The Map Equation Goes Neural: Mapping Network Flows with Graph Neural Networks

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too long; didn't listen

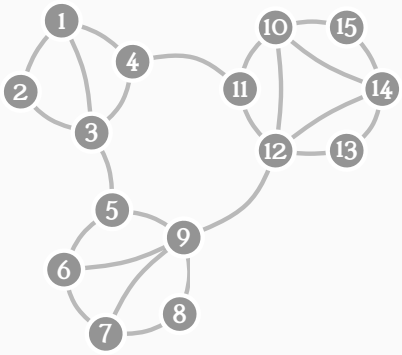
map equation + graph neural networks

Idea: leverage advances in deep learning for deep graph clustering with an information-theoretic objective function from network science – the map equation

The Map Equation

→ Rosvall and Bergstrom; PNAS 2008

The Map Equation



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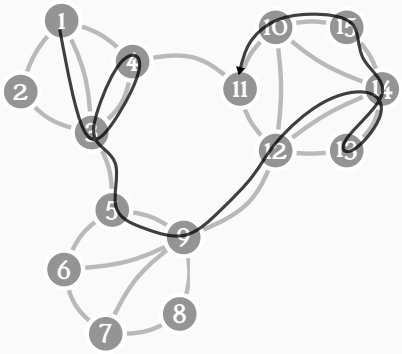

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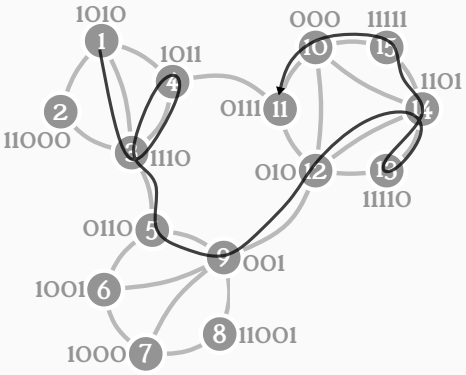

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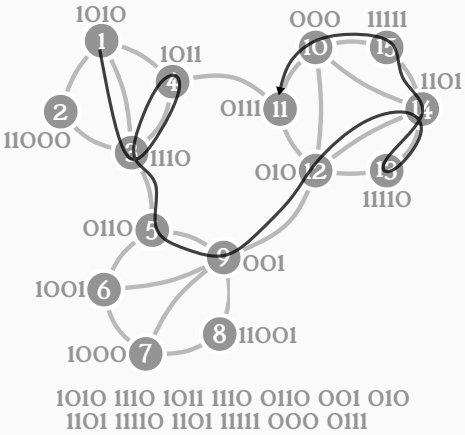
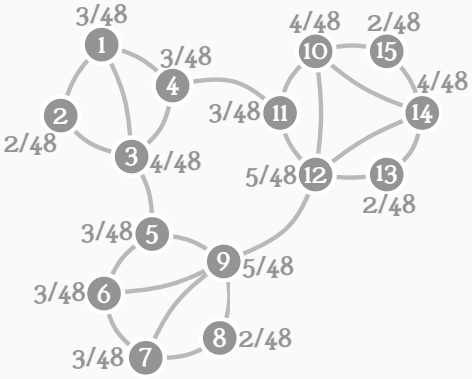


Description length

$$H(P) = -\sum_{v \in V} p_v \log_2 p_v \text{ bits} \qquad (1)$$

The Map Equation



Description length

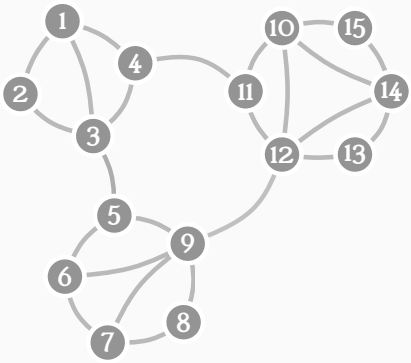
$$H(P) = -\sum_{v \in V} p_v \log_2 p_v \text{ bits} \tag{1}$$

Visit rates

$$p_v = \sum_{u \in V} p_u t_{uv} \qquad t_{uv} = \frac{w_{uv}}{\sum_{v \in V} w_{uv}} \tag{2}$$

But we are interested in communities...

The Map Equation



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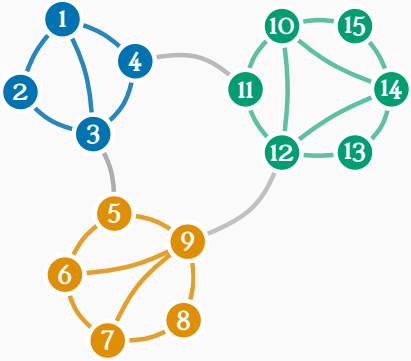

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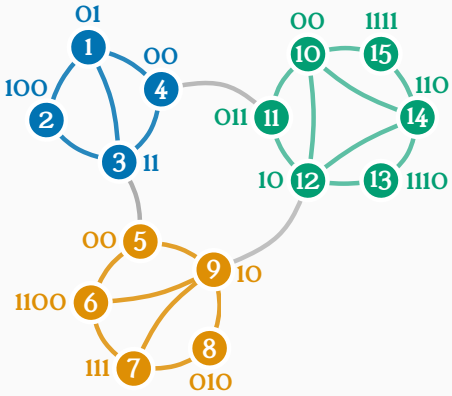

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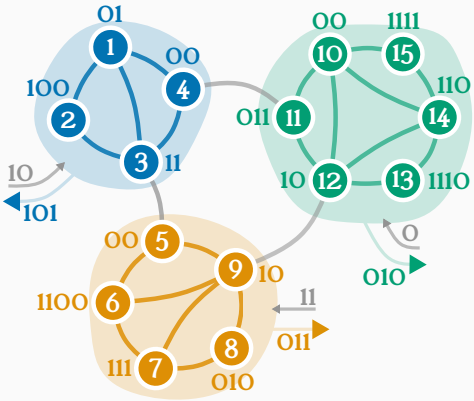

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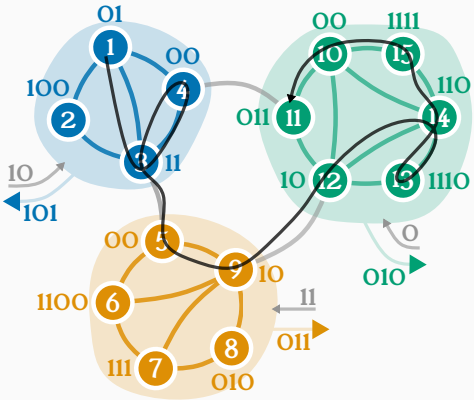

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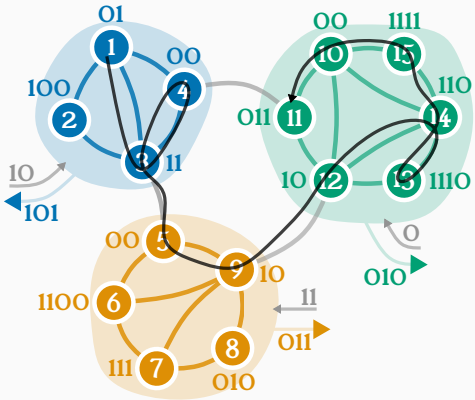


1001 11 00 11 101 1100 10 011010
110 1110 110 1111 00 011

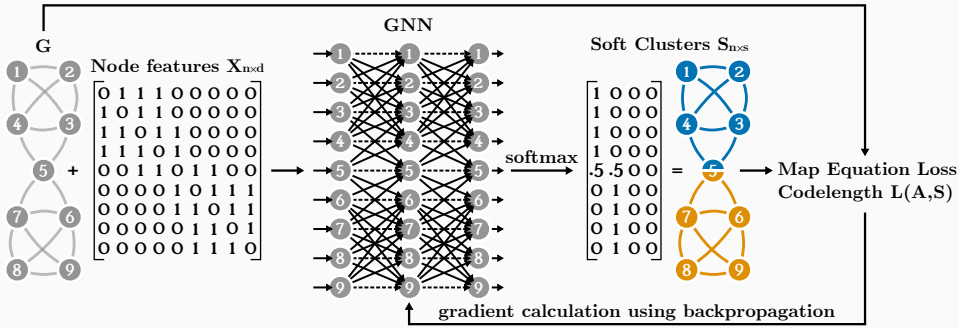
$$L(\mathrm{M}) = qH(Q) + \sum_{\mathrm{m}\in\mathrm{M}} p_{\mathrm{m}} H(P_{\mathrm{m}}) \rightarrow \min$$

Minimum Description Length (MDL) Principle

The Map Equation Goes Neural

The Map Equation Goes Neural

- We introduce a soft cluster assignment matrix for differentiability
  → overlapping modules
- We implement the differentiable map equation in tensor form
  → clustering loss for (G)NNs
- Optimisation with gradient descent means differentiating the codelength with respect to soft cluster assignments



The Map Equation Goes Neural

Compute visit rates from graph's transition matrix $\mathbf{T}$ and normalised node in-degrees $\mathbf{d}^{\text{in}}$

$$\mathbf{p}^{(t+1)} \leftarrow \frac{\alpha}{W_{\text{tot}}}\mathbf{d}^{\text{in}} + (1-\alpha)\,\mathbf{p}^{(t)}\mathbf{T} \qquad \text{and set} \qquad \mathbf{p}^{(0)} = \mathbf{d}^{\text{in}}$$

Compute flow matrix $\mathbf{F}$ and flows between clusters $\mathbf{C}$, given cluster assignments $\mathbf{S}$

$$\mathbf{F} = \frac{\alpha}{W_{\text{tot}}}\mathbf{A} + (1-\alpha)\,\text{diag}\,(\mathbf{p})\,\mathbf{T} \qquad \mathbf{C} = \mathbf{S}^{\top}\mathbf{F}\mathbf{S}$$

Define terms

$$q = 1 - \text{tr}\,(\mathbf{C}) \quad \mathbf{q}_{\text{m}} = \mathbf{C}\mathbf{1}_{\text{s}} - \text{diag}\,(\mathbf{C}) \quad \mathbf{m}_{\text{exit}} = (\mathbf{1}_{\text{s}}^{\top}\mathbf{C})^{\top} - \text{diag}\,(\mathbf{C}) \quad \mathbf{p}_{\text{m}} = \mathbf{q}_{\text{m}} + \mathbf{1}_{\text{s}}^{\top}\mathbf{C}$$

Assemble the map equation

$$L\,(\mathbf{A}, \mathbf{S}) = q \log_2 q - (\mathbf{q}_{\text{m}} \log_2 \mathbf{q}_{\text{m}})\,\mathbf{1}_{\text{s}} - (\mathbf{m}_{\text{exit}} \log_2 \mathbf{m}_{\text{exit}})\,\mathbf{1}_{\text{s}} - (\mathbf{p} \log_2 \mathbf{p})\,\mathbf{1}_{n} + (\mathbf{p}_{\text{m}} \log_2 \mathbf{p}_{\text{m}})\,\mathbf{1}_{\text{s}}$$

Evaluation

Evaluation – Setup

Datasets

- LFR networks with 1000 nodes, planted communities, and various mixing parameters
- Real networks from PyTorch Geometric, PyTorch Geometric Signed Directed, and Open Graph Benchmark (OGB)

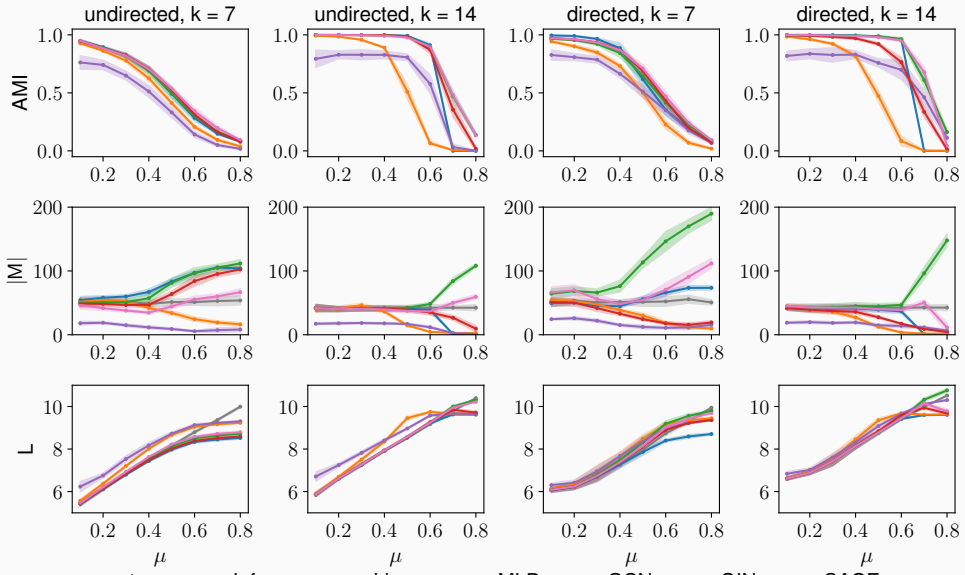
Community Detection

Neuromap with different (G)NN architectures

- Simple linear layer and MLP
- GCN, GIN, SAGE with 2 layers

Baselines: Infomap, DMoN, NOCD, DiffPool, MinCut, Ortho

Results – directed



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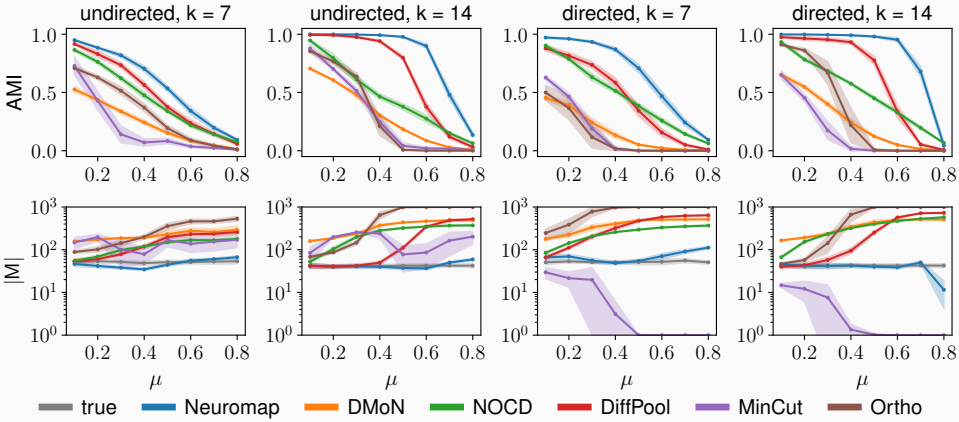
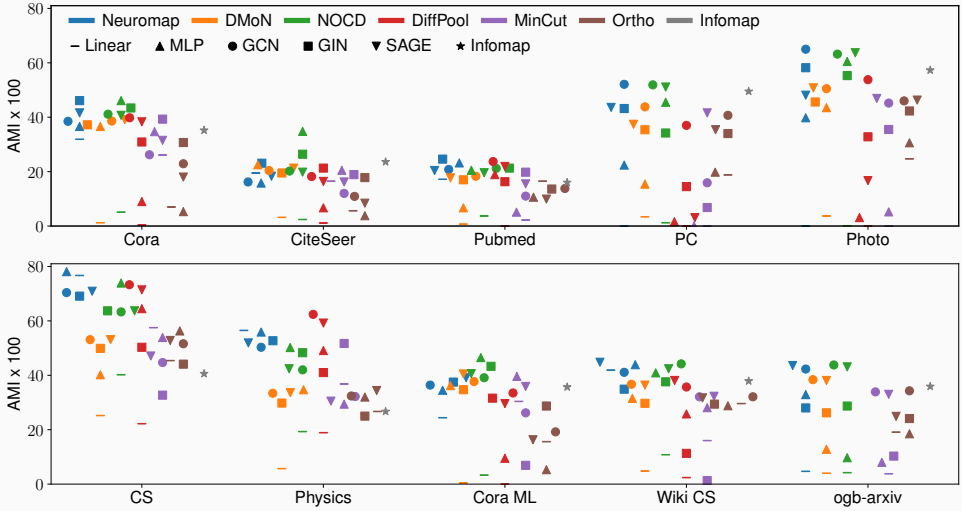


Here: SAGE, more architectures in the paper!

Results – real-world networks



Complete tabulated and additional results in the paper!

Conclusion

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Motivation

Combine the best of both worlds: deep community detection with MDL

Our Approach

We make the map equation differentiable by introducing soft cluster assignments, and optimise it with (G)NNs and gradient descent.

Results

- Community-detection performance depends on the chosen (G)NN architecture
- Soft cluster assignments produce overlapping communities
- No explicit regularisastion needed, MDL is sufficient!
- Neuromap performs competitively against recent deep clustering approaches
- Additional benefit: enables fast experimentation with map equation adaptions!

Thank you for your attention!