Machine learning of percolation models using graph convolutional neural networks

Hua Tian,1 Lirong Zhang,1 Youjin Deng,3,4,5,∗ and Wanzhou Zhang2,3,6,†

1College of Information and Computer, Taiyuan University of Technology, Taiyuan 030024, China
2College of Physics, Taiyuan University of Technology, Shanxi 030024, China
3Hefei National Laboratory for Physical Sciences at the Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei 230026, China
4Shanghai Research Center for Quantum Sciences, Shanghai 201315, China
5MinJiang Collaborative Center for Theoretical Physics, College of Physics and Electronic Information Engineering, Minjiang University, Fuzhou 350108, China
6CAS Key Laboratory for Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China

(Dated: July 8, 2022)

Percolation is an important topic in climate, physics, materials science, epidemiology, finance, and so on. Prediction of percolation thresholds with machine learning methods remains challenging. In this paper, we build a powerful graph convolutional neural network to study the percolation in both supervised and unsupervised ways. From a supervised learning perspective, the graph neural network simultaneously and correctly trains data of different lattice types, such as the square and triangular lattices. For the unsupervised perspective, combining the graph convolutional neural network and the confusion method, the percolation threshold can be obtained by the “W” shaped performance. The finding of this work opens up the possibility of building a more general framework that can probe the percolation-related phenomenon.

Introduction.— More than half a century ago, S.R. Broadbent and J.M. Hammersley proposed the percolation model[1]. It can help one understand physics [2], materials science [3], complex networks [4, 5], epidemiology [6], geology climate [7], quantum computation [8], and other fields [9, 10]. Many classical statistical physics models can be mapped to the correlated percolation models [11–15] in geometric perspectives. In 2016, M. Roger et al. and M. Troyer et al. successfully used neural networks (NN) to identify the different phases of both classical and quantum statistical matter[16, 17]. Since then, supervised machine learning (ML) methods have also been used to study a large number of phase transitions [18]. Meanwhile, attempts are being made to study the phase transition using unsupervised ML methods. These methods include principal component analysis methods [19], t-distributed stochastic neighbor embedding methods [20], diffusion mapping methods [21, 22], the confusion scheme [23] and auto-encoders [24].

For the percolation model, the supervised learning is able to predict the percolation threshold and determine critical exponents [25, 26]. However, by entering the occupied states of the site percolation, the NN cannot distinguish the lattice types that the configurations come from. In addition, for unsupervised learning, despite a great success application in correlated systems, such as the Ising model, however, it can not detect the percolation thresholds properly [27–30]. Specifically, an occupied state for the site percolation model is not percolating for the square lattice (a), but it can be percolating for the triangular lattice (b). A neural network (NN) is unable to distinguish between these two cases.

For the site percolation, the connection information between sites is an important factor in determining the percolation threshold and must be encoded in the training set. Otherwise, the NN is fed only the occupied states of sites and then cannot distinguish the different lattice structures. In addition, there is a spanning cluster in the system when percolation occurs, and percolation is a non-local feature that is difficult to be captured by a NN [30]. This problem may seem to simple, but the percolation model has many important applications in various fields and the solution to this problem is non-trivial.

The previous work [30] modified the input datasets of percolation configurations with well-characterized datasets, i.e., the diluted Ising model. In this paper, we choose another option, modifying not the dataset but the machine learning framework, that is, turning the NN into a more powerful graph convolutional neural network (GCN) [31]. GCN is a deep learning-based scheme that operates on a graph, in such a way that the graph encodes both the state of the site and the connection information.
The main idea of this work. (a) The three snapshots, graph representation containing sites \{v_i\} and \{e_{ij}\} and the embedding layer, (b) are the convolution and pooling layers, (c) are the full connection layer and the output layer. Supervised learning results in an ‘X’-shaped curve and unsupervised learning corresponds to a ‘W’-shaped neural network performance.

The GCN performs a convolution operation with the feature (usually a vector) of the surrounding nodes and the edges between the nodes, and then iteratively updates the feature information of each node. After \(l\) times of convolution, each node contains the feature of its \(l\)-order neighboring nodes, and the local features of the configuration are extracted.

The main highlights of this article are the following two points. (I) For supervised learning, we can build a more general framework, that can simultaneously determine percolation thresholds for different lattices, such as triangular lattices and square lattices. Datasets with different lattice structures can participate in the training simultaneously. Extending to other lattices is also straightforward and feasible. (II) For unsupervised learning, information about connections between sites is fed to the GCN and correlations between sites are captured to a large extent. Using the unsupervised method \[32\], we can get a percolation threshold that cannot be obtained by the NN unsupervised method \[30\]. In addition, technologically, we use state-of-the-art graph convolution and soft allocation of learnable pooling \[32\] to build our GCN.

The basic framework of the method. — Figure 2 shows the training process of a batch, consisting of the following three steps, (a) data input, (b) graph convolution and pooling and (c) output, respectively.

(a) Data input. In Figs. 2 (a1)-(a2), we generate the configurations and represent them as directed graphs. For site-percolation on a square lattice, the configuration is obtained via randomly occupying sites according to a certain probability \(p_i \in [p_{\min}, p_{\max}]\). Three snapshots are shown with the occupation probabilities \(p = 0.2, 0.593\) (percolation threshold) and 0.8 respectively. In the configuration, the sites are denoted as the nodes \{v_i\}, and the connections between sites are denoted as directed edges \({e_{v_i, v_j}}\), where \(i\) and \(j\) are the indexes of the sites. The feature of \(e_{v_i, v_j}\) can be marked by \(attr_{v_i, v_j}\) and it is assigned to 1, when the node \(v_i\) and node \(v_j\) are occupied at the same time; on the contrary, \(attr_{v_i, v_j}\) is assigned to 0. Figure 2 (a3) describes an embedding implemented by a small two-layer fully connected network. In the first layer, there are 2 neurons. The first neuron indicates the occupation status of the \(i\)-th node and the second indicates the occupation probability. These 2 neurons are then mapped to the second layer with more neurons. Their values are labeled as \(b_i^1\) (a vector), and are prepared for the next layer of graph convolution. The embedding is done in order to allow better performance of our training because the richer features are considered.

(b) Convolution and pooling. In Fig. 2 (b1), the convolution is performed and the basic idea is from Ref. \[33\]. GCN learns the features from neighboring nodes through the edges. The features of each node, \(b_i^1\), are updated by convolution of the features of neighboring nodes \(h_j^{(l-1)}\).
In Figs. 2 (b2), in a specified graph collapse way, a 3-layering module [32], based on the graph hierarchical pooling. In Fig. 2 (b2), the pooling is performed [32]. From a $3 \times 3$ graph, one obtains a super node, representing the feature of the whole graph.

(c) Output. In Fig. 2(c1), the final classification result is obtained by training the full connection neural network. In Fig. 2(c2), the results of the output neuron have an “X” shape output for supervised learning. For the unsupervised method, one determines the true $p_c$ by the position of the peak of “W” shaped performance [23]. The algorithm for a batch of training is shown in appendix I.

Convolution and pooling in more detail. In each convolution layer, the features on the neighboring nodes and edges are concatenated together, i.e., $z_{ij}^l = h_{vi}^l \oplus h_{v_j}^l \oplus \text{attr}_{vi,v_j}$, where $\oplus$ represents the concatenation operation. Then, the convolution is performed by [33],

$$m_{vi}^l = \sum_{v_j \in N(v_i)} \sigma(z_{ij}^l W_f^l + b_f^l) \odot g(z_{ij}^l W_s^l + b_s^l), \quad (1)$$

where $\{v_j | v_j \in N(v_i)\}$ represents the collection of adjacent nodes of node $v_i$, $W$ is the weight matrix and $b$ is the bias, $l \in \{1, 2, 3, \cdots\}$ represents the convolution of layer number, $\sigma(\cdot)$ is the sigmoid function $\sigma(x) = \frac{1}{1 + e^{-x}}$, $g(\cdot)$ is the softplus function $g(x) = \log(1 + e^x)$. Finally, the new feature $h_{vi}^{l+1}$ is updated by $h_{vi}^{l+1} = h_{vi}^l + m_{vi}^l$.

In the pooling layer, we use a differentiable graph pooling module [32], based on the graph hierarchical pooling. In Figs. 2 (b2), in a specified graph collapse way, a $3 \times 3$ graph becomes a new graph with $2 \times 2$ nodes and finally collapses to a super node. The way of graph collapse can be realized by a cluster assignment matrix $S \in R^{nk \times nk+1}$ is used and given by

$$S^{(k)} = \text{softmax} \left( \text{GCNConv}_{\text{pooling}} \left( A^{(k)}, X^{(k)} \right) \right), \quad (2)$$

where $X^{(k)}$ is the feature vector of the super node in the $k$-th pooling layer. The operator GCNConv used in pooling is from Ref. [34], its specific definition is as follows,

$$\text{GCNConv}_{\text{pooling}} : X^{k+1} = \hat{D}^{-\frac{1}{2}} \hat{A} \hat{D}^{-\frac{1}{2}} X^k \Theta, \quad (3)$$

where $\hat{A} = A + I$ denotes the adjacency matrix with inserted self-loops for the super-nodes and $\hat{D}_{ii} = \sum_{j=0} A_{ij}$ is diagonal degree matrix. $\Theta$ is the filter parameter matrix representing the probability that the node is assigned to any clusters (super nodes) for the next hierarchical pooling layer. Then, one has to calculate the feature $X^{(k+1)}$ and the adjacency matrix $A^{(k+1)}$ of the next layer, by the equations as follows,

$$X^{(k+1)} = S^{(k)}^T X^{(k)} \in R^{nk+1 \times d}, \quad (4)$$

$$A^{(k+1)} = S^{(k)}^T A^{(k)} S^{(k)} \in R^{nk+1 \times nk+1}. \quad (5)$$

In general, the iteration obeys the flow as in equation $A^{(k)}, X^{(k)} \xrightarrow{\text{GCN}} S^{(k)} \rightarrow A^{(k+1)}, X^{(k+1)}$.

Message passing. The previous operations of convolution and pooling are implemented based on the message passing mechanism [35], by which one can obtain information from “adjacent” nodes, and realize the “convolution” operation on the graph and aggregate the information of surrounding nodes. The message passing consists of the delivery and the readout steps. During the delivery step, the feature $h_{vi}^l$ of each node $v_i$ is updated according to Eq. 6 and Eq. 7 given by,

$$m_{vi}^l = \sum_{v_j \in N(v_i)} M_l(h_{vi}, h_{v_j}, e_{v_i,v_j}), \quad (6)$$

$$h_{vi}^l = U_l(h_{vi}^{l-1}, m_{vi}^l), \quad (7)$$

where $M_l(\cdot)$ is the aggregate function, and $U_l(\cdot)$ is the update function. In Figs. 3 (a) and (b), when $l = 1$, the site 13 absorbs messages from its four neighbors 12, 14, 8, and 18. At the same time, these neighbors also absorb information from their respective neighborhoods, i.e., $h_{vi}^l$ is replaced with $h_{vi}^0$. For the second iteration, $l = 2$, site 13 indirectly grabs information from the next nearest neighbors, connected by the dashed blue lines. In the readout stage, the function $R(\cdot)$ is used to calculate the feature vector of the whole graph as follows,

$$y = R(\{h_{vi}^l | v \in V(G)\}), \quad (8)$$

where $R(\cdot)$ sums features from all nodes and it can be some learnable differentiable function, for example, the pooling function.
Confusion method.— For the percolation controlled by \( p \), the configurations represented in graphs can be classified into percolating at \( p \geq p_c \) and non percolating \( p \leq p_c \). Therefore, if one separates the data with different \( p \) into two classes, the separation according to \( p_c \) results in the largest differences between the two classes, therefore leads to a high classification accuracy obtained by our GCN. The idea of the confusion method [23] here is to find such performance peaks, which is helpful to detect the percolation threshold. To perform this method, one has to prepare a dataset first. We divide the parameter range \( [p_{\text{min}}, p_{\text{max}}] \) into \( N_p \) parameters \( \{p_i\} \) and generate \( N_s \) configurations at each parameter \( p_i \). This gives us totally \( N = N_p \times N_s \) configurations. Then, one can make the trial labels and perform training and testing. The \( p_i \) is chosen as the trial threshold for generating trial labels, and all graphs generated with \( p_j < p_i \) are specified as the label 0, and the rest are specified as label 1. One repeats the previous two operations with all trial thresholds \( \{p_i\} \) in the range \( [p_{\text{min}}, p_{\text{max}}] \), and would output the performance curve as expected. A binary classification GCN as shown in Fig. 2.

Results.— Our first idea is to build a general GCN that can predict the percolation thresholds of different lattices simultaneously, i.e., we train the GCN using the input graphs with a fixed number of nodes but different numbers of edges simultaneously, which is impossible for a NN. To test and validate the idea, we first study site percolation models on the triangular and square lattices using supervised machine learning methods.

The results are shown in Fig. 4 (a). We see the two “X” shaped outputs for triangular lattices (TL) and square lattices (SL). The lattice sizes are \( L = 8, 12, 16, 20 \), respectively. In the training dataset, 100 configurations are generated for each lattice type (SL, TL) under each \( p_i \). The data set of different lattice types but the same size of configurations are fed into the same neural network to participate in training. The same network, however, can predict the thresholds on different types of lattices simultaneously, which is impossible to achieve with non-graph networks. The obtained threshold is 0.488(2) for the TL and 0.58(1) for the SL by the inset in Fig. 4 (a). The accuracy can continue to be improved by better training of the neural network. We also test the bond percolation and the predictions are also acceptable, but not shown.

The second idea is to predict the percolation threshold using unsupervised learning. In Fig. 4(b), using the confusion method [23, 29, 30], we obtain the performance with the “W” shape. In these datasets, there are 100 -1000 configurations per \( p_i \) with \( p_i \in [0, 1] \) interval of 0.1. The lines are the real data, which is the average of 20 bins. The colorful bands also mark the error bars. The location of the peak of the “W” shaped curve is the percolation threshold, which is around \( p_c = 0.593 \). In the simulation, to get a better result for the confusion method, in addition to putting \( p_i \) in the embedding, we also put degree centrality in the feature for each node in the embedding, which is defined as

\[
dc = \frac{\text{degree}(v_i)}{(n_{\text{total}} - 1)},
\]

where \( \text{degree}(v_i) \) is the degree of the node \( v_i \), \( n_{\text{total}} \) is the total number of nodes. The features such as properties of edges, occupation probability, and degree centrality make the network perform better.

Conclusion and Outlook.— In conclusion, using the advantages of graph neural networks, we have solved a difficult problem since the year 2017 [23, 25–27, 29, 30]. The NN can not distinguish the different structures of lattices if the site status are fed. Fortunately, the GCN captures the information about the connections between the sites, as well as global features like lattice percolation. We show a possibility that the GCN can act as a general framework that can simultaneously detect the percolation threshold on different lattices in a supervised manner. The intersection in the “X” shaped output curves
is the critical point. For unsupervised machine learning, the position of the “W”-shaped performance also reflects the predicted percolation threshold well. At the technical level, we build a graph neural network suitable for lattice statistical physical models such as the percolation model. Our work is helpful for the extension of GCN to many percolation-related topics. Further, we build a more general neural network to train physical systems with fixed nodes but different topologies.

Acknowledgments We thank for the valuable discussion from Tzu-Chieh Wei about the confusion method, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions. W.Z. was supported by the Hefei National Research Center for Physical Sciences at the Microscale (KF2021002), and Peng Huanwu Center’s Visiting Scientist Program for 2022 by Institute of Theoretical Physics, Chinese Academy of Science, Beijing. L.Z. and H.T. were supported by NSFC under Grant No. 11625522, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions. W.Z. was supported by the Visiting Scientist Program for 2022 by Institute of Theoretical Physics, Chinese Academy of Science, Beijing. L.Z. and H.T. were supported by NSFC under Grant No. 11625522, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions. W.Z. was supported by the Visiting Scientist Program for 2022 by Institute of Theoretical Physics, Chinese Academy of Science, Beijing. L.Z. and H.T. were supported by NSFC under Grant No. 11625522, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions. W.Z. was supported by the Visiting Scientist Program for 2022 by Institute of Theoretical Physics, Chinese Academy of Science, Beijing. L.Z. and H.T. were supported by NSFC under Grant No. 11625522, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions. W.Z. was supported by the Visiting Scientist Program for 2022 by Institute of Theoretical Physics, Chinese Academy of Science, Beijing. L.Z. and H.T. were supported by NSFC under Grant No. 11625522, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions. W.Z. was supported by the Visiting Scientist Program for 2022 by Institute of Theoretical Physics, Chinese Academy of Science, Beijing. L.Z. and H.T. were supported by NSFC under Grant No. 11625522, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions. W.Z. was supported by the Visiting Scientist Program for 2022 by Institute of Theoretical Physics, Chinese Academy of Science, Beijing. L.Z. and H.T. were supported by NSFC under Grant No. 11625522, and also thank Junyin Zhang, Bo Zhang and Longxiang Liu for useful discussions.

*Corresponding author: yjdeng@ustc.edu.cn
†Corresponding author: zhangwanzhou@tyut.edu.cn

[1] S. Broadbent and J. M. Hammersley, Percolation processes. i. crystals and mazes (1957).
[2] R. G. Larson, L. E. Scriven, and H. T. Davis, Percolation theory of residual phases in porous media, Nature 268, 409 (1977).
[3] K. P. Krishnaraj and P. R. Nott, Coherent force chains in disordered granular materials emerge from a percolation of quasilinear clusters, Phys. Rev. Lett. 124, 198002 (2020).
[4] O. Riordan and L. Warnke, Explosive Percolation Is Continuous, Science 333, 322 (2011).
[5] M. Li, R.-R. Liu, L. Liu, M.-B. Hu, S. Xu, and Y.-C. Zhang, Percolation on complex networks: Theory and application, Physics Reports 907, 1 (2021), percolation on complex networks: Theory and application.
[6] M. E. J. Newman, Spread of epidemic disease on networks, Phys. Rev. E 66, 016128 (2002).
[7] J. Fan, J. Meng, Y. Ashkenazy, S. Havlin, and H. J. Schellnhuber, Climate network percolation reveals the expansion and weakening of the tropical component under global warming, Proceedings of the National Academy of Sciences 115, E12128 (2018), https://www.pnas.org/doi/pdf/10.1073/pnas.1811068115.
[8] M. Pant, D. Towsley, D. Englund, and S. Guha, Percolation thresholds for photonic quantum computing, Nature Communications 10, 1070 (2019).
[9] X. Feng, Y. Deng, and H. W. J. Blöte, Percolation transitions in two dimensions, Phys. Rev. E 78, 031136 (2008).
[10] W. Huang, P. Hou, J. Wang, R. M. Ziff, and Y. Deng, Critical percolation clusters in seven dimensions and on a complete graph, Phys. Rev. E 97, 022107 (2018).
[11] C. M. Fortuin and P. W. Kasteleyn, On the random-cluster model: I. Introduction and relation to other models, Physica 57, 536 (1972).
[12] C. Fortuin, On the random-cluster model ii. the percolation model, Physica 58, 393 (1972).
[13] M. E. Fisher, Magnetic critical point exponents—their interrelations and meaning, J. Appl. Phys. 38, 981 (1967).
[14] A. Coniglio and W. Klein, Clusters and Ising critical droplets: a renormalisation group approach, J. Phys. A Math. Theor. 13, 2775 (1980).
[15] C.-K. Hu, Percolation, clusters, and phase transitions in spin models, Phys. Rev. B 29, 5103 (1984).
[16] J. Carrasquilla and R. G. Melko, Machine learning phases of matter, Nature Physics 13, 431 (2017).
[17] G. Carleo and M. Troyer, Solving the Quantum Many-Body Problem with Artificial Neural Networks, Science 355, 602 (2017), arXiv:1606.02318 [cond-mat, physics:quant-ph].
[18] G. Carleo, I. Cirac, K. Cranmer, L. Daudet, M. Schuld, N. Tishby, L. Vogt-Maranto, and L. Zdeborová, Machine learning and the physical sciences, Rev. Mod. Phys. 91, 045002 (2019).
[19] L. Wang, Discovering phase transitions with unsupervised learning, Phys. Rev. B 94, 195105 (2016).
[20] L. van der Maaten and G. Hinton, Visualizing data using t-sne, Journal of Machine Learning Research 9, 2579 (2008).
[21] J. F. Rodriguez-Nieva and M. S. Scheurer, Identifying topological order through unsupervised machine learning, Nat. Phys. 15, 790 (2019).
[22] M. S. Scheurer and R.-J. Slager, Unsupervised machine learning and band topology, Phys. Rev. Lett. 124, 226401 (2020).
[23] E. P. L. Van Nieuwenburg, Y.-H. Liu, and S. D. Huber, Learning phase transitions by confusion, Nat. Phys. 13, 435 (2017).
[24] J. Shen, W. Li, S. Deng, and T. Zhang, Supervised and unsupervised learning of directed percolation, Phys. Rev. E 103, 052140 (2021).
[25] W. Zhang, J. Liu, and T.-C. Wei, Machine learning of phase transitions in the percolation and XY models, Physical Review E 99, 032142 (2019).
[26] D. Bayo, A. Honecker, and R. A. Römer, Machine learning the 2d percolation model, Journal of Physics: Conference Series 2207, 012057 (2022).
[27] S. Cheng, F. He, H. Zhang, K.-D. Zhu, and Y. Shi, Machine learning percolation model, arXiv preprint arXiv:2101.08928 (2021).
[28] W. Zhang, J. Liu, and T.-C. Wei, Machine learning of phase transitions in the percolation and XY models, Phys. Rev. E 99, 032142 (2019).
[29] R. Xu, W. Fu, and H. Zhao, A new strategy in applying the learning machine to study phase transitions, arXiv preprint arXiv:1901.00774 (2019).
[30] J. Zhang, B. Zhang, J. Xu, W. Zhang, and Y. Deng, Machine learning for percolation utilizing auxiliary Ising variables, Physical Review E 105, 024144 (2022).
[31] J. Zhou, G. Cui, S. Hu, Z. Zhang, C. Yang, Z. Liu, L. Wang, C. Li, and M. Sun, Graph neural networks: A review of methods and applications, AI Open 1, 57 (2020).
[32] R. Ying, J. You, C. Morris, X. Ren, W. L. Hamilton, and J. Leskovec, Hierarchical Graph Representation Learning with Differentiable Pooling, arXiv:1806.08804 [cs, stat]
Algorithm 1 A batch of training

Initialize conv_num=L; pool_num=k; len_G=|V|
Input: percolation snapshots
Output: Category probability \( p_1, p_2 \)

1: data input
   Generate percolation graph representation \( G \)
   \( \forall i, j \), Initialize \( \{v_i|v_i \in V(G)\}, \{e_{ij}|e_{ij} \in E(G)\}\)
   \( \forall i, j \), use FCN to get new node embedding \( h^0_{v_i} \)

2: data processing
   for num=0 to conv_num do:
      \( \forall i, j \), \( z^l_{v_i} = \text{concat}(h^l_{v_i}, h^l_{v_j}, e_{v_i,v_j}) \)
      \( h^l_{v_i} = h^{l-1}_{v_i} + \sum \sigma(\text{MLP}(z^l_{v_i})) \odot g(\text{MLP}(z^l_{v_i})) \)
   for len_G to 1 do:
      \( G^k = \text{DiffPool}(G^{k-1}) \)

3: data output
   \( p_1, p_2 = \text{Softmax}(\text{MLP}(G^k)) \)
end

II. AN EXAMPLE OF HARD CLUSTER NUMBER ASSIGNMENT

FIG. 5. Graph collapse example. A 9-node graph is collapsed into a 4-super-node graph. The three nodes (1, 2, 5) in blue become a super node. The nodes in the pink shadow, green shadow and yellow shadow are performed similarly

The matrix \( A \) and \( S \) are shown as follows,

\[
A^{(0)} = \begin{bmatrix}
0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \\
\end{bmatrix},
S^{(0)} = \begin{bmatrix}
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\end{bmatrix},
\]

where \( S_{ij} = 1 \) if and only if node \( i \) belongs to the cluster \( j \) or the super node \( j \). Using the transformation \( S^T A S \), one gets a new adjacency matrix \( A^{(1)} \) defined as

\[
A^{(1)} = S^{(0)T} A^{(0)} S^{(0)} = \begin{bmatrix}
4 & 3 & 5 & 0 \\
3 & 2 & 1 & 2 \\
5 & 1 & 4 & 2 \\
0 & 2 & 0 & 0 \\
\end{bmatrix},
\]

where 4, 3, 5 in the first row means the super node 1 is connected to the super nodes 1, 2, 3, which is consistent with the description in Fig. 5. \( A^{(1)} \) is an new adjacency matrix with weights.