Mean-field theory of graph neural networks in graph partitioning

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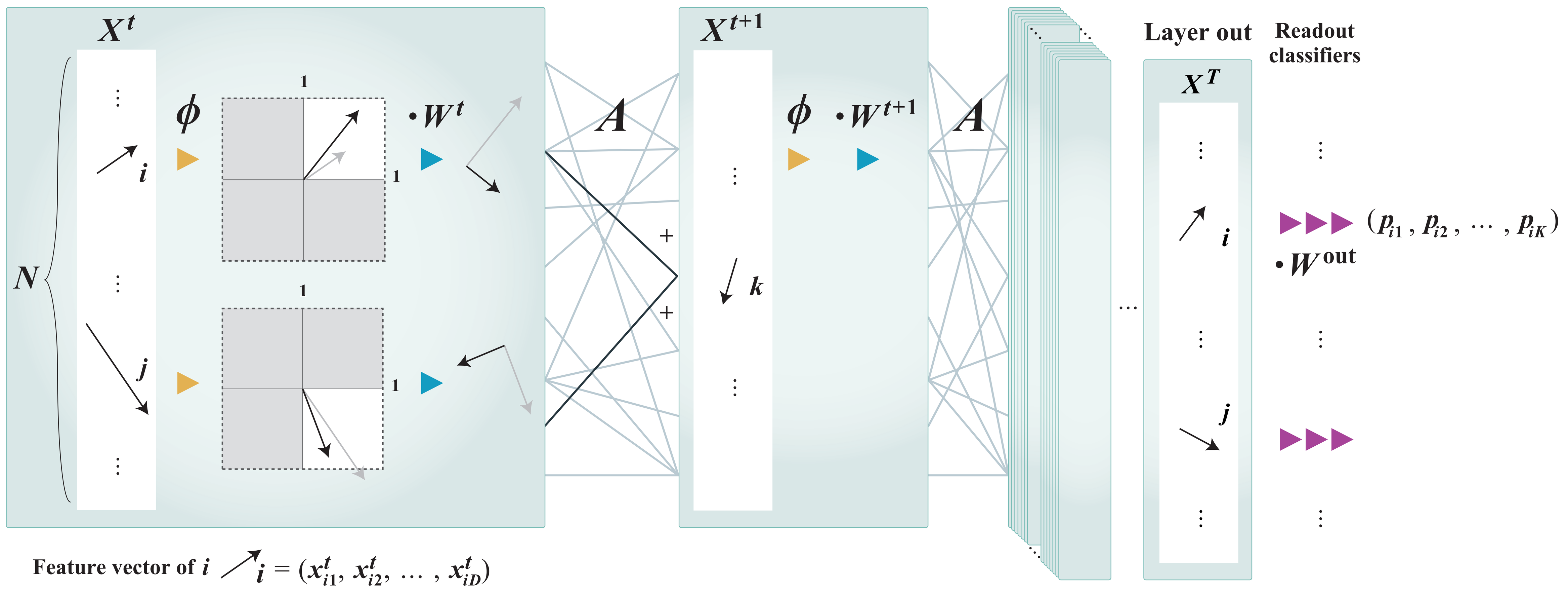
Background

When Graph Neural Networks (GNN) perform well, is it thanks to

- learning of model parameters (e.g., backprop.)? or
- architecture of the model (nonlinear structure + input graph) itself?

Question

For a simple graph partitioning problem, does a GNN already perform well without training?
Can we evaluate the performance analytically?



A *minimal* GNN (untrained)

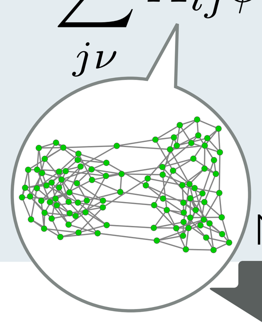
Random N×D matrix
$X^0 \equiv [x^0_{i\mu}]$

tanh(x)

$$x^{t+1}_{i\mu} = \sum_{j\nu} A_{ij}\phi\left(x^t_{j\nu}\right) W^t_{\nu\mu}$$

untrained GNN

Gaussian random matrix
$W^t_{\nu\mu} \sim \mathcal{N}(0, 1/D)$



N×N adjacency matrix

$X^T = [x^T_{i\mu}]$
Classify using the k-means

Classification of D-dim vectors

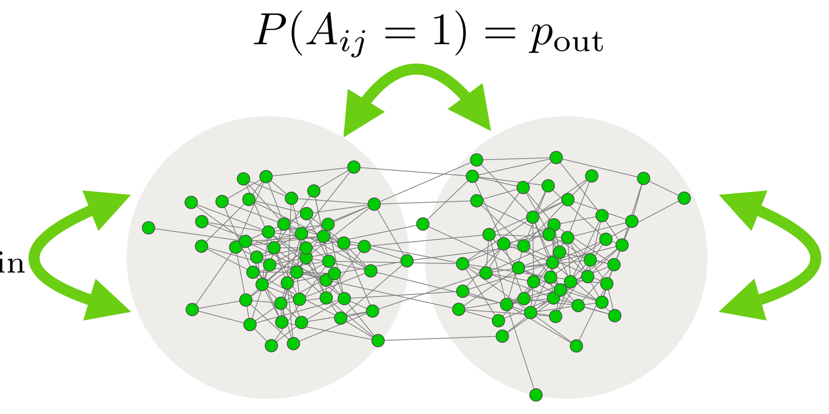
Stochastic block model inference

Graph partitioning

$|V| = N$

$P(A_{ij} = 1) = p_{\mathrm{out}}$

$P(A_{ij} = 1) = p_{\mathrm{in}}$



$P(A_{ij} = 1) = p_{\mathrm{in}}$

(equal-size groups)

c = average degree

$$\epsilon \equiv \frac{p_{\mathrm{out}}}{p_{\mathrm{in}}}$$

GNN is related to many other algorithms

$$x^{t+1}_{i\mu} = \sum_j M_{ij}\,\varphi\left(\sum_\nu \phi(x^t_{j\nu})W^t_{\nu\mu}\right) + b^t_{i\mu}$$

algorithm	domain	M	$\phi(x)$	$\varphi(x)$	W^t	b^t	$\{W^t, b^t\}$ update
untrained GNN	V	A	tanh	$I(x)$	random	omitted	not trained
trained GNN [KipfWelling2016]	V	$I-L$	ReLu	$I(x)$	trained	omitted	trained via backprop.
Spectral method	V	L	$I(x)$	$I(x)$	QR	/	updated at each layer
EM + BP	E	B	softmax	$\log(x)$	learned	learned	learned via M-step

Mean-field（Martin-Siggia-Rose formalism）

[A Crisanti, HJ Sommers, and H Sompolinsky, (1990)]

We introduce a group-wise (macroscopic) state variable.

$$\mathrm{x}^t_{\sigma\mu} \equiv (\gamma_\sigma N)^{-1} \sum_{i\in V_\sigma} x^t_{i\mu}$$

$\mathrm{x}^t = [\mathrm{x}^t_{\sigma\mu}]$ (2×D matrix)

$\sigma \in \{1, 2\}$ group label

The state equation

$$P(\mathrm{x}^{t+1}) = \left\langle \prod_{\sigma\mu} \delta\left(\mathrm{x}^{t+1}_{\sigma\mu} - \frac{1}{\gamma_\sigma N}\sum_{i\in V_\sigma}\sum_{j\nu} A_{ij}\phi(x^t_{j\nu})W^t_{\nu\mu}\right)\right\rangle_{A, W^t, X^t}$$

Averages w.r.t.

- graph(stochastic block model)
- $W^t_{\nu\mu} \sim \mathcal{N}(0, 1/D)$
- state in the previous layer *t*

Covariance matrix of x^t in the limit of T = ∞

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \qquad B = \frac{N}{4}\begin{pmatrix} p_{\mathrm{in}} & p_{\mathrm{out}} \\ p_{\mathrm{out}} & p_{\mathrm{in}} \end{pmatrix}$$

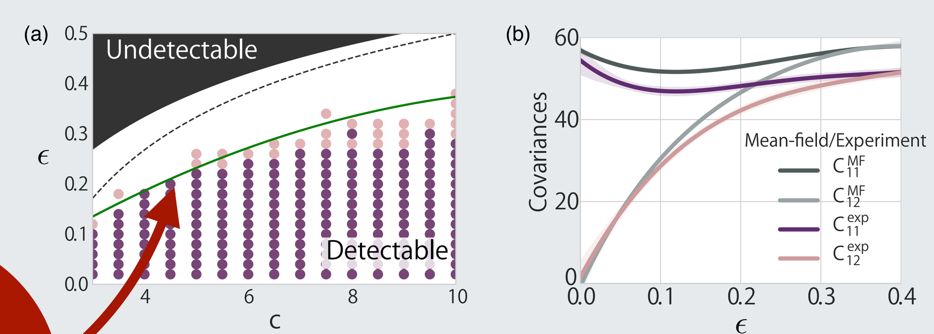
Self-consistent equation w. r. t. C

$$C_{\sigma\sigma'} = \frac{1}{\gamma_\sigma\gamma_{\sigma'}} \sum_{\tilde{\sigma}\tilde{\sigma}'} B_{\sigma\tilde{\sigma}}B_{\sigma'\tilde{\sigma}'} \int \frac{d\mathrm{x}\, \mathrm{e}^{-\frac{1}{2}\mathrm{x}^\top C^{-1}\mathrm{x}}}{(2\pi)^{\frac{N}{2}}\sqrt{\det C}}\, \phi(\mathrm{x}_{\tilde{\sigma}})\phi(\mathrm{x}_{\tilde{\sigma}'})$$

Numerical experiments

Comparison of the (*algorithmic*) *detectability limit estimates* between the mean-field result & numerical experiments

Behaviors of $C = [C_{\sigma\sigma'}]$



(algorithmic) detectability limit
The limit such that an algorithm cannot identify statistically significant groups.

$C_{11} \simeq C_{12}$
overlap ~ 0.5

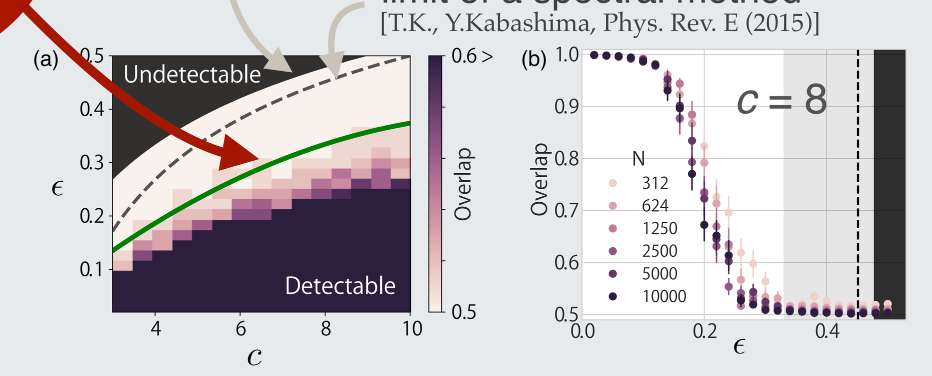
Mean-field estimate

information-theoretic limit
[E.Mossel, J.Neeman, and A.Sly, Probab. Theory Relat. Fields (2015)]

limit of a spectral method
[T.K., Y.Kabashima, Phys. Rev. E (2015)]

Behaviors of the overlaps

overlap = fraction of correctly classified vertices



Even a minimal GNN performs well, indeed.

A trained GNN

(This is not the only way, and probably not the best way.)

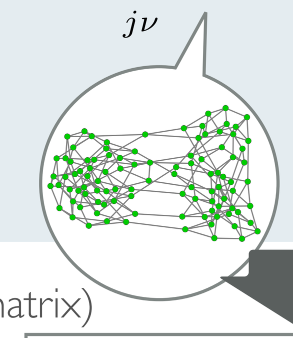
random N×D matrix
$X^0 \equiv [x^0_{i\mu}]$

tanh(x)

$$x^{t+1}_{i\mu} = \sum_{j\nu} A_{ij}\phi\left(x^t_{j\nu}\right) W^t_{\nu\mu}$$

trained GNN

Back prop.



N×N adjacency matrix

(D×2 matrix)

Read out classifier W^{out}

error function

learn from the “correct” label

normalized mutual information
error function

$$a_{i\sigma} = \sum_\mu x_{i\mu}W^{\mathrm{out}}_{\mu\sigma} \qquad p_{i\sigma} \equiv \mathrm{softmax}(a_{i\sigma})$$

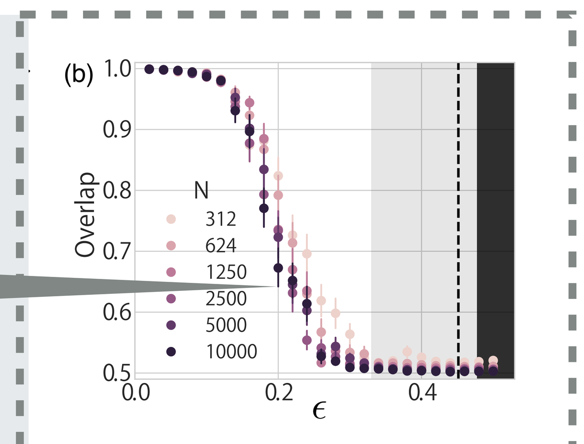
$$P_{\sigma\hat{\sigma}} = \frac{1}{N}\sum_{i=1}^N P(i\in V_\sigma, i\in V_{\hat{\sigma}}) = \frac{1}{N}\sum_{i\in V_\sigma} p_{i\hat{\sigma}},$$

$$P_\sigma = \sum_{\hat{\sigma}} P_{\sigma\hat{\sigma}} = \gamma_\sigma,$$

$$\mathrm{NMI}\left([P_{\sigma\hat{\sigma}}]\right) = 2\left(1 - \frac{\sum_{\sigma\hat{\sigma}} P_{\sigma\hat{\sigma}}\log P_{\sigma\hat{\sigma}}}{\sum_\sigma \gamma_\sigma\log\gamma_\sigma + \sum_{\sigma\hat{\sigma}} P_{\sigma\hat{\sigma}}\log\sum_\sigma P_{\sigma\hat{\sigma}}}\right)$$

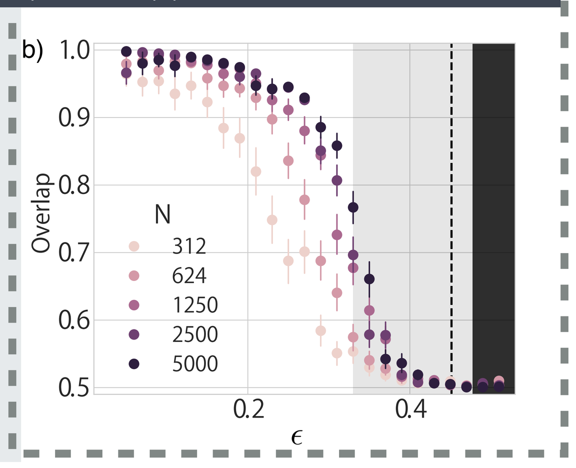
untrained GNN

Performance deteriorates because of the k-means.



The transition points appear to be the same…!

trained GNN



Chainer
+ Batch normalization
+ ResNet