The Grouped Two-Sided Orthogonal Procrustes Problem

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Introduction

- Given matrices A, B the <u>*orthogonal Procrustes problem*</u> seeks an orthogonal matrix that satisfies

$$R^* = \arg \min_{R \in O(n)} ||AR - B||_f^2$$

- Useful as a geometric transformation to correct for rotational distortions between two datasets

- This paper considers a constrained version of the <u>*Two-sided orthogonal Procrustes problem*</u>: Given symmetric matrices C, C_r , find an orthogonal matrix that satisfies:

$$R^* = \arg \min_{R \in O(n)} ||R^T C R - C_r||_f^2$$

Applications

- Covariance (or correlation) matrix matching

- Graph matching problems
  - C, C_r are adjacency matrices of weighted graphs
  - Goal: identify permutation of the vertices of one graph that best matches the adjacency matrices:

$$P^* = \arg\min_P ||P^T C P - C_r||_f^2$$

Hard problem: combinatorial

  - **Umeyama's method**:
    1. Relax permutation constraint to an orthogonal transformation constraint (two-sided Procrustes)
    2. Find closest permutation matrix to the orthogonal matrix by the Hungarian algorithm

Orthogonal Procrustes Solutions

- For orthogonal Procrustes problem,

$$R^* = \arg \min_{R \in O(n)} ||AR - B||_f^2$$

  - Solution obtained by SVD of $A^T B$

- For two-sided orthogonal Procrustes problem,

$$R^* = \arg \min_{R \in O(n)} ||R^T C R - C_r||_f^2$$

  - Family of solutions may be expressed in terms of the eigendecompositions: $C = V \Lambda V^T, C_r = V_r \Lambda_r V_r^T$

$$R^* = V D V_r^T$$

  - where D is a any diagonal matrix with diagonal entries in $\{+1, -1\}$

Grouped Two-Sided Procrustes

- Graph vertices are sometimes attributed with side information that facilitate solving the two-sided Procrustes problem
- ***This paper*** considers the case when the vertices can be parcellated into groups

- Examples:
  - When the graph represents an object, vertices can be grouped based on part label
  - When there is a spatial configuration to the vertices, a grouping may be derived based on a region-based segmentation

Problem Formulation

- Assume each dataset is parcellated into M groups
  - For each point i, let $g(i) \in \{1, \ldots, M\}$ denote the group it belongs to

- Goal: estimate M orthogonal transformations (one for each group) that satisfy:

$$R^* = \arg \min_{R=\mathrm{diag}(R_1,\ldots,R_M)} ||R^T C R - C_r||_f^2$$

- Denote this as the ***grouped*** two-sided orthogonal Procrustes problem
  - Reduces to the standard two-sided problem when M=1

Problem Formulation

- Grouped version is a constrained two-sided problem
  - Subject to an additional set of linear constraints:

$$[R]_{pq} = 0 \text{ if } g(p) \neq g(q)$$

- Benefits of the grouping structure:
  - Constraints serve to regularize the optimization
  - The grouping structure imposes prior knowledge on the problem
  - Reduction in the number of estimation parameters

Solution Method Initialization

- For M>1, an iterative solution must be pursued
- Let: C_{ii}, C_{ii}^r denote the *within-region* similarity structures
  C_{ij}, C_{ij}^r denote the *across-region* similarity structures

- A logical initialization is to only consider within-region similarities
  - Problem decouples into M two-sided Procrustes problems: $$R_m = V_{mm} D_m {V_{mm}^r}^T$$
  - where $C_{mm} = V_{mm} \Sigma_{mm} {V_{mm}}^T$ and $C_{mm}^r = V_{mm}^r \Sigma_{mm}^r {V_{mm}^r}^T$

Solution Method

- Goal: Improve on initial estimates by incorporating across-region similarities

- Our proposed algorithm is a two-step process:
  1. Solve for $(D_1, \ldots, D_M)$ by matching across-region similarities
     - Diagonal entries $(\{+1, -1\})$ can be approximated by MAXCUT
  2. Fine-tune initial orthogonal estimates by a greedy selection strategy
     - Updates are progressively built up as a product of Givens rotations
     - Can be seen as 2x2 block coordinate descent

Solution Method (Step 2)

- <u>Model assumption</u>: observed C is a perturbed version of the template:

$$C = RC_rR^T + E$$

- Due to noise, the eigenvectors of the observed within-region similarities C_{mm} are perturbed versions of the true eigenvectors

- Modify the estimate for group m by:

$$R_m = V_{mm}U_mD_m{V_{mm}^r}^T$$

- where $V_{mm}U_m$ serves as an improved estimate for the eigenvectors of C_{mm}

Solution Method (Step 2)

- Let $U = \mathrm{diag}(U_1, \ldots, U_M)$
- U is estimated by matching both the within-region and the across-region similarities
- <u>Greedy approach</u>: model U at iteration t as:

$$U_t = U_{t-1} \underline{U_{p_t q_t}(\theta_{p_t q_t})}$$

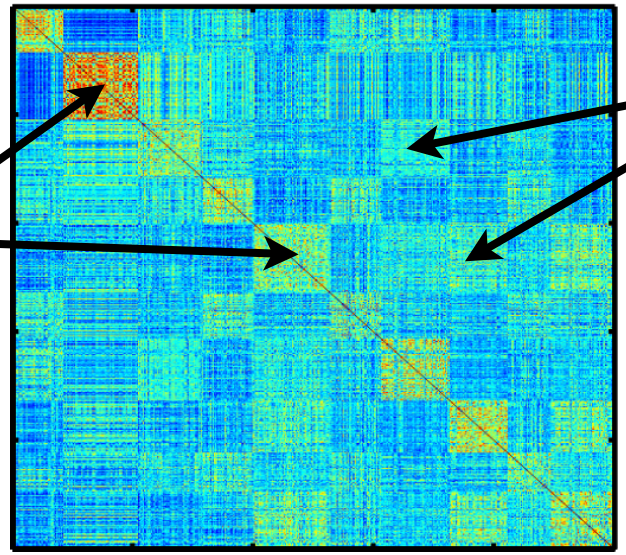
Givens rotation matrix that rotates p_t ,q_t through an angle θ_t

- For t = 1,2,…
  - Choose p_t, q_t (such that $g(p_t) = g(q_t)$) by a greedy selection strategy
  - Select the rotation angle θ_t by a line search that maximizes decrease in objective

Results

- Algorithm was tested on 2 datasets:
  - MNIST handwritten digits (parcellated by digit)
  - YaleB face database (parcellated by identity)
- Each group m was transformed by a random orthogonal matrix A_m and corrupted by additive noise

MNIST Similarity Structure

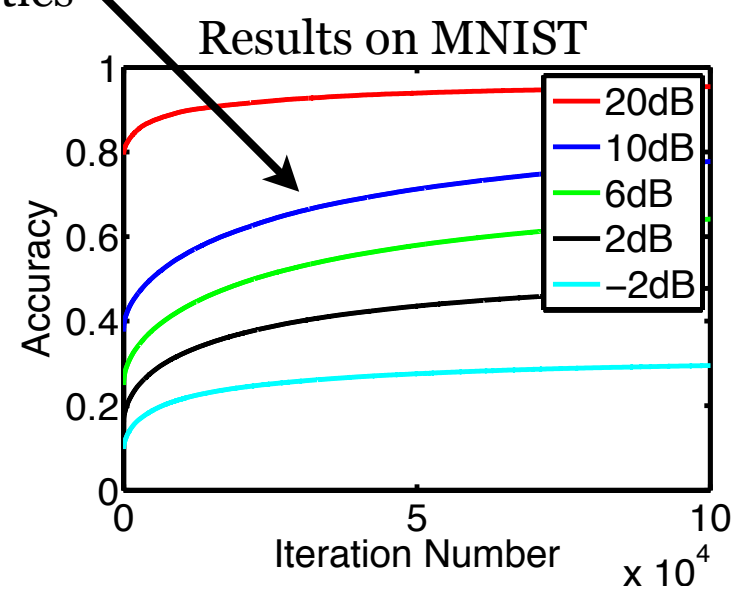


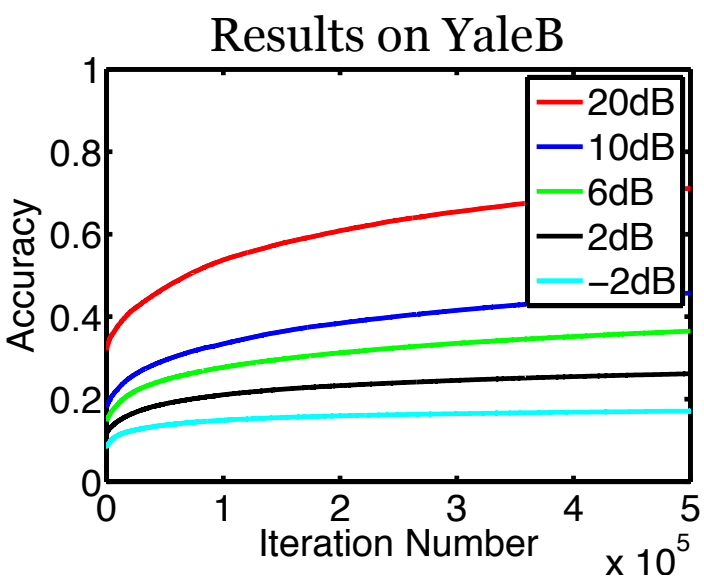
Results

- Accuracy measure between true and estimated transformations:

$$\text{Accuracy} = \frac{1}{N}\sum_{m=1}^{M} \text{trace}(\hat{A}_m^T A_m) \quad \text{(N=total \# datapoints)}$$

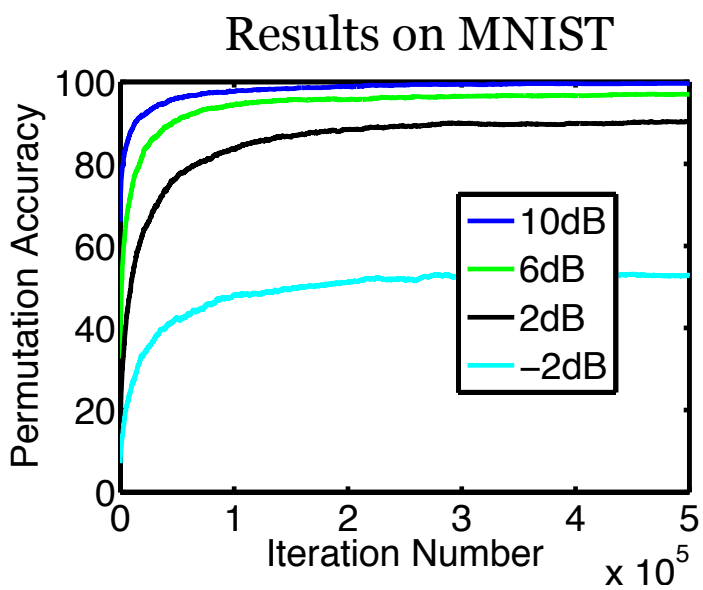
Improvement over iterations shows the usefulness of across-region similarities

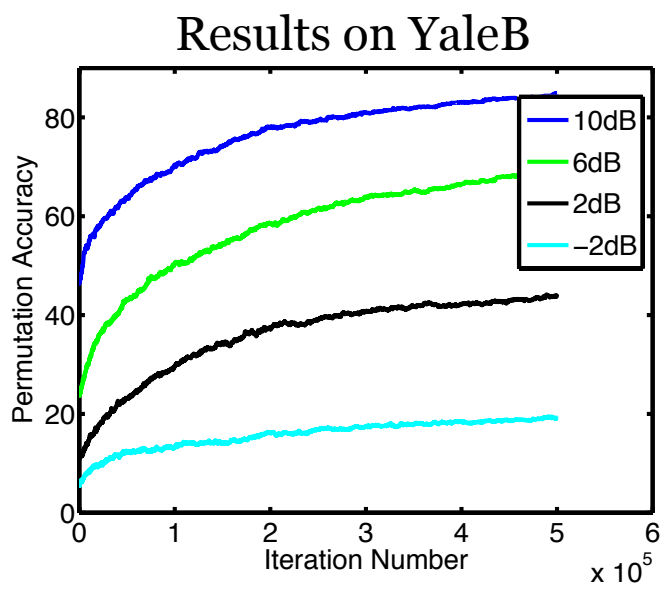




Results (Graph matching problem)

- Each group was transformed by a random permutation and perturbed with noise
- Hungarian algorithm was run to estimate optimal permutation matrix from estimated orthogonal transformation





Conclusion

- We posed the grouped version of the two-sided orthogonal Procrustes problem
- Proposed an algorithm that is both computationally efficient and simple to implement
- Results of the algorithm on simulations show that the algorithm effectively utilizes the grouping structure to greatly improve estimation accuracy in the presence of noise

Thanks!

(Extra slides)

Results (Compared with Umeyama)

	Permutation Accuracy (%) - MNIST	
SNR	Umeyama's Method	Proposed Algorithm
10dB	32.8%	97.6%
6dB	13.5%	94.5%
2dB	7.2%	83.4%
-2dB	4.1%	46.5%

	Permutation Accuracy (%) - YaleB	
SNR	Umeyama's Method	Proposed Algorithm
10dB	29.1%	71.4%
6dB	12.7%	50.2%
2dB	6.1%	29.4%
-2dB	3.4%	14.1%