ISF Research Grant Application 2026: Multimodal Representation Learning from Unpaired Data

Principal Investigator:
Uri Shaham
Department of Computer Science, Bar Ilan University

1 Scientific Background

The ability to integrate and reason across multiple data modalities is a central frontier in modern ~~artificial intelligence~~. As applications increasingly involve diverse sensory or semantic inputs—such as text, images, speech, molecular structures, and biological measurements—there is growing demand for multimodal representation learning ~~(MMRL)~~: learning joint embeddings that capture shared semantics across modalities. This capability is foundational to many recent successes in AI, from vision-language models like CLIP [28] and GPT-4V, to biomedical applications such as protein structure prediction or multi-omics data integration.

However, most advances in ~~MMRL~~ rely heavily on paired supervision: large-scale datasets of aligned samples across modalities (e.g., image–text pairs, audio–video clips). In contrast, many scientific and real-world datasets are unpaired, weakly paired, or noisily aligned. For instance, patient data may include structured clinical tests, free-text notes, and medical images collected asynchronously and with missing links; environmental sensors may capture time series from different locations and modalities with no direct correspondences. The vast majority of multimodal data remains underutilized simply because it lacks perfect alignment.

This project aims to develop a principled and unified framework for multimodal representation learning from unpaired data, grounded in mathematical theory and scalable algorithms. We identify three core challenges that arise in the absence of paired supervision: (i) how to learn shared structure when only partial or noisy correspondences are available; (ii) how to extract statistically correlated components across modalities without access to paired samples; and (iii) how to fuse disparate modality-specific representations into a coherent joint embedding space. These challenges are addressed through three tightly connected technical objectives:

1. **Learning shared representations from ~~weakly-paired~~ data,** leveraging partial or probabilistic alignment to guide robust cross-modal embedding;
2. **Unpaired canonical correlation analysis ~~(CCA)~~,** formulating a new framework for discovering correlated structure from fully unpaired samples;
3. **Unpaired representation fusion,** designing methods to integrate independently trained modality-specific embeddings into a unified representation space.

Each objective tackles a distinct aspect of the unpaired ~~MMRL~~ problem, yet together they contribute to a comprehensive, theoretically grounded approach for learning with multimodal data in real-world settings. The methods developed will build on various mathematical tools from spectral geometry, statistics,

operator theory and optimization, and will be evaluated both empirically and analytically to ensure interpretability, stability, and generalization. While grounded in geometric and spectral methods, this proposal addresses a fundamental challenge in modern AI — the ability to learn unified representations from disjoint, unaligned, or siloed data. Our methods are broadly applicable across science and technology domains where aligned multimodal data is costly or unavailable, making them valuable tools for scalable, data-efficient, and privacy-aware AI systems

1.1 ~~Current approaches for representation Learning from unpaired data~~

Approaches such as CycleGAN [51] and domain-adversarial training [12] aim to align the marginal distributions of different modalities by fooling a discriminator into believing that mapped samples come from a shared domain. While attractive, such approaches come with serious drawbacks, such as instability, mode collapse, and lack of guarantees. Specifically, in scientific applications—where spurious correlations are common and precise interpretation matters—these drawbacks limit the reliability of adversarial approaches.

A second line of work aims at aligning marginal distributions by matching statistical or geometric patterns. Typically, such models implicitly make rigid assumptions, such as structural isomorphism or metric compatibility across modalities, which is problematic when modalities differ in information content, noise, or sampling.

Contrastive methods have seen success in paired settings, and some efforts extend them to unpaired data using heuristic pseudo-pairing strategies. While popular, such methods are mostly heuristic and may introduce noisy or biased pseudo-labels, which may result in embeddings that ~~may~~ capture correlations that do not reflect true cross-modal semantics.

To summarize, across all these approaches, common limitations emerge: ~~A~~ reliance on implicit or fragile alignment signals, lack of generality across domains and modalities, and absence of rigorous theoretical guarantees for shared structure discovery in the unpaired setting. These limitations highlight the need for a new class of methods—mathematically grounded, computationally efficient, and broadly applicable across scientific domains—which this proposal aims to develop.

Multimodal representation learning from unpaired data is rapidly becoming a central research focus, with several fascinating recent contributions that explore representation learning strategies in the absence of direct supervision in various domains, e.g., [22, 47, 49, 13, 25, 48, 1, 36, 38]. This growing body of work highlights both the promise and the complexity of the unpaired setting, motivating the need for new methods that are both mathematically principled and practically ~~effective.~~"

1.2 Scientific Potential and AI for Science

Beyond algorithmic innovation, the ability to learn from unpaired multimodal data has transformative potential for AI for science. In scientific domains—such as biology, neuroscience, geophysics, and materials science—data is often multimodal but rarely aligned. Developing methods that can integrate genomics and imaging, or correlate text-based reports with sensor data, without relying on curated pairings, can unlock rich, latent structure in complex systems. Moreover, such methods support key scientific goals: hypothesis generation, data-driven discovery, and interpretable modeling of high-dimensional processes.

In line with emerging trends toward weak supervision, modality fusion, and foundation models, this project aims to establish the mathematical and algorithmic foundations for robust multimodal learning in the absence of explicit labels or pairs—broadening the reach of AI into previously inaccessible or underutilized scientific data regimes.

2 Research Objectives and Expected Significance

The overarching aim of this project is to establish a principled foundation for **multimodal representation learning under weak or absent pairing**. Whereas current multimodal learning methods largely assume abundant aligned data, our goal is to design mathematical frameworks and scalable algorithms that remain effective when correspondences are scarce, noisy, or entirely missing. This requires resolving fundamental challenges of discovering shared latent structure without explicit supervision, defining meaningful cross-modal correlation when the problem is ill-posed, and integrating both shared and modality-specific information without paired examples. The three objectives below each tackle one of these challenges, together forming a coherent program that advances both the theoretical underpinnings and practical applicability of multimodal learning from unpaired data.

Objective 1: Learning Shared Representations from ~~Weakly-Paired~~ Data

This objective aims to develop a theoretical and algorithmic framework for learning shared representations across modalities under weak supervision. A shared representation is a common latent space in which instances from different modalities that convey the same underlying information are mapped to the same—or nearby—points. In many practical settings, such as in science, medicine, and human-centered data, such correspondences are not fully available: data may be only coarsely aligned, sparsely paired, or entirely unpaired. This objective addresses the challenge of learning shared representations in these ~~weakly paired~~ regimes by exploiting the **universality of embedding geometries**—the observation that meaningful structure in each modality can be captured in a way that is stable, comparable, and aligned across domains. By enabling the discovery of shared latent structure without relying on strong pairing assumptions, this objective contributes to broadening the scope and robustness of multimodal representation learning in real-world, weakly supervised environments.

Objective 2: ~~Unpaired Canonical Correlation Analysis (CCA)~~

The second objective is to establish a framework for discovering maximally correlated representations across modalities **without access to paired data**. Canonical ~~Correlation Analysis~~ (CCA) is an extremely popular algorithm for learning representations of multimodal data, widely used by practitioners in numerous areas in data science and machine learning. CCA traditionally requires paired samples to identify projections that reveal shared latent structure between two views. In the absence of such pairing, the problem becomes fundamentally ill-posed, as many joint distributions can be consistent with a given pair of marginals. This objective addresses the challenge by introducing a principled criterion for selecting among ~~these~~; namely, the joint distribution that **maximizes cross-modal correlation**. We show that this ~~joint~~ can be characterized as the solution to an optimal transport problem, augmented with orthogonality constraints to ensure the resulting embeddings behave analogously to classical CCA projections. Beyond the theoretical formulation, this objective also includes the **development of efficient and scalable algorithms** for computing such ~~unpaired CCA~~ embeddings, enabling practical application to large-scale multimodal datasets. This contributes both foundational insights and computational tools to the broader effort of multimodal representation learning from unpaired data.

Objective 3: Unpaired Representation Fusion

The third objective is to develop a framework for fusing representations across modalities in the absence of pairing, under the assumption that different modalities carry both shared and modality-specific information. In contrast to approaches that focus solely on common latent structure, this objective seeks to learn rich represen-

tations that integrate the full informational content of all modalities—capturing both what is shared and what is unique. Achieving this without access to paired data requires novel strategies for aligning and combining modalities. A key innovation in our approach is the use of artificially generated pairs, which serve as anchors for bridging modalities without relying on real correspondences. This departs fundamentally from CycleGAN-style methods, which rely on bidirectional consistency losses and implicitly assume strong information overlap. By relaxing this assumption, our goal is to enable more flexible and expressive multimodal fusion that reflects the complexity of real-world data. This objective advances multimodal representation learning by addressing a central, yet underexplored, challenge: how to integrate complementary signals from unpaired sources into a unified representation space.

2.1 Expected ~~significance~~

Multimodal data is pervasive across science and technology — from medical diagnostics that combine imaging, text, and molecular data, to autonomous systems that process visual, auditory, and spatial signals. Yet in many real-world settings, paired multimodal data is rare or unavailable, severely limiting the applicability of standard multimodal learning approaches. This project addresses this fundamental challenge by developing mathematically grounded and practically effective methods for learning from unpaired multimodal data, thereby expanding the scope and usability of machine learning in real-world contexts.

On the scientific level, the project is expected to make fundamental contributions to the theory of multimodal representation learning. It introduces new frameworks for learning shared and fused representations without supervision, grounded in tools from optimal transport, spectral theory, and statistical dependence. These contributions go beyond heuristic or adversarial approaches by offering a principled understanding of when and how unpaired modalities can be aligned and integrated — filling an important gap in the literature. The project is also expected to yield new algorithmic paradigms that are scalable, robust, and broadly applicable.

From a practical standpoint, the outcomes of this research will be relevant across domains that involve heterogeneous and unaligned data sources. In biomedicine, for example, the ability to integrate genomic, imaging, and clinical text data without requiring aligned patient samples could lead to more holistic diagnostic and prognostic models. In climate science, combining satellite imagery with sensor readings and textual reports can support more comprehensive environmental monitoring. In human-computer interaction, learning from unpaired speech, gesture, and visual input can enable more adaptive and multimodal AI agents.

Moreover, the project aligns with broader trends in AI that prioritize data efficiency, robust generalization, and cross-modal understanding. By enabling flexible and modular representation learning from unpaired data, it supports the development of AI systems that are more adaptable to real-world complexity, including scenarios where supervised data is scarce or privacy constraints prevent alignment.

In summary, this project has the potential to advance both the foundations of machine learning and its practical reach across scientific and technological domains, making multimodal AI more broadly accessible, theoretically principled, and capable of addressing high-impact challenges in science and society.

3 Detailed Description of the Proposed Research

3.1 Working Hypotheses

This project is guided by the following hypotheses:

Main Hypothesis (~~overarching aim~~): It is possible to develop a principled framework for multimodal representation learning that does not rely on paired data by leveraging universal geometric properties of embeddings, optimal transport formulations of correlation, and novel strategies for representation fusion. Under this framework, meaningful shared structure across modalities can be consistently identified even in the absence of explicit correspondences.

Hypothesis 1 (Objective 1 – ~~Weakly-Paired~~ Data): Embedding geometries across different modalities exhibits universal structures that can be aligned in a shared latent space. Even when correspondences are coarse, sparse, or noisy, these universal properties enable recovery of semantically consistent shared representations.

Hypothesis 2 (Objective 2 – ~~Unpaired CCA~~): Among the many joint distributions consistent with two marginal distributions, the one that maximizes cross-modal correlation corresponds to the true latent alignment. This joint can be recovered through an optimal transport formulation with orthogonality constraints, yielding ~~unpaired CCA~~ embeddings with theoretical guarantees and scalability.

Hypothesis 3 (Objective 3 – Unpaired Fusion): Multimodal fusion that integrates both shared and modality-specific information is feasible without paired data, provided that artificial anchor pairs are introduced. These anchors enable alignment across modalities without requiring strict overlap assumptions, thereby supporting more expressive and flexible multimodal representations than ~~cycle-consistency-based-based~~ methods.

3.2 Learning Shared Representations from ~~Weakly-Paired~~ Data

Multimodal representation learning aims to construct a common embedding space in which samples from different modalities that convey the same underlying information are mapped to similar representations. In most existing frameworks, this goal is achieved through fully paired supervision, where each sample in one modality is matched with its exact counterpart in the other. However, in many practical settings—such as medicine, scientific research, or human behavior modeling—pairing between modalities is sparse, noisy, or entirely missing. This objective aims to develop a theoretically grounded framework for learning shared representations under weak supervision, leveraging the intrinsic geometry of each modality to guide alignment.

3.2.1 Rationale

Mathematical Motivation. Modern pre-trained unimodal foundation models have a proven ability to represent semantics. For example, two given images have close embeddings if their semantic meaning is similar, and far apart otherwise. These similarities can be captured by a random walk process on the samples' representations. This suggests that a random walk process defined on such unimodal representations should largely correspond to semantic similarity. Therefore, we can expect random walks defined on different unimodal representations that capture semantics well to be highly similar. Random walk processes are finite analogs of diffusion operators. Thereby, the similarity of random walks that are constructed from different, modality-dependent representations implies that the eigenfunctions of the corresponding diffusion operators will have universality properties (i.e., ~~modality-invariance~~) [7]. Therefore, constructing a spectral embedding (SE) based on the leading eigenvectors of random walks, which are viewed as discrete approximations of the leading eigenfunctions of diffusion operators [3, 31], enables us to take advantage of this concept even in the absence of paired data.

We formalize our assumption as follows. Let $\mathcal{M}$ be a latent, underlying semantic manifold, and let f, g be two transformations, such that $f(\mathcal{M})$ and $g(\mathcal{M})$ represent the two modalities from which we observe samples.

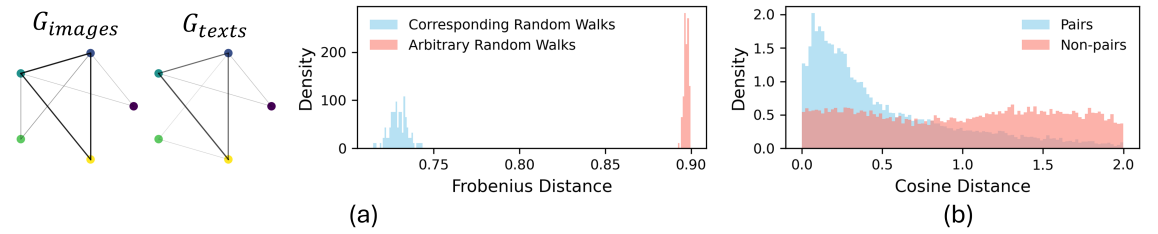


Figure 1: **Empirical demonstration of universality.** (a) Distances between corresponding random walks on image and text graphs from MSCOCO, compared to distances to randomly shuffled (non-matching) walks. Although constructed independently from unimodal features, corresponding walks exhibit significantly greater similarity. (b) Distances between paired and unpaired points in the shared space of aligned 2D ~~spectral embeddings (~~SEs~~)~~. Paired points are consistently closer, indicating that the independently learned SEs capture analogous structure across modalities.

There is a body of work specifying conditions under which the spectral properties of $\mathcal{M}$ are preserved under f, g. For example, if f, g have bounded distortion and bounded Ricci curvature, the corresponding eigenfunctions of the Laplace-Beltrami operator on $f(\mathcal{M})$ and $g(\mathcal{M})$ are similar in the L_∞ sense [5].

Intuitively, our assumption states that the diffusion operators defined on each modality are relatively similar. This assumption is also empirically supported in recent ~~works~~ [17, 10, 14]. Then, universality is enabled through the eigenfunction preservation properties of the similar diffusion operators. Namely, the eigenfunctions of these operators will be universal, in the sense of ~~modality-invariance~~ (see Figure 1).

In practice, the ability to learn Laplacian eigenfunctions is obtained via SpectralNet [29], a previous work of the PI. ~~While trained to compute the eigenvectors of the graph Laplacian of its training data, being a generalizable parametric map makes it a practical means to compute the eigenfunctions of the Laplacian operator (and thus also of the Diffusion operator), viewing the eigenvectors as a discretization of the eigenfunctions [3, 31].~~ Crucially, we train SpectralNet on unimodal data only; hence, no paired data is needed to learn the Laplacian eigenfunctions, i.e., our universal embedding functions.

Overview. In a recent preprint of ours [41], ~~we propose and explore a novel pipeline, named Spectral Universal Embedding (SUE).~~ SUE consists of three steps: SE, ~~CCA and MMD~~. First, it maps each pre-trained unimodal embedding space into its corresponding eigenspace, to retrieve the global structure of each modality [2, 24, 32]. Using SpectralNet [29], this is done parametrically, allowing generalization to test data. ~~Noteworthy,~~ SE is not unique, as eigenvalues with multiplicity p can yield any basis spanning the p-dimensional eigenspace and even single eigenvectors may differ by sign.

To resolve the SE ambiguity and provide additional linear alignment, we use CCA on a minimal number of paired samples. However, as ~~the~~ CCA ~~purposefully~~ considers a limited number of samples, and the SEs differ by more than an orthogonal transformation, we strengthen the cross-modal alignment using a ~~Maximum Mean Discrepancy (~~MMD~~)~~ residual network [30]. This kind of network architecture was originally proposed (by the PI) for batch-effect removal by minimizing the empirical MMD value of two distributions. Namely, we view the two low-dimensional representations as similar distributions and learn a (close to identity) non-linear shift to align the distributions. The MMD serves as the last step to fine-tune the alignment. Notably, MMD loss does not require paired data, which enables the utilization of the full unpaired dataset. Figure 2 depicts SUE.

3.2.2 Uncovering SUE

In this section, we formularize SUE, roughly described in ~~Sec~~ 3.2.1. ~~A summary of the~~ steps of the SUE algorithm ~~is~~ outlined in Algorithm 1.

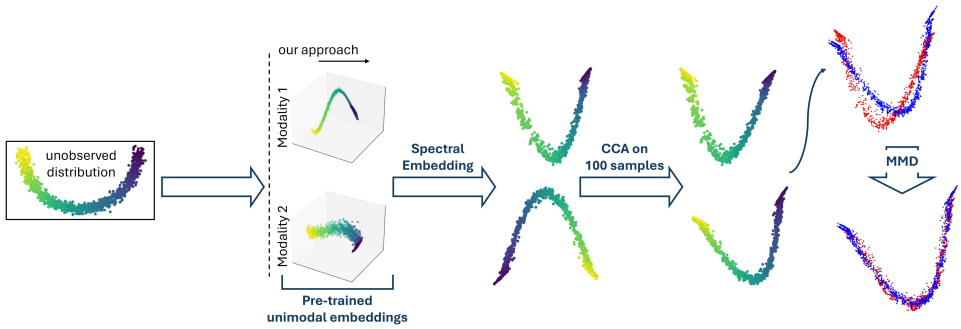


Figure 2: ~~SUE's overview~~. The modalities (represented by their unimodal embeddings) represent an unobserved universal (semantic) distribution; the SE is capable of retrieving this universal structure, up to rotations; CCA on a minimal number of pairs enable linear alignment between the modalities, but not sufficient for a joint universal embedding; the MMD then fixes the misalignment between the modalities, integrating them into the universal embedding space.

Notations. Throughout this section, we will use the following notations. Let $\mathcal{X} \subseteq \mathbb{R}^{d_1}, \mathcal{Y} \subseteq \mathbb{R}^{d_2}$ be sets of unpaired pre-trained unimodal embeddings of sizes n_1, n_2, ~~resp.~~ Accordingly, denote $\mathcal{X}_p = \{x_1, \ldots, x_m\} \subseteq \mathcal{X}, \mathcal{Y}_p = \{y_1, \ldots, y_m\} \subseteq \mathcal{Y}$ to be sets of paired embeddings. Importantly, $m \ll n_1, n_2$. Let $k \geq r$ be two pre-chosen dimensions for the SE and final universal representations.

Approach. Given $\mathcal{X}, \mathcal{Y}$, we train two independent SpectralNet models $S_\mathcal{X} : \mathcal{X} \to \mathbb{R}^k$, $S_\mathcal{Y} : \mathcal{Y} \to \mathbb{R}^k$ to approximate the k-dimensional SE of each modality. ~~Due to~~ the non-uniqueness of the SE, $S_\mathcal{X}$ and $S_\mathcal{Y}$ might differ by sign and basis of each eigenspace.

To address this ambiguity we utilize $\mathcal{X}_p$ and $\mathcal{Y}_p$. Specifically, we employ CCA on $\big(S_\mathcal{X}(\mathcal{X}_p), S_\mathcal{Y}(\mathcal{Y}_p)\big)$ to obtain the projections $Q_\mathcal{X}, Q_\mathcal{Y} \in \mathbb{R}^{k \times r}$. These projections are used to align $S_\mathcal{X}(\mathcal{X})$ and $S_\mathcal{Y}(\mathcal{Y})$. The linearly aligned SEs approximations can be written as $\tilde{S}_\mathcal{X} := Q_\mathcal{X} \circ S_\mathcal{X}$, $\tilde{S}_\mathcal{Y} := Q_\mathcal{Y} \circ S_\mathcal{Y}$.

Then, we learn a residual neural network $F_\theta : \mathbb{R}^r \to \mathbb{R}^r$ to bring the distribution of the linearly aligned SEs as close as possible. Specifically, we minimize the squared MMD between the two empirical distributions

$$\mathcal{L}_{\text{MMD}} = \frac{1}{m_1^2} \sum_{x_i, x_j \in \mathcal{X}} \kappa(\tilde{x_i}, \tilde{x_j}) - \frac{1}{m_1 m_2} \sum_{x_i \in \mathcal{X}, y_j \in \mathcal{Y}} \kappa(\tilde{x_i}, \tilde{y_j}) + \frac{1}{m_2^2} \sum_{y_i, y_j \in \mathcal{Y}} \kappa(\tilde{y_i}, \tilde{y_j}), \tag{1}$$

where m_1, m_2 are the corresponding batch sizes, κ is a universal kernel (e.g., ~~RBF~~ kernel), and $\tilde{x_i} = \tilde{S}_\mathcal{X}(x_i)$, $\tilde{y_i} = \tilde{S}_\mathcal{Y}(y_i)$. The final functions can be written as $f_\mathcal{X} := \tilde{S}_\mathcal{X}$, $f_\mathcal{Y} := F_\theta \circ \tilde{S}_\mathcal{Y}$.

Given a new test point y_t, ~~sampled from the same distribution as $\mathcal{Y}$, we simply propagate it through $f_\mathcal{Y}$, and similarly to~~ a test point sampled from the $\mathcal{X}$ distribution.

Algorithm 1: ~~Spectral Universal Embedding (~~SUE~~)~~

Input: Unpaired sets of pre-trained unimodal embeddings $\mathcal{X} \in \mathbb{R}^{n_1 \times d_1}$ and $\mathcal{Y} \in \mathbb{R}^{n_2 \times d_2}$, and paired sets $\mathcal{X}_p$ and $\mathcal{Y}_p$ of size $m \geq 0$

Output: Maps $f_\mathcal{X} : \mathbb{R}^{d_1} \to \mathbb{R}^r$, $f_\mathcal{Y} : \mathbb{R}^{d_2} \to \mathbb{R}^r$ approximating the universal embedding from each modality

1 Train $S_\mathcal{X}, S_\mathcal{Y}$

2 Perform CCA on $\big(S_\mathcal{X}(\mathcal{X}_p), S_\mathcal{Y}(\mathcal{Y}_p)\big)$ to obtain projections $Q_\mathcal{X}, Q_\mathcal{Y} \in \mathbb{R}^{k \times r}$

3 Train a residual neural network $F_\theta : \mathbb{R}^r \to \mathbb{R}^r$ to minimize the MMD loss $\mathcal{L}_{\text{MMD}}$ (Eq. 1)

4 Return the maps:

$$f_\mathcal{X} := Q_\mathcal{X} \circ S_\mathcal{X}, \quad f_\mathcal{Y} := F_\theta \circ Q_\mathcal{Y} \circ S_\mathcal{Y}$$

5 At inference time, propagate the sample x or y through the appropriate map $f_\mathcal{X}(x)$ or $f_\mathcal{Y}(y)$

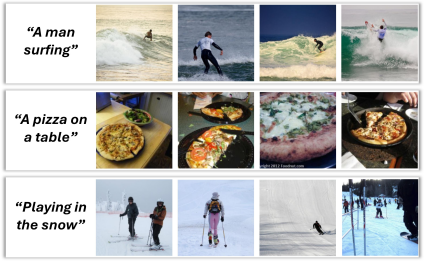


Figure 3: **Almost exclusively unpaired image retrieval.** Retrieved images for custom captions on the MSCOCO dataset, trained with 100 pairs and 10k non-pairs. The retrieved images are highly similar semantically to the text queries, even though almost no pairs were available during training.

Table 1: **Retrieval results.** Results with few paired samples on vision-language (🏞📝) and vision-vision (🏞🏞) datasets from each modality to another: image-to-text (I2T), text-to-image (T2I), edges-to-shoes (E2S), shoes-to-edges (S2E); by SUE and Contrastive. The Imp. column states the relative mean improvement of SUE over Contrastive learning. Using the same small number of pairs, SUE significantly outperforms the popular paired ~~method.~~ **SUE substantially relies on unpaired data.**

	#paired		SUE (ours) R@1	SUE (ours) R@5	SUE (ours) R@10	Contrastive R@1	Contrastive R@5	Contrastive R@10	Imp.
MSCOCO 🏞📝	100	I2T	5.75	21.50	34.25	1.50	8.50	13.00	+257.20%
		T2I	5.25	18.25	33.25	0.80	5.80	12.20	
Flickr30k 🏞📝	500	I2T	4.25	19.75	32.00	3.00	9.50	16.20	+103.32%
		T2I	5.75	22.00	32.75	2.50	9.80	15.00	
Polyvore 🏞📝	500	I2T	6.00	22.75	32.25	3.20	13.8	22.5	+55.67%
		T2I	4.75	20.75	32.00	4.00	11.50	23.00	
Edges2Shoes 🏞🏞	50	E2S	4.00	16.00	25.25	1.0	5.50	14.00	+200.51%
		S2E	3.50	17.00	27.00	0.80	6.00	12.80	

3.2.3 Preliminary Results

In this section, we provide a demonstration of SUE for ~~vision-language~~ retrieval (Figure 3, Table 1). Additional results demonstrating capabilities in zero-shot classification and image manipulation are not provided~~,~~ due to space limitations. In addition, Figure 4 demonstrates that SUE is designed to benefit from unpaired data~~,~~ by ~~analyzing~~ the effects of different numbers of paired and unpaired instances on the performance of SUE.

Unpaired ~~samples~~. ~~Fig.~~ 4b shows the impact of additional unpaired samples. This ~~experiment~~ is of significant interest, as unpaired samples are usually considered unusable in the multimodal setting for point-to-point matching. The results indicate that additional *unpaired* data significantly enhances retrieval results. This opens the door for a new ~~regime~~ of multimodal ~~learning – using~~ unpaired data with only a minimal number of available pairs.

Paired ~~samples~~. ~~Fig.~~ 4c depicts the results of an analogous experiment examining the effect of the number of paired samples required for the CCA step, with the unpaired samples held constant. As expected, a minimal number of paired samples are required for good results (∼500 in this case of Flickr30k). However, SUE does not rely on additional pairs, as increasing their number above the minimum required is redundant. This outcome highlights the potential for learning significant cross-modal embeddings while focusing on unpaired data, which ~~is~~ much easier to obtain.

3.2.4 Future Directions

The proposed method advances multimodal learning by showing that meaningful shared representations can be learned from structure alone, without explicit correspondence. This opens the door to broader deployment of

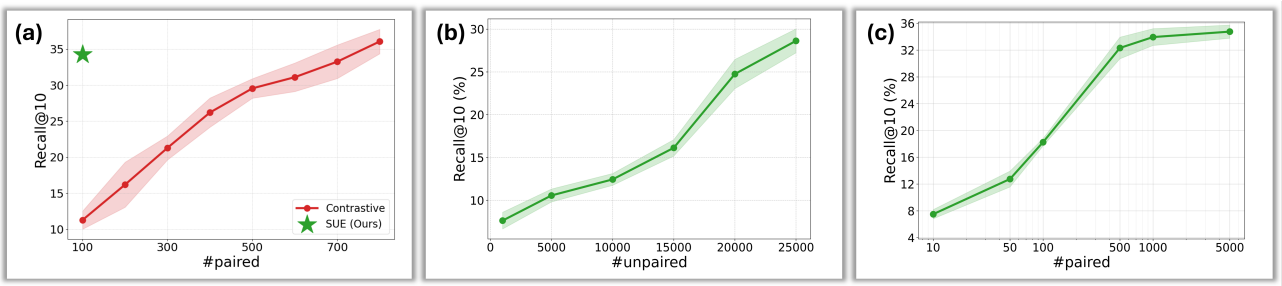


Figure 4: **(a) Contrastive requires an order of magnitude more pairs to achieve similar results as SUE in the weakly-paired regime.** Recall@10 results on MSCOCO by SUE (with 100 pairs) and Contrastive with various numbers of pairs. SUE exploits unpaired data to outperform contrastive learning when limited pairs are available. An order of magnitude more pairs are required to achieve similar results with contrastive learning; (b-c) Effect of #unpaired and #paired samples on Recall@10 results on image retrieval on the Flickr30k dataset. **(b) SUE improves as the amount of unpaired data is increased. (c) SUE relies on non-pairs instead of pairs.** SUE relies minimally on paired data, while substantially on unpaired data, enabling it to enhance its performance with additional unpaired samples, which are much easier to obtain.

multimodal models in settings where data collection is siloed, incomplete, or ~~privacy-constrained~~.

As part of this objective, we plan to:

- **Task 1.1**: Formalize conditions under which spectral alignment is provably possible.
- **Task 1.2**: Extend the method to handle multiple modalities~~, by~~ using multiview CCA machinery
- **Task 1.3**: Apply the method to real-world scientific datasets, such as multi-omics, medical imaging + text, sensor fusion, graphs, and time series
- **Task 1.4**: Investigate manifold-alignment methods, e.g., [8] as a pre-processing step, to expand the applicability of SUE to new modalities.
- **Task 1.5**: Investigate robustness to modality-specific distortions and distribution shifts.
- Investigate the applicability of SUE to unpaired multimodal causal discovery tasks, by replacing contrastive learning [23, 44].
- ~~**Task 1.6:** Most importantly, the following objective proposes the development of an unpaired CCA technique. While important in its own right, an immediate application of it would be to turn SUE into a fully unpaired method, as the pairs are used in the SUE pipeline only in CCA.~~

Ultimately, this objective offers a new paradigm for multimodal learning: instead of relying on dense supervision, we extract and align universal geometric structure, enabling robust, interpretable, and scalable learning in weakly supervised environments.

3.3 Objective 2: ~~Unpaired Canonical Correlation Analysis (CCA)~~

3.3.1 ~~Overview of this objective.~~

Despite recent progress in leveraging unpaired data, no principled extension of CCA to the unpaired setting exists. Our aim is to bridge this gap by establishing a theoretical connection between distributional divergences and correlation, and by formulating a provable equivalence to CCA that holds without access to paired samples. In particular, our theoretical analysis reveals that the Wasserstein distance plays a central role in this equivalence [35]. Specifically, the 2-Wasserstein distance between two marginal distributions P_X, P_Y can be shown to be equivalent to the correlation of their maximally correlated joint distribution, which we denote by $\mathrm{MCJ}(P_X, P_Y)$.

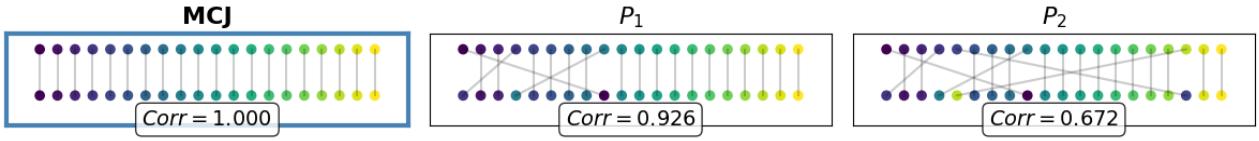


Figure 5: **MCJ.** A demonstration of Maximum Correlation Joint between two uniform distributions. Many joints are possible, but the left joint maximizes the correlation and indeed is the MCJ.

This insight leads to proposing an approach for unpaired CCA, which we term UCCA, operating by finding linear orthogonal projections for each view, with minimal Wasserstein distance. An important preliminary result of ours (Theorem 3.3) states that, under mild assumptions,

$$\mathrm{UCCA}(P_X, P_Y) = \mathrm{CCA}\big(\mathrm{MCJ}(P_X, P_Y)\big).$$

Intuitively, this means that UCCA recovers the CCA solution of a specific, highly meaningful joint distribution of P_X, P_Y.

Building on this theoretical foundation, we aim to develop a practical algorithm that can learn shared representations in fully unpaired settings. The reformulation of correlation maximization as a distribution matching problem enables the application of tools from Riemannian geometry and manifold optimization to the problem of correlation maximization in the unpaired setting. Specifically, we define the following tasks:

- **Task 1.1**: **Theoretical Connection between Wasserstein Distance and CCA:** We aim to prove a formal link between minimizing the Wasserstein distance between two distributions and maximizing the correlation under their maximally correlated joint. This result provides a bridge between optimal transport and classical correlation-based methods.
- **Task 1.2**: **Unpaired Canonical Correlation Analysis (UCCA):** Based on our theoretical insights, we aim to introduce a fully unpaired variant of CCA. This practical tool enables correlation-based learning without any paired data by connecting Wasserstein distance, correlation, and optimization in a unified framework.
- **Task 1.3**: **Unpaired Nonlinear Shared Representation Learning:** Finally, by integrating our weakly-paired and unpaired techniques, we aim to construct a fully unpaired multimodal learning framework capable of learning nonlinear shared representations.

3.3.2 Previous work on Unpaired CCA.

Timilsina et al. [34] proposed a provable framework for unpaired shared component analysis, although its connection to correlation remains unclear. An earlier attempt by Hoshen and Wolf [15] introduced an unpaired variant of CCA; however, their method is unstable and requires multiple runs to obtain satisfactory results, as noted in their own work. Additionally, no implementation is publicly available, limiting its reproducibility and practical use. On a more theoretical front, the concept of a maximally correlated joint distribution has been studied in depth [9, 18, 33], and its connection to optimal transport is well established [35]. However, the link between this joint and the classical CCA algorithm has not been formally drawn.

3.3.3 Preliminary theoretical results

While in the weakly-paired domain, we have developed and assessed a method to capture a universal embedding, in the unpaired domain, our current results are mostly theoretical. To understand our theoretical result,

we first need to define a few terms.

Definition 3.1. *The ~~Maximum Correlation Joint (MCJ)~~ of two whitened ~~distribution~~ P_X, P_Y is*

$$MCJ(P_X, P_Y) = \arg \sup_{P_{XY} \in \mathcal{J}(P_X, P_Y)} TC(P_{XY})$$

where $\mathcal{J}(P_X, P_Y)$ is the set of all joint distributions of P_X and P_Y, and $TC(P_{XY})$ is the sum of correlations between the corresponding dimensions.

A demonstration of the MCJ is depicted in ~~Fig.~~ 5. Def. 3.1 lets us reformulate the known connection between Wasserstein distance and correlation, as follows.

Proposition 3.2. *Let P_X, P_Y be whitened probability measures, then*

$$TC\big(MCJ(P_X, P_Y)\big) = d - \frac{1}{2} W_2(P_X, P_Y)^2$$

where $W_2(P_X, P_Y)$ is the 2-Wasserstein distance between P_X, P_Y.

That is, the 2-Wasserstein distance between the marginal distributions P_X, P_Y of two views corresponds to the correlation between the ~~maximally correlated joints~~ of the marginal distributions. For readability, we skip a few formal definitions here~~,~~ and intuitively define $\text{MCJ}_{\mathcal{F}}(P_X, P_Y)$ as the "best" MCJ of P_X, P_Y in terms of total correlation~~,~~ over all projections in a function class $\mathcal{F}$. ~~We also denote by UCCA our algorithm for unpaired CCA. That is, minimizing~~ the Wasserstein distance over all orthogonal projections from $\mathbb{R}^d$ to $\mathbb{R}^k$. By that, we can finally state our novel result, which is

Theorem 3.3. *Let P_X, P_Y be whitened probability measures. Under mild assumptions,*

$$UCCA(P_X, P_Y) = CCA(MCJ_{V_k(\mathbb{R}^n)}(P_X, P_Y))$$

Intuitively, Thm. 3.3 states that our UCCA algorithm is equivalent to CCA on a specific joint of P_X, P_Y - the best MCJ of their projections.

3.4 Objective 3: Unpaired Representation Fusion

3.4.1 ~~Overview of this objective.~~

The prevailing paradigm in multi-view representation learning, particularly in contrastive self-supervised methods, is to extract only the *shared* information between views while suppressing view-specific information. While this is effective for achieving invariance, it inevitably discards the complementary and unique signals that each modality provides. In contrast, our objective in this case is not merely to align views by eliminating differences, but rather to *fuse* them in a way that leverages both the shared structure and the unique information contained in each view. This richer fusion is critical in settings where each modality contributes distinct yet meaningful aspects of the underlying phenomenon. Crucially, we aim at learning such unified representations across views in the absence of any pairwise correspondences.

Specifically, we plan to achieve this by thinking of each view as a diffusion operator constructed from its data manifold. Using previous methods of the PI for generalizable ~~spectral embeddings~~ [29, 4, 42], we generalize the eigenfunctions of each operator to evaluate across all views, yielding *artificially parallel* diffusion maps. These are then summed into a fused operator that encodes both global and view-specific geometry, serving as a surrogate for true cross-view relationships.

3.4.2 Previous work on unpaired cross-domain learning.

In the cross-modal setting, cycle-consistency frameworks such as CycleGAN [51] and StarGAN [6] have been applied to learn mappings between unpaired domains. While successful in some settings, these techniques often struggle to preserve fine-grained structure, are difficult to train, and typically rely on implicit distributional assumptions. Moreover, they do not explicitly model the geometric or spectral structure of the data.

A few recent works address unpaired multi-view scenarios by designing methods for specific tasks such as clustering or classification. These methods are typically not designed for learning a unified representation and instead construct task-driven models that operate on a cluster level or seek weak correspondences indirectly. In clustering, methods based on matrix factorization, graph matching, tensor learning, manifold learning, pseudo labeling, or contrastive learning operate at the cluster level or seek weak correspondences indirectly [45, 37, 20, 19, 50, 21, 43, 39, 46, 16, 40]. While these approaches provide practical solutions in constrained settings, they are not general-purpose multi-view learning frameworks and do not support representation learning that integrates both shared and unique information across modalities.

3.4.3 Mathematical layout.

Artificial parallelism via functional maps. Consider two manifolds $\mathcal{M}, \mathcal{N}$, representing two modalities, and an arbitrary injective map $T : \mathcal{M} \to \mathcal{N}$. A functional map [27, 11] T_F is an operator between function spaces $\mathcal{F}(\mathcal{M})$ and $\mathcal{F}(\mathcal{N})$ consisting of real-valued functions over each manifold so that if $f \in \mathcal{F}(\mathcal{M})$ and $y \in \mathcal{N}$ then $T_F(f)(y) = f(T^{-1}(y))$. Conveniently, for any T, the functional map T_F is linear, and can be expressed as a matrix C describing the transformation in terms of bases of $\mathcal{F}(\mathcal{M})$ and $\mathcal{F}(\mathcal{N})$. Specifically, if $f \in \mathcal{F}(\mathcal{M})$ with basis expansion

$$f = \sum_i a_i^{\mathcal{M}} \phi_i^{\mathcal{M}} = \mathbf{a}^{\mathcal{M}} \Phi^{\mathcal{M}}$$

and $g = T_F(f)$ be its corresponding functional in $\mathcal{F}(\mathcal{N})$:

$$g = \sum_i a_i^{\mathcal{N}} \phi_i^{\mathcal{N}} = \mathbf{a}^{\mathcal{N}} \Phi^{\mathcal{N}}$$

The functional map C gives a convenient translation between their basis coefficients $\mathbf{a}^{\mathcal{N}} = C\mathbf{a}^{\mathcal{M}}$. A well-chosen basis (typically Laplacian eigenfunctions) has the property that a small number of basis elements are often sufficient to represent smooth functions to a high accuracy, resulting in a matrix C of a relatively small size.

Our idea is to use a functional map, trained in an unsupervised manner, in order to create artificial pairs for samples from a single modality. Such artificial pairs might allow us to use methods for paired data like contrastive learning or fusion approaches, as if the data were originally paired, such as a recent work of the PI [41].

Learning fused representations. We plan to use the artificially paired data to learn a fused representation combining information from both modalities. Such a representation can be used for downstream tasks, requiring information from all modalities. However, assuming that the above idea will allow us to generate pairs for all unimodal samples is probably too naive. A more probable scenario is that only a small portion of the pairs will be reliable.

Our plan is to use the fused representation to train models for downstream tasks. The parameters of such models will naturally encode information about all modalities. In inference time, however, we will encounter

only unpaired data (i.e., each data sample is expected to be unimodal). To overcome this, we plan to learn encoders from each unimodal space to the joint space. This will allow us to artificially complement information from other views to unimodal samples.

We therefore define the following tasks

- **Task 1.1**: **Design supervised descriptors.** For example, in the supervised case, where partial correspondence is available, one way to design descriptors is via the assumption that Dirac functions are mapped to Dirac functions, and local bumps are mapped to local bumps.
- **Task 1.2**: **Design unsupervised descriptors:** Recently, [11] has also used them for representation learning. However, they report a significant gap between the performance with supervised and unsupervised descriptors. As a by-product of this research objective, we plan to design improved unsupervised descriptors, possibly by leveraging spectral properties.
- **Task 1.3**: **Subset selection for functional map training:** For example, in the supervised case, this might be done via selecting Diracs and bumps that are faithfully represented as combinations of a small number of basis elements.
- **Task 1.4**: **Selection reliable artificial pairs for learning the fused representation :** Specifically, this will involve developing an approach for distinguishing reliable pairs from less reliable ones, possibly via reconstruction or cycle consistency terms.
- **Task 1.5**: **Application of the above pipeline for scientific discovery :** One attractive applicative domain is multi-omics data. Specifically, we will explore the benefits of the proposed pipeline over approaches like matching of domain conversion, e.g., [26].

3.4.4 Preliminary results

In preliminary experimental results, we successfully represented bump functions using 128 Laplacian eigenfunctions on real-world data. This demonstrates that a compact spectral basis is sufficient to capture local patterns, supporting our hypothesis that functional maps preserve locality by mapping bumps to bumps. Building on this, we are now generating artificial cross-modal pairs using the same framework, with encouraging non-trivial results. We have also implemented a scalable Gromov–Wasserstein manifold alignment objective (see Section 3.9) to further stabilize learning. Together, these results suggest that our spectral framework effectively captures cross-modal correspondences in unpaired settings and provide a strong foundation for extending the approach to higher-dimensional and geometrically complex modalities.

3.5 Plan of Evaluation

The success of this project will be evaluated through a combination of theoretical analysis, algorithmic development, and empirical validation across synthetic and real-world multimodal datasets. Each of the three objectives will be assessed according to the following criteria:

Objective 1: Learning Shared Representations from Weakly-Paired Data We will evaluate the quality of the learned shared representations by measuring cross-modal retrieval performance, alignment consistency, and robustness to pairing noise. Benchmark comparisons will be made against state-of-the-art methods in weakly supervised and semi-supervised multimodal learning. Theoretical evaluation will involve proving conditions under which universality guarantees hold and deriving error bounds on the recovered embeddings.

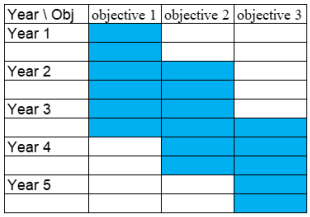
Objective 2: ~~Unpaired Canonical Correlation Analysis~~ The effectiveness of the proposed ~~unpaired CCA~~ framework will be assessed through correlation recovery, representation disentanglement, and computational efficiency. Empirical experiments will test the approach on standard unpaired datasets such as cross-lingual word embeddings, image-text pairs, and audio-visual benchmarks. We will also evaluate the practicality of the algorithm under distribution shifts and limited sample regimes.

Objective 3: Unpaired Representation ~~Fusion~~ Evaluation will focus on the ability of the model to capture both shared and modality-specific information without supervision. We will design proxy tasks such as zero-shot classification, few-shot transfer, and multimodal completion to quantify the utility of fused representations. Comparisons will include baselines based on CycleGAN-like models, mixture-of-experts, and late fusion methods.

In all cases, evaluation will include ablation studies to isolate the effect of key components and scalability tests on large datasets. Additionally, we will measure generalization to unseen modalities or domains and validate performance under imperfect or noisy input distributions. The outcomes of the project — including theoretical findings, new algorithms, and empirical benchmarks — will be made available through open-source implementations, peer-reviewed publications, and reproducible research artifacts, allowing the broader community to validate, adopt, and extend the work.

3.6 Work Plan

The work will be performed by the PI, two Ph.D. students, and two M.Sc. students. One Ph.D. student will work on objectives 1 and 3, and the other on objective 2. One M.Sc. student will work on objective 1 and the other on objective 3. Both students will work on objective 2.



3.7 Expected Results and Broader Impact

This project aims to make foundational contributions to multimodal representation learning under minimal supervision, with broad implications for both the development and responsible deployment of AI systems. By enabling learning from unpaired and weakly aligned data, the proposed research lowers the barrier to applying machine learning in domains where annotation is costly, infeasible, or restricted by privacy, such as healthcare, environmental science, and public policy. These capabilities are especially important for democratizing access to AI in settings where high-quality labeled datasets are not available. Furthermore, the project advances representation learning in a direction that favors modularity, adaptability, and data efficiency, promoting the development of AI systems that are more transparent, robust, and ~~privacy-aware~~. By reducing reliance on manual supervision and exploiting structure in unpaired data, the proposed methods open opportunities for scientific discovery in fields that increasingly rely on multimodal measurements but lack aligned data —such as genomics, neuroscience, and climate modeling. In doing so, this work contributes to the broader goal of using AI not only to build better models, but also to accelerate progress in science and improve societal outcomes through data integration and cross-modal reasoning.

3.8 Resources

I am a statistician by training, with a solid background in mathematics and algorithms, and 20 years of experience in machine and deep learning research, both in the industry and academia. As such, I bring a holistic, multi-view perspective, along with a rich toolbox to each of the research objectives. My research is multi-disciplinary at its core, as it requires knowledge of multiple fields such as machine learning, applied mathematics, computer science, and engineering. Perhaps the best evidence of the multi-disciplinary nature of my research is the papers I publish, which include both rigorous mathematical proofs and practical methods applied to challenging real-world problems. ~~MY~~ research team currently consists of one Ph.D. student and 14 M.Sc. students. In the past months, four M.Sc. students have graduated, all with publications in major machine learning venues. I credit much of the productivity and creativity of the group to the fruitful discussions and close interactions between the research group members, which I highly encourage, and all the projects described in this research proposal are important elements of my team's research. I also maintain collaborations with several researchers in other departments at Bar Ilan, in other universities in Israel, at also in several US universities, such as Yale and ~~UCSD~~. I am convinced that both my team at Bar Ilan University and I are well-suited to meet the challenges of this ambitious and fascinating research proposal.

3.9 Potential Pitfalls and Alternative Strategies

While the proposed research rests on solid theoretical foundations, we recognize several challenges that may arise in practice and outline alternative strategies to mitigate them.

For Objective 1, a potential pitfall is that in certain scientific domains, unlike in vision or language, the underlying manifolds may not exhibit sufficient natural alignment across modalities. This could hinder the identification of shared latent structure using universal embedding geometries alone. As a contingency, we will investigate manifold alignment pre-processing techniques that explicitly enforce geometric comparability prior to shared embedding, thereby enhancing robustness across heterogeneous domains.

For Objective 2, a key challenge is the computational complexity of optimizing optimal transport (OT) objectives, which can become prohibitive in high-dimensional settings. To address this, we will explore alternative divergence measures, such as the ~~Maximum Mean Discrepancy (~~MMD~~)~~ and other kernel-based criteria, that can serve as tractable surrogates while still capturing cross-modal dependencies, and with which the PI is experienced [30]. These alternatives provide a flexible pathway to balance theoretical rigor with computational feasibility.

For Objective 3, an anticipated limitation is that the functional map framework, while powerful in computer graphics, may not generalize efficiently to other types of multimodal data. As a workaround, we will incorporate Gromov–Wasserstein alignment tools that compare relational structures across manifolds without requiring direct correspondences. This offers a more general mechanism for aligning modality-specific spaces and ensures that the fusion framework remains broadly applicable beyond geometric domains.

By identifying these potential pitfalls in advance and proposing viable alternatives, the project is designed with built-in adaptability, ensuring progress even if initial approaches encounter limitations.

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