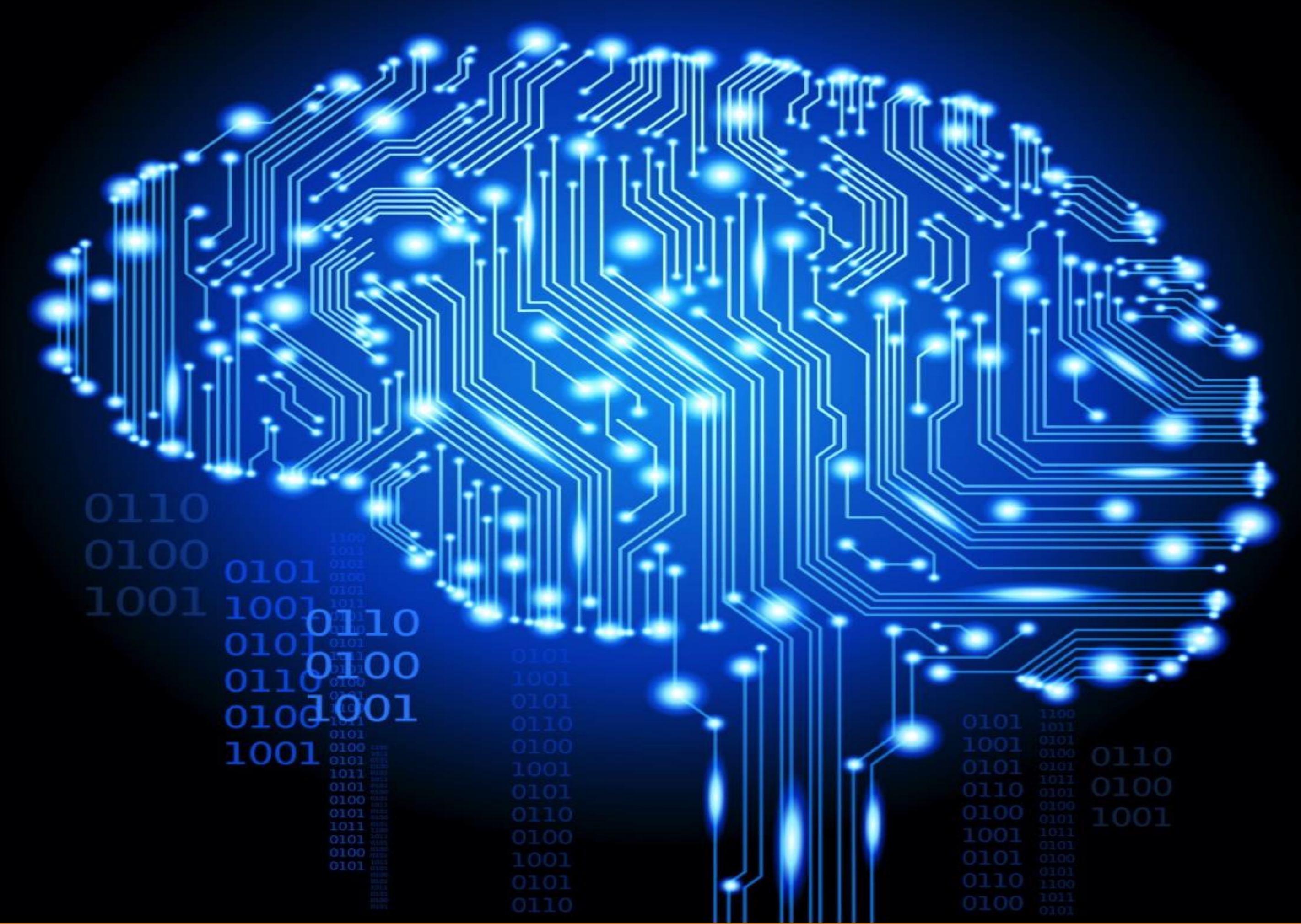


Lecture 7: Graph Neural Networks

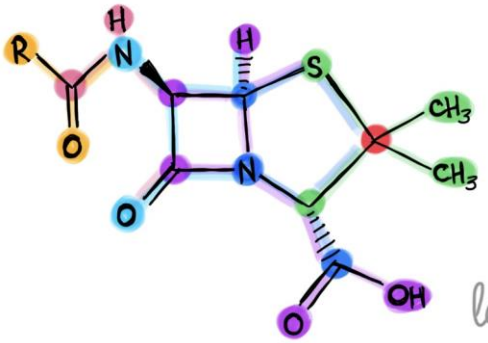
Efstratios Gavves

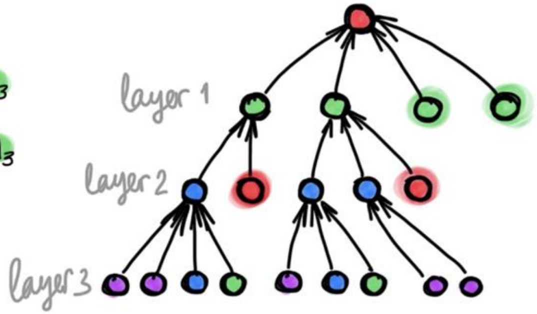
Lecture overview

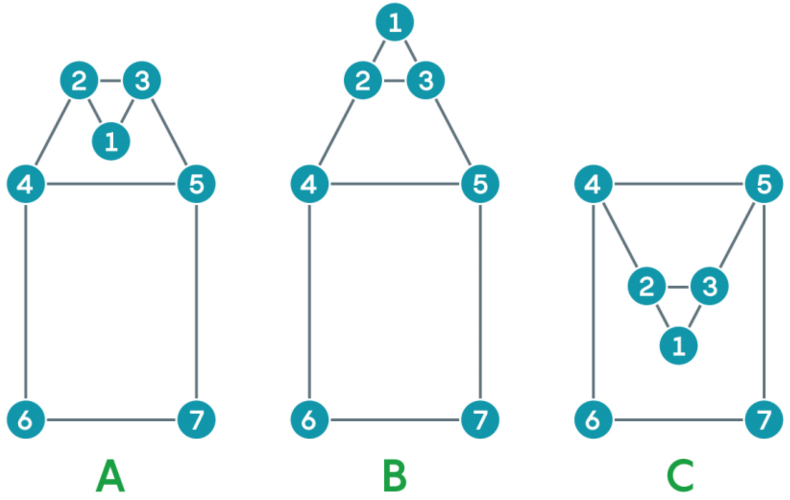
- What makes graphs special?
- Revisiting graphs
- Revisiting convolutions
- Spectral graph convolutions
- Spatial graph convolutions

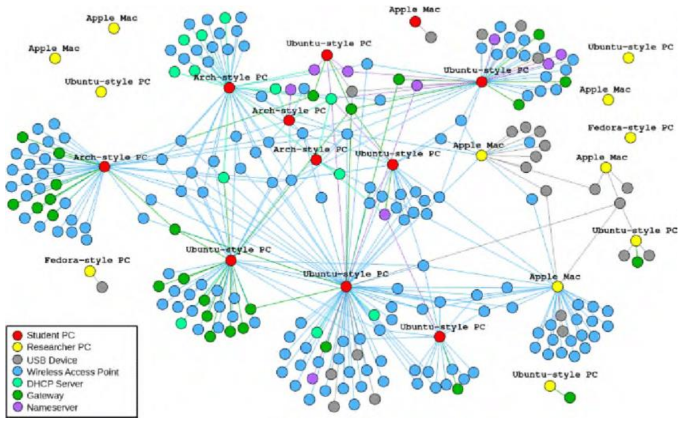
What are graphs?

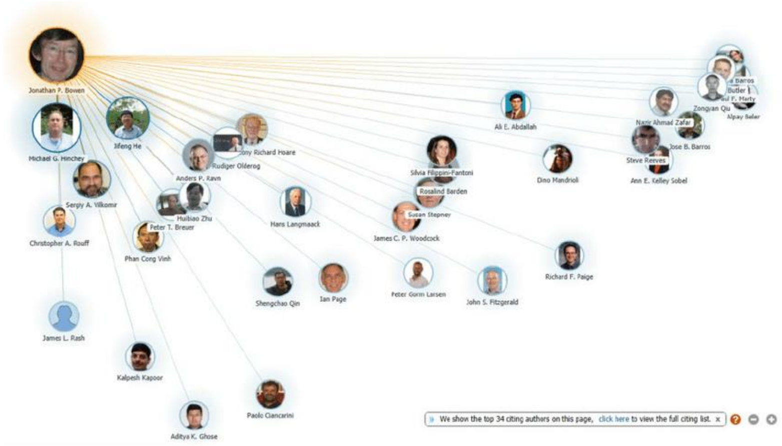
- Data structures of sets of variables (or objects) connected with each other



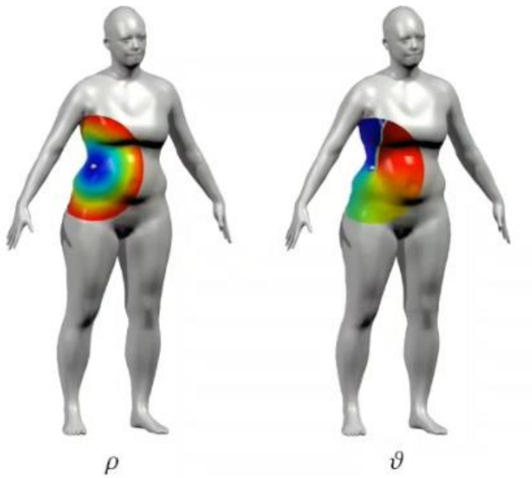


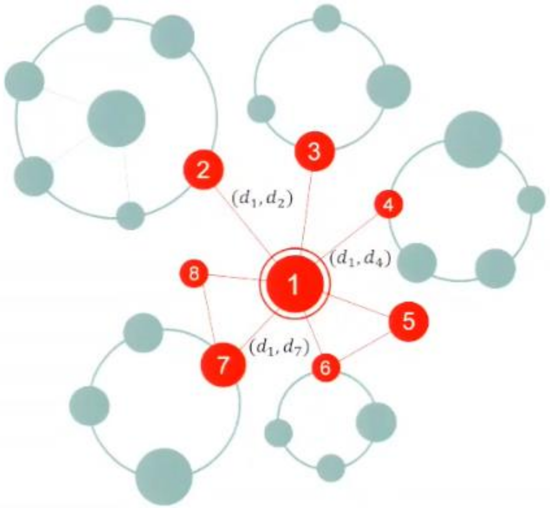


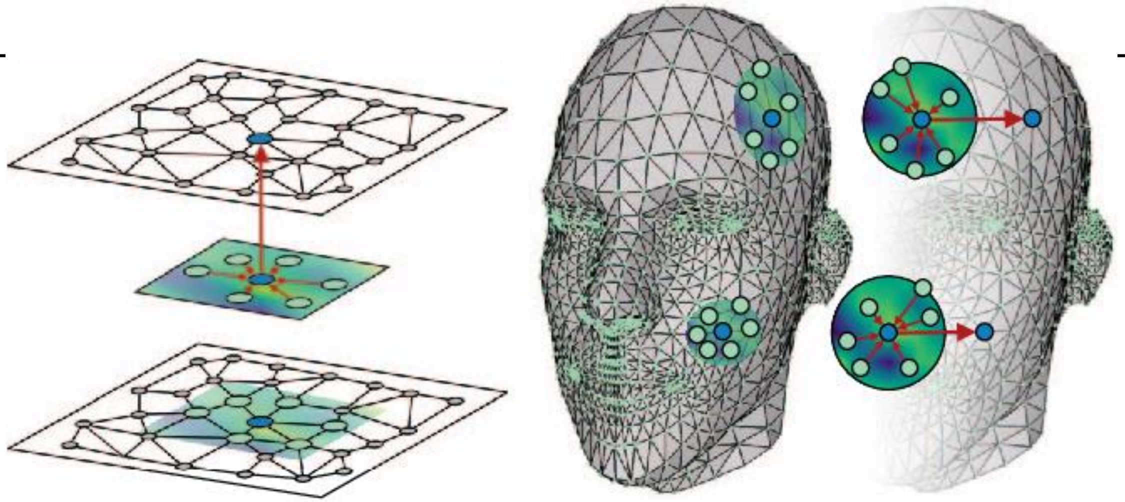




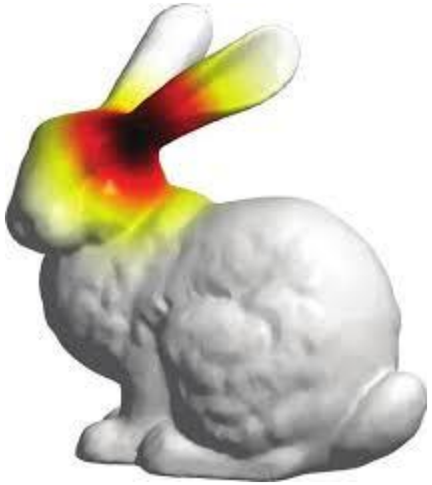
Graphs as geometry

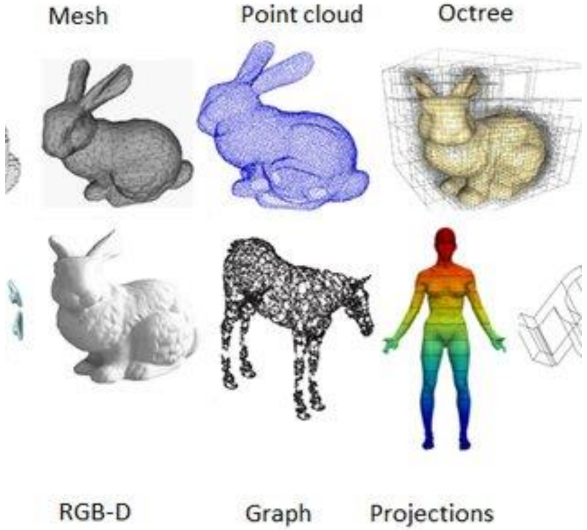






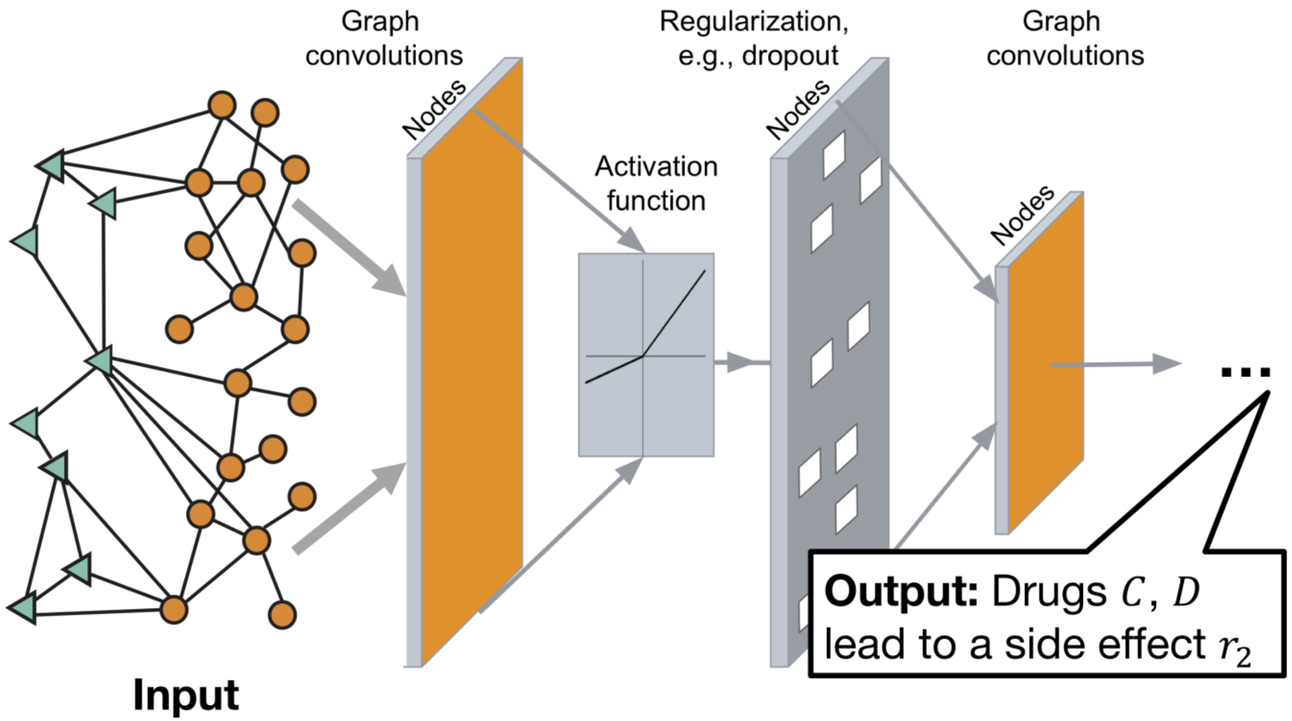
(a) Filtering of graphs (b) Filtering of meshes

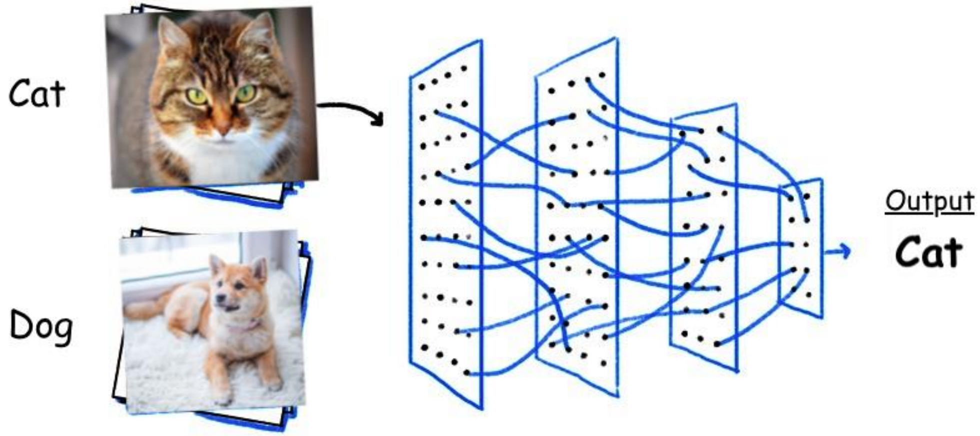




Classifying graphs

- Making predictions at the level of a graph
- Even an image can be thought as regular graph (grid)



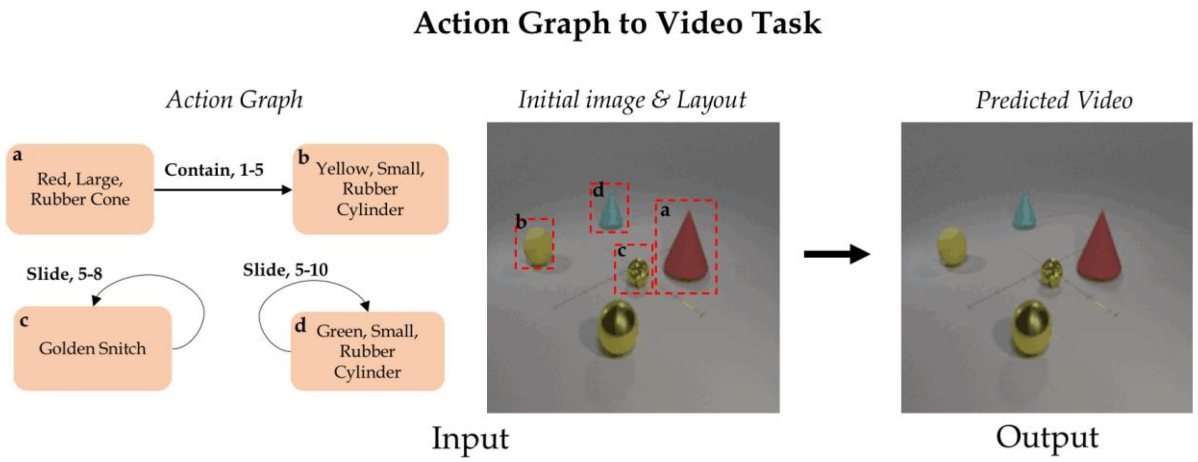


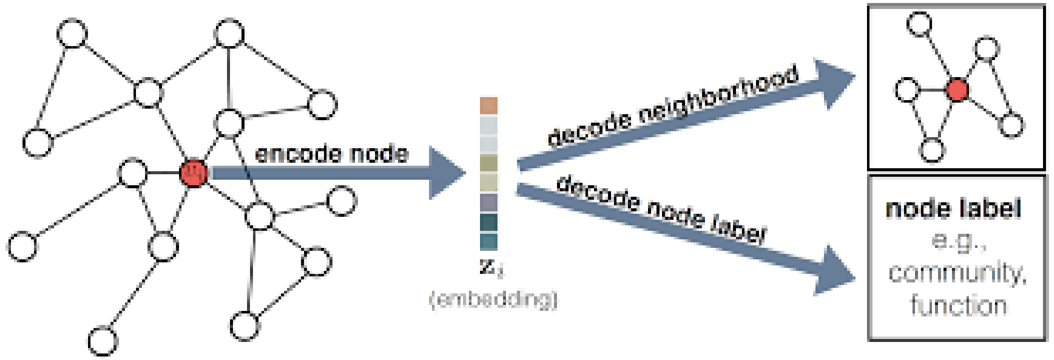
Classifying nodes

- E.g., who is likely to have coronavirus?
- Or which pixel nodes correspond to car or a pedestrian?

Classifying edges

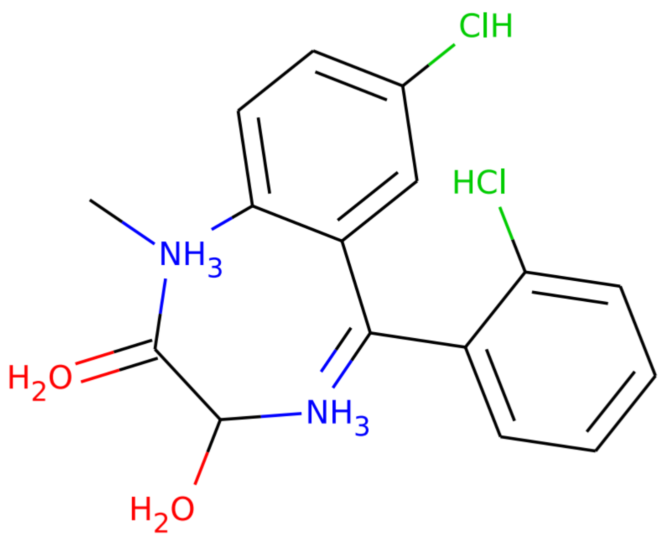
- E.g., actions between objects
- Filling missing edges



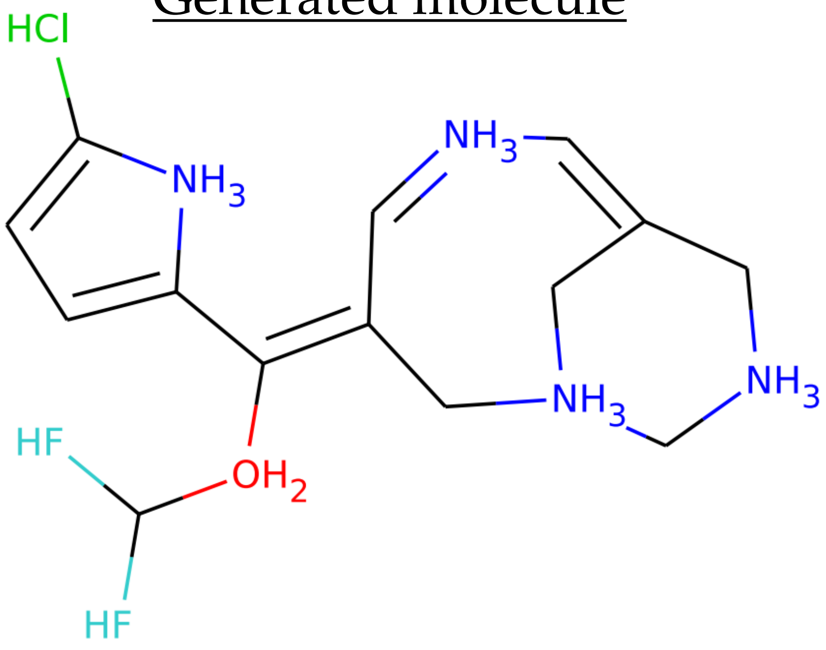


Graph generation

<u>Example molecule</u>



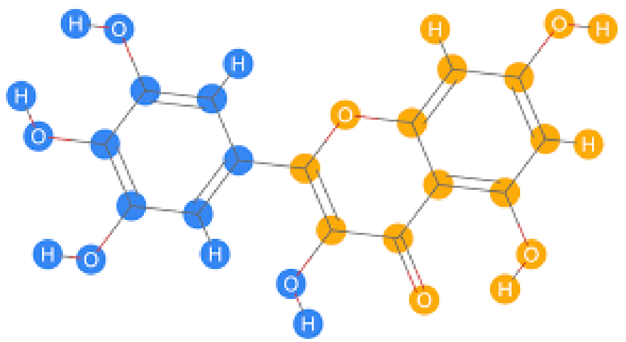
<u>Generated molecule</u>



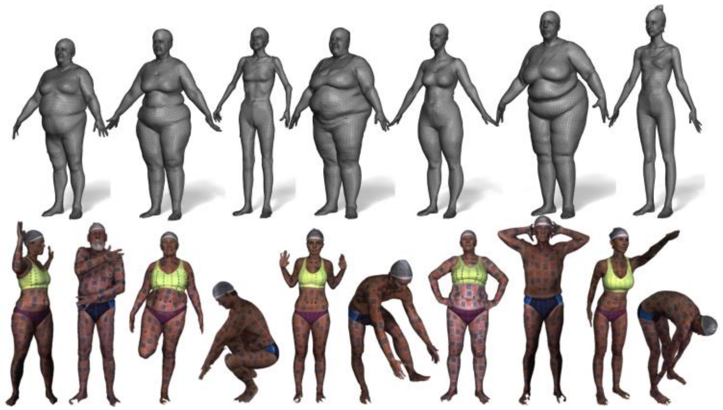
P. Lippe, E. Gavves, Categorical Normalizing Flows via Continuous Transformations, in submission to ICLR 2021

Graphs can be static, varying, or even evolving with time

- Molecule graphs do not change



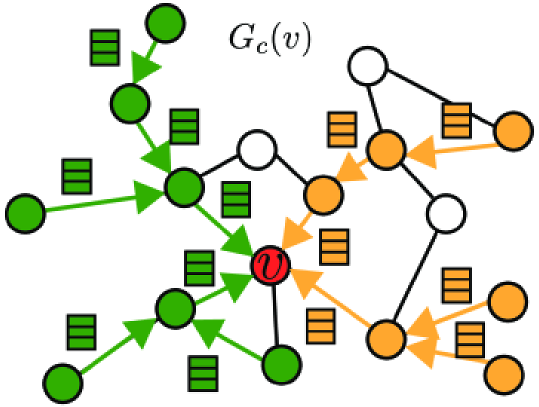
- 3D mesh grids can deform



- Graph relations between objects change continuously

Regular structures vs graphs

- Regular structures are subsets of graphs
  - E.g., images are grid graphs



- Convolution + pooling
- Local neighborhood: fixed window
- Constant number of neighbors
- With fixed ordering
- Translation equivariance
- $O(n)$ per layer complexity

- Message passing + coarsening
- Local neighborhood: 1-hop
- Different number of neighbors
- No ordering of neighbors
- Local permutation equivariance
- $O(n)$ per layer complexity