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

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too long; didn't listen

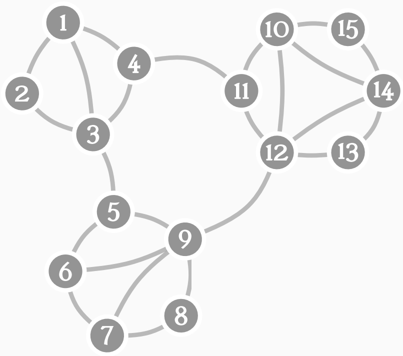
map equation + graph neural networks

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

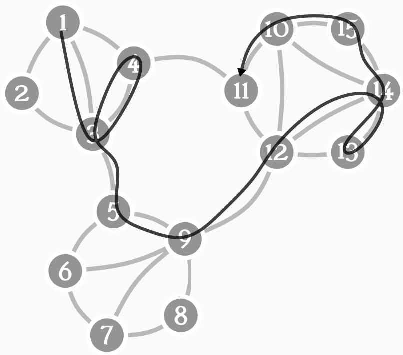
The Map Equation

$\longrightarrow$ Rosvall and Bergstrom; PNAS 2008

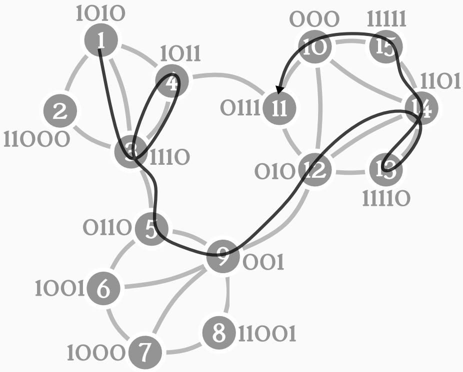
The Map Equation



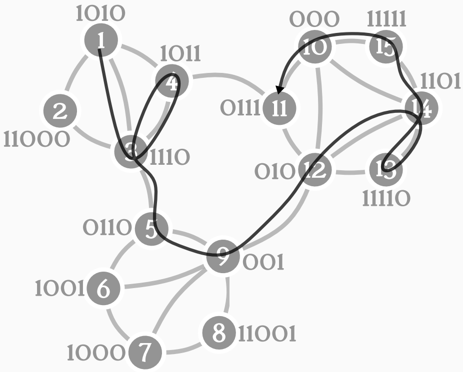
The Map Equation



The Map Equation



The Map Equation



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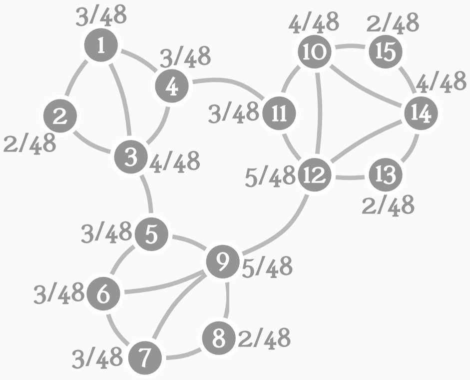
Description length

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

The Map Equation



Description length

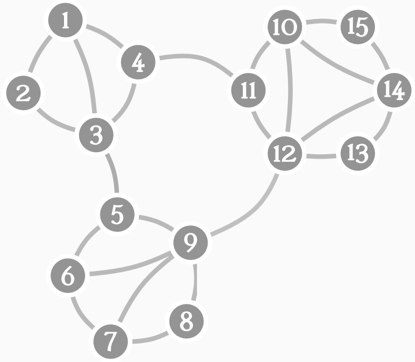
$$H(P) = -\sum_{v \in V} p_v \log_2 p_v \text{ bits} \tag{1}$$

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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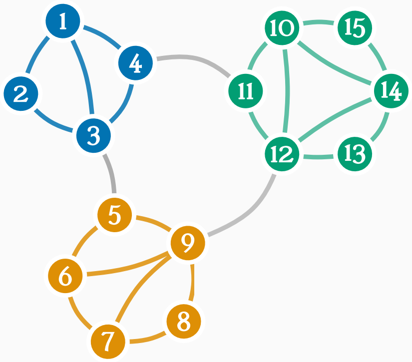
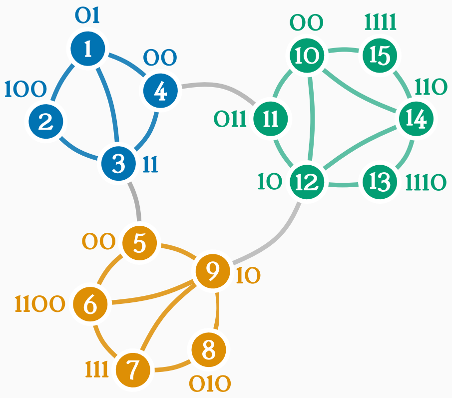
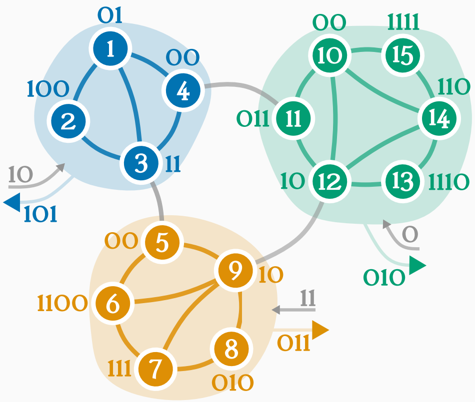


The Map Equation





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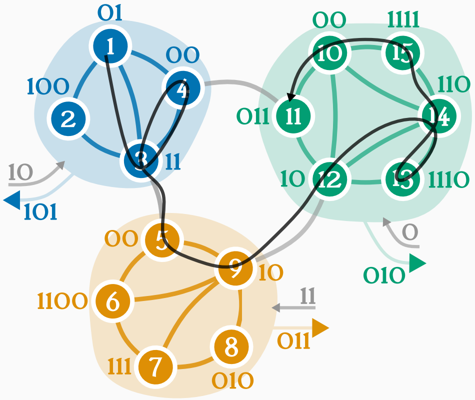
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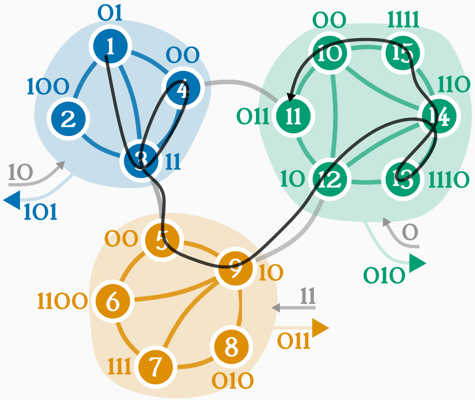

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$$L(M) = qH(Q) + \sum_{m \in M} p_m H(P_m) \to \min$$

Minimum Description Length (MDL) Principle

The Map Equation Goes Neural

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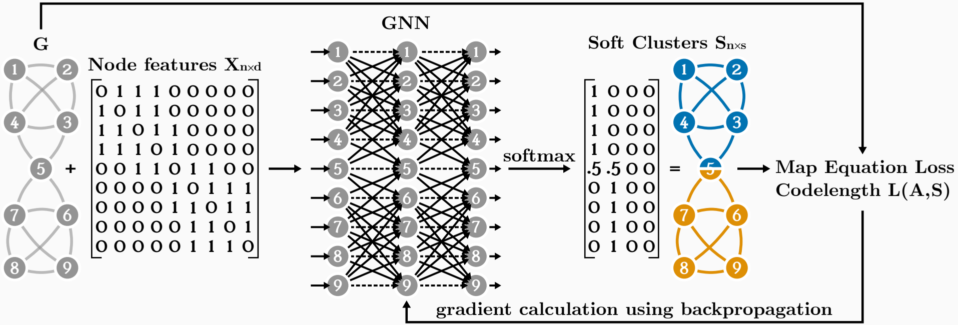
- We introduce a soft cluster assignment matrix for differentiability
  $\rightarrow$ overlapping modules
- We implement the differentiable map equation in tensor form
  $\rightarrow$ clustering loss for (G)NNs
- Optimisation with gradient descent means differentiating the codelength with respect to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

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

Assemble the map equation

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

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)

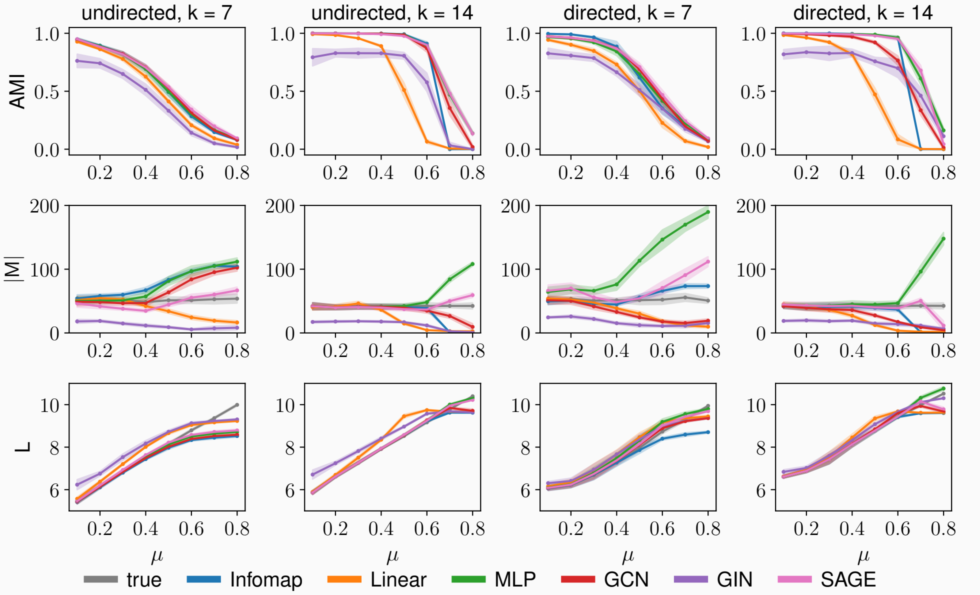
Community Detection

Neuromap with different (G)NN architectures

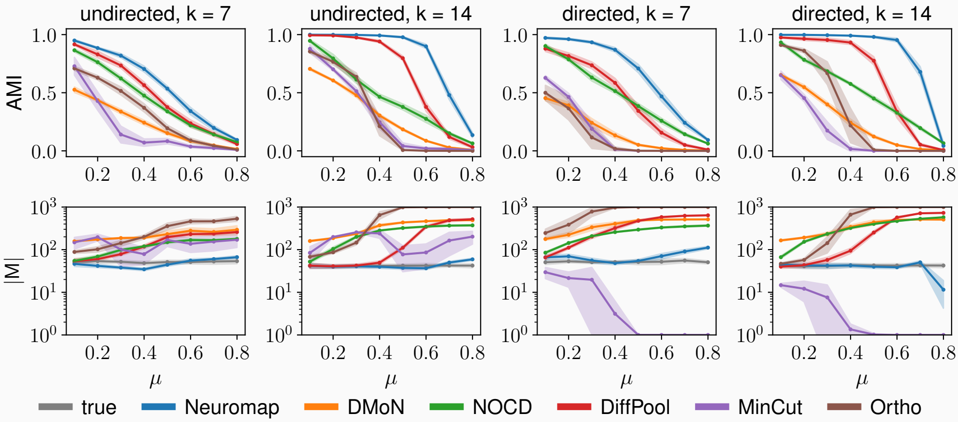
- Simple linear layer and MLP
- GCN, GIN, SAGE with 2 layers

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

Results – directed

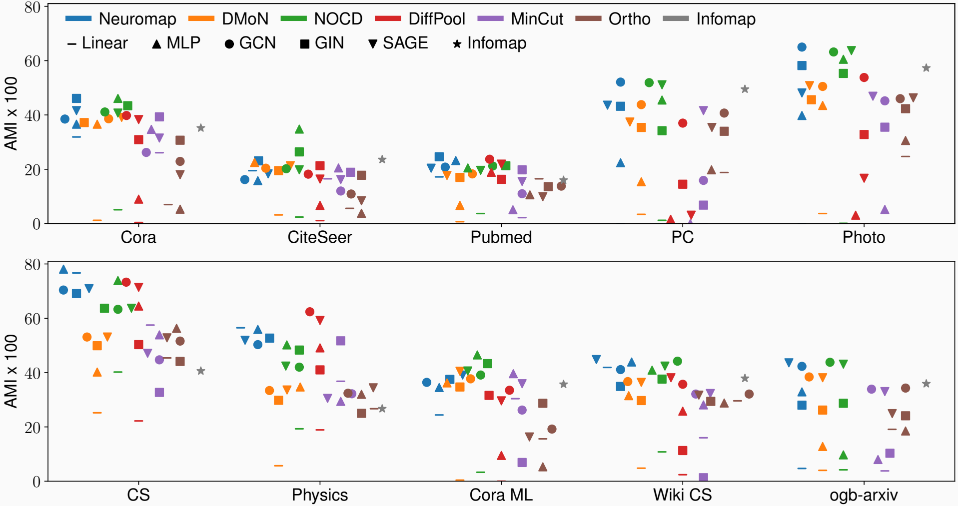


Results – directed



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!