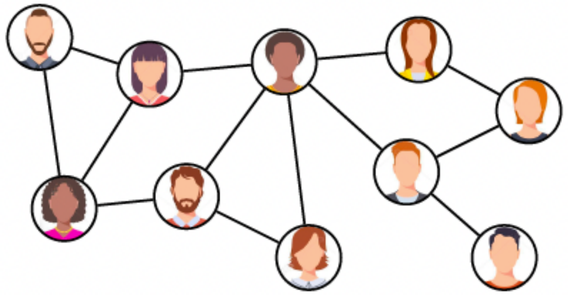
Kick-off Meeting

Foundations of Supervised Machine Learning with Graphs

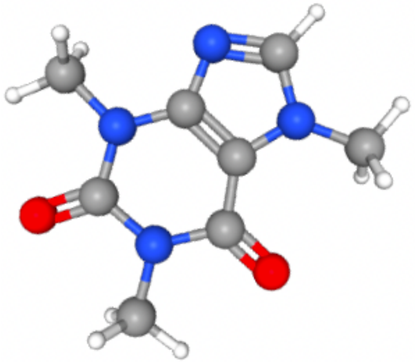
Seminar (Master): WS 22/23, Christopher Morris, RWTH Aachen University

Motivation: Graph data

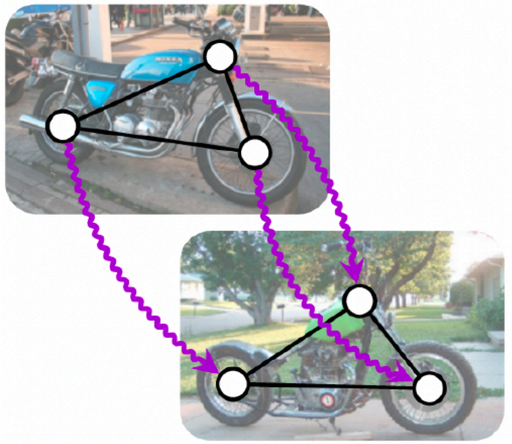
Graphs are everywhere…



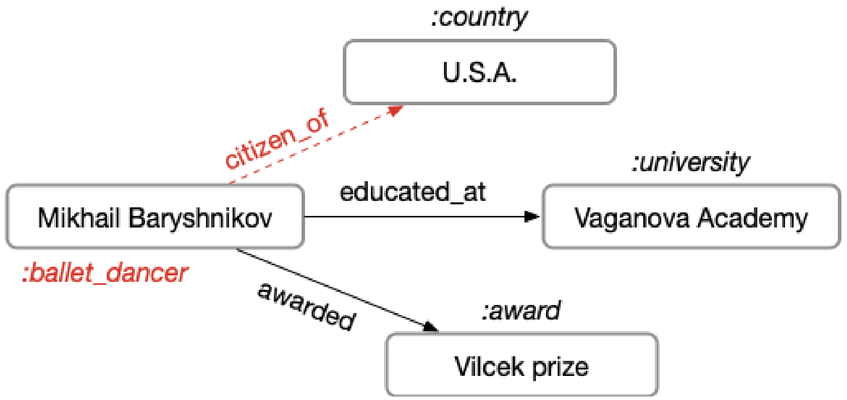
Social Networks



Chemical Molecules



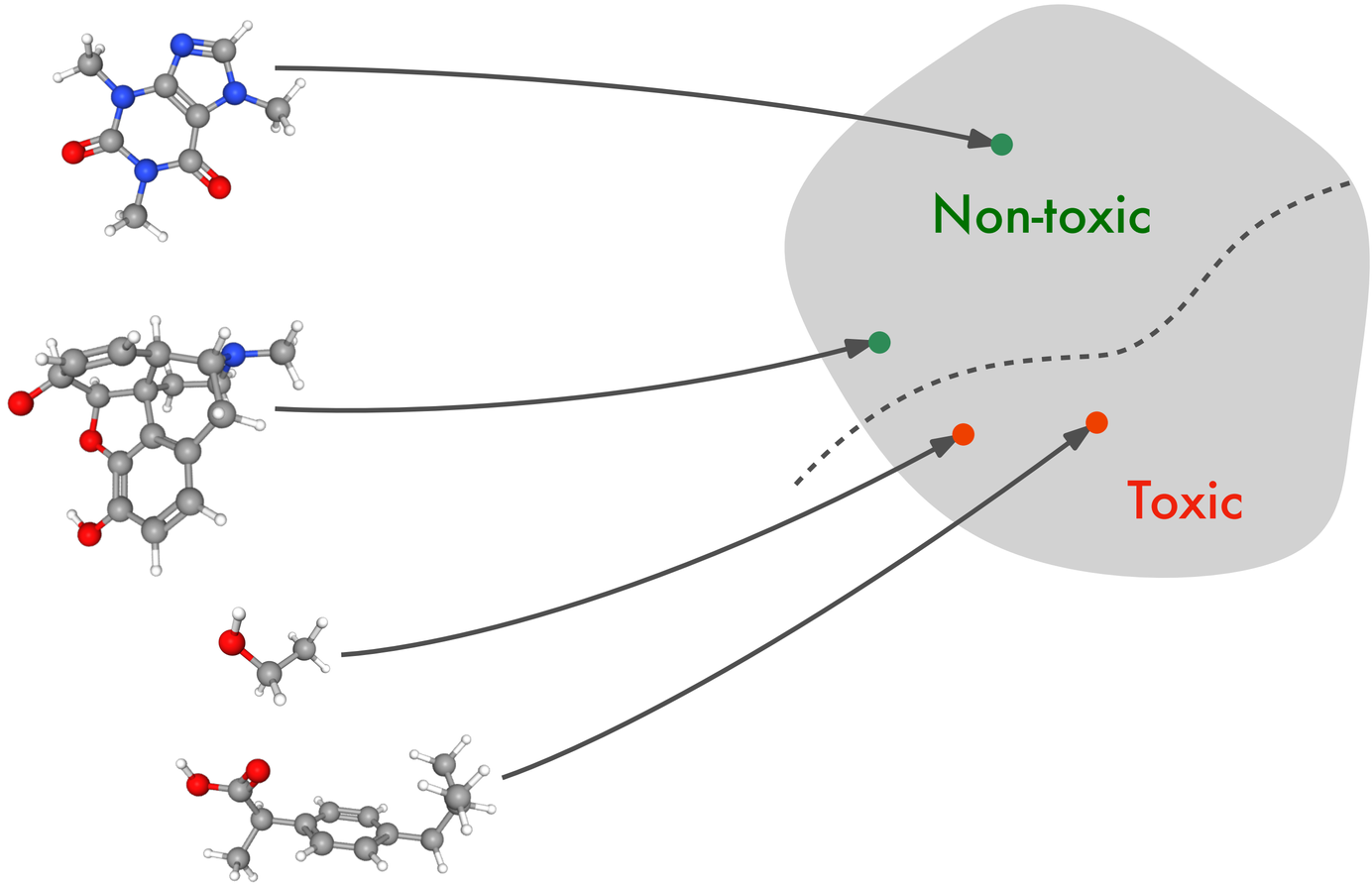
Computer Vision



Knowledge Bases

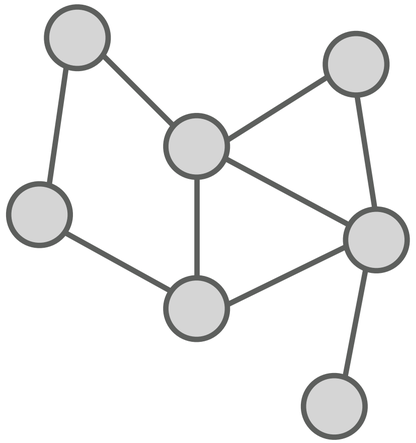
Motivation: A first example

Learning of molecular properties

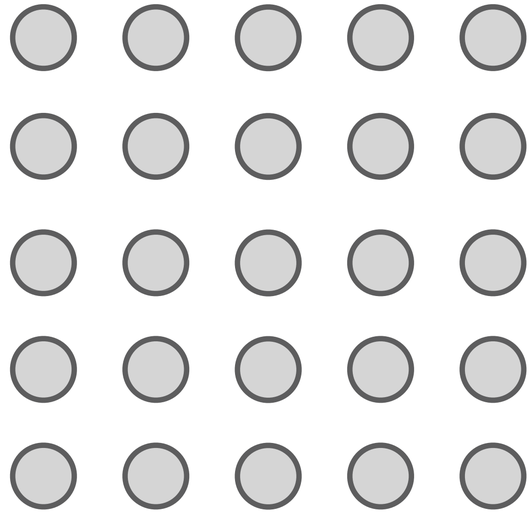


Challenges of graph-structured data

Graphs versus images



versus



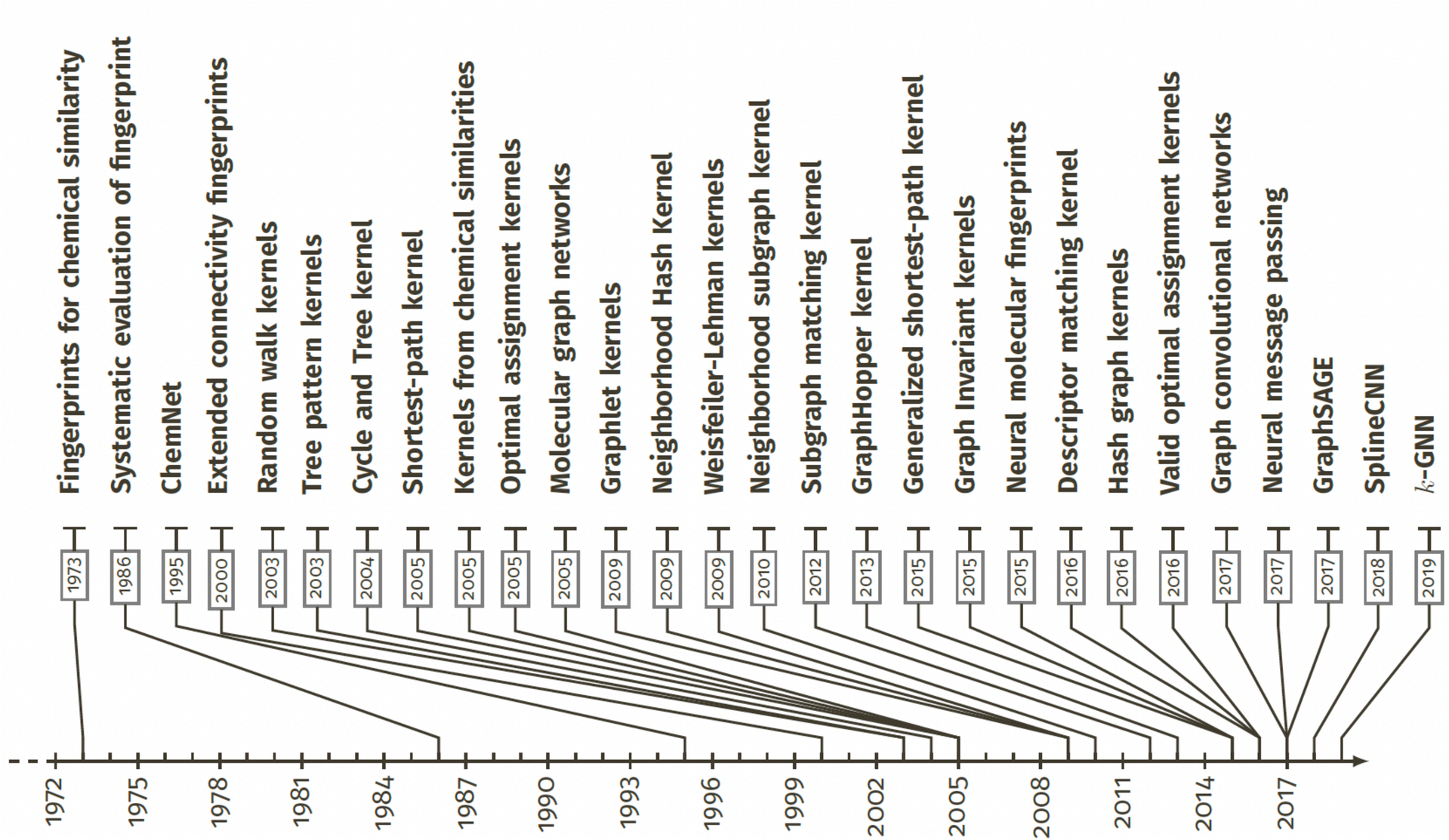
Graph:
Non-regular structure

Image:
Regular structure

Insight

Graphs *do not* have a *regular structure*.

Research on Machine Learning with Graphs



Research on Machine Learning with Graphs

Substantial number of papers published in the last 60 years. However, …

- Methods are mostly designed in an ad-hoc way, driven mostly by intuition.
- No established theory:
  - Which graph properties can methods capture? (*Expressivity*)
  - Does the method generalize beyond the training set? (*Generalization)*
  - …
- *Only in the last five years theoretical papers appeared.*

Seminar Organization

Overview and requirements for passing

You will get a paper assigned, and have to...

- Give a 30-minute-long talk about your assigned paper
- Write a 12- to 15-page detailed report about your assigned paper, using the LaTeX template.
- Peer-review your fellow students' reports.
- Attend all meetings and actively participate.
- Plagiarism leads to failing the seminar.

Seminar Organization

Talks

Aim of your talk is to...

- Give a 30-minute polished presentation about your assigned paper, i.e.,
  - You should provide an overview of your assigned paper.
  - Highlight most important concepts and ideas.
  - If possible explore one key concept in more detail.
  - The target audience are your fellow students.
  - Strive for clarity. Make your talk as understandable as possible, strive for a mix of formal correctness and intuition.

Seminar Organization

Reports

Aim of your report is to...

- Give a detailed overview of the assigned paper.
- 12 to 15 pages, using the provided LaTeX template.
- Strive for clarity and formal correctness.

Seminar Organization

Peer review of reports

You get one report assigned from your fellow student…

- Annotate the PDF with corrections, comments, and suggestions and improvements.
- Additionally submit a half-page report, reporting on the quality of the report and summarize suggested changes and comments.
- Aim is to help your fellow student improve his or her manuscript.

Seminar Organization

Time line and dates

- 10.11.2022, 24:00: Submission of report drafts
- 01.12.2022, 24:00: Submission of reports for peer review
- 14.12.2022, 24:00: Submission of peer reviews
- 20.12.2022, 10:00: In person meeting, discussion of peer reviews
- 09.01.2023, 24:00: Submission of revised reports
- 16.01.2023, 24:00: Feedback by the organizers
- 31.01.2023, 24:00: Submission of final reports
- 10.02.2023, 24:00: Submission of presentation slides
- 16.02.2023, 10:00: Talks

Seminar Organization

Papers

1. Equivariant Subgraph Aggregation Networks
2. Provably Powerful Graph Networks
3. Weisfeiler and Leman Go Sparse: Towards Scalable Higher-order Graph Embeddings
4. Weisfeiler and Leman Go Walking: Random Walk Kernels Revisited
5. Graph Neural Networks with Local Graph Parameters
6. Generalization and Representational Limits of Graph Neural Networks
7. Agent-based Graph Neural Networks
8. What Functions Can Graph Neural Networks Generate?
9. Affinity-Aware Graph Networks