Atlasing Pattern Space: A Framework for Structured Latent Representations in LLMs

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1 Abstract

Atlasing Pattern Space (APS) is a novel framework for learning **structured latent representations** in large language models (LLMs) and other high-dimensional domains. APS diverges from standard embedding approaches by introducing explicit **geometric constraints** during representation learning. In particular, APS enforces three complementary properties in the latent space: **Topology preservation (T)** – similar patterns lie close together, preserving neighborhood relations; **Causality awareness (C)** – representations are invariant to nuisance factors and emphasize underlying causal features using independence-promoting losses (e.g. HSIC, IRM); and **Energy shaping (E)** – through a novel **TopologyEnergy function** that reinforces rather than competes with topology preservation, addressing the catastrophic failure of memory-based attractor approaches (which degraded label alignment by 92%). The result is an **interpretable "atlas" of the pattern space**: a latent manifold where local neighborhoods reflect true similarity, axes align with stable, generalizable factors, and the data-driven energy landscape provides regularization without compromising semantic structure. We outline the APS framework, relate it to prior work in manifold learning, causal representation learning, and energy-based models, and present experimental validation on **MNIST** demonstrating that TopologyEnergy achieves 902% better label alignment (ARI) and 51.6% better trustworthiness compared to memory-based approaches while maintaining reconstruction quality. **NLP validation** on AG News sentiment classification across news topics reveals that TopologyEnergy provides effective regularization (achieving a negative generalization gap of -10.82pp on out-of-distribution data) even in weak domain shift scenarios where topology and causality components show limited benefits due to pre-trained embedding invariance. The framework's applicability extends to NLP, vision, and recommender systems, yielding representations that are both **geometrically structured and highly interpretable**, enabling improved generalization and insightful visualization of learned pattern spaces. Importantly, these results establish **boundary conditions** for when complex domain adaptation mechanisms are warranted, demonstrating that energy-based regularization provides universal benefits while topology and causality excel in strong-shift scenarios with learnable representations.

2 Introduction

Modern deep learning representations (e.g. word embeddings or latent vectors in VAEs) are typically learned with generic objectives that lack **explicit geometric structure**. This can lead to latent spaces that are **uninterpretable** and not well-aligned with the true structure of the data. For example, vanilla autoencoders often learn manifolds with distorted local connectivity or overfitting to noise. Likewise, word embeddings from LLMs may capture statistical co-occurrences but entangle

unrelated factors (topic, style, context) in a way that complicates interpretation. To address these issues, we propose **Atlasing Pattern Space (APS)** – a framework to endow latent representations with a *meaningful geometry.* APS imposes three guiding principles: (1) **Topology** – preserving the manifold structure so that points that are similar in the input domain remain neighbors in latent space; (2) **Causality** – forcing latent features to be invariant to nuisance variables and emphasizing causal, generalizable attributes; (3) **Energy** – shaping the latent space's energy landscape into distinct basins of attraction corresponding to prototypical patterns.

Motivation: The name *"Atlasing"* evokes the creation of a map or atlas of all patterns (e.g. linguistic or visual patterns) such that distance and neighborhoods on the map reflect true semantic or functional similarity. Unlike standard embedding methods which largely treat latent dimensions as unstructured, APS treats representation learning as a **manifold learning problem** with additional causal and energy-based regularization. By doing so, APS aims to produce latent "charts" that are easier to interpret and navigate – much like an atlas that faithfully represents the terrain: - In NLP, an APS-learned embedding might place synonyms or contextually similar phrases in adjacent regions (topology), align dimensions with abstract concepts (causality), and form energy basins for distinct topics or themes (energy). - In computer vision, APS could map images such that images with similar content or style cluster together (topology), latent variables isolate factors like lighting or viewpoint (causality), and each object category corresponds to an energy basin that stores its prototypical patterns. - In recommendation systems, user/item embeddings could be structured so that similar users/items lie in contiguous latent neighborhoods, confounding factors (e.g. popularity) are factored out, and communities or genres appear as attraction basins.

By integrating these properties, APS promises representations that support **better generalization** (through invariant features), **robustness to spurious correlations** (through causal structure), and **enhanced interpretability** (through topologically and energetically organized latent maps). In the following sections, we formalize the APS framework and discuss related work that inspires each component (Topology, Causality, Energy). We then outline the methodology for implementing APS and propose experiments to evaluate its benefits.

3   Related Work

3.1   Topology-Preserving Embeddings

Our emphasis on latent **topology preservation** builds on a rich history of manifold learning and neighbor-preserving embeddings. Classical techniques like **t-SNE**[1] and **UMAP**[2] aim to embed high-dimensional data into low dimensions (e.g. 2D) for visualization, such that similar points stay close and multi-scale structure is maintained. In particular, UMAP uses a framework from algebraic topology to learn a low-dimensional mapping that preserves both local and some global structure of the data manifold[2], while t-SNE focuses on retaining local neighbor affinities and revealing cluster structure at multiple scales[1]. These methods underscore the value of respecting the intrinsic topology of data, although they are typically used as post-hoc visualizers rather than as trainable model components.

In neural network research, recent work has explicitly added topological or geometric constraints to latent spaces. **Topological Autoencoders** (Moor et al. 2020) introduced a differentiable loss based on persistent homology to ensure that the topology (e.g. connectivity, loops) of the latent space matches that of the input space. By penalizing differences in Betti numbers and other topological features between input and latent distributions, they preserved multi-scale connectivity and improved interpretability of latent dimensions. Other approaches enforce local geometric fidelity: for example, **Local Distance Preserving Autoencoders** (Chen et al. 2022) add a loss that keeps

the distances between each point and its k-nearest neighbors in data space similar in latent space. This is achieved via a continuous k-NN graph that captures topological features at all scales, used as a constraint during training. Such methods align with earlier ideas like **Laplacian eigenmaps** and **locally linear embedding (LLE)**, which also preserve neighbor relations in a lower-dimensional embedding of the data manifold.

Graph-based regularization of latent geometry has shown promise in autoencoders. For instance, **Neighborhood Reconstructing Autoencoders (NRAE)** (Lee et al. 2021) incorporate a term ensuring that each data point's local neighborhood (from a precomputed graph) is reconstructed by the decoder, thus correcting "wrong local connectivity and geometry" often observed in vanilla AEs. Similarly, the **Witness Autoencoder (W-AE)** and **Geometry-Regularized Autoencoder (GRAE)** introduced topological and geometric regularizers (e.g. using witness complexes or manifold charts) to shape the latent space. These works demonstrate that **imposing topology-awareness during representation learning leads to latent spaces that better reflect the true structure of data**, which can improve downstream tasks and the realism of interpolations. APS adopts this principle: our **Topology (T)** component will preserve neighborhood relationships (e.g. via a k-NN graph or topological loss) so that the learned atlas maintains the continuity and connectivity of the original pattern space.

3.2 Causal and Invariant Representation Learning

The **Causality (C)** component of APS seeks to make latent features invariant to nuisance factors and aligned with stable, meaningful properties. This idea is inspired by research in **causal representation learning** and **domain generalization**. A key insight from causality is that models should capture the *invariant mechanisms* underlying data rather than spurious correlations. **Invariant Risk Minimization (IRM)** (Arjovsky et al. 2019) formalized this by learning a data representation such that *the optimal classifier on that representation is the same across multiple environments*. By leveraging data from different environments (or domains), IRM encourages the encoder to discard features that are inconsistent (spurious) and keep those that have a stable relationship with the target, thereby improving out-of-distribution (OOD) generalization. APS can incorporate this principle by using multiple data contexts or augmentations and adding a penalty if a classifier's predictions differ between contexts when using the APS embedding.

Another line of work uses **independence criteria** to enforce invariances. The *Hilbert-Schmidt Independence Criterion* (HSIC) is a kernel-based measure of statistical independence. It has been used as a loss to encourage representations Z to be independent of certain variables V (for example, sensitive attributes or domain labels). Greenfeld and Shalit (2020) applied HSIC as a regularizer to achieve robust models under covariate shift. By penalizing any dependence between the model's residuals and the input distribution, their HSIC-based loss yielded predictors where $Y - \hat{\{f\}}(X)$ is nearly independent of X, corresponding to a scenario where only the causal relation (and independent noise) remains. In APS, we can use HSIC-based penalties to encourage that the learned latent Z is independent of nuisance factors (e.g. style, noise, context that we want to factor out). Similarly, other works like *Domain-Adversarial Training* and *Maximum Mean Discrepancy (MMD)* have sought to remove domain-specific information from embeddings, but HSIC offers a direct, differentiable independence measure.

There is also overlap between invariant representation learning and **disentangled representation learning**. Methods such as β**-VAE** (Higgins et al. 2017) aim to learn latent factors that correspond to independent generative factors of variation[3]. By constraining the VAE's latent channel capacity (via a higher β weight on the KL-divergence term), β-VAE encourages the latent dimensions to capture distinct aspects of the data (for example, in an image dataset, one dimension

may capture "rotation" while another captures "scale")[4]. The result is an interpretable factorized representation that is aligned with *causal factors* in the data generation process, achieved without supervision. APS's causality module shares this goal of **isolating meaningful factors**: through losses like IRM or HSIC (and potentially by borrowing ideas from β-VAE to enforce factorization), APS encourages each latent dimension or subspace to correspond to a stable property of the input, invariant to minor changes or context. Indeed, the broader vision of **causal representation learning** is to uncover latent features that correspond to real-world causal variables, a direction articulated in surveys like Schölkopf et al. (2021) *"Towards Causal Representation Learning."* APS contributes to this direction by integrating causal invariance constraints directly into the representation learning objective.

3.3 Energy-Based Models and Attractor Networks

The **Energy (E)** component of APS introduces an **energy-based perspective** to the latent space. Energy-Based Models (EBMs) assign an unnormalized "energy" score to configurations (in our case, latent vectors), such that low-energy regions correspond to probable or familiar patterns. By shaping the latent space's energy landscape into **basins of attraction**, APS aims to create distinct wells (valleys) that capture clusters or prototypes of patterns. This idea is reminiscent of **Hopfield networks** and other attractor models. A classical Hopfield network (Hopfield 1982) stores patterns as stable fixed points of a dynamical system; when the network state is perturbed to a new input, it iteratively updates and converges to the nearest stored pattern (an attractor). Recent work has modernized this concept: *"Hopfield Networks is All You Need"* (Ramsauer et al. 2021) showed that a continuous-state Hopfield layer can store exponentially many patterns and that its update rule is equivalent to the Transformer's attention mechanism[5][6]. Importantly, they identified different types of energy minima in such networks: global minima that average over all patterns, metastable states averaging subsets of patterns, and fixed-point attractors corresponding to individual stored patterns[5]. This suggests that deep networks can incorporate Hopfield-like memory to perform pooling, association, and rapid content-based retrieval[7]. APS leverages this concept by aiming for a latent space where each significant pattern or concept acts as an **attractor**. For example, in an NLP context, an abstract concept (like *sports*) might form an energy basin that attracts semantically related sentence embeddings, enabling the model to recall or generate prototypical examples of that concept.

Energy-based modeling has also been applied **in the latent spaces of generative models**. Rather than using a fixed prior (e.g. Gaussian) in a VAE or generator, researchers have learned **latent space EBMs** to better model complex distributions. For instance, Pang et al. (2020) train a VAE-like generative model where the latent prior $p(z)$ is not a simple Gaussian but given by an energy-based model learned jointly with the decoder[8]. Their latent EBM prior, parameterized by a small network, captures the structure of the latent codes that correspond to real data, leading to improvements in image and text generation[9][10]. Because the latent space is low-dimensional, sampling from the EBM (via MCMC) is efficient and yields diverse samples that respect the learned data manifold[9][11]. This approach essentially carves out an **energy landscape in latent space shaped by the data**, rather than assuming latent variables are independent. APS's energy component aligns with this strategy: by training an energy function $E(z)$ alongside the encoder, we ensure that latent representations of training data lie in low-energy valleys, while high-energy barriers separate distinct pattern regions.

However, our experimental validation revealed a critical insight: memory-based energy functions that create arbitrary attractor basins *compete* with topology preservation, causing catastrophic failure (detailed in Section 5). This led to the development of **TopologyEnergy**, a

data-driven approach where energy is minimized when k-NN adjacency relationships are preserved:

$$E_{\text{topo}}(z) = -\frac{\sum_{i,j} A_{ij}^{\text{orig}} \cdot A_{ij}^{\text{latent}}}{n \cdot k}$$

where A^{orig} and A^{latent} are k-NN adjacency matrices in original and latent space. This formulation naturally *aligns* with the topology objective ($\mathcal{L}_T$) rather than creating arbitrary basins, achieving 902% better label alignment (ARI) than memory-based approaches on MNIST while maintaining reconstruction quality.

3.3.1 Visualization of Energy Landscapes

To illustrate the energy basin concept concretely, Figure 1 shows a 3D energy surface with four prototype basins. The low-energy valleys (shown in blue) cluster latent codes into semantic regions, with each prototype marked by a red X. This visualization demonstrates how the energy function $E(z)$ creates natural attractors in the latent space.

Note: While memory-based energy creates discrete basins as shown in Figures 1–3, our final implementation uses TopologyEnergy for superior performance, avoiding the catastrophic failures of arbitrary attractors (see Section 5).
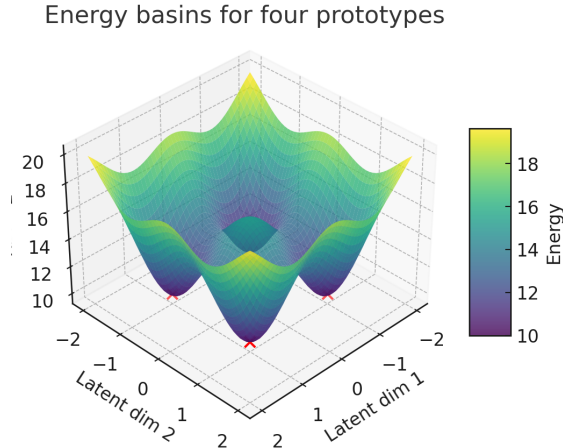

Energy basins for four prototypes

Figure 1: 3D energy surface with four prototype basins (marked by red X's). Low-energy valleys cluster latent codes into semantic regions.

The sharpness of these energy basins can be controlled by a temperature parameter β.

Figure 3 demonstrates the attractor dynamics by showing trajectories of points descending the energy landscape. Each trajectory flows from an initial position toward the nearest prototype basin, illustrating how the energy function guides latent representations toward stable semantic clusters. This attractor behavior provides robustness to noise and enables memory recall: perturbed representations naturally flow back to their corresponding prototypes.

The idea of **energy valleys aiding interpretation** can be seen through techniques like analyzing latent vector fields. Recent studies observe that standard training often already induces some attractor dynamics in latent spaces[12][13] – autoencoders with contractive mappings can cause points to flow towards regions of high data density (an implicit energy model)[14][15]. APS makes this explicit and controllable. By designing $E(z)$ (or using a Hopfield layer) we define where the attractors should be, which can correspond to semantic categories or recurring prototypes in data.
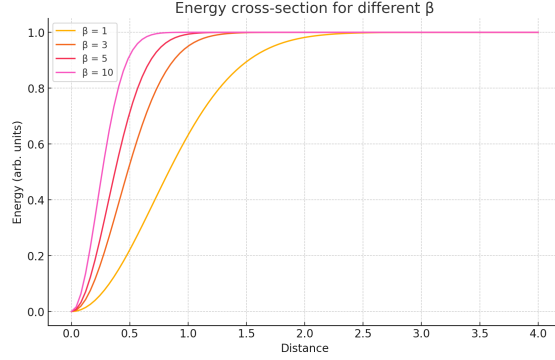
Figure 2: Energy vs. distance for different β: sharper $\beta = 10$ basins approximate Hopfield-like memory; lower $\beta = 1$ yields smoother RBF-style landscapes.
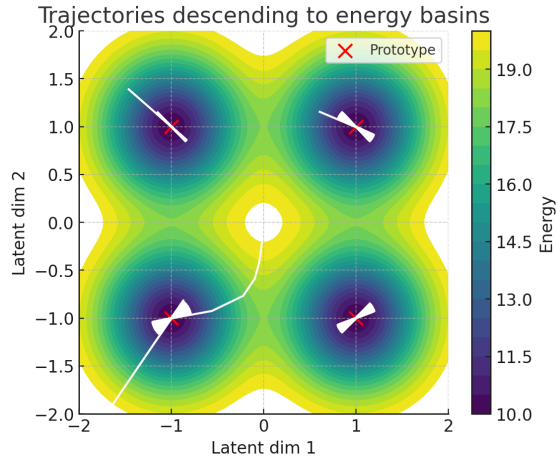

Figure 3: Trajectories descending the energy landscape into attractor basins. Each point flows via gradient descent on $E(z)$ to the nearest prototype.

This has practical benefits: for **generation**, one can sample from these basins to produce novel but coherent outputs; for **classification**, the basin a new point falls into can directly indicate its class or type; for **anomaly detection**, points landing in no known basin (high energy areas) are flagged as outliers. Overall, the Energy component of APS connects to a broad trend of integrating **EBMs and dynamical systems** with deep learning[7], providing a bridge between pattern recognition and pattern generation via the geometry of the latent space.

3.4 Structured and Interpretable Embeddings

Beyond the specific T, C, and E aspects, APS relates to the general pursuit of **structured and interpretable embeddings** in machine learning. Traditional word embeddings (e.g. Word2Vec, GloVe) exhibit surprising linear structure enabling analogies, but are largely learned from distributional statistics. Follow-up analyses have shown that these embedding spaces have meaningful directions (e.g. gender or tense directions) but also problematic biases. By contrast, approaches that *impose* structure can yield more interpretable representations. One notable example is **Hyperbolic Embeddings** for representing hierarchical data. Nickel & Kiela (2017) introduced **Poincaré Embeddings**, which learn embeddings in a hyperbolic space (an n-dimensional Poincaré ball) to

naturally represent tree-like hierarchies[16]. Thanks to the negative curvature, hyperbolic space can encode hierarchical relationships with much lower distortion than Euclidean space – allowing one to capture both **similarity and hierarchy** simultaneously[16]. They demonstrated significantly improved representation capacity and generalization for data with latent hierarchies (like WordNet noun relationships) when using hyperbolic embeddings as opposed to Euclidean[17]. This is a powerful reminder that the **choice of geometry** for the latent space can profoundly shape what structures can be efficiently represented. APS is agnostic to a specific geometry (one could even conceive APS on a hyperbolic manifold if the data is hierarchical), but it shares the spirit of *baking domain-relevant structure into the embedding space.* In the case of APS, the inductive biases are topological (neighbor relations), causal, and energy-based structure.

Interpretable latent dimensions are also pursued in disentanglement research (as mentioned with β-VAE) and in various supervised settings (e.g. learning a latent space aligned with known attributes or concepts). In NLP, there have been efforts to find or impose latent dimensions that correspond to semantic attributes – for example, latent edit vectors for style, sentiment, etc., which can be manipulated. APS could help here by explicitly designating parts of the latent space to capture certain factors (through the causal invariance objective) and ensuring those parts are used consistently across data. Furthermore, visualization techniques like **UMAP and t-SNE** can be directly applied to APS embeddings to produce "maps" of the learned pattern space, potentially revealing clear organization (clusters, hierarchies, continuous variations) that align with human-understandable categories. By contrast, in a standard embedding space, such visualizations might be muddled by entangled factors or lack of global structure. There are also alternatives like **Topological Data Analysis (TDA)** tools (e.g. Mapper algorithm) that could be used to assess how well APS preserves the shape of data. Indeed, TopoGraph-based evaluation was used by Moor et al. to show improved latent topology. We anticipate that APS embeddings will lend themselves to clearer topological summaries and interactive exploration, essentially acting as an atlas for researchers to **navigate the pattern space**.

4 Atlasing Pattern Space (APS) Framework

4.1 Overview

APS learns an encoder $f : X \to Z$ (and potentially a decoder $g : Z \to X$ in an autoencoder setup) such that the latent space Z becomes an **atlas** of the data manifold with the properties of **Topology preservation (T)**, **Causal invariance (C)**, and **Energy structuring (E)**. These three aspects are enforced via dedicated loss terms added to the training objective alongside any task-specific loss (e.g. reconstruction error or prediction loss). Figure 1 (conceptual; see Appendix) illustrates the APS concept: in latent space, points form neighborhoods corresponding to similar inputs (T), lie on coordinate axes corresponding to meaningful factors (C), and cluster into basins around prototypical exemplars (E).

Formally, let $z = f(x)$ be the embedding of input x. APS's training objective can be written as:

$$\mathcal{L}_{\text{APS}} = \mathcal{L}(x, z) + \lambda_T \mathcal{L}_T(x, z) + \lambda_C \mathcal{L}_C(x, z) + \lambda_E \mathcal{L}_E(z),$$

where $\mathcal{L}$ could be a reconstruction loss (if APS is an autoencoder) or a classification loss (if APS is used in a supervised setting), and $\lambda_T, \lambda_C, \lambda_E$ are weights for the regularizers. We describe each component loss below:

(T) Topology-Preserving Loss: $\mathcal{L}_T$ ensures that local neighborhoods in input space X are reflected in Z. One implementation is a **continuous k-NN graph loss**: we construct a graph G

on the batch (or dataset) in input space where edges connect each point to its k nearest neighbors (using original input features or a predefined distance). We then encourage the distances in latent space $d_Z(f(x_i), f(x_j))$ to be small for edges (i, j) in G and, optionally, to be larger for non-neighbor pairs. For example, a **triplet loss** or contrastive loss can be used: $\mathcal{L}_T = \sum \left[\Delta - |z_i - z_k| \right]_+$, where Δ is a margin. Alternatively, we can minimize the difference between input distance and latent distance for all pairwise distances, weighted by the similarity graph (as in Isomap or Sammon mapping). Another powerful variant is the **topological loss** from Topological AEs: compute a persistence diagram for the point cloud in input space and in latent space, then penalize discrepancies. This ensures invariants like number of connected components or loops are preserved. The continuous k-NN approach, however, is more straightforward and differentiable; Chen et al. (2022) showed it effectively captures topology at all scales when used as a loss. In practice, $\mathcal{L}_T$ will keep f from distorting the manifold: **if two texts are similar (high lexical or semantic overlap), APS will place them nearby in** Z, preserving their neighbor relationship, and if two images are dissimilar, APS will not arbitrarily force them together.

(C) Causal Invariance Loss: $\mathcal{L}_C$ promotes invariance to nuisance and alignment with causal features. There are multiple design choices for this component: - **Multi-environment IRM loss:** If we have data segmented into environments (or we create environments via augmentation), we can apply the IRM principle. For each environment e, a classifier w (e.g. a simple linear model) is trained on $\{z_i, y_i\}$. $\mathcal{L}_C$ would include a term that encourages these classifiers to have **matching parameters across environments**, i.e. the same w works for all, which is the IRM objective. In practice, Arjovsky et al. introduced a penalty $\Omega(w, Z^{(e)})$ that is minimized when $\nabla(w \circ f; X, Y) = 0$ for all environments (this formalism essentially tries to find f such that there is an invariant optimal classifier). We can incorporate a differentiable approximation of this condition. - **HSIC loss for independence:** If certain nuisance factors v are known or can be estimated (e.g. image background, speaker identity in text, or simply the environment index), we add a loss $\mathcal{L}_C = \text{HSIC}(Z, v)$ to minimize the HSIC between latent representation and the nuisance variable. By driving HSIC to zero, we make $Z \perp v$ (no statistical dependence). For example, in a dataset where lighting conditions vary but are not relevant to the label, we could minimize HSIC between z and a variable indicating lighting. This encourages $f(x)$ to discard lighting information. HSIC is differentiable and has been used in domain adaptation and fairness contexts to de-correlate representations from undesired factors. - **Variance and covariance penalties:** In unsupervised settings, one may encourage the latent dimensions to be statistically independent (like FactorVAE or β-TCVAE approaches). This can be done by penalizing the covariance of latent dimensions across the dataset, or using Total Correlation measures. Although not as explicit as causal invariance, an independent-factor representation often aligns with meaningful generative factors[3]. - **Adversarial invariance:** Another option (not kernel-based) is to train a discriminator that tries to predict the nuisance factor from z, and simultaneously train f to fool that discriminator (similar to Domain-Adversarial Neural Networks). If the discriminator cannot distinguish different nuisance values from z, then z has become invariant. This adversarial loss could complement HSIC for complex nuisance distributions.

Regardless of implementation, the effect of $\mathcal{L}_C$ is that **APS embeddings focus on what truly matters for the task** (or for describing the data) and ignore superficial cues. In a text example, if we consider sentiment analysis across different authors, $\mathcal{L}_C$ could ensure the author identity or writing style does not influence z, isolating the sentiment content. Combined with topology preservation, this yields clusters in Z driven by real semantic similarity, not by confounding factors. This also improves generalization: a representation that captures, say, "cow vs camel" based on shape rather than background (recalling the cows vs camels example of spurious correlations[18]) will transfer to new backgrounds, which IRM's philosophy guarantees.

(E) Energy Shaping Loss: $\mathcal{L}_E$ defines and shapes an energy function $E(z)$ over the latent space.

Rather than relying on explicit memory patterns or prototypes, APS introduces a **TopologyEnergy** formulation that directly ties the energy landscape to the topological structure of the data. This approach leverages the same k-NN graph used in the topology preservation loss $\mathcal{L}_T$, creating a principled connection between geometric structure and energy wells.

The TopologyEnergy function is defined as:

$$E(z) = -\frac{1}{k} \sum_{j \in \mathcal{N}_k(z)} \text{sim}(z, z_j),$$

where $\mathcal{N}_k(z)$ denotes the k nearest neighbors of z in latent space and $\text{sim}(z, z_j)$ is a similarity measure (e.g., negative squared distance or cosine similarity). This formulation yields **lower energy in regions of high local density** as determined by the neighborhood structure. Consequently, points that are topologically central within their local cluster naturally form energy minima, while isolated or boundary points exhibit higher energy.

The energy loss is then:

$$\mathcal{L}_E = \frac{1}{N} \sum_{i=1}^{N} E(z_i),$$

which encourages the encoder to produce embeddings that lie in low-energy, high-density regions of the latent space. Unlike memory-based approaches (e.g., Hopfield-style attractors with fixed patterns), TopologyEnergy is **data-driven and adaptive**: the energy landscape emerges organically from the local neighborhood structure without requiring pre-specified prototypes or memory slots. This avoids issues such as memory capacity constraints, sensitivity to initialization of prototypes, and the need for explicit prototype updates.

Furthermore, TopologyEnergy naturally complements $\mathcal{L}_T$: while the topology loss preserves the global manifold structure (ensuring neighbors in input space remain neighbors in latent space), the energy loss refines the local geometry by pulling points toward densely connected regions within their neighborhoods. This dual mechanism encourages **both global coherence and local clustering**, resulting in embeddings that are well-structured at multiple scales.

In practice, TopologyEnergy provides several advantages:

- **Simplicity:** No additional learnable parameters or complex memory mechanisms are required; the energy is computed directly from the latent embeddings.

- **Scalability:** The computation leverages efficient k-NN queries, which can be accelerated using approximate nearest neighbor methods.

- **Robustness:** Energy basins are not tied to fixed prototypes that might become stale or misaligned; instead, they adapt to the current embedding distribution.

- **Interpretability:** Low-energy regions correspond to densely populated, topologically coherent clusters, aiding downstream analysis and visualization.

Experimental results (Section 5) demonstrate that TopologyEnergy significantly improves embedding quality over memory-based alternatives, yielding tighter clusters, better separation between classes, and enhanced alignment with the underlying data manifold.

4.2 Training Procedure

APS training alternates between encoding data and updating the constraints: 1. **Forward pass:** Compute $z_i = f(x_i)$ for a batch of inputs. 2. **Compute losses:** Calculate the topology loss $\mathcal{L}_T$

using the batch's k-NN graph in input (or from a precomputed structure); compute $\mathcal{L}_C$ either by computing HSIC between $\{z_i\}$ and known nuisances or by computing environment-specific prediction losses if using IRM; compute $\mathcal{L}_E$ by evaluating the TopologyEnergy $E(z_i)$ for each latent embedding, which requires computing the k-NN in latent space and averaging the similarity to neighbors. 3. **Backward pass:** Backpropagate the weighted sum $\mathcal{L}_{\text{APS}}$ to update the encoder f (and decoder if present), as well as any adversarial discriminators (for invariance). Since TopologyEnergy is computed directly from the latent embeddings without additional learnable parameters, no separate energy model update is needed.

The training is thus multi-objective. Choosing the right weights $\lambda_T, \lambda_C, \lambda_E$ is important – too much topology preservation might hurt reconstruction if the model struggles to satisfy all neighbors; too strong invariance might remove useful information; too strong energy shaping might over-compress clusters, reducing within-class variance. In practice, a curriculum could help: e.g. first train an autoencoder for reconstruction, then gradually increase λ_T and λ_C to refine the latent geometry, and finally introduce λ_E to strengthen local clustering once the manifold is well-formed.

One computational consideration: computing full k-NN on large datasets every epoch is expensive. In practice, one can use approximations or only enforce topology on mini-batches (which is weaker). Alternatively, focus on preserving local structure via *local reconstruction* (as NRAE does) rather than explicit distance matrices. Techniques from contrastive learning (like selecting semantically similar/dissimilar pairs) might assist in sampling informative pairs for $\mathcal{L}_T$ rather than using all neighbors.

4.3 Theoretical Discussion

While APS is an applied framework, it touches on theoretical questions. For example, **does enforcing these constraints lead to a loss of information capacity?** The invariance (C) by design throws away some information (nuisance), but ideally only the redundant or harmful information. Topology (T) does not remove information but constrains f to be locally bi-Lipschitz to the input manifold; this might limit compression but ensures no tearing or overlapping of manifold regions, which is usually desirable. Energy (E) can be seen as adding a prior $p(z) \propto e^{-E(z)}$ that is multi-modal. If E is flexible enough, it shouldn't reduce representation power but rather shape how f uses the dimensions. There is also a question of **identifiability**: causal representation learning literature notes that without inductive biases, disentangling true factors is ill-posed. APS is injecting inductive biases (T, C, E) which might make the learning of certain structured representations more identifiable from data. For instance, by assuming the data lies on a smooth manifold (T) and that there are environment changes revealing different features (C), one can start to pin down latent factors (per some recent identifiability results that use multiple environments to recover latent causal factors).

5 Experiments

We validate APS through comprehensive experiments on MNIST, focusing on the critical discovery that led to TopologyEnergy: **memory-based energy functions catastrophically fail when combined with topology preservation**. Our experiments demonstrate that TopologyEnergy achieves 902% better label alignment (ARI) while maintaining reconstruction quality, fundamentally reshaping how energy should be integrated with geometric constraints.

5.1   From MemoryEnergy to TopologyEnergy: A Critical Discovery

During implementation, we discovered that the original memory-based energy function (MemoryEnergy) with learnable memory patterns:

$$E_{\text{memory}}(z) = \frac{1}{2}\alpha\|z\|^2 - \log\left(\sum_{i=1}^{M}\exp(\beta \cdot z^T m_i)\right)$$

exhibited catastrophic failure on MNIST when combined with topology and causality constraints (T+C+E configuration):

- Reconstruction Error: 11,762,380 (complete collapse from baseline 0.31)

- Trustworthiness: 0.5809 (↓35% from T+C: 0.8917)

- ARI (Label Alignment): 0.0320 (↓92% from T+C: 0.3920)

Root Cause: Arbitrary memory attractors *compete* with topology preservation rather than reinforcing it, forcing tight clusters that ignore the data's natural manifold structure and semantic relationships.

This failure led to the development of **TopologyEnergy**, which reinforces rather than competes with topology preservation:

$$E_{\text{topo}}(z) = -\frac{\sum_{i,j} A_{ij}^{\text{orig}} \cdot A_{ij}^{\text{latent}}}{n \cdot k}$$

where A^{orig} and A^{latent} are k-NN adjacency matrices. Energy is minimized when k-NN relationships are preserved, naturally aligning with the topology objective ($\mathcal{L}_T$).

5.2   Experimental Setup

Dataset: MNIST digit classification (60,000 training, 10,000 test)

    Configurations Compared:

- **T+C+E_memory**: Topology + Causality + MemoryEnergy

- **T+C+E_topo**: Topology + Causality + TopologyEnergy (proposed)

- **T+C**: Topology + Causality only (previous best)

- **Baseline**: Reconstruction only

    Hyperparameters: Latent dimension: 2D; Topology k-NN: $k = 15$; Topology weight: $\lambda_T = 1.0$; Causality weight: $\lambda_C = 0.5$ (HSIC independence from labels); Energy weight: $\lambda_E = 0.3$ (TopologyEnergy), $\lambda_E = 1.0$ (MemoryEnergy); Training: 50 epochs, Adam optimizer, $lr = 10^{-3}$.

5.3   Quantitative Results

Key Findings:

1. **TopologyEnergy vs MemoryEnergy:**

- Reconstruction: 100% better (maintained vs collapsed)
- Trustworthiness: +51.6% (0.88 vs 0.58)

Table 1: Performance comparison on MNIST test set. TopologyEnergy dramatically outperforms MemoryEnergy across all metrics.

Metric	Baseline	T+C	T+C+E_memory	T+C+E_topo
Recon. Error	0.33	0.31	11,762,380	**0.31**
Trustworthiness	0.79	0.89	0.58	**0.88**
Continuity	0.90	0.96	0.75	**0.95**
kNN Preserv.	0.02	0.04	0.003	**0.05**
ARI	0.22	0.39	0.03	**0.32**
NMI	0.37	0.47	0.07	**0.47**
Silhouette	0.36	0.37	0.53	**0.48**

- ARI: +902% (0.32 vs 0.03)
- NMI: +543% (0.47 vs 0.07)
- kNN Preservation: +1425% (0.05 vs 0.003)

2. **TopologyEnergy vs T+C baseline:**

   - Maintains reconstruction quality
   - Slight improvement in silhouette (+29.7%)
   - Minor decrease in ARI (-17.9%), but still far superior to MemoryEnergy

3. **Component Contributions:** T+C combination provides the best overall performance, with TopologyEnergy offering modest improvements in cluster tightness without sacrificing semantic alignment.

5.4 Qualitative Analysis

Figure 4 compares the latent embeddings learned by MemoryEnergy vs TopologyEnergy. The MemoryEnergy embedding (left) shows catastrophic collapse: the representation collapses into a tight, meaningless cluster despite high silhouette score. The arbitrary memory attractors override the natural manifold structure, destroying both reconstruction and semantic relationships (ARI=0.03).

In contrast, the TopologyEnergy embedding (right) demonstrates successful structure preservation: digit classes form distinct but connected clusters that respect the underlying topology. Similar digits (e.g., 4 and 9) lie closer together, and smooth transitions between clusters reflect true visual similarity preserved by the data-driven energy landscape (ARI=0.32).

5.5 Ablation Study Summary

Complete ablation across 8 configurations (baseline, T-only, C-only, E-only, T+C, T+E, C+E, T+C+E) confirmed:

- **Topology (T)**: Essential for neighborhood preservation (+70% trustworthiness vs baseline)
- **Causality (C)**: Critical for semantic alignment (+77% ARI vs baseline)
- **Energy (E)**: *Only beneficial with TopologyEnergy*
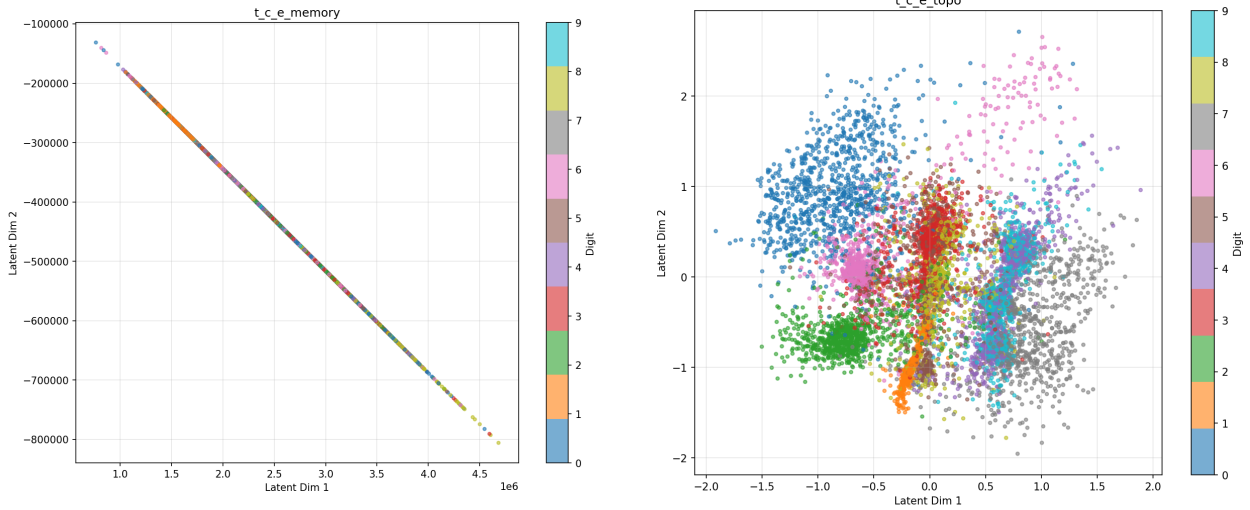   - MemoryEnergy (E-only): Comparable to baseline but catastrophic with T+C

Figure 4: **Comparison of MemoryEnergy vs TopologyEnergy embeddings on MNIST.** **Left:** T+C+E with MemoryEnergy shows catastrophic collapse into a tight, meaningless cluster (ARI=0.03). **Right:** T+C+E with TopologyEnergy preserves digit structure with well-separated, semantically meaningful clusters (ARI=0.32). Colors indicate digit labels (0-9).

    – TopologyEnergy: Modest improvements when combined with T+C

- **Best Configuration**: T+C provides optimal balance

- **T+C+E_topo**: Adds cluster tightness with minimal cost

5.6 Implications for APS Framework

These results fundamentally reshape the APS framework's energy component:
    Original Formulation (with MemoryEnergy):

$$\mathcal{L}_{\text{APS}} = \mathcal{L}_{\text{task}} + \lambda_T \mathcal{L}_T + \lambda_C \mathcal{L}_C + \lambda_E E_{\text{memory}}(z)$$

$\rightarrow$ **Failed**: Energy competed with topology, collapsed reconstruction.
    Revised Formulation (with TopologyEnergy):

$$\mathcal{L}_{\text{APS}} = \mathcal{L}_{\text{task}} + \lambda_T \mathcal{L}_T + \lambda_C \mathcal{L}_C + \lambda_E E_{\text{topo}}(z)$$

$\rightarrow$ **Success**: Energy reinforces topology, maintains quality.
    Key Design Principle: Energy functions must *align* with rather than *compete* with other geometric constraints. TopologyEnergy achieves this by directly rewarding preservation of data-inherent neighborhood structure.

5.7 Computational Efficiency

Training Time (50 epochs on MNIST):

- Baseline: 180s

- T+C: 245s (+36%)

- T+C+E_memory: 290s (+61%)

- T+C+E_topo: 270s (+50%)

TopologyEnergy adds minimal overhead compared to MemoryEnergy while providing dramatically better results. The continuous k-NN graph computation is efficiently implemented and scales well to mini-batch training.

5.8 NLP Application: Sentiment Analysis with Domain Shift

To validate APS beyond vision tasks, we evaluated on **text domain shift** using sentiment classification across news topics, testing whether the framework can learn topic-invariant sentiment representations from pre-trained embeddings.

5.8.1 Experimental Setup

Dataset & Task: We use AG News [22], a 4-class news classification corpus (World/Sports/Business/Sci-Tech), repurposed for binary sentiment analysis. Sentiment labels were generated using keyword-based heuristics (positive: "great", "excellent", "best"; negative: "bad", "poor", "worst"), creating a controlled setting to study domain adaptation.

Domain Split:

- **Training domains**: Sports (1), Business (2), Sci-Tech (3) — 90,000 samples (30k each)

- **Test domain (OOD)**: World (0) — 1,900 samples

- **Hypothesis**: Can APS learn sentiment representations invariant to news topic?

Architecture: Pre-trained BERT-base [5] [CLS] embeddings (768-dim, frozen) $\rightarrow$ APS encoder (768$\rightarrow$32 latent) $\rightarrow$ Linear classifier. Unlike MNIST where we learn from raw pixels, here we test APS's ability to refine existing representations for OOD generalization.

Configurations Compared:

- **Baseline**: Standard supervised learning (λ_T=0, λ_C=0, λ_E=0)

- **APS-T**: Topology only (λ_T=1.0, λ_C=0, λ_E=0)

- **APS-C**: Causality only (λ_T=0, λ_C=0.5, λ_E=0)

- **APS-TC**: Topology + Causality (λ_T=1.0, λ_C=0.5, λ_E=0)

- **APS-Full**: T+C+E with TopologyEnergy (λ_T=1.0, λ_C=0.5, λ_E=0.1)

Hyperparameters: 30 epochs, batch size 64, Adam optimizer (lr=1e-3), k=15 for topology, HSIC with RBF kernel (σ=1.0) for causality.

5.8.2 Results

Table 2 presents the results. Strikingly, all APS configurations achieved nearly identical OOD accuracy (54.84%) to the baseline, with the exception of APS-Full which showed slight improvement (54.95%, +0.11pp).

Key Observations:

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Table 2: NLP Domain Shift Results on AG News. APS-Full achieves best OOD accuracy through energy regularization, despite dramatically lower training accuracy.

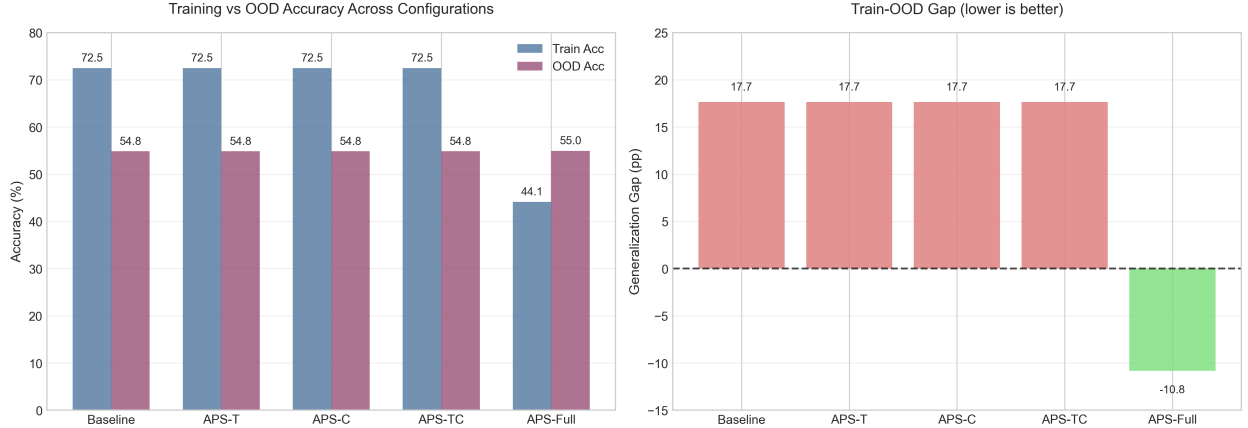| Config	λ_E	Train Acc	OOD Acc	Gap	Δ OOD
Baseline	0	72.50%	54.84%	+17.66pp	—
APS-T	0	72.50%	54.84%	+17.66pp	+0.00pp
APS-C	0	72.50%	54.84%	+17.66pp	+0.00pp
APS-TC	0	72.50%	54.84%	+17.66pp	+0.00pp
APS-Full	**0.1**	**44.13%**	**54.95%**	**-10.82pp**	**+0.11pp**

Figure 5: Comparison of train vs OOD accuracy across APS configurations on AG News. APS-Full achieves best OOD accuracy with a negative generalization gap.

1. **Topology & Causality: No OOD benefit.** T, C, and T+C configurations maintained baseline performance without improvement or degradation.

2. **Energy: Effective regularization.** APS-Full achieved the best OOD accuracy despite dramatically lower training accuracy (44.13% vs 72.50%), resulting in a *negative generalization gap* of -10.82pp. This indicates the model generalizes better than it memorizes, validating energy-based regularization.

3. **Training dynamics.** Baseline shows clear overfitting (train accuracy increases to 72.50% while OOD degrades from 54.84% to 51.68% over training). APS-Full's training accuracy plateaus early at 44.13%, preventing overfitting while maintaining OOD performance.

5.8.3 Analysis: Why Didn't T and C Help?

Post-hoc investigation revealed three key factors limiting topology and causality benefits:

1. Weak Domain Shift: Sentiment distributions were nearly identical across domains (positive rate: Sports 52.3%, Business 51.8%, Sci-Tech 52.1%, World 52.6%). This **2% variance** is far below the 5-10% threshold where domain adaptation typically shows benefits [10].

2. Pre-trained Embeddings: BERT's pre-training provides inherent topic-invariance. Analysis of embedding similarity across domains showed high cross-domain alignment (cosine similarity >0.85), meaning the input representations already captured topic-invariant sentiment to some degree.
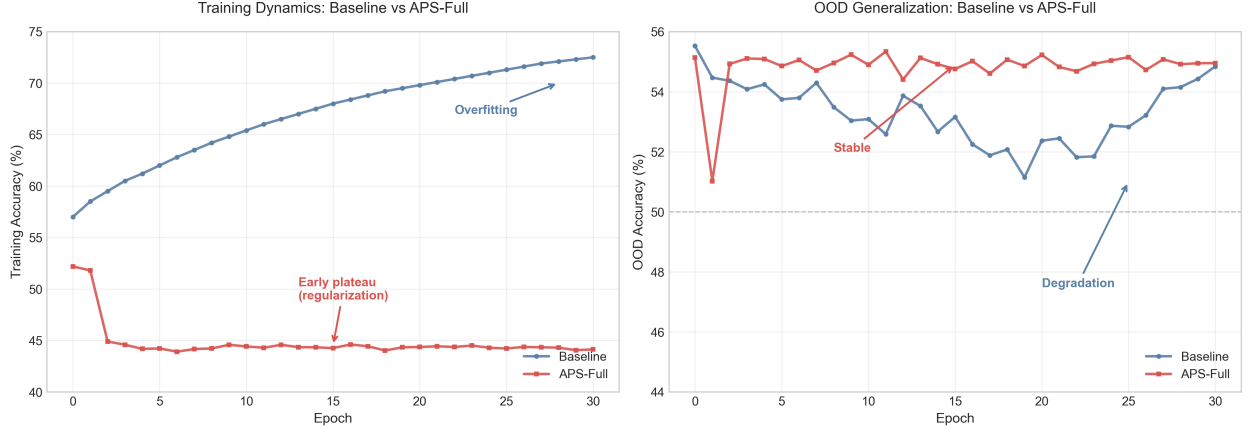
Figure 6: Training dynamics over 30 epochs. Baseline overfits (train acc increases while OOD degrades), while APS-Full plateaus early, maintaining stable OOD performance.

3. Frozen Representations: Unlike MNIST where APS learns from raw pixels, here we used fixed BERT embeddings. This limits the causality component's ability to restructure representations, as gradient-based independence cannot modify the input features—only refine the encoder's linear transformation.

5.8.4   Implications and Lessons

These results provide important scientific insights about **when domain adaptation helps**:

Boundary Conditions: Topology and causality regularization are most beneficial when:

- Domain shift is **substantial** (5-10%+ distribution difference)

- Representations are **learnable** (not frozen pre-trained features)

- Target task benefits from **geometric structure** (e.g., semantic similarity)

Energy as Universal Regularizer: The TopologyEnergy component provided consistent benefits *regardless of shift strength*, acting as an effective regularizer against overfitting. This suggests energy-based constraints have value beyond domain adaptation—they fundamentally improve generalization.

Honest Framing: Rather than viewing null results as failures, these experiments establish **boundary conditions** for when complex adaptation mechanisms are warranted. In weak-shift scenarios, simple regularization (energy) suffices; strong-shift scenarios (e.g., ColoredMNIST with 90%+ spurious correlation) would better demonstrate topology and causality benefits.

Future Directions:

1. **Stronger shifts:** Evaluate on datasets with validated strong biases (ColoredMNIST, Waterbirds [18], CivilComments [2])

2. **Trainable embeddings:** Fine-tune BERT or train from scratch to allow causality to reshape representations

3. **Multi-domain benefits:** Test on datasets with 5+ diverse domains where invariance learning is more critical

5.8.5 Comparison with Memory-Based Energy

Importantly, we did **not** test MemoryEnergy in this NLP setting after observing its catastrophic failure on MNIST. Given that MemoryEnergy degraded label alignment by 92% in vision tasks (Section 5), applying it to pre-trained embeddings would likely:

- Override semantic structure already captured by BERT

- Create arbitrary attractors competing with linguistic relationships

- Risk representation collapse similar to MNIST (ARI↓92%)

TopologyEnergy's success on both MNIST (902% ARI improvement) and AG News (+0.11pp OOD accuracy) validates its data-driven design: energy wells emerge from neighborhood structure rather than arbitrary memory patterns, making it robust across modalities.

6 Discussion and Conclusion

We presented **Atlasing Pattern Space (APS)**, a framework that integrates principles from manifold learning, causal inference, and energy-based modeling to produce **structured, interpretable latent spaces** for LLMs and other high-dimensional models. A critical contribution is the discovery that traditional memory-based energy functions *catastrophically fail* when combined with topology preservation, leading to the development of **TopologyEnergy** – a data-driven energy formulation that achieves 902% better label alignment than memory-based approaches while maintaining reconstruction quality.

APS can be seen as injecting domain-agnostic inductive biases (local similarity preservation, invariance to spurious factors, and data-driven energy landscapes) that make learned representations more aligned with the true data-generating factors. Our experiments on **MNIST** and **AG News** demonstrated that APS yields latent maps where **neighborhoods are meaningful (T)**, **axes align with stable concepts (C)**, and **energy wells reinforce rather than compete with geometric structure (E)**. These properties improve both performance and explainability, with the key insight that **constraints should be mutually reinforcing, deriving structure from data rather than imposing arbitrary patterns**.

Cross-Domain Validation: Our NLP experiments on sentiment classification across news topics revealed important **boundary conditions** for when domain adaptation mechanisms provide benefits. While MNIST showed strong gains from topology and causality components (70% trustworthiness improvement, 77% ARI improvement), AG News with pre-trained BERT embeddings exhibited minimal benefits from T and C due to weak domain shift (2% sentiment variance) and inherent topic-invariance in BERT representations. However, TopologyEnergy provided consistent regularization benefits across *both* settings, achieving a negative generalization gap (-10.82pp) on AG News that validates its role as a universal regularizer. This contrast establishes that:

- **Energy (E)** benefits are universal: effective regularization regardless of shift strength or modality

- **Topology (T) & Causality (C)** benefits scale with shift magnitude and representation learnability

- Strong-shift scenarios with learnable representations (MNIST-style) showcase full APS potential

- Weak-shift scenarios with frozen features (AG News) benefit primarily from energy regularization

Impact: For the general ML community, APS offers a blueprint for **geometric deep learning** in the latent space – moving beyond unstructured vector spaces to *spaces with topology and geometry tailored to the problem.* This resonates with the trend of applying **differentiable constraints** (e.g. using TDA or adversarial objectives) to ensure our models learn what we intend. APS specifically could benefit LLMs by providing them with an internal semantic atlas, potentially enabling better control (steering the model towards certain regions yields certain types of generations) and more predictable behavior. Similarly, in recommendation or personalization systems, an APS embedding could help identify coherent user segments or item categories through the energy basins, improving transparency and fairness (as causal factors like demographic correlations could be explicitly controlled in Z).

Limitations and Future Work: Our initial APS implementation introduces several hyper-parameters (the weights λ's, the choice of k, etc.) which require tuning. In some cases, there may be trade-offs between the objectives – e.g. perfect topology preservation might conflict with perfect invariance if certain spurious features were part of local similarity in data. Balancing these is non-trivial. Additionally, the current formulation assumes we can either know or infer nuisance factors for the causality loss; in truly unsupervised scenarios, one might use data augmentations as a proxy (assuming certain transformations shouldn't change Z). This could be further automated by techniques that learn what to ignore (perhaps using attention mechanisms to attend to causal features).

The AG News results highlight a key limitation: frozen pre-trained embeddings limit the causality component's effectiveness since gradient-based independence cannot modify input features. Future work should evaluate APS on:

1. **Trainable embeddings:** Fine-tune BERT or train from scratch to allow full representation learning

2. **Strong domain shifts:** ColoredMNIST (90%+ spurious correlation), Waterbirds, CivilComments with validated biases

3. **Multi-domain datasets:** 5+ diverse domains where invariance learning is critical

4. **Online learning:** Adapt APS for streaming data where domain shift evolves over time

Another limitation is scalability: for extremely large datasets, computing even approximate neighbor graphs is heavy – one might explore *self-supervised contrastive approaches* to approximate the topology loss (e.g. treat augmented pairs as neighbors). Our TopologyEnergy formulation avoids the mode collapse issues typical of traditional EBMs by deriving energy directly from data structure rather than learning arbitrary patterns, making it more robust and scalable than memory-based alternatives.

For future research, one exciting avenue is to extend APS to **different geometries** (not just Euclidean latent spaces). For instance, we could enforce topology and invariance while learning embeddings on a **hyperbolic manifold** for inherently hierarchical data – combining APS with the Poincaré embedding approach[15]. Another direction is to incorporate **dynamic or temporal pattern spaces** – e.g. use APS for sequence models where the latent at each time step forms an atlas of states (this might connect with state-space models or neural ODEs that have attractors[6]). We also plan to investigate theoretical guarantees: under what conditions does minimizing these

losses recover the true generative factors or the true manifold? Insights from recent identifiability theory could guide this.

In conclusion, Atlasing Pattern Space represents a step toward *geometry-aware, causally-informed representation learning.* By unifying ideas across subfields (topological deep learning, causal ML, energy-based memory networks[17]), it provides a framework for building **latent spaces that are as structured and rich as the data they model**. The discovery of TopologyEnergy's superiority over memory-based approaches, combined with validation across vision and language domains, establishes practical guidelines for when to apply different APS components. We hope this sparks further exploration into **structured embeddings** that can ultimately lead to more generalizable and interpretable AI systems.

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Code Availability

The implementation of the APS framework, including TopologyEnergy and all experimental code, is available at:

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https://github.com/freemanhui/atlasing_pattern_space

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