Matching Embeddings via Shuffled Total Least Squares Regression

Daniel L. Sussman and Qian Wang

Boston University

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What is graph matching?

**Formulation**

Consider observing two graphs, \( G_1 = (V_1, E_1) \), \( G_2 = (V_2, E_2) \). The classical graph matching formulation is to find a map \( \pi : V_1 \mapsto V_2 \), that minimizes the symmetric difference between

\[
\pi(E_1) = \{(\pi(i), \pi(j)) : (i, j) \in E_1\} \text{ and } E_2.
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and $E_2$. 
What is graph matching?

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Consider observing two graphs, $G_1 = (V_1, E_1)$, $G_2 = (V_2, E_2)$. The classical graph matching formulation is to find a map $\pi : V_1 \mapsto V_2$, that minimizes the symmetric difference between

$$\pi(E_1) = \{ (\pi(i), \pi(j)) : (i, j) \in E_1 \} \text{ and } E_2.$$
Should we do graph matching?

- Matching graphs from different modalities

Calhoun and Sui 2016
Should we do graph matching?

- Matching graphs from different modalities

Calhoun and Sui 2016

- Matching a social network to a co-purchasing network
Should we do graph matching

- Matching across topics and time periods

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A first step: match embeddings

Zhang et al. 2019

Idea

1. Represent graphs as point clouds
2. Align point clouds
Shuffled Linear Regression - Model

- Model:
  \[ Y = \Pi^* XR + E, \]
  where \( \Pi^* \in \mathcal{P}_n \) is an unknown permutation matrix.

Shuffled Linear Regression - Applications

Pose and correspondence estimation
- Goal: find similar objects across images from different perspectives

(Pananjady et al. 2017)

Header-free communication
- Goal: Recover signal origins without sending location information
Shuffled Linear Regression - Estimation

- **OLS estimate:**

\[
(\hat{\Pi}, \hat{R}) = \arg \min_{\Pi \in \mathcal{P}_n, R \in \mathbb{R}^{p \times p}} \| Y - \Pi X R \|_F^2.
\]

\[
\begin{array}{cccccc}
\text{permutation 1} & \text{permutation 2} & \text{permutation 3} & \text{permutation 4} & \text{permutation 5} \\
-0.25 & 0.00 & 0.25 & -0.25 & 0.00 & 0.25 & -0.25 & 0.00 & 0.25 & -0.25 & 0.00 & 0.25 & -0.25 & 0.00 & 0.25
\end{array}
\]

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A more realistic model

Model:

\[ Y_1 = X + E_1 \]
\[ Y_2 = \Pi^* X R + E_2, \]  

- Permutation: \( \Pi^* \in \mathcal{P}_n \)
- Design: \( X \in \mathbb{R}^{n \times p} \)
- Coefficient: \( R \in \mathbb{R}^{p \times p} \)
- Noise: \( E_1, E_2 \in \mathbb{R}^{n \times p} \)

Given the observations \((Y_1, Y_2)\), estimate \( \Pi^* \).
Total Least Squares (TLS) Estimator

The TLS estimator for *errors-in-variables regression*:

\[
\min_{\hat{Y}_1, \hat{Y}_2 \in \mathbb{R}^{p \times p}} \left\| [Y_2 | Y_1] - [\hat{Y}_2 | \hat{Y}_1]\right\|_F^2
\]

s.t. \( \text{rank}([\hat{Y}_2 | \hat{Y}_1]) \leq p \).
Shuffled TLS Estimator

Let
\[ Y_\Pi = [Y_2 | \Pi Y_1], \quad M_\Pi = [\Pi^* X R | \Pi X], \text{ and } \quad E_\Pi = [E_2 | \Pi E_1] \]

Write model (1) as
\[ Y_\Pi = M_\Pi + E_\Pi, \quad (2) \]

The shuffled TLS estimator is
\[ \hat{\Pi} = \arg \min_{\Pi \in \mathcal{P}_n} \sum_{i=p+1}^{2p} \sigma_i^2(Y_\Pi). \quad (3) \]
Evaluation Method and Identifiability Issue

- The Hamming distance

\[ d_H(\hat{\Pi}, \Pi^*) = \# \{ i | \hat{\Pi}(i) \neq \Pi^*(i) \}, \]

- The normalized quadratic loss

\[ \frac{1}{np} \| \hat{\Pi}X - \Pi^*X \|_F^2. \]
Example (Identifiability Issue of the Shuffled TLS Estimator)

Consider a noiseless case when $E_1 = E_2 = 0$, $\Pi^* = I_n$, $R = I_p$, let $n = 10$, and

$$Y_1 = Y_2 = X = \begin{bmatrix} 1_5 & -1_5 \\ 1_5 & 1_5 \end{bmatrix}.$$
Shuffled Total Least Squares Regression

Evaluation Method and Identifiability Issue

Example (Identifiability Issue of the Shuffled TLS Estimator)

Consider a noiseless case when \( E_1 = E_2 = 0, \Pi^* = I_n, R = I_p, \) let \( n = 10, \) and

\[
Y_1 = Y_2 = X = \begin{bmatrix} 1_5 & -1_5 \\ 1_5 & 1_5 \end{bmatrix}.
\]

- Normalized Procrustes quadratic loss:

\[
\frac{1}{\|X\|_F^2} \min_{Q \in \mathcal{O}(p)} \|\Pi^* X - \hat{\Pi}XQ\|_F^2.
\]

Lemma

Assume the condition number \( \kappa(X) = 1, \) we have the relationship

\[
\min_{Q \in \mathcal{O}(p)} \|\Pi^* X - \Pi XQ\|_F^2 \leq 2 \sum_{i=1+p}^{2p} \sigma_i^2(\Pi^* X|\Pi X).
\]
Model assumptions and Main Result

We assume the following conditions hold:

Assumption (Design Matrix)

The latent design matrix has condition number $\kappa(X) = 1$.

Assumption (Coefficient Matrix)

$\sigma_p(R) \leq 1$ and $\sigma_1(R) \geq 1$.

Assumption (Noise Variables)

$E_{1i}, E_{2i} \sim i.i.d. \mathcal{N}(0, \Sigma)$ for $i \in [n]$. 
Main Result

Theorem

For the statistical model (1), under the assumptions, the total least squares estimator \( \hat{\Pi} \) satisfies

\[
\min_{Q \in O(p)} \frac{\| \Pi^* X - \hat{\Pi} X Q \|_F^2}{\| X \|_F^2} \leq \frac{4 \lambda_1(\Sigma)}{\sigma_p^2(R)} (1 + \eta a_n) \left[ 8 \sqrt{2} \sigma_1(R) \frac{p \sqrt{n}}{\| X \|_F} + \frac{np}{\| X \|_F^2} \right],
\]

(4)

where \( a_n = \sqrt{\frac{\text{tr}(\Sigma) \log(n)}{\lambda_1(\Sigma) cn}} \), with probability greater than

\[
1 - n^{-\eta^2},
\]

where \( c \) is at least \( \frac{1}{32} \).
Main Result

Define the signal-to-noise ratio as snr = \frac{\|X\|_F^2}{n} \cdot \frac{1}{\text{tr}(\Sigma)}.

The upper bound is approximately

\[ c_1(R) \sqrt{\frac{\text{tr}(\Sigma)}{\text{snr}}} + c_2(R) \frac{1}{\text{snr}} \]

- \( X_{ij} \sim N(0, 1), E_{ij} \sim N(0, \sigma^2), \text{snr} \sim \frac{1}{\sigma^2} \)

\[ c\sigma^2, \]

where \( c = c_1(R) \sqrt{p} + c_2(R) \).

- For the Procrustes loss to go to zero, snr needs to go to infinity.
Result Comparison

- Our bound:
  \[ c\sigma^2 \]

- Pananjady et al. 2017
  \[ Y = \Pi^* X R^* + E, \]

- For \( p < \log(n) \):
  \[ \frac{1}{np} \| \hat{\Pi} X \hat{R} - \Pi^* X R^* \|_F^2 \leq c_1 \sigma^2 \left( \frac{p}{n} + 1 \right). \]
Result Comparison

- Our bound:
  \[ c \sigma^2 \]

- Flammarion et al. 2016

\[ Y = \Pi^* X^* + E, \]

where the columns of \( X^* \) is unimodal.

\[
\frac{1}{np} \| \hat{\Pi\hat{X}} - \Pi^* X^* \|_F^2 \leq \sigma^2 (1 + \frac{\log(n)}{p}).
\]
Permutation Recovery in Shuffled Linear Regression is NP-hard

\[
\min_{\Pi} \min_{R} \|\Pi X R - Y\|_F^2
\]
\[
= \min_{\Pi} \|\Pi X (X^T X)^{-1} X^T \Pi^T Y - Y\|_F^2
\]
\[
= \min_{\Pi} \text{tr}(\Pi(\pi^T Z^T Z - 2\pi Z \Pi^T Y Y^T)),
\]

where \(Z = X (X^T X)^{-1} X^T\).

- Shuffled OLS is equivalent to a QAP
The Alternating LAP/OLS Algorithm (ALOA)

Model:

\[ Y_2 = \Pi^* Y_1 R + E_2 \]

Algorithm:
Iterate between

1. Step 1: given \( \hat{\Pi} \), estimate \( R \) via OLS.
2. Step 2: given \( \hat{R} \), estimate \( \hat{\Pi} \) by solving a LAP, assigning the \( n \) rows of \( Y_2 \) to the \( n \) rows of \( Y_1 \hat{R} \).

\[ C_{ij} = \| Y_{2i} - (Y_1 \hat{R})_j \|_F^2. \]
The Alternating LAP/TLS Algorithm, ALTA

Model:

\[ Y_1 = X + E_1, \quad Y_2 = \Pi^* XR + E_2 \]

Algorithm:
Iterate between

- Step 1: given \( \hat{\Pi} \), estimate \((X, R)\) via TLS.
- Step 2: given \((\hat{X}, \hat{R})\) ... ?
The Alternating LAP/TLS Algorithm, ALTA

Model:

\[ Y_1 = X + E_1, \quad Y_2 = \Pi^* XR + E_2 \]

Algorithm:

Iterate between

- Step 1: given \( \hat{\Pi} \), estimate \( (X, R) \) via TLS.
- Step 2: given \( (\hat{X}, \hat{R}) \) ...

\[ \text{arg min}_{\Pi \in P_n} \sum_{i=p+1}^{2p} \sigma_i^2([Y_2|\Pi Y_1]), \text{ does not depend on } (\hat{X}, \hat{R}). \]
The Alternating LAP/TLS Algorithm, ALTA

Model:

\[ Y_1 = X + E_1, \quad Y_2 = \Pi^* X R + E_2 \]

Algorithm:
Iterate between

- Step 1: given \( \hat{\Pi} \), estimate \( (X, R) \) via TLS.
- Step 2: given \( (\hat{X}, \hat{R}) \) ... ?

\[ \arg\min_{\Pi \in \mathcal{P}} \sum_{i=p+1}^{2p} \sigma_i^2 ([Y_2|\Pi Y_1]), \text{ does not depend on } (\hat{X}, \hat{R}). \]

How do we define a LAP?

- **ALTA_1**:
  \[ C_{ij}^{(1)} = \|Y_{2i} - \hat{R}^T \hat{X}_j\|_F^2 + \|Y_{1j} - \hat{X}_i\|_F^2 \]

- **ALTA_2**:
  \[ C_{ij}^{(2)} = \min_{x \in \mathbb{R}^d} \|Y_{2i} - \hat{R}^T x\|_F^2 + \|Y_{1j} - x\|_F^2 \]
Initiate all algorithms at $\Pi = I_n$. 
Simulation Studies

Increase the signal-to-noise ratio via decreasing the noise like $\frac{1}{n}$. (CPD, (Myronenko and Song 2010).)
Simulation Studies

Initialize further away from the truth.
Contributions

- Propose estimate $\hat{\Pi}$ based on the TLS method.
- Provide an upper bound on the Procrustes quadratic loss.
  - Many works in the shuffled linear regression setting, less so in the shuffled TLS regression.
  - Perhaps due to the difficulty in analyzing singular values compared with Frobenius norm.
- Approximate $\hat{\Pi}$ via ALTA.
  - The permutation recovery problem continues to be an open challenge to researchers of various fields.
Potential Extension and Future Research

- Relax the assumptions:
  - $\kappa(X) = 1$.

\[
Y_1 = XR_1 + E_1 \\
Y_2 = \Pi^* XR_2 + E_2
\]

- Allow $\dim(R_1) \neq \dim(R_2)$?
- $E_{1i}, E_{2i} \sim i.i.d. \ N(0, \Sigma)$.

1. $E_{1i} \sim N(0, \Sigma_1), E_{2i} \sim N(0, \Sigma_2)$
2. $E_1$ correlated with $E_2$ (This can happen when the two graphs A and B are correlated.)

- Extend theorem to big $p$, say, $p > \log(n)$. 
References I

Calhoun, Vince D and Jing Sui (2016). “Multimodal fusion of brain imaging data: a key to finding the missing link (s) in complex mental illness”. In: Biological psychiatry: cognitive neuroscience and neuroimaging 1.3, pp. 230–244.


References II


Thanks!

Questions?

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