Towards Precision Medicine with Graph Representation Learning

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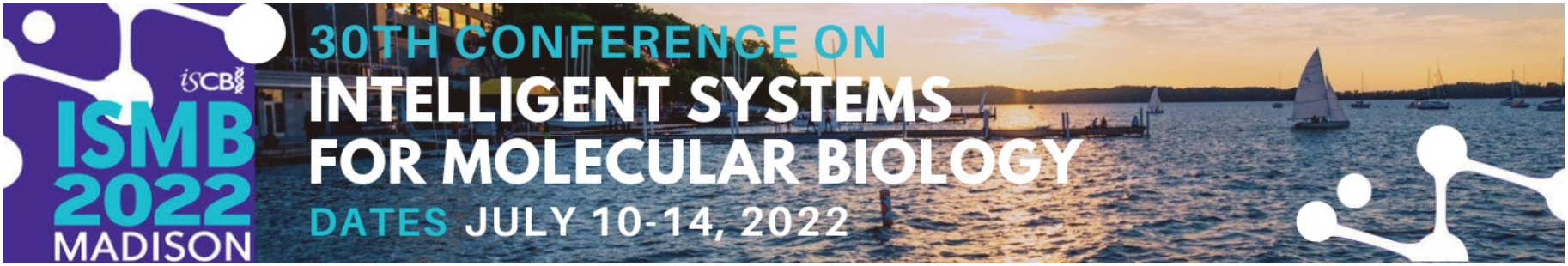


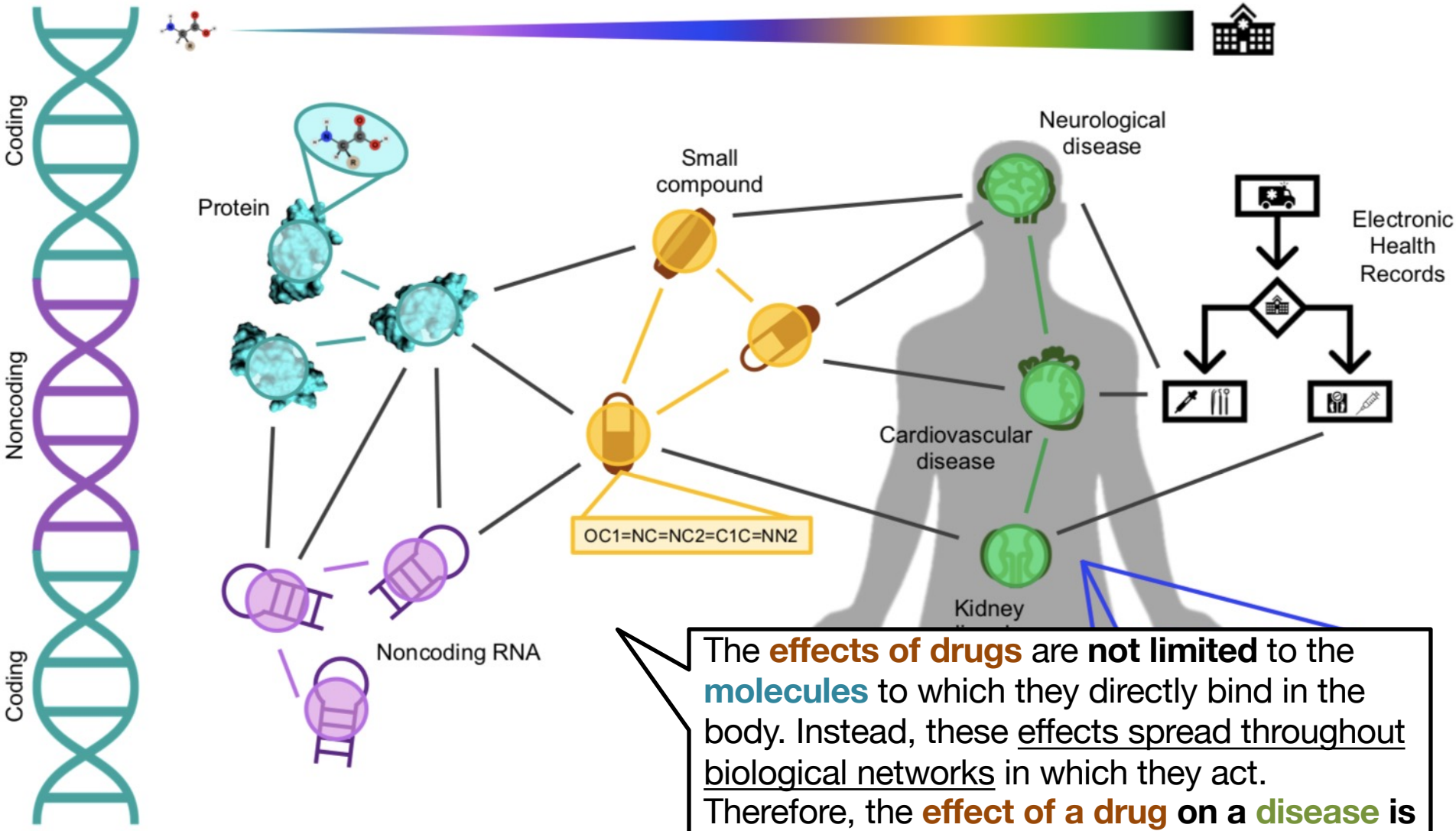
Tutorial VT4

July 7, 2022 at 9am – 1pm CDT

All tutorial materials are available at

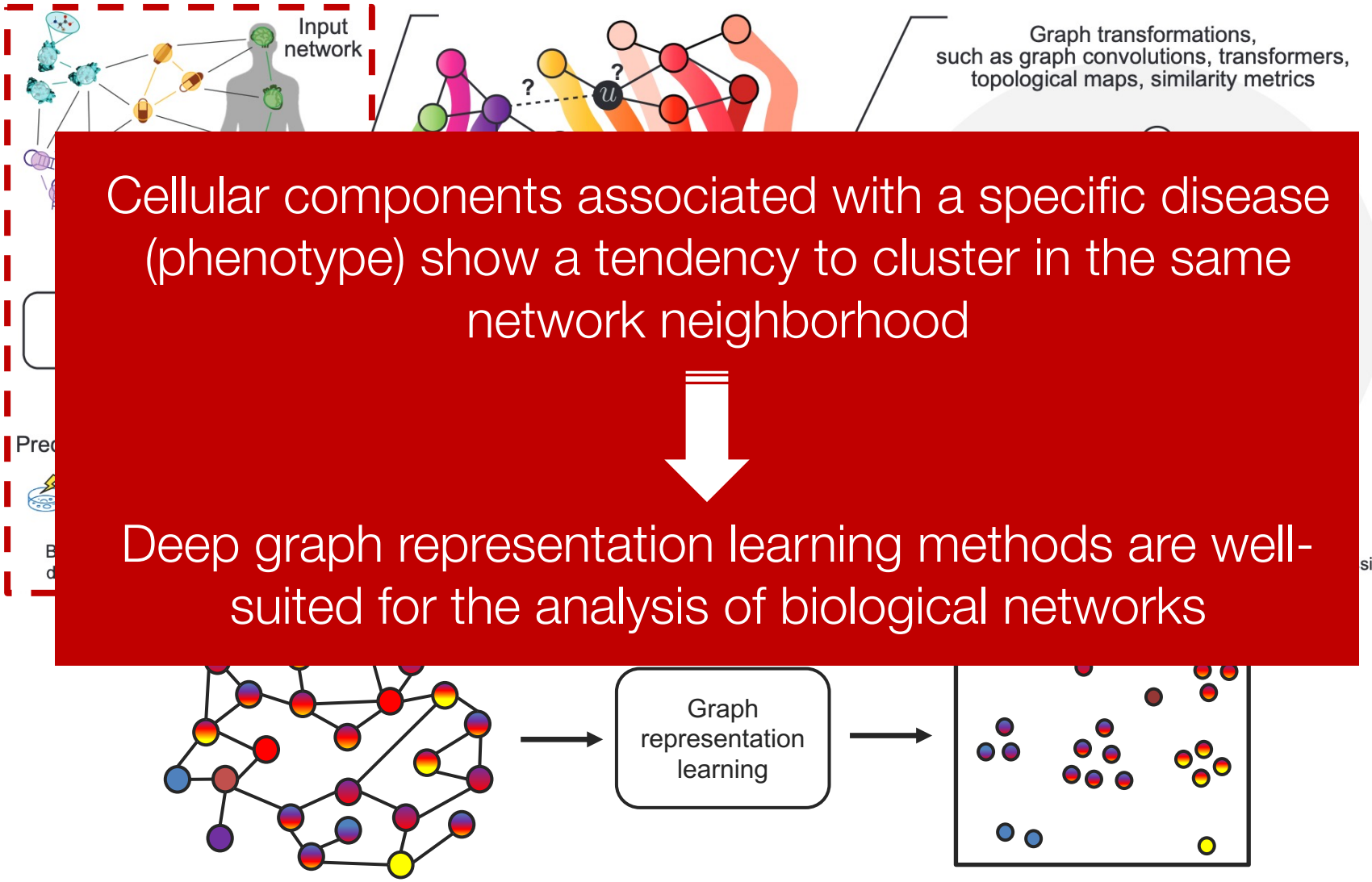
zitniklab.hms.harvard.edu/biomedgraphml

Biology is interconnected



The **effects of drugs** are **not limited** to the **molecules** to which they directly bind in the body. Instead, these effects spread throughout biological networks in which they act. Therefore, the **effect of a drug** **on a disease** **is inherently a network phenomenon**

Graph representation learning realizes key network principles for data-rich biomedicine



Graph Representation Learning for Biomedicine, *Nature Biomedical Engineering* (in press), 2022, arXiv:2104.04883

This Tutorial

✓ 1. Methods: Network diffusion, shallow network embeddings, and graph neural networks

✓ 2. Applications: Fundamental biological discoveries and precision medicine

3. Outlook: Future directions and Q&A session

4. Hands-on exercises: Demos, implementation details, tools, and tips

Future directions

Q&A Session

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4. Hands-on exercises: Demos, implementation details, tools, and tips

Hands-on Exercises

Please refer to:

<Insert link to GitHub repo/notebook>

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✓ 2. Applications: Fundamental biological discoveries and precision medicine

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✓ 4. Hands-on exercises: Demos, implementation details, tools, and tips

Resources

- Books & survey papers
  - William Hamilton, *Graph Representation Learning* (morganclaypool.com/doi/abs/10.2200/S01045ED1V01Y202009AIM046)
  - Li et al., Graph Representation Learning for Biomedicine (arxiv.org/abs/2104.04883)

- Keynotes
  - Michael Bronstein, “Geometric Deep Learning: The Erlangen Programme of ML” (ICLR 2021 keynote) (youtube.com/watch?v=w6Pw4MOzMuo)

- Software & packages
  - PyTorch Geometric
  - NetworkX
  - Stanford Network Analysis Platform (SNAP)

Resources

- Conferences & summer schools
  - London Geometry and Machine Learning Summer School (logml.ai)
  - Learning on Graphs Conference (logconference.github.io)

- Tutorials & code bases
  - Pytorch Geometric Colab Notebooks (pytorch-geometric.readthedocs.io/en/latest/notes/colabs.html)
  - Zitnik Lab Graph ML Tutorials (github.com/mims-harvard/graphml-tutorials)
  - Stanford University's CS224 (web.stanford.edu/class/cs224w)

- Datasets
  - Precision Medicine Oriented Knowledge Graph (PrimeKG) (zitniklab.hms.harvard.edu/projects/PrimeKG)
  - Therapeutic Data Commons (TDC) (tdcommons.ai)
  - BioSNAP (snap.stanford.edu/biodata/)
  - Open Graph Benchmark (OGB) (ogb.stanford.edu)