Optimising network efficiency in the epidemic scenario

With Deep Epidemic Efficiency Network (DEEN)

Magdalena Proszewska, Michał Bujak,
Rafał Kucharski, Marek Śmieja, Jacek Tabor

Jagiellonian University, Kraków, Poland

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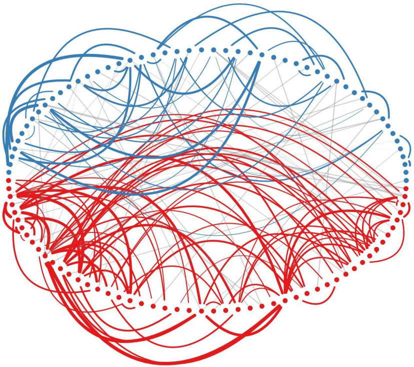
Aim of the study

We aim to **reduce virus spreading** in a system represented by the **graph** structure while **maintaining the highest utility** levels. Deep Epidemic Efficiency Network (DEEN) model:

- based on Graph Convolutional Neural Network with a novel loss function;
- outputs a graph partition maximising utility at a set epidemic threshold;
- applicable to real-life problems, validated against three scenarios;
- capable of maintaining close to the original utility with a great reduction in the spreading potential.

Method showcase

Ride-pooling service with 150 travellers in NYC. **Decomposition** of graph into **two clusters** resulted in **decrease of the performance 3%** and **increase in the epidemic threshold by 170%**.



Notation

- $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ - system: weighted, directed graph;
- $\mathbf{A} = (\mathbf{A}_{ij}) \in \mathrm{R}^{|\mathcal{V}| \times |\mathcal{V}|}$ - adjacency matrix with weights;
- $\Delta = (\Delta_{ij}) \in \{0, 1\}^{|\mathcal{V}| \times |\mathcal{V}|}$:

$$\Delta_{ij} = \begin{cases} 1, & \mathbf{A}_{ij} > 0 \\ 0, & \mathbf{A}_{ij} \leq 0. \end{cases}$$

- Decomposition $\mathcal{H}$ for $\mathcal{G}$ is a subgraph (i.e. $\mathcal{V}_{\mathcal{H}} = \mathcal{V}, \mathcal{E}_{\mathcal{H}} \subseteq \mathcal{E}$) consisting of disconnected components, i.e. $\mathcal{H} = \bigcup_{j \leq k} \mathcal{H}_j$ such that:
  - $\mathcal{V}_{\mathcal{H}} = \bigcup_{j \leq k} \mathcal{V}_{\mathcal{H}_j}$,
  - $\mathcal{E}_{\mathcal{H}} = \bigcup_{j \leq k} \mathcal{E}_{\mathcal{H}_j}$,
  - $\mathcal{V}_{\mathcal{H}_i} \cap \mathcal{V}_{\mathcal{H}_j} = \emptyset$ for $i \neq j$.

  The set of decompositions of graph $\mathcal{G}$ we denote as $\mathcal{D}(\mathcal{G})$.

Utility Function

Utility function **effectiveness of the** network **system** given by the graph. To ensure **applicability** of the algorithm to a variety of scenarios, we make the following assumption of the utility function:

1. may not have a closed-form analytical solution;
2. can be approximated with link weights;
3. is evaluated with an external (black-box) algorithm.

Following postulates by Dawar[1], we assume that the utility function $U : \mathcal{G} \to [0, +\infty)$ is **non-increasing** with respect to the **edge removal**, i.e.

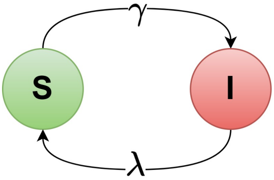
$$\mathcal{H} \subseteq \mathcal{G} \implies U(\mathcal{H}) \leq U(\mathcal{G}).$$

In particular,

$$\mathcal{H} \in \mathcal{D}(\mathcal{G}) \implies U(\mathcal{H}) \leq U(\mathcal{G}).$$

[1] Dawar, Bera, and Goyal, *High-utility itemset mining for subadditive monotone utility functions*

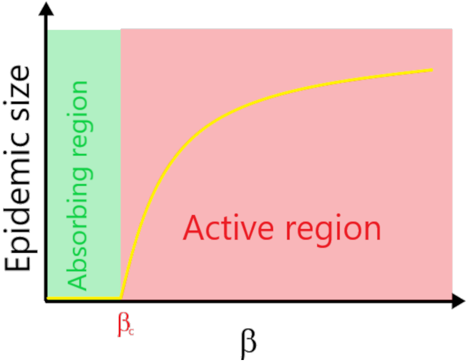
SIS model



- **S** - Susceptible
- **I** - Infected
- γ - Infection rate
- $\boldsymbol{\lambda}$ - Recovery rate

$\boldsymbol{\beta} = \gamma/\lambda$ - Effective transmission rate

We seek the critical effective transmission β_c rate where the epidemic is absorbed with time.



Epidemic threshold

The critical effective transmission depends on the topology of the graph. Hence, we denote it as $ET(\mathcal{G})$.
To account for the different nodes' degrees, we apply the heterogeneous mean-field approach. Following results by Wang[2], for a connected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$,

$$ET(\mathcal{G}) = \frac{\sum_{v \in \mathcal{V}} \deg(v)}{\sum_{v \in \mathcal{V}} \deg(v)^2}.$$

The considered graph $\mathcal{G}$ is not always connected. For the not connected graph $\mathcal{G}$, let $\mathcal{G} = \bigcup_{i \leq K} \mathcal{G}_i$, where $G_i = (\mathcal{V}_i, \mathcal{E}_i)$ is connected for $i \leq K$ and $\mathcal{G}_i \cap \mathcal{G}_j = \emptyset$ for $i \neq j$. We denote $C(\mathcal{G}) = \{\mathcal{G}_i : i \leq K\}$. Then,

$$ET(\mathcal{G}) = \sum_{i \leq K} \frac{|\mathcal{V}_i|}{|\mathcal{V}|} ET(\mathcal{G}_i).$$

[2] Wang et al., "Unification of theoretical approaches for epidemic spreading on complex networks"

Optimisation problem

Input:

- weighted graph $\mathcal{G}$;
- target epidemic threshold β_c;
- utility function U (unknown to us).

Output:

Decomposition $\mathcal{H}_{\max} \in \mathcal{D}(\mathcal{G})$ defined as:

$$\begin{aligned} \max_{\mathcal{H} \in \mathcal{D}(\mathcal{G})} \quad & U(\mathcal{H}), \\ \text{s.t.} \quad & ET(\mathcal{H}) \geq \beta_c. \end{aligned} \tag{1}$$

Model architecture

The framework is realised using **Graph Convolutional Neural Networks** (GCNN) (Kipf and Welling[3]) with the **output** later defines by the **softmax**.
To include information about the node features itself, we modify the weight matrix before passing to the GCNN:

$$\widehat{\mathbf{A}} = \mathbf{A} + \delta \mathbf{I},$$

where $\delta \in \mathbb{R}_+$ (as suggested by Lampert[4]). The GCNN returns the assignment matrix $\mathbf{S} \in \mathbb{R}^{|\mathcal{V}| \times K}$:

$$\mathbf{S} = \mathrm{softmax}(\mathrm{GCNN}(\widehat{\mathbf{A}})),$$

where $K \in \mathbb{N}_+$ is the resulting number of clusters.
Unlike Kipf and Welling, we do experience over-smoothing, hence we do not apply Laplacian normalisation.

[3] Kipf and Welling, *Semi-Supervised Classification with Graph Convolutional Networks*

[4] Lampert and Scholtes, *The Self-Loop Paradox: Investigating the Impact of Self-Loops on Graph Neural Networks*

Loss function

We construct the loss function so to incorporate three factors:

- utility maximisation;
- epidemic threshold maximisation;
- prevent degenerate solutions.

Utility loss

Motivation:

1. represent system performance;
2. differentiable;
3. quickly and analytically computable;
4. be generally applicable.

Reasons 2, 3 and 4 encouraged us to propose a formula which does not include the exact utility formulation in a given problem. Furthermore, our algorithm can find a solution in a setting where the true utility function is unknown.

Utility loss formula

Let $S = [s_i]^T_{i \leq |\mathcal{V}|}$. $s_i \in \mathbb{R}^K$ represents cluster assignment of i-th node.

$$\mathcal{L}_u(\mathbf{S}; \mathbf{A}) = \frac{1}{|\mathcal{V}|} \sum_{i=1}^{|\mathcal{V}|} \sum_{j=1}^{|\mathcal{V}|} a_{ij} (1 - s_i s_j^T)$$

$\mathcal{L}_u(\mathbf{S}; \mathbf{A})$ forces nodes connected by an edge of high weight to be in the same cluster.

$$\mathcal{L}_u(\mathbf{S}; \mathbf{A}) = \frac{1}{|\mathcal{V}|} \mathbf{e}^T (\mathbf{A} \odot (\mathbf{e}\mathbf{e}^T - \mathbf{S}\mathbf{S}^T))\mathbf{e},$$

where $\odot$ denotes element-wise multiplication.
Proper (local) manipulation of the graph edges' weights additionally prevents the creation of isolated nodes.

Virus spreading loss

We aim to **maximise the epidemic threshold**. Softmax is a continuous assignment, hence we approximate the nodes' degree in the continuous form too.

$$d_i = \sum_{j=1}^{|\mathcal{V}|} \sum_{k=1}^{K} \Delta_{ij} \cdot s_{ik} \cdot s_{jk}$$

$$\mathbf{d} = \text{diag}(\Delta^T \mathbf{S}\mathbf{S}^T)$$

Then, we define the virus spreading loss for a connected graph as

$$\mathcal{L}_{vs}(\mathbf{S}; \mathbf{A}) = -\frac{\|\mathbf{d} + \mathbf{e}\|_1}{\|\mathbf{d} + \mathbf{e}\|_2^2}.$$

Virus spreading loss

$$\mathcal{L}_{vs}(\mathbf{S};\mathbf{A}) = -\frac{\|\mathbf{d}+\mathbf{e}\|_1}{\|\mathbf{d}+\mathbf{e}\|_2^2}$$

Presence of $\mathbf{e}$ (self-loop with weight 1) prevents $\mathcal{L}_{vs} \xrightarrow{d\to 0} -\infty$.
For graph $\mathcal{G}$ comprised of $C(\mathcal{G})$ connected components,

$$\mathcal{L}_{vs}(\mathbf{S};\mathbf{A}) = \sum_{(\mathcal{V}_i,\mathcal{E}_i)\in C(\mathcal{G})} \frac{|\mathcal{V}_i|}{|\mathcal{V}|}\mathcal{L}_{vs}(\mathbf{S}^{(i)};\mathbf{A}^{(i)}),$$

where $\mathbf{S}^{(i)}$ and $\mathbf{A}^{(i)}$ represent the assignment and weight matrices for the graph $\mathcal{G}_i$, respectively.

Collapse regularisation

Collapse regularisation proposed by Tsitsulin[5]:

- prevents the trivial decomposition;
- otherwise the algorithm finds local minima (empty clusters) that trap the gradient;
- does not dominate optimisation of the main objective.

Let $||A||_F = \sqrt{\sum_{i \leq m, j \leq n} |a_{ij}|^2}$ denote the Frobenius norm.

$$\mathcal{R}_c(\mathbf{S}) = \frac{\sqrt{K}}{|\mathcal{V}|} \left\| \sum_i \mathbf{S}_i^\top \right\|_F - 1$$

[5] Tsitsulin et al., *Graph Clustering with Graph Neural Networks*

Final loss formula

$$\mathcal{L}_{DEEN}(\mathbf{S};\mathbf{A}) = \mathcal{L}_u(\mathbf{S};\mathbf{A}) + \lambda\mathcal{L}_{vs}(\mathbf{S};\mathbf{A}) + \mathcal{R}_c(\mathbf{S})$$

- λ balances virus spreading and performance;
- high λ prioritise epidemic prevention;
- low λ favours performance;
- in all our experiment we recognised $\lambda = 0.4$ as the optimal level.

Solving optimisation problem

To conduct calculation we need to fix the number of clusters:

- large number yield more components, hence lowering the transmission;
- small number helps to maintain connectivity required for better performance.

To find the optimal level for a target epidemic threshold, we conduct a binary search to find the least number of clusters that exceeds the given level. For technical reasons, we also apply the maximum number of clusters which we consider as a hyperparameter.

Modularity

For an adjacency matrix A of an undirected graph $\mathcal{G}$ with n nodes and m edges, cluster assignments $c_1, \ldots, c_n$,

$$\mathcal{Q} = \frac{1}{2m} \sum_{ij} [\mathbf{A}_{ij} - \frac{d_i d_j}{2m}] \delta(c_i, c_j).$$

Greedy algorithms:

- progressive by Clauset-Newman-Moore[6];
- regressive by Girvan-Newman[7].

[6] Clauset, Newman, and Moore, "Finding community structure in very large networks"

[7] Newman, "Fast algorithm for detecting community structure in networks"

Baselines

Another analytical approach is **spectral clustering**. Vectors associated with positive eigenvalues of spectrum of the graph Laplacian point to minimal cuts.

GNN baselines:

- MinCutPool[8]: approximate the minimum K-cut;
- Just Balance GNN[9]: minimise local quadratic variation;
- DMoN[10]: maximise modularity.

[8] Bianchi, Grattarola, and Alippi, *Spectral Clustering with Graph Neural Networks for Graph Pooling*

[9] Bianchi, "Simplifying Clustering with Graph Neural Networks"

[10] Tsitsulin et al., *Graph Clustering with Graph Neural Networks*

Hyperparameters

For each experiment we use the same architecture and nearly the same hyperparameters.

- 3 non-normalised graph convolutional layers, 1 dense layer;
- ReLU activation after each layer;
- Adam optimiser with learning rate 0.001;
- train till convergence (2000 epochs);
- maximum number of clusters: $\frac{n}{2}$ for transportation experiment, 32 otherwise (for larger graphs).

Three cases

In the experimental part, we analyse three potential real-world applications.

1. **Ride-pooling**: We limit potential combinations of travellers who can share a ride. Our goal is to minimise the pandemic risk while maintaining benefits associated with the ride-pooling service.
2. **Country regions**: Given the region map of Poland, we seek an optimal decomposition (cross-regional lockdown) such that the business and educational exchange is unimpeded, while the pandemic risk is reduced.
3. **Peer-to-peer**: For Gnutella P2P file sharing network, we aim to minimise the computer virus infection risk while maintaining high connectivity between peers.

Case I: Ride-pooling

Setting: Ride-pooling is a transportation service similar to standard taxi, with an additional perk that travellers share parts of their trips. The spatio-temporal distribution of travellers' requested trips creates a compatibility graph, where travellers of similar origin-destination paths (and time) are connected.
Aim: Decompose the compatibility graph in a manner such that the vehicle mileage reduction is maximised and the epidemic threshold is exceeded.
Edge weights:

$$w(v,u) = \frac{d(v) + d(u) - d(v,u)}{d(v) + d(u)},$$

$d(v,u)$ - vehicle mileage when u and v travel together, $d(u)$ - distance when u travels alone.
True utility: External black-box[11].

[11] For creation of the compatibility and utility we rely on Kucharski and Cats, "Exact matching of attractive shared rides (ExMAS) for system-wide strategic evaluations".

Case II: Country regions

Setting: We represent a map of 3000 regions of Poland as a graph, where neighbouring regions are connected. Each region is characterised by its population.
Aim: Optimise an optimal cross-regional lockdown such that the work and education exchange between regions remains stable and the risk of pandemic is reduced.
Edge weights:

$$w(v,u) = \left(\frac{p(v)}{2 \cdot \max_{w \in \mathcal{N}(u)} p(w)} + \frac{p(u)}{2 \cdot \max_{w \in \mathcal{N}(v)} p(w)} \right).$$

True utility: We follow the accessibility formulas by Levison[12]:

$$U(v, \mathcal{R}_v) = \sum_{u \in \mathcal{R}_v / \{v\}} \frac{p(v) \cdot p(u)}{d(u,v)},$$

where $p(u)$ is the population, $d(u,v)$ denotes distance between centres of regions and $\mathcal{R}_v$ denotes regions reachable from v.

[12] Levinson, "Accessibility and the journey to work"

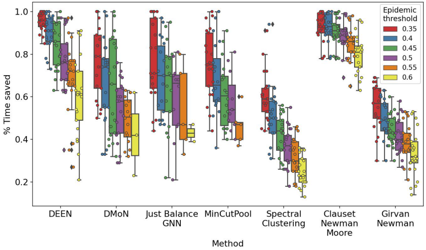
Case III: P2P network

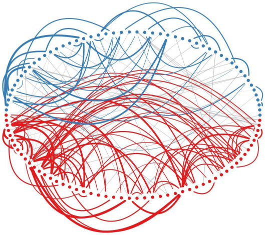
Setting: Gnutella peer-to-peer file sharing snapshots create a vast network. We assume hosts are prone to computer viruses spread via the network.
Aim: Maintain possibly many connections while reducing the risk of computer virus spreading.
Edge weights:

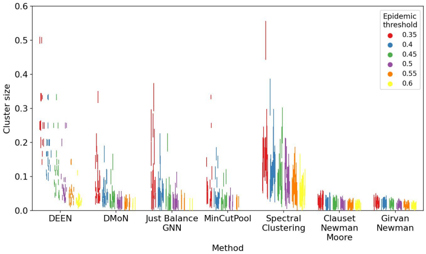
$$w(v,u) = \frac{1}{2 \cdot deg(v)} + \frac{1}{2 \cdot deg(u)}.$$

True utility: The fraction of preserved edges.

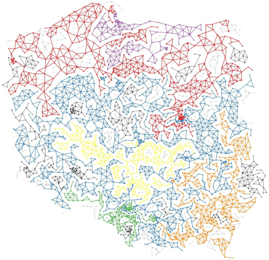
Case I: Ride-pooling



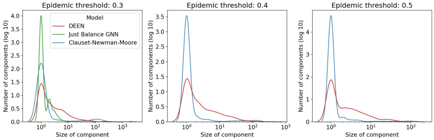




Case II: Regions in Poland

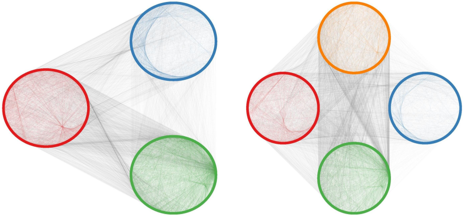


Epidemic threshold	0.3	0.4	0.5
DEEN	0.37	0.36	0.28
DmoN	-	-	-
Just Balance GNN	0.61	-	-
MinCutPool	-	-	-
Clauset-Newman-Moore	0.31	0.29	0.26



Case III: P2P Network

	Utility			Clusters size (AVG $\pm$ SD)		
Epidemic threshold	0.4	0.5	0.6	0.4	0.5	0.6
DEEN	0.38	0.28	0.22	0.25 ± 0.01	0.17 ± 0.01	0.14 ± 0.01
DMoN	0.53	0.43	–	0.36 ± 0.09	0.29 ± 0.08	–
Just Balance GNN	0.59	0.39	–	0.42 ± 0.02	0.28 ± 0.06	–
MinCutPool	0.76	–	–	0.47 ± 0.13	–	–
Clauset-Newman-Moore	0.33	0.26	0.22	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00



Ablation study