Research Summary: Statistical Algorithms for Complex Data

Junhyoung Chung

Department of Statistics, Seoul National University

Research 001: Operator Fused Optimal Transport

Research question: Is it possible to design a fused transport framework that is simultaneously (i) **convex** and computationally tractable, (ii) sensitive to **feature information**, and (iii) capable of preserving the intrinsic **geometric** structure of the domains?

Contributions

- **Convex objective design.** Develop a new loss function (1) formulated as a **convex objective**, guaranteeing efficient and globally optimal solutions.
- **Graph-to-Metric space extension.** Extend the convex relaxation techniques of graph matching problems to the operator level, thereby generalizing the problem from aligning two graphs to aligning two **metric spaces**.
- **Scalable solver with guarantees.** Use a projection-free Frank–Wolfe algorithm for the empirical convex quadratic program, and derive an optimization-statistical error bound.

Convex Structural Penalty

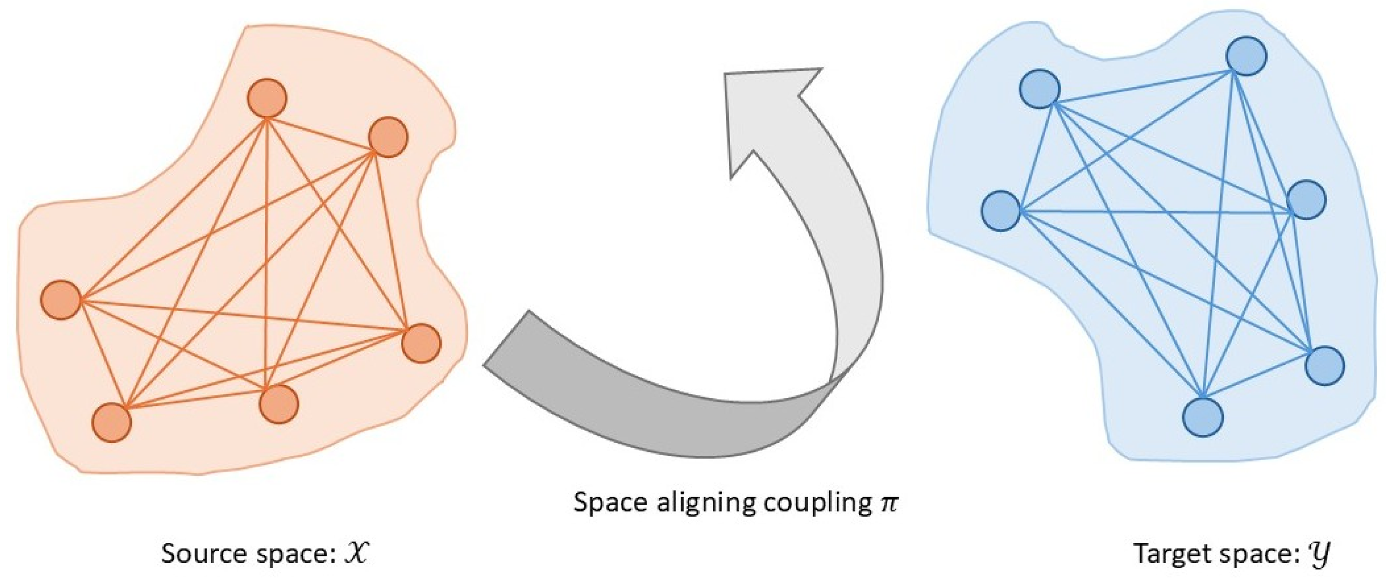


Figure: A coupling π that aligns two spaces $\mathcal{X}$ and $\mathcal{Y}$

- Let $(\mathcal{X}, d_{\mathcal{X}}, \mathbb{P}_X)$ and $(\mathcal{Y}, d_{\mathcal{Y}}, \mathbb{P}_Y)$ be connected and compact metric measure spaces.
- The Gromov–Wasserstein (GW) discrepancy is powerful for matching problems between heterogeneous spaces:

$$\pi^* = \underset{\pi \in \Pi(\mathbb{P}_X, \mathbb{P}_Y)}{\arg\min} \; \mathbb{E}_{\pi \otimes \pi}\left[|d_{\mathcal{X}}(X, X') - d_{\mathcal{Y}}(Y, Y')|^2\right].$$

- However, the GW loss is highly **non-convex** with respect to π.

Motivation: Convex Relaxation in Graph Matching

- Let A_X and A_Y be the adjacency matrices of G_X and G_Y, respectively. The standard graph matching problem of finding a permutation matrix P such that $A_X \approx PA_YP^\top$ can be written as minimizing $\|A_X - PA_YP^\top\|_F^2$, which is equivalent to $\|A_XP - PA_Y\|_F^2$.
- Relaxing P to a soft assignment matrix Π in the Birkhoff polytope then yields the convex quadratic program $\min_\pi \|A_X\Pi - \Pi A_Y\|_F^2$.
- We lift this idea from the graph domain to the **operator level alignment** for general metric spaces.

Our Penalty: $\|D_{\mathbb{P}_X}T_\pi - T_\pi D_{\mathbb{P}_Y}\|_{\mathrm{HS}}^2$.

- $D_{\mathbb{P}_X}$ **(Distance operator):**
  - This operator encodes the distance information within the metric space $(\mathcal{X}, d_{\mathcal{X}})$, analogous to the adjacency matrix (A_X) in graph matching.
  - Definition: $(D_{\mathbb{P}_X}f)(x) = \mathbb{E}_{\mathbb{P}_X}[d_{\mathcal{X}}(x, X)f(X)]$.
- T_π **(Alignment operator):**
  - This operator represents the **soft assignment** or alignment between the two spaces, generalizing the permutation matrix (P) or soft assignment matrix (Π).
  - Definition: $(T_\pi g)(x) = \mathbb{E}_\pi[g(Y) \mid X = x]$.

Main Results

Theorem 1 (Convexity). For $0 \le \alpha \le 1$, the following is a convex optimization problem:

$$\inf_{\pi \in \Pi(\mathbb{P}_X, \mathbb{P}_Y)} \underbrace{(1-\alpha)\mathbb{E}_\pi\left[\|f_{\mathcal{X}}(X) - f_{\mathcal{Y}}(Y)\|_2^2\right] + \frac{\alpha}{2}\|D^\kappa_{\mathbb{P}_X}T_\pi - T_\pi D^\kappa_{\mathbb{P}_Y}\|_{\mathrm{HS}}^2}_{=\mathcal{L}(\pi)}. \tag{1}$$

- We additionally introduce an feature space $M \subset \mathbb{R}^k$, into which the source $X \sim \mathbb{P}_X$ and target $Y \sim \mathbb{P}_Y$ are mapped via continuous feature functions $f_{\mathcal{X}} : \mathcal{X} \to M$ and $f_{\mathcal{Y}} : \mathcal{Y} \to M$.

Proposition 1 (Isometry consistency). Let $T : \mathcal{X} \to \mathcal{Y}$ be a bijective measurable map, and consider $\pi = (\mathrm{Id}, T)_\# \mathbb{P}_X$. Then,

$$\|D_{\mathbb{P}_X}T_\pi - T_\pi D_{\mathbb{P}_Y}\|_{\mathrm{HS}}^2 = 0 \iff d_{\mathcal{Y}}(T(x), T(x')) = d_{\mathcal{X}}(x, x') \text{ for } \mathbb{P}_X \otimes \mathbb{P}_X\text{-a.e. } (x, x').$$

- The above proposition shows that the proposed structural penalty favors isometry transport plans, while ensuring convexity.
- More generally, the penalty vanishes iff $D_{\mathbb{P}_X}T_\pi = T_\pi D_{\mathbb{P}_Y}$, that is, if φ is an eigenfunction of $D_{\mathbb{P}_Y}$ with eigenvalue λ, then

$$D_{\mathbb{P}_X}(T_\pi\varphi) = T_\pi(D_{\mathbb{P}_Y}\varphi) = \lambda T_\pi \varphi,$$

  forcing an alignment of their geometric eigenstructures.

Theorem 2 (Consistency). Under regularity conditions, the error of the solution $\hat{\pi}$ from the empirical loss $\mathcal{L}_n(\pi)$ relative to the true optimal loss $\mathcal{L}(\pi)$ is bounded by:

$$\left|\mathcal{L}_n(\hat{\pi}) - \inf_{\pi \in \Pi(\mathbb{P}_X, \mathbb{P}_Y)} \mathcal{L}(\pi)\right| \le \underbrace{\frac{8\alpha\, n}{(T+1)}}_{\text{Optimization error}} + C \underbrace{\left(W_2^{d_{\mathcal{X}}}(\mathbb{P}_X, \hat{\mathbb{P}}_X) + W_2^{d_{\mathcal{Y}}}(\mathbb{P}_Y, \hat{\mathbb{P}}_Y)\right)}_{\text{Statistical error}},$$

Research 002: Graphical Models under Data Contamination

Research question: Can we design a robust statistical algorithm to estimate causal structures using graphical models, given that the data often suffers from **measurement errors** and other forms of **contamination** in fields like biology, social science, and environmental science?

Contributions

- **Identifiability.** Propose two complementary sets of conditions that identify true causal graph up to its Markov equivalence class (MEC), even in the presence of data contamination.
  - **Condition 1 (Anchored-frugality)**: Requires the Gaussian assumption on the true data distribution, but does not require prior knowledge of the contamination process.
  - **Condition 2 (Geometry-faithfulness)**: Is distribution-free, but requires prior knowledge of the contamination process (e.g., the structure or type of noise).
- **Consistency.** Design consistent MEC learning algorithms.

Anchored Directed Acyclic Graphical (DAG) Models

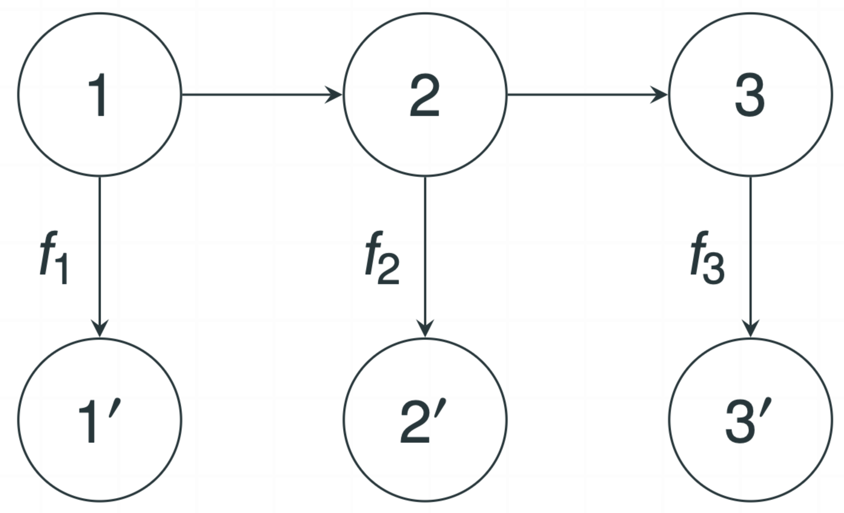


Figure: 3-node anchored DAG

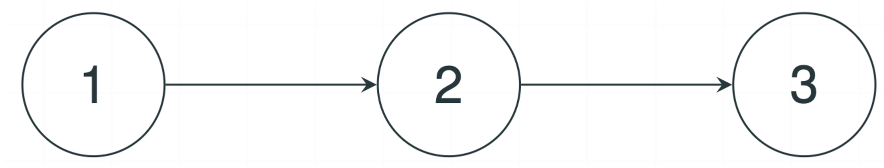


Figure: True latent DAG

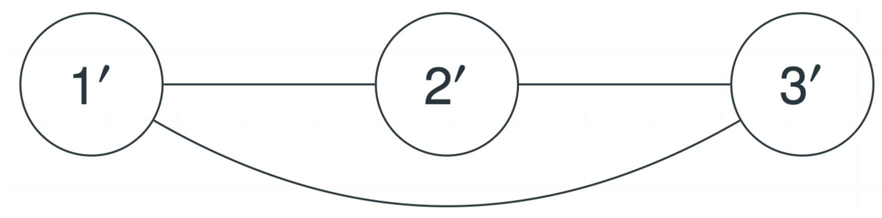


Figure: Contaminated graph

- Let $Z \in \mathbb{R}^d$ be a latent random vector generated by a linear structural equation model (SEM):

$$Z = BZ + E,$$

  where B is the edge weight matrix, and E is a mean zero random vector with finite variance.
- We assume that B is strictly lower-triangular, excluding cyclic relationships within Z.
- In anchored DAG models, we do not observe Z directly, but rather its imperfect realizations, denoted by the observed random vector $X \in \mathbb{R}^d$.
- The relationship is defined element-wise:

$$X_j = f_j(Z_j), \quad \forall j \in \{1, \ldots, d\},$$

  where each f_j can be either deterministic or a stochastic mapping.
- Anchored DAG models encompass a wide range of contamination models:
  - **Additive measurement error models.** $X_j = Z_j + \Psi_j$ with $\mathbb{E}(\Psi_j) = 0$ and $\mathbb{E}(\Psi_j^2) < \infty$.
  - **Dropout models.** $X_j = \Psi_j Z_j$ with $\Psi_j \sim \mathrm{Bernoulli}(p_j)$.
  - **Discretized models.** $X_j = \sum_{k=1}^K a_k I(Z_j \in S_k)$, where $S_1, \ldots, S_K$ form a partition of $\mathbb{R}$.

Identifiability

Condition 1 (Anchored-frugality). Let Z be Gaussian, and suppose that X is contaminated by additive measurement errors, such that its covariance matrix is $\Sigma^X = \Sigma^Z + \Sigma^\Psi$, where Σ^Ψ is diagonal. Among all possible corrections $\Sigma^X - \mathrm{diag}(\eta^2) \in \mathcal{S}^d_{++}$, the graph induced by the resulting covariance matrix Σ^Z exhibits the sparsest structure. Here, $\mathcal{S}^d_{++}$ is the set of $d \times d$ positive definite matrices.

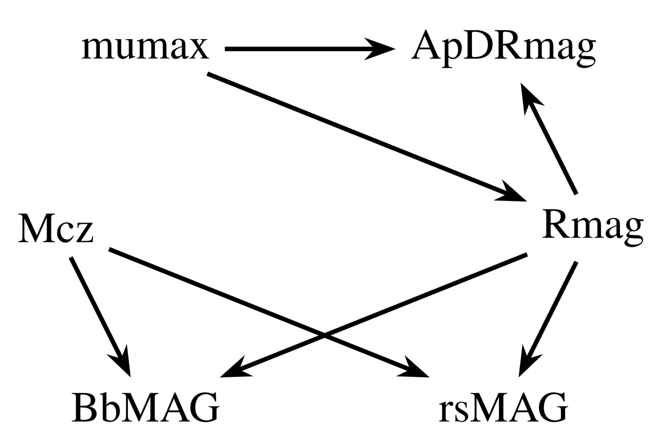
Condition 2 (Geometry-faithfulness). Assume that the latent covariance matrix Σ^Z can be recovered from the known moment relationships between X and Z. The geometry-faithfulness requires that the d-separation relationships between nodes perfectly encode the orthogonal relationships among the latent random vector Z, that is,

$$i \text{ and } j \text{ are d-separated by a set } S \iff Z_i - \Sigma^Z_{iS}(\Sigma^Z_{SS})^{-1}Z_S \text{ and } Z_j - \Sigma^Z_{jS}(\Sigma^Z_{SS})^{-1}Z_S \text{ are uncorrelated.}$$

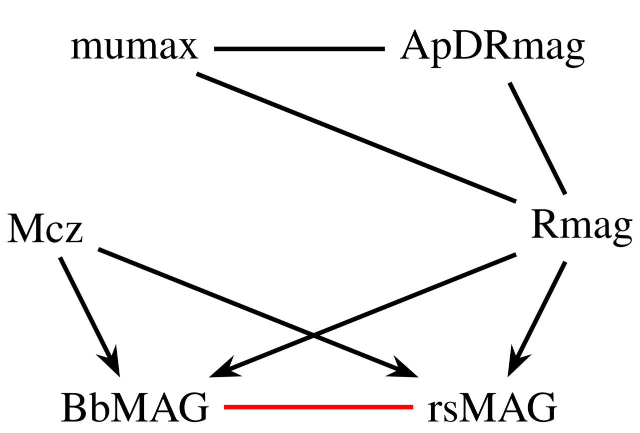
- Anchored-frugality is deeply aligned with Occam's razor: among all candidate structures obtained after correcting for variability, the simplest one reveals the true relationships.
- Geometry-faithfulness replaces the conditional independence relationships in the standard faithfulness by linear orthogonality.
- Under linear SEMs, both conditions are valid except for a set of Lebesgue measure zero.

Theorem 1 (Identifiability). Under Condition 1 or 2, the latent graph is identifiable up to its MEC.

Real-World Application: Galaxy Brightness Measurements



(a) True DAG



(b) Estimated MEC

References

- Chung, J., Ahn, Y., Shin, D., & Park, G. (2025). Learning distribution-free anchored linear structural equation models in the presence of measurement error. *Journal of the Korean Statistical Society*.
- Shin, J., Chung, J., Hwang, S., & Park, G. (2025). Discovering causal structures in corrupted data: frugality in anchored Gaussian DAG models. *Computational Statistics & Data Analysis*.