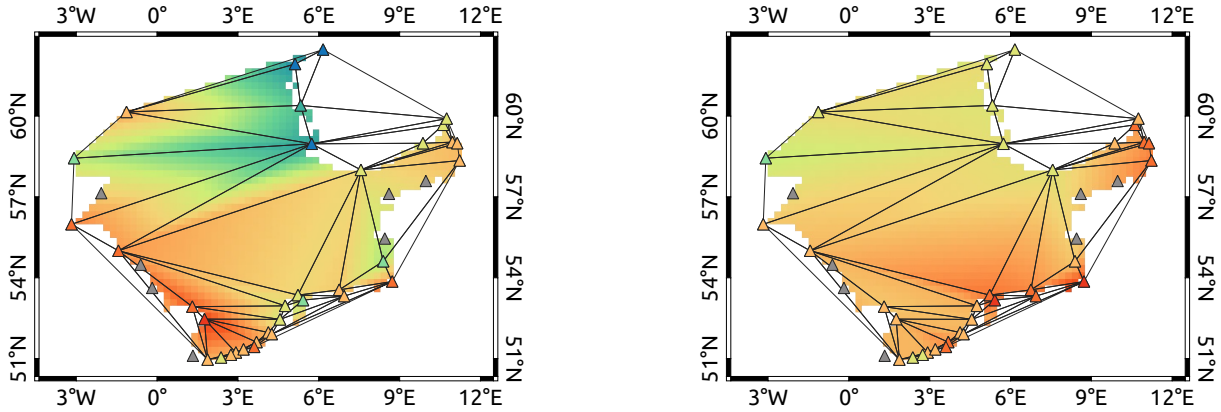
Observing coastal sea-level change from satellite altimetry



→ bicriteria shortest path

Joint work with Jürgen Kusche (Univ. Bonn)

Triangulations for Sea Surface Reconstruction



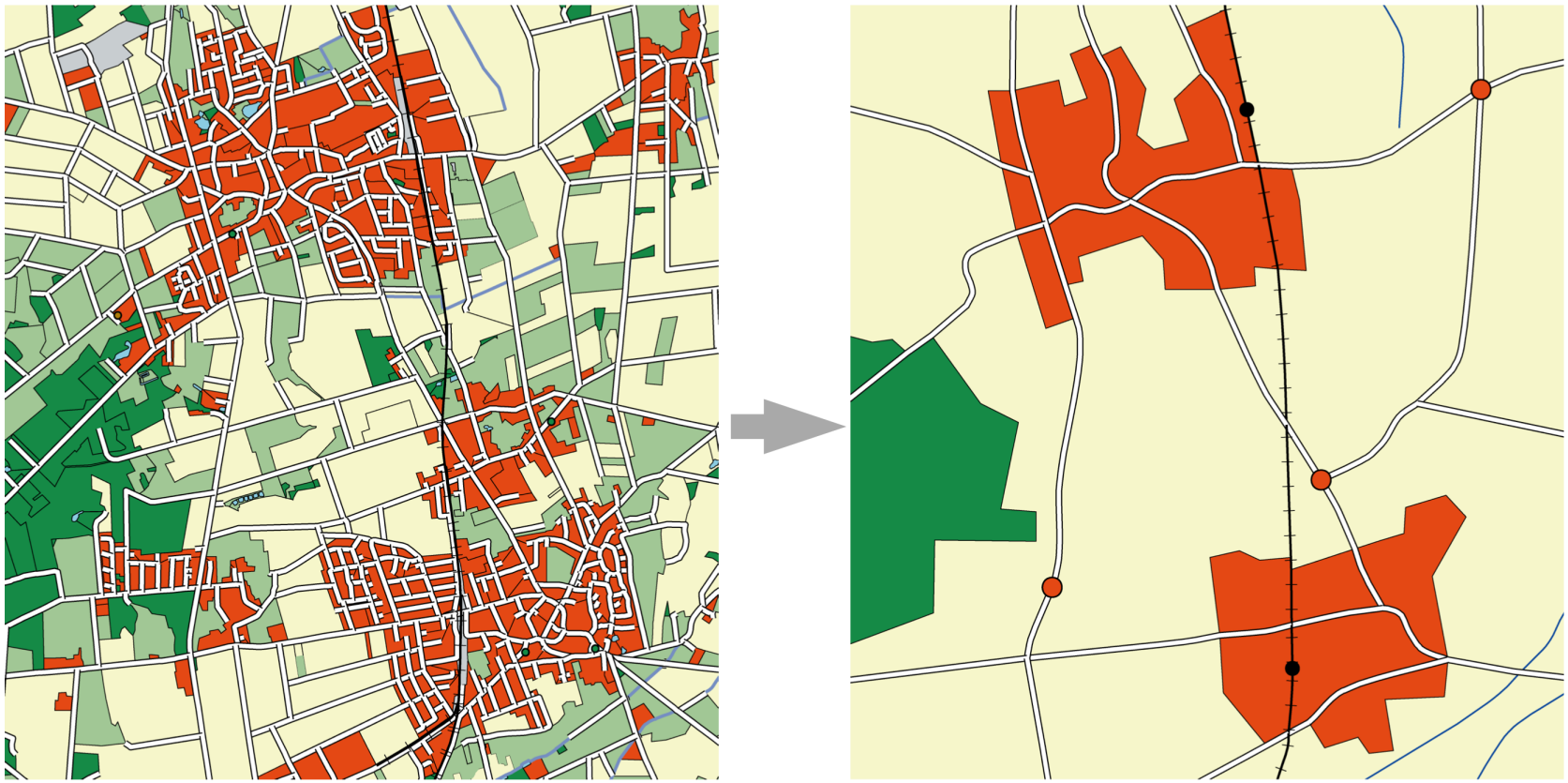
Error for reconstruction of June 2010 and May 2015
from triangulation June 2015 for North Sea Data Set

Idea of approach

- compute a min-error triangulation of the tide gauge stations to approximate the altimetry data
- use that triangulation to interpolate between tide gauge stations at epochs where no altimetry data is available

Nitzke, Niedermann, Fenoglio-Marc, Kursche, Haunert 2021; Arutyunova, Driemel, Haunert, Haverkort, Kusche, Langetepe, Mayer, Mutzel, Röglin 2022

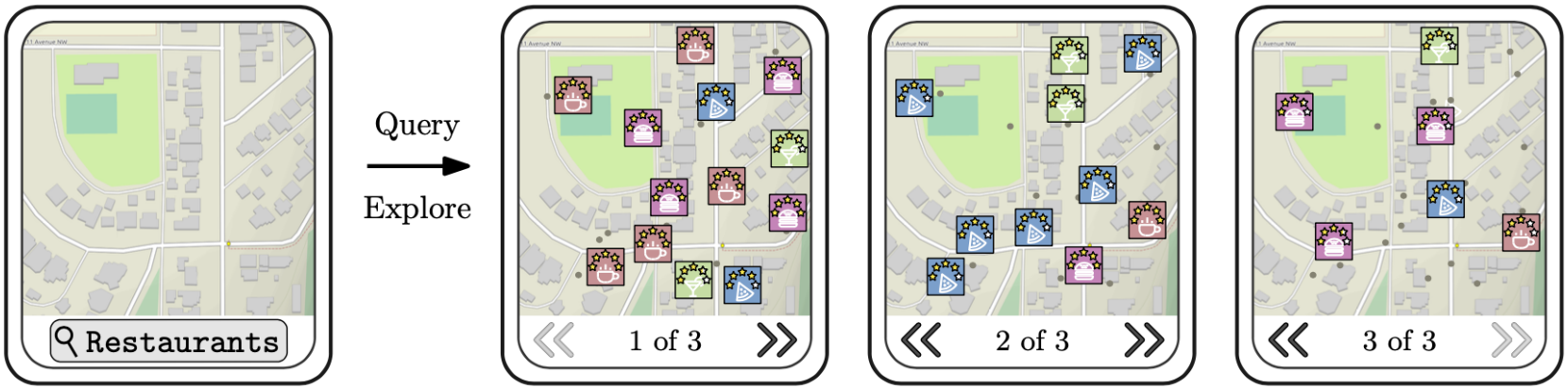
Map Generalization in Cartography



Graph problems, e.g., shortest path, bicriteria optimization, minimum cut

Source: Jan-Henrik Haunert (Univ. Bonn)

Map Labelling in Cartography



Multi-page labelling: minimize number of pages

$\Rightarrow$ Vertex Coloring Problem

Source: Gedicke, Jabrayilov, Niedermann, Mutzel, Haunert 2021