Quadratic Assignment Problem with Reinforcement Learning

The quadratic assignment problem

[Image of 2 graphs]

[Demonstrate assignment and show how to compute value]

[mention traditional algorithms and scaling problems to motivate machine learning]

Mathematical formulation [?]

...

Graph Neural Networks

[Image showing weighted graph -> Icon for messages on edges (message transformation) -> Arrows from messages to nodes (aggregation)]

$$\mathbf{x}_i' = \psi \left(\mathbf{x}_i, \sum_{j \in \mathcal{N}(i)} \phi(\mathbf{x}_j, \mathbf{e}_{ij}) \right)$$

Reinforcement learning environment

State	Input graphs
Actions	Pairs of nodes
Reward	(Negative) cost that becomes fixed after pair has been assigned
Next state	Graph after pair has been assigned

Q Network

Predicts the best achievable value after taking an action

[image]

1. Encode graph structure into node embeddings with two separate GNNs
2. For every pair of nodes, compute predicted value after assignment

Representing previously assigned nodes in graph

Options:

- Add a binary feature to the node
- Use special network to encode nodes
- Compute an equivalent subproblem for the remaining nodes

Subproblems after assignment

[Image to illustrate the approach]

Requires heterogenous graph neural network

Limitations of Graph Neural Networks

[Show triangle and rectangle graph that a GNN cannot distinguish]

Isomorphism can be represented as QAP, but GNN cannot solve it

Oversmoothing of node embeddings

Remedies for GNN limitations

- More expressive GNNs (incorporating higher-order structures, initializing node features to be distinguishable)
  - Computationally expensive, harder to train
- Normalization layers to force distance between node embeddings
  - Possibly strong distortion with few nodes
  - Eliminate global information contained in nodes
- Local search

Evaluation

[reward plot on single instance]

[reward plot on random problem distribution]

[q value compared to stochastic/optimal q values]

Open questions

- What is the impact of state representation on performance?
- Which patterns does the GNN need to be able to recognize? How to choose training data?
- What is the heuristic learned by the agent?
- How import is exploration in this task?

Not enough time to talk about

- QAP normalization (scale and shift invariance) / diagonal elimination
- REINFORCE agent
- Details about experiments and evaluation
- Edge weight histogram idea
- Directed graphs
- Details and impact of normalization layers