Topics in Graph Deep Learning

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Table of Contents:

Permutation Invariant induced Representations

Consider the equivalence relation $\sim$ on $\mathbb{R}^{n\times d}$ indiced by the group of permutation S_n: for any $X, X' \in \mathbb{R}^{n\times d}$,

$$X \sim X' \quad \Leftrightarrow \quad X' = PX \ , \ \text{for some } P \in S_n$$

Let $\mathbb{M} = \mathbb{R}^{n\times d}/\sim$ be the quotient space endowed with the natural distance induced by Frobenius norm $\|\cdot\|_F$

$$d(\hat{X}_1, \hat{X}_2) = \min_{P\in S_n} \|X_1 - PX_2\|_F \quad , \quad \hat{X}_1, \hat{X}_2 \in \mathbb{M}.$$

Permutation Invariant induced Representations

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The Problem: Construct a Lipschitz embedding $\hat{\alpha} : \mathbb{M} \to \mathbb{R}^m$, i.e., an integer $m = m(n,d)$, a map $\alpha : \mathbb{R}^{n\times d} \to \mathbb{R}^m$ and a constant $L = L(\alpha) > 0$ so that for any $X, X' \in \mathbb{R}^{n\times d}$,

1. If $X \sim X'$ then $\alpha(X) = \alpha(X')$
2. If $\alpha(X) = \alpha(X')$ then $X \sim X'$
3. $\|\alpha(X) - \alpha(X')\|_2 \leq L\, d(\hat{X}, \hat{X}')$

Motivation (1)

Graph Learning Problems

Consider data graphs such as: social networks, transportation networks, citation networks, chemical networks, protein networks, biological networks, etc. Each such network is modeled as a (weighted) graph $(\mathcal{V}, \mathcal{E}, A)$ of n nodes, and a set of feature vectors $\{x_1^T, \cdots, x_n^T\} \subset \mathbb{R}^d$ that form the matrix $X = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} \in \mathbb{R}^{n \times d}$.

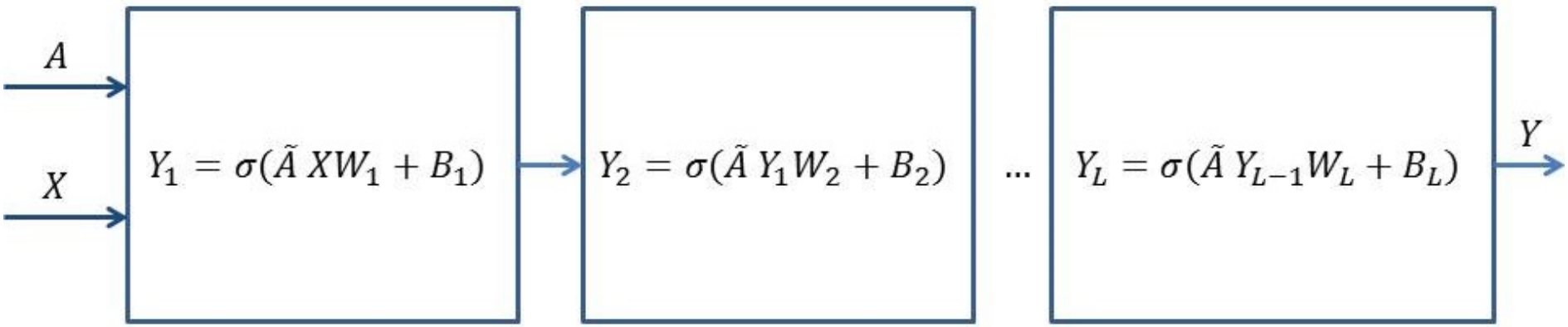
Two important problems involving a map $f : (A, X) \to f(A, X)$:

1. classification: $f(A, X) \in \{1, 2, \cdots, c\}$
2. regression/prediction: $f(A, X) \in \mathbb{R}$.

In each case we expect the task to be invariant to vertices permutation: $f(PAP^T, PX) = f(A, X)$, for every $P \in S_n$.

Motivation (2)

Graph Convolutive Networks (GCN), Graph Neural Networks (GNN)



GCN (Kipf and Welling ('16)) uses $\tilde{A} = I + A$, where A is the adjacency matrix, or the graph weight matrix; GNN uses $\tilde{A} = p(A)$, polynomial in adjacency matrix, or weight matrix. L-layer GCN has parameters $(p_1, W_1, B_1, \cdots, p_L, W_L, B_L)$.

Motivation (2)

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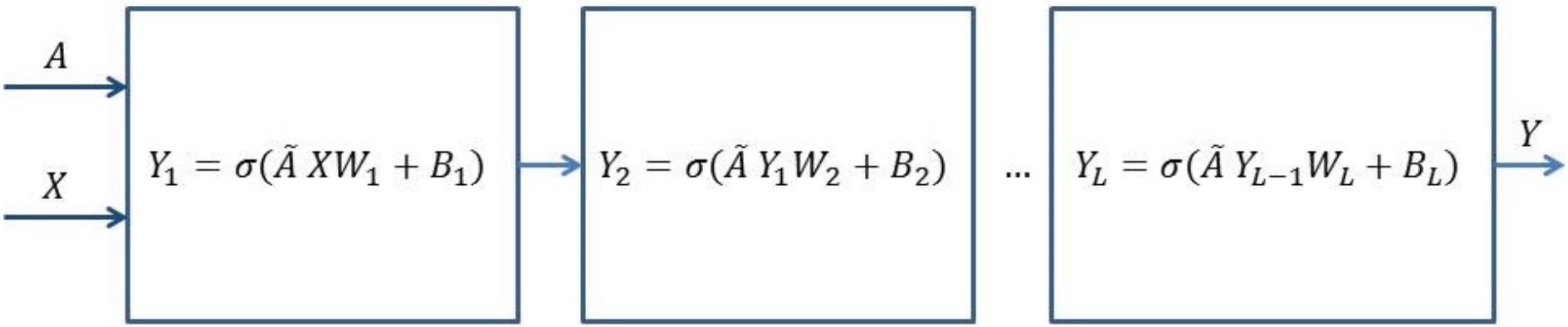

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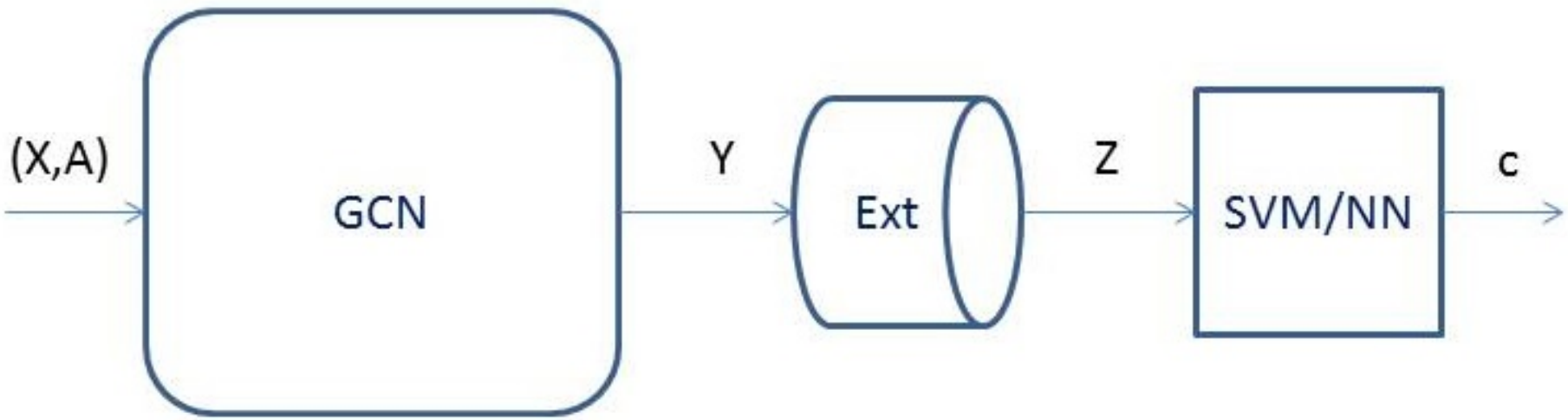
Note the *covariance property*: for any $P \in O(n)$ (including S_n), $(A, X) \mapsto (PAP^T, PX)$ and $B_i \mapsto PB_i$ then $Y \mapsto PY$.

Motivation (3)

Deep Learning with GCN

The two learning tasks (classification or regression) can be solved by the following scheme:



where *Ext* is a permutation invariant feature extractor, and SVM/NN is a single-layer or a deep neural network (Support Vector Machine or a Fully Connected Neural Network).

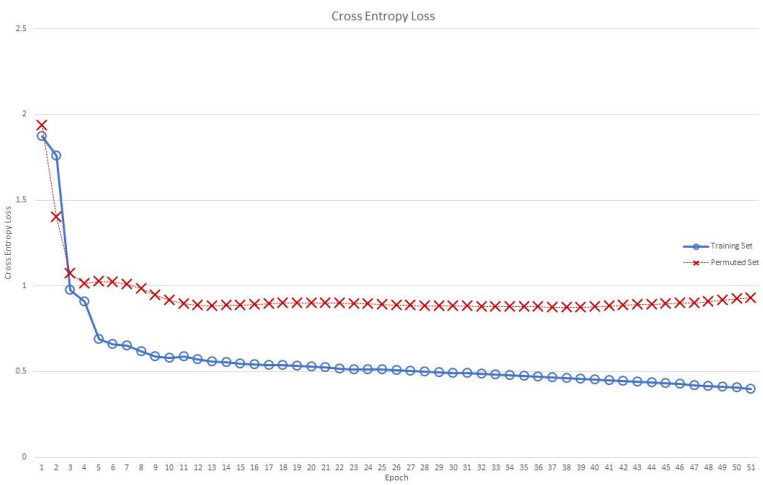
The purpose of this (part of the) talk is to analyze the *Ext* component.

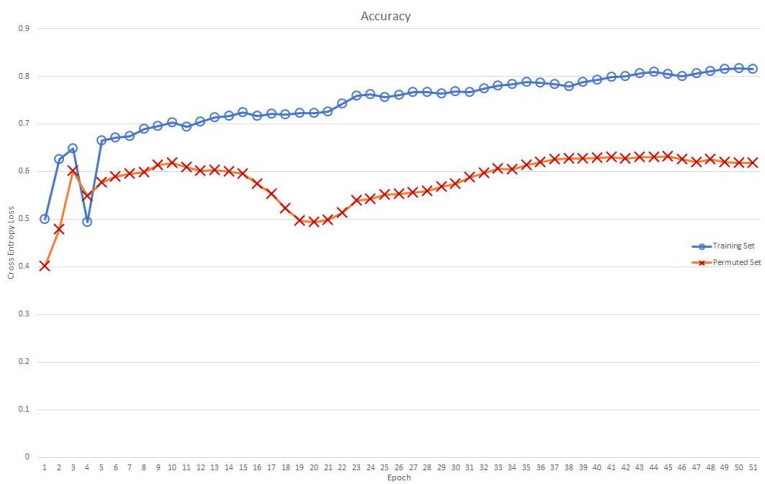
Motivation (4)

Enzyme Classification Example

Protein Dataset where task is classification into *enzyme* vs. *non-enzyme*.
Dataset: 450 enzymes and 450 non-enzymes.
Architecture (ReLU activation):

- GCN with $L = 3$ layers and $d = 25$ feature vectors in each layer;
- No Permutation Invariant Component: *Ext* = *Identity*
- Fully connected NN with dense 3-layers and 120 internal units.





The Measure Theoretic Embedding

First approach: Consider the map

$$\mu : \mathbb{M} \to \mathcal{P}(\mathbb{R}^d) \quad , \quad \mu(X)(x) = \frac{1}{n} \sum_{k=1}^{n} \delta(x - x_k)$$

where $\mathcal{P}(\mathbb{R}^d)$ denotes the convex set of probability measures over $\mathbb{R}^d$, and δ denotes the Dirac measure.
Clearly $\mu(X') = \mu(X)$ iff $X' = PX$ for some $P \in S_n$.

Main drawback: $\mathcal{P}(\mathbb{R}^d)$ is infinite dimensional!

Finite Dimensional Embeddings

Architectures

Two classes of extractors [Zaheer et.al.17' -'Deep Sets']:

1. Pooling Map – based on Max pooling
2. Readout Map – based on Sum pooling

Finite Dimensional Embeddings

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1. Pooling Map – based on Max pooling
2. Readout Map – based on Sum pooling

Intuition in the case $d = 1$:

Max pooling:

$$\lambda : \mathbb{R}^n \to \mathbb{R}^n \quad , \quad \lambda(x) = x^{\downarrow} := (x_{\pi(k)})_{k=1}^n \ , \ x_{\pi(1)} \geq x_{\pi(2)} \geq \cdots \geq x_{\pi(n)}$$

Finite Dimensional Embeddings

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Sum pooling:

$$\sigma : \mathbb{R}^n \to \mathbb{R}^n \quad , \quad \sigma(x) = (y_k)_{k=1}^n \ , \ y_k = \sum_{j=1}^n \nu(a_k, x_j)$$

where kernel $\nu : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, e.g. $\nu(a, t) = e^{-(a-t)^2}$, or $\nu(a = k, t) = t^k$.

Pooling Mapping Approach

Fix a matrix $R \in \mathbb{R}^{d\times D}$. Consider the map:

$$\Lambda : \mathbb{R}^{n\times d} \to \mathbb{R}^{n\times D} \equiv \mathbb{R}^{nD} \quad , \quad \Lambda(X) = \lambda(XR)$$

where λ acts columnwise (reorders monotonically decreasing each column). Since $\Lambda(\Pi X) = \Lambda(X)$, then $\Lambda : \widehat{\mathbb{R}^{n\times d}} \to \mathbb{R}^{n\times D}$.

Theorem

For any matrix $R \in \mathbb{R}^{n,d+1}$ so that any $n \times n$ submatrix is invertible, there is a subset $Z \subset \widehat{\mathbb{R}^{n\times d}}$ of zero measure so that $\Lambda : \widehat{\mathbb{R}^{n\times d}} \setminus Z \to \mathbb{R}^{n\times d+1}$ is faithful (i.e., injective).

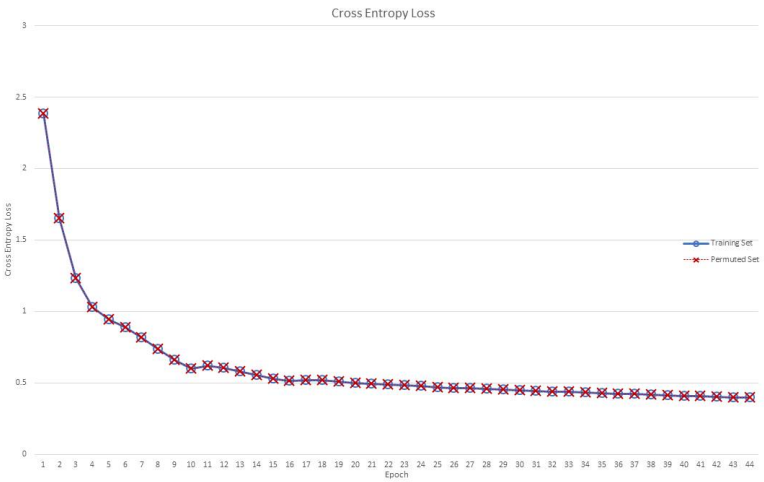
No known tight bound yet as to the minimum $D = D(n, d)$ so that there is a matrix R so that Λ is faithful (injective).
However, due to local linearity, if Λ is faithful (injective), then it is stable.

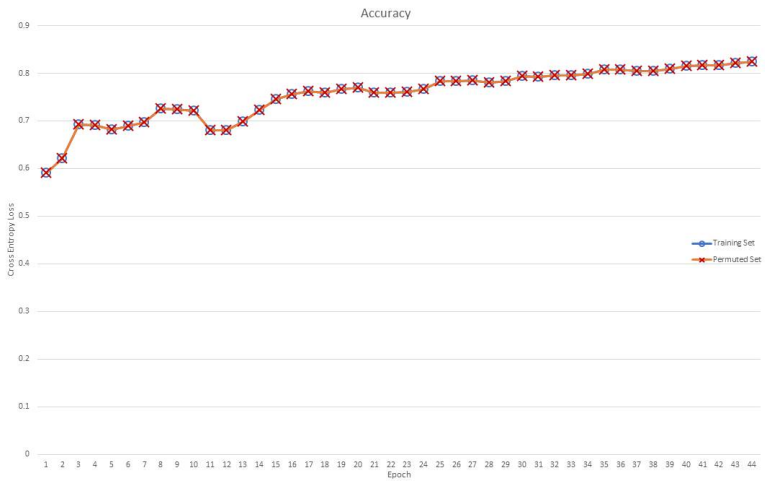
Enzyme Classification Example

Extraction with Hadamard Matrix

Protein Dataset where task is classification into *enzyme* vs. *non-enzyme*.
Dataset: 450 enzymes and 450 non-enzymes.
Architecture (ReLU activation):

- GCN with $L = 3$ layers and $d = 25$ feature vectors in each layer;
- $Ext = \Lambda$, $Z = \lambda(YR)$ with $R = [I\ Hadamard]$. $D = 50$, $m = 50$.
- Fully connected NN with dense 3-layers and 120 internal units.





Readout Mapping Approach

Kernel Sampling

Consider:

$$\Phi : \mathbb{R}^{n\times d} \to \mathbb{R}^m \quad , \quad (\Phi(X))_j = \sum_{k=1}^{n} \nu(a_j, x_k) \text{ or } (\Phi(X))_j = \prod_{k=1}^{n} \nu(a_j, x_k)$$

where $\nu : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a kernel, and $x_1, \cdots, x_n$ denote the rows of matrix X.

Known solutions: If $m = \infty$, then there exists a Φ that is globally faithful (injective) and stable on compacts.

Interesting mathematical connexion: On compacts, some kernels ν define Repreducing Kernel Hilberts Spaces (RKHSs) and yield a decomposition

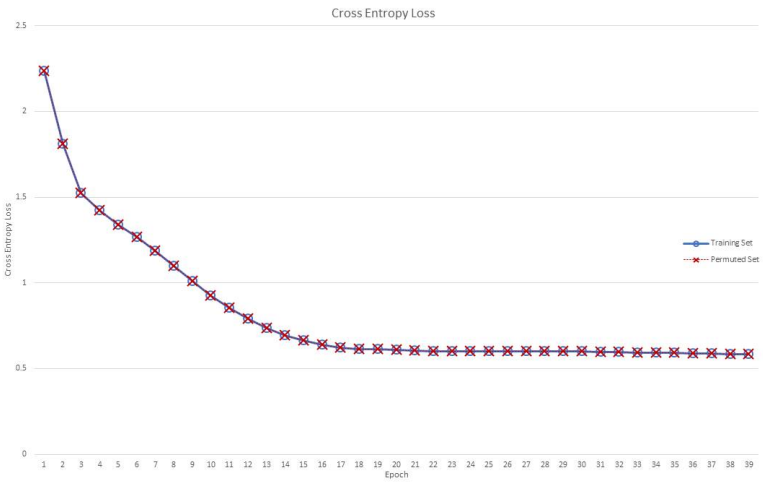
$$(\Phi(X))_j = \sum_{p\geq 1} \sigma_p f_p(a_j) g_p(X)$$

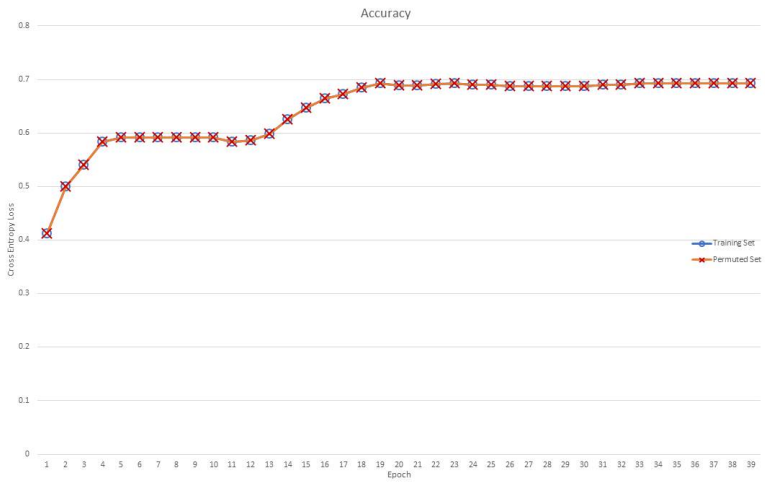
Enzyme Classification Example

Feature Extraction with Exponential Kernel Sampling

Protein Dataset where task is classification into *enzyme* vs. *non-enzyme*.
Dataset: 450 enzymes and 450 non-enzymes.
Architecture (ReLU activation):

- GCN with $L = 3$ layers and $d = 25$ feature vectors in each layer;
- $Ext : Z_j = \sum_{k=1}^{n} exp(-\pi \|y_k - z_j\|)$ with $m = 120$ and z_j random.
- Fully connected NN with dense 3-layers and 120 internal units.





Readout Mapping Approach

Polynomial Expansion - Quadratics

Another interpretation of the moments for $d = 1$: coefficients of linear expansion

$$P(X) = \frac{1}{n}\sum_{k=1}^{n}(X - x_k)^n = X^n + \sum_{k=1}^{n} a_k X^{n-k}$$

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For $d > 1$, consider the quadratic d-variate polynomial:

$$\begin{aligned} P(Z_1, \cdots, Z_d) &= \prod_{k=1}^{n}\left((Z_1 - x_k(1))^2 + \cdots + (Z_d - x_k(d))^2\right) \\ &= \sum_{p_1,\ldots,p_d=0}^{2n} a_{p_1,\ldots,p_d} Z_1^{p_1} \cdots Z_d^{p_d} \end{aligned}$$

Encoding complexity:

$$m = O\begin{pmatrix} 2n+d \\ d \end{pmatrix} \sim (2n)^d.$$

Readout Mapping Approach

Polynomial Expansion - Quadratics (2)

A more careful analysis of $P(Z_1, ..., Z_d)$ reveals a form:

$$P(Z_1, ..., Z_d) = t^n + Q_1(Z_1, ..., Z_d)t^{n-1} + \cdots + Q_{n-1}(Z_1, ..., Z_d)t + Q_n(Z_1, ..., Z_d)$$

where $t = Z_1^2 + \cdots + Z_d^2$ and each $Q_k(Z_1, ..., Z_d) \in \mathbb{R}_k[Z_1, ..., Z_d]$. Hence one needs to encode:

$$m = \left(\begin{array}{c} d+1 \\ 1 \end{array} \right) + \left(\begin{array}{c} d+2 \\ 2 \end{array} \right) + \cdots + \left(\begin{array}{c} d+n \\ n \end{array} \right) = \left(\begin{array}{c} d+n+1 \\ n \end{array} \right) - 1$$

number of coefficients.

Readout Mapping Approach

Polynomial Expansion - Linear Forms

One can do even better than that!
Consider the n linear forms $\lambda_k(Z_1, ..., Z_d) = x_k(1)Z_1 + \cdots x_k(d)Z_d$.
Consider the polynomial in variable t with coefficients in $\mathbb{R}[Z_1, ..., Z_d]$:

$$P(t) = \prod_{k=1}^{n}(t - \lambda_k(Z_1, ..., Z_d)) = t^n - e_1(Z_1, .., Z_d)t^{n-1} + \cdots (-1)^n e_n(Z_1, ..., Z_d)$$

The elementary symmetric polynomials $(e_1, ..., e_n)$ are in 1-1 correspondence (Newton-Girard theorem) with the moments:

$$\mu_p = \sum_{k=1}^{n} \lambda_k^p(Z_1, ..., Z_d) \quad , \quad 1 \leq p \leq n$$

Readout Mapping Approach

Polynomial Expansion - Linear Forms (2)

Each μ_p is a homogeneous polynomial of degree p in d variables. Hence to encode each of them one needs $\begin{pmatrix} d+p-1 \\ p \end{pmatrix}$ coefficients. Hence the total embedding dimension is

$$m = \begin{pmatrix} d \\ 1 \end{pmatrix} + \begin{pmatrix} d+1 \\ 2 \end{pmatrix} + \cdots + \begin{pmatrix} d+n-1 \\ n \end{pmatrix} = \begin{pmatrix} d+n \\ n \end{pmatrix} - 1$$

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For $d = 1$, $m = n$ which is optimal.

For $d = 2$, $m = \frac{n^2+3n}{2}$. Is this optimal?

Algebraic Embedding
Encoding using Complex Roots

Idea: Consider the case $d = 2$. Then each $x_1, \cdots, x_n \in \mathbb{R}^2$ can be replaced by n complex numbers $z_1, \cdots, z_n \in \mathbb{C}$, $z_k = x_k(1) + ix_k(2)$.
Consider the complex polynomial:

$$Q(z) = \prod_{k=1}^{n}(z - z_k) = z^n + \sum_{k=1}^{n} \sigma_k z^{n-k}$$

which requires n complex numbers, or $2n$ real numbers.

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Open problem: Can this construction be extended to $d \geq 3$?
Remark: A drawback of polynomial (algebraic) embeddings: [Cahill'19] showed that polynomial embeddings of translation invariant spaces cannot be bi-Lipschitz.

Quadratic Optimization Problems

Approach

Consider two symmetric (and positive semidefinite) matrices $A, B \in \mathbb{R}^{n\times n}$. The *quadratic assignment problem* asks for the solution of

$$\begin{aligned} &\textit{maximize} && \textit{trace}(\Pi A \Pi^T B) \\ &\text{subject to:} && \\ &\Pi \in S_n && \end{aligned}$$

where *Input* stands for a given set input data, and S_n denotes the symmetric group of permutation matrices.

Idea: Use a two-step procedure:

1. Perform a latent representation of the Input Data using a Graph Convolutive Network (or Graph Neural Network);
2. Solve the Linear Assignment Problem for an appropriate cost matrix to obtain an estimate of the optimal Π.

QAP
Motivation

Consider two $n \times n$ symmetric matrices A, B. In the alignment problem for quadratic forms one seeks an orthogonal matrix $U \in O(n)$ that minimizes

$$\|UAU^T - B\|_F^2 := trace((UAU^T - B)^2) = \|A\|_F^2 + \|B\|_F^2 - 2trace(UAU^T B).$$

The solution is well-known and depends on the eigendecomposition of matrices A, B: if $A = U_1 D_1 U_1^T$, $B = U_2 D_2 U_2^T$ then

$$U_{opt} = U_2 U_1^T \quad , \quad \|U_{opt} A U_{opt}^T - B\|_F^2 = \sum_{k=1}^{n} |\lambda_k - \mu_k|^2,$$

where $D_1 = diag(\lambda_k)$ and $D_2 = diag(\mu_k)$ are diagonal matrices with eigenvalues ordered monotonically.

QAP
Motivation 2

The challenging case is when U is constrained to belong to the permutation group. In this case, the previous minimization problem

$$\min_{U \in S_n} \|UAU^T - B\|_F$$

turns into the QAP:

$$\max_{U \in S_n} trace(UAU^T B).$$

In the case A, B are graph Laplacians (or adjacency matrices), an efficient solution to this optimization problem would solve the graph isomorphism problem, one of the remaining milenium problems: decide if two given graphs are the same modulo vertex labelling.

Prior work to discrete optimizations using deep learning

- Direct approach to discrete optimization: Pointer Networks (Ptr-Nets) utilize sequence-to-sequence Recurrent Neural Networks [Vinyals'15];
- Reinforcement learning and policy gradients: [Bello'16]
- Graph embedding and deep Q-learning: [Dai'17]
- QAP using graph deep learning: [Nowak'17] utilizes siamese graph neural networks that act on A and B independently to produce embeddings E_1 and E_2; then the product $E_1 E_2^T$ is transformed into a permutation matrix through soft-max and cross-entropy loss.

Results of this presentation: [R.B.,N.Haghani,M.Singh] SPIE 2019.

Shift Invariance Properties

Consider $A = A^T$ and $B = B^T$ (no positivity assumption).

Lemma

The QAP associated to (A, B) has the same optimizer as the QAP associated to $(A - \lambda I, B - \mu I)$, where $\lambda, \mu \in \mathbb{R}$.

Indeed, the proof of this lemma is based on the following direct computation:

$$trace(\Pi(A-\lambda I)\Pi^T(B-\mu I)) = trace(\Pi A \Pi^T B) - \mu trace(A) - \lambda trace(B) + n\lambda\mu$$

A consequence of this lemma is that, without loss of generality, we can assume $A, B \geq 0$. In fact, we can shift the spectrum to vanish the smallest eigenvalues of A, B.

The case of Rank One

Assume now $A = aa^T$ and $B = bb^T$ are non-negative rank one matrices. Then:

$$trace(\Pi A \Pi^T B) = |b^T \Pi a|^2 = (trace(\Pi a b^T))^2 = \frac{1}{trace(AB)}(trace(\Pi AB))^2$$

In this case we obtain the explicit solution to the QAP:

Lemma

Assume $A = aa^T$ and $B = bb^T$ are rank one. Then the QAP optimizer is the optimizer of one of the following two optimization problems:

$$\begin{array}{ll} \textit{maximize} & trace(\Pi C) \\ \textit{subject to:} & \\ \Pi \in S_n & \end{array} \quad \text{or} \quad \begin{array}{ll} \textit{minimize} & trace(\Pi C) \\ \textit{subject to:} & \\ \Pi \in S_n & \end{array}$$

where $C = AB$.

Linear Assignment Problems

Given a cost matrix $C \in \mathbb{R}^{n \times n}$, the *Linear Assignment Problem* (LAP) is defined by:

$$\begin{aligned} &\textit{maximize} && \textit{trace}(\Pi C) \\ &\text{subject to:} && \\ &\Pi \in S_n && \end{aligned}$$

Without loss of generality, max can be replace by min, for instance by solving LAP for $-C$.

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Without loss of generality, max can be replace by min, for instance by solving LAP for $-C$.

The key observation is that LAP can be solved efficiently by a linear program. Specifically, the convexification of LAP produces the same optimizer:

$$\begin{array}{c} \textit{maximize} \quad \textit{trace}(WC) \\ \text{subject to:} \\ W_{i,j} \geq 0 \ , \ 1 \leq i,j \leq n \\ \sum_{i=1}^{n} W_{i,j} = 1 \ , \ 1 \leq j \leq n \\ \sum_{j=1}^{n} W_{i,j} = 1 \ , \ 1 \leq i \leq n \end{array}$$

Diagonal Matrices

Another case when we know the exact solution is when A and B are diagonal matrices. Say $A = diag(a)$ and $B = diag(b)$. Then

$$trace(\Pi A \Pi^T B) = trace(diag(\Pi a) diag(b)) = trace(\Pi a b^T) = trace(\Pi C)$$

where $C = ab^T$.

Lemma

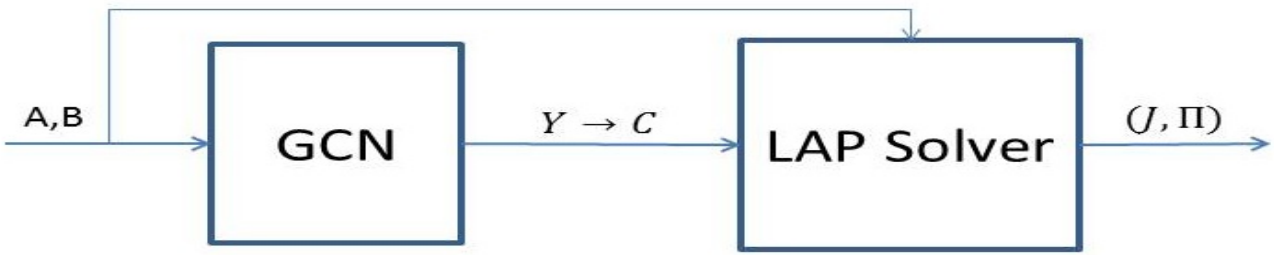
If $A = diag(a)$ and $B = diag(b)$ then the solution of the QAP is given by the solution of the LAP

$$\begin{aligned} &maximize && trace(\Pi C) \\ &subject\ to: && \\ &\Pi \in S_n && \end{aligned}$$

where $C = ab^T$.

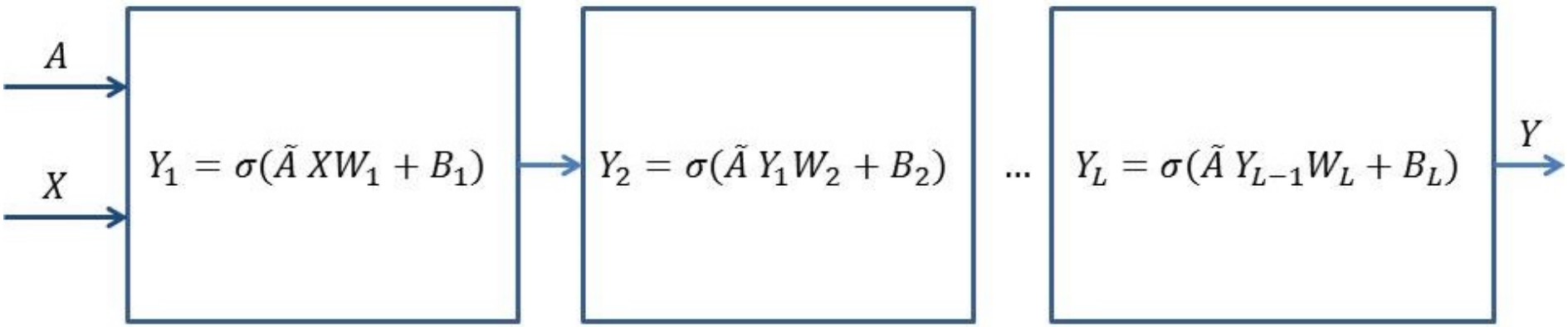
Approach

Graph Deep-Learning Based Approach: First convert the input data (A, B) into a cost matrix C, and then solve two LAPs, one associated to C the other associated to $-C$. Finally choose the permutation that produces the larger objective function.
The conversion step $(A, B) \mapsto C$ is performed by a Graph Convolutional Network (GCN).



Graph Convolutional Networks (GCN)

Kipf and Welling (2016) introduced a network structure that performs local processing according to a modified adjacency matrix:



Here $\tilde{T} = I + T$, where T is an input adjacency matrix, or graph weight matrix. The L-layer GCN has parameters $(W_1, B_1, W_2, B_2, \cdots, W_L, B_L)$. As activation map σ we choose the ReLU (Rectified Linear Unit).

The Specific GCN Architecture

For the QAP associated to matrices (A, B) we design a specific GCN architecture:

$$X = \begin{bmatrix} A & 0 \\ B & 0 \end{bmatrix}, \quad \tilde{T} = \begin{bmatrix} I_n & \frac{1}{\|A\|_F \|B\|_F} AB \\ \frac{1}{\|A\|_F \|B\|_F} BA & I_n \end{bmatrix} \tag{2.1}$$

where the 0 matrices in X are designed to fit the appropriate size of W_1. For σ we choose the ReLU (Rectified Linear Unit) function in each layer except for the last one; in the last layer we do not use any activation function (i.e., $\sigma = Identity$). The biases $B_1, \cdots, B_L$ are chosen of the form $B_k = 1 \cdot \beta_k^T$, i.e., each row β_k^T is repeated.

GCN Guarantee

The following result applies to this network.

Theorem

Assume $A = aa^T$ *and* $B = bb^T$ *are rank one with* $a, b \geq 0$, *and consider the GCN with* L *layers and activation map ReLU as described above. Then for any nontrivial weights* $W_1, \cdots, W_L$ *and zero biases* $B_1, \cdots, B_L = 0$ *the network output* Y *partitioned* $Y = \begin{bmatrix} Y^1 \\ Y^2 \end{bmatrix}$ *into two blocks of* n *rows each, satisfies* $Y^1 Y^{2T} = \gamma AB$, *for some constant* $\gamma \in \mathbb{R}$. *In particular, the max-LAP and min-LAP applied to the latent representation matrix* $C = Y^1 Y^{2T}$ *are guaranteed to produce the optimal solution of the QAP.*

Reference Algorithms

We compare the GCN based optimizer with two different algorithms.
1. The *AB Method* bypasses the GCN block. Thus $Y = X$ and the cost matrix inputted into the LAP solver is simply $C = AB$ (hence the name of the method). Similar to the GCN approach, the AB Method is exact on rank 1 inputs. But there is no adaptation of the cost matrix for other input matrices.
2. The *Iterative* algorithm is based on alternating max-LAP or min-LAP as follows:

$$\Pi_{k+1} \in \left\{ \begin{array}{ll} \text{argmax} & trace(\Pi A \Pi_k^T B) \\ \Pi \in S_n & \end{array} \right. , \left. \begin{array}{ll} \text{argmin} & trace(\Pi A \Pi_k^T B) \\ \Pi \in S_n & \end{array} \right\}$$

where $\Pi_0 = I$ (identity), and the choice of permutation at each k is based on which permutation produces a larger $trace(\Pi A \Pi^T B)$.

Comparison with Ground Truth

Results for $2 \leq n \leq 10$ and raw data normal distributed

Average relative difference w.r.t. maximum objective function:

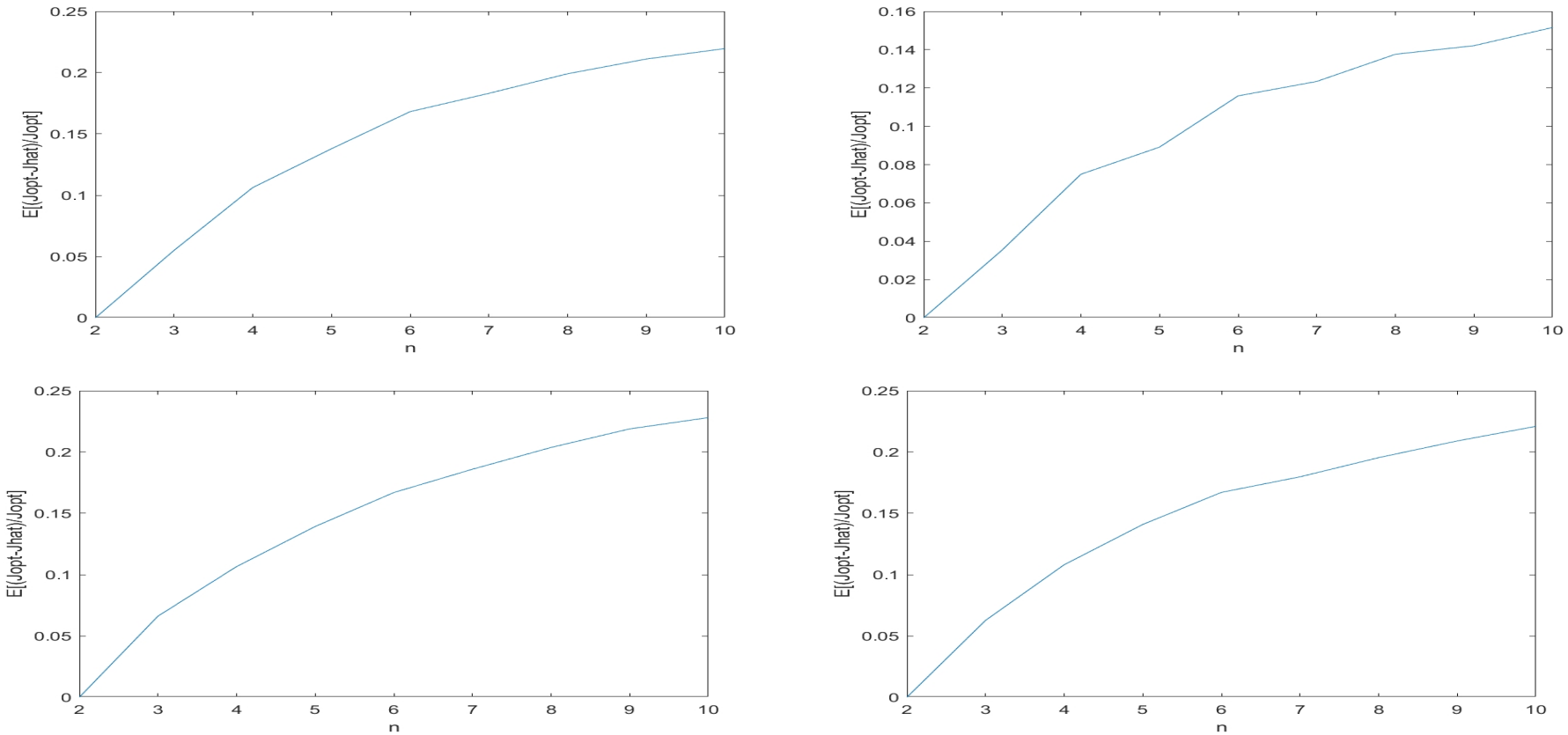


Figure: Top left: ABMethod, Top right: Iterative algorithm, Bottom left: GCN with L=2 layers and bais, Bottom right: GCN with $L = 3$ layers and bias

Comparison with Ground Truth

Results for $2 \leq n \leq 10$ and raw data uniform distributed

Average relative difference w.r.t. maximum objective function:

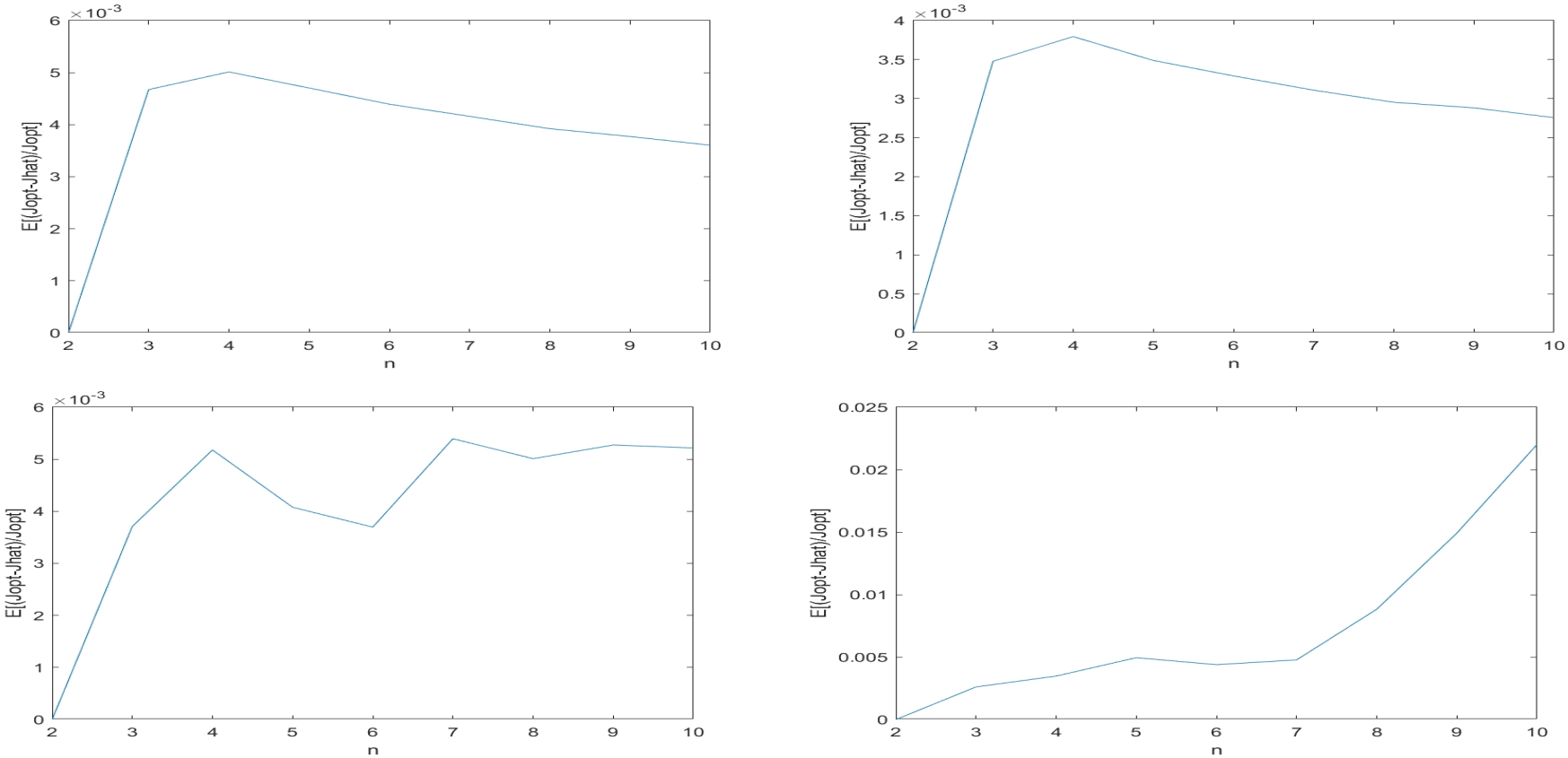


Figure: Top left: ABMethod, Top right: Iterative algorithm, Bottom left: GCN with L=2 layers and bais, Bottom right: GCN with $L = 3$ layers and bias

Relative Comparison

Results for $n = 100$ and $n = 200$ with raw data normal distributed

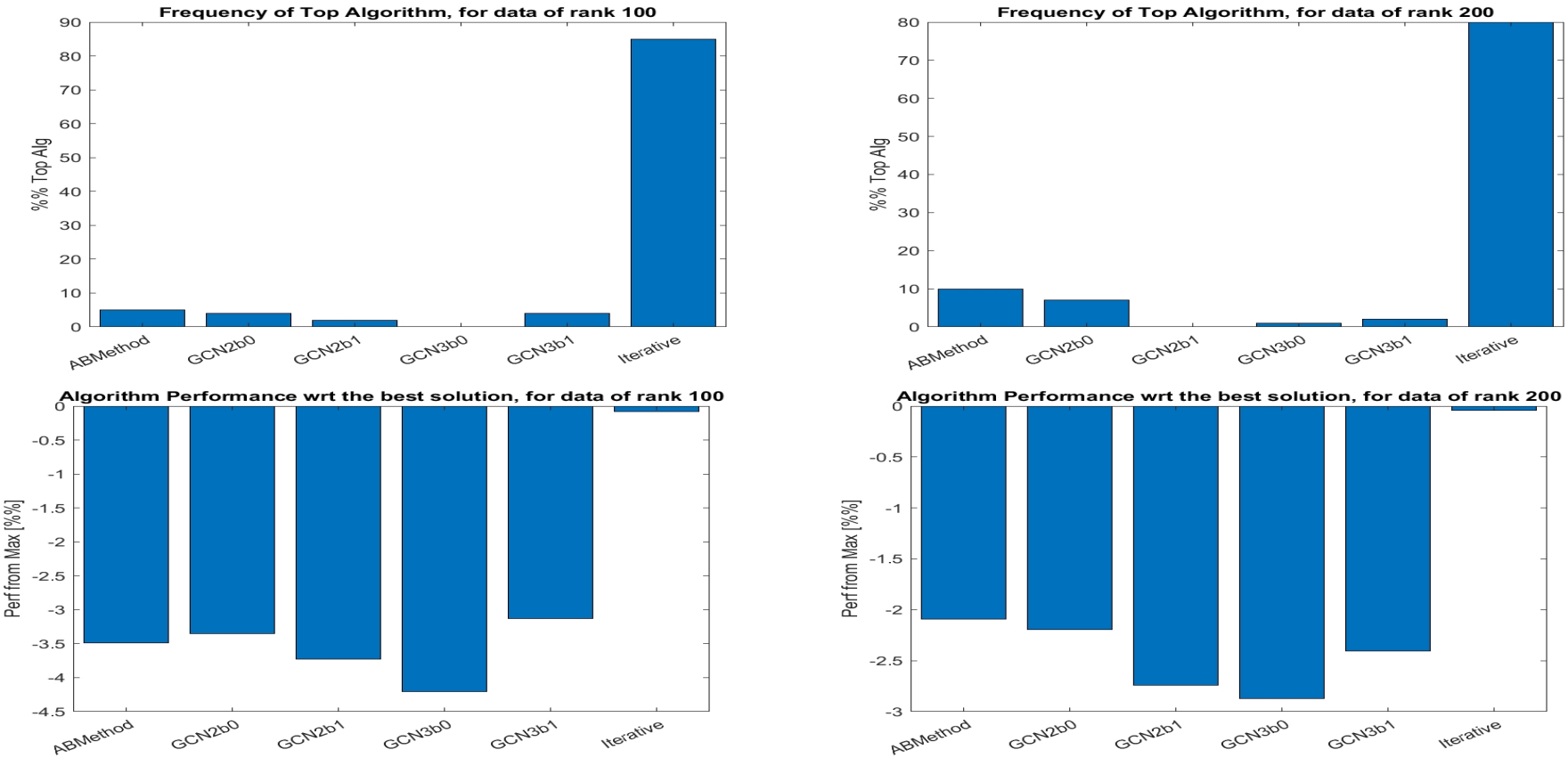


Figure: Top row: Frequency of optimal algorithm for $n = 100$ (left), and $n = 200$ (right). Borrom row: Relative performance [%] to the best algorithm for $n = 100$ (left) and $n = 200$ (right)

Relative Comparison

Results for $n = 100$ and $n = 200$ with raw data normal distributed

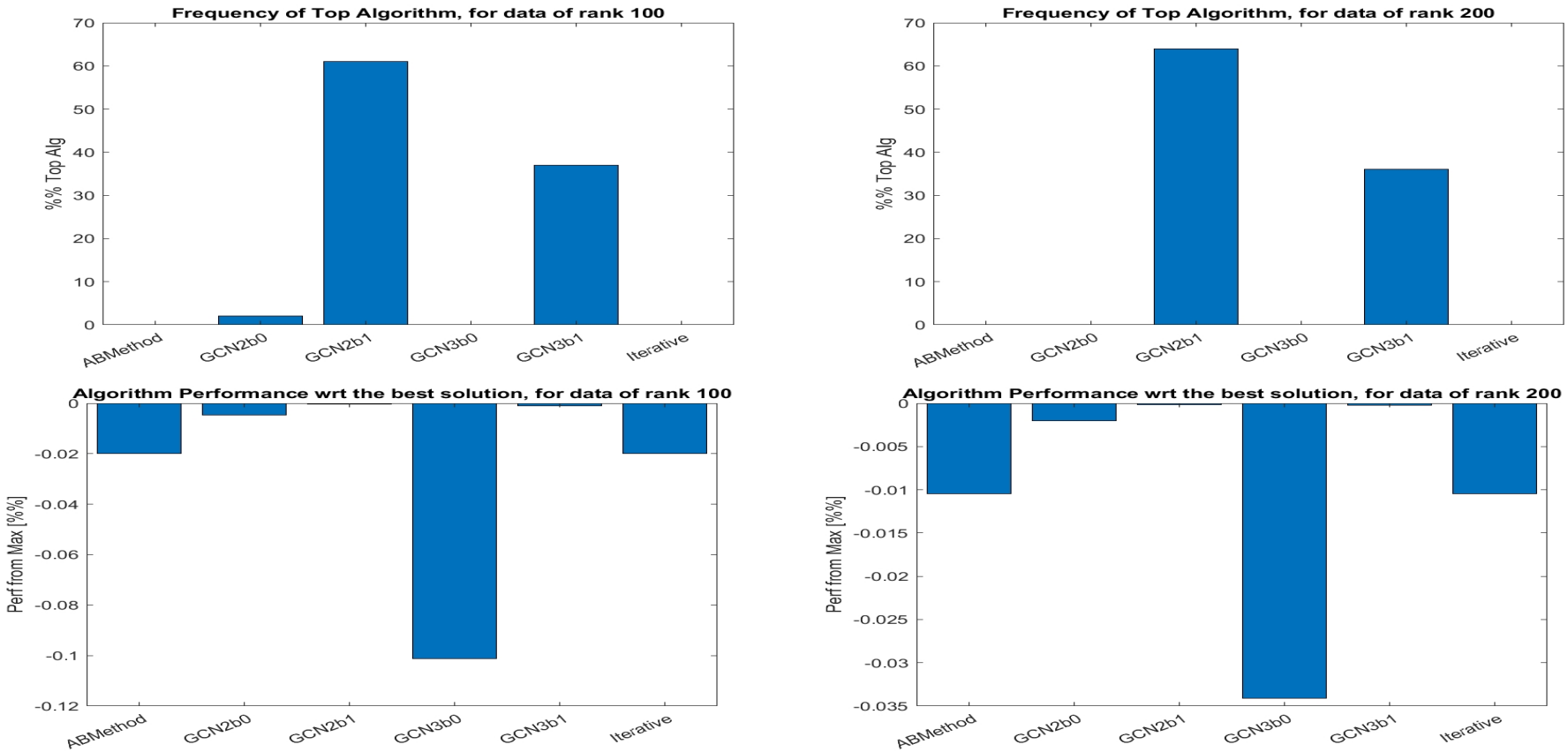


Figure: Top row: Frequency of optimal algorithm for $n = 100$ (left), and $n = 200$ (right). Borrom row: Relative performance [%] to the best algorithm for $n = 100$ (left) and $n = 200$ (right)

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