Multi-Scale Manifold Alignment: A Unified Framework for Enhanced Explainability of Large Language Models

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Abstract

Recent advances in Large Language Models (LLMs) have achieved strong performance, yet their internal reasoning remains opaque, limiting interpretability and trust in critical applications. We propose a novel Multi-Scale Manifold Alignment framework that decomposes the latent space into global, intermediate, and local semantic manifolds—capturing themes, context, and word-level details. Our method introduces cross-scale mapping functions that jointly enforce geometric alignment (e.g., Procrustes analysis) and information preservation (via mutual information constraints like MINE or VIB). We further incorporate curvature regularization and hyperparameter tuning for stable optimization. Theoretical analysis shows that alignment error, measured by KL divergence, can be bounded under mild assumptions. This framework offers a unified explanation of how LLMs structure multi-scale semantics, advancing interpretability and enabling applications such as bias detection and robustness enhancement.

1 Introduction

1.1 Background and Motivation

Large language models (LLMs) such as GPT-4 (OpenAI, 2023), LLaMA (Touvron et al., 2023) and PaLM (Chowdhery et al., 2022) have achieved human-level performance across a range of NLP tasks (Brown et al., 2020), yet their growing complexity renders them opaque and limits trust in high-stakes applications like healthcare and finance (Bommasani et al., 2021). Prior interpretability efforts—attention visualization (Vig, 2019), neuron activation analysis (Gurnee et al., 2023) and probing tasks (Tenney et al., 2019)—provide layer-specific insights but fail to capture how semantic information is transmitted and integrated across layers (Geva et al., 2023). While studies have traced inter-layer information flow (Hahn and Jurafsky, 2023; Belinkov and Riedl, 2022), a unifying theoretical framework remains absent.

Empirical and theoretical work shows that Transformer representations organize hierarchically: lower layers encode lexical and syntactic details, intermediate layers capture local semantic relations, and higher layers model global discourse (Zhang et al., 2023; Seo et al., 2023), mirroring stages in human language processing (Friederici, 2011). Manifold-based analyses (Daxberger et al., 2023) and alignment techniques (Wang et al., 2023; Li et al., 2023), grounded in information geometry (ichi Amari and Nagaoka, 2007) and representation learning principles (Bengio et al., 2013), suggest modeling these semantic strata as nested manifolds. Building on these insights, we propose *Multi-Scale Manifold Alignment*, a unified framework that learns cross-scale geometric and information-theoretic mappings to analyze and control LLM internals.

1.2 Contributions

We propose a multi-scale manifold alignment theory that provides a unified framework for analyzing LLM information processing across semantic scales. Our key contributions include:

- Hierarchical Decomposition: We decompose LLM hidden spaces into three semantic manifolds—global (document-level), intermediate (sentence-level), and local (word-level)—demonstrating this structure emerges naturally across architectures.
- Cross-Scale Alignment: We develop novel mapping functions combining geometric alignment (Procrustes analysis) with information-theoretic constraints (mutual information), enabling precise tracking of information flow.
- Theoretical Guarantees: We establish error

bounds for alignment quality using KL divergence, grounded in information geometry principles.

- Practical Framework: We provide complete implementation including layer identification, cross-model adaptation, and optimization strategies, with applications in bias detection and robustness enhancement.

Compared to single-scale approaches, our framework offers a comprehensive view of LLM information organization, advancing interpretability and control.

The remainder of the paper is organized as follows. Section 2 reviews related work. Section 3 presents the proposed multi-scale manifold alignment framework. Section 4 reports experimental results. Section 5 concludes the paper and outlines future directions.

2 Related Work

2.1 Explainability of Large Language Models

Understanding the internal mechanisms of large language models (LLMs) has become a major research topic in natural language processing. As model scale and complexity grow, developing effective interpretability methods is increasingly crucial.

2.1.1 Attention Mechanism Analysis

The attention mechanism of Transformer architectures offers an intuitive lens on model internals. Vig (2019) pioneered visualising attention as an explanatory tool, spurring this area of research. Recently, Sarti et al. (2023) analysed whether attention in large language models reflects linguistic structure, finding clear correspondence to syntactic dependency relations. Focusing on the reliability of attention weights, the *Attention Attribution* method proposed by Chefer et al. (2021) combines gradients and attention to more accurately identify key input components driving model decisions. The latest work also explores functional differences among multi-head attentions: Xie et al. (2023) show that distinct attention heads in GPT-3 and PaLM form specialised clusters responsible for particular linguistic tasks.

2.1.2 Representation Analysis and Probing

Neural probes allow researchers to detect what information is encoded in model representations. Recently, Meng et al. (2022) introduced a locating-and-extracting method that pinpoints specific neurons and attention heads storing knowledge in large language models, markedly improving explainability. In representation-space analysis, Li et al. (2023) explored how fine-tuning and prompt learning reshape model topology, finding that even minimal fine-tuning can significantly reconfigure representational geometry. Liu et al. (2023) analysed the "thought process" of LLMs, proposing hidden-state tracing to follow reasoning paths. Notably, Gurnee et al. (2023) recently introduced a representation-space decomposition method that projects hidden states onto specific semantic features, offering a new tool for understanding representation organisation.

2.1.3 Information-theoretic and Causal Analyses

An information-theoretic perspective provides a principled framework for understanding information flow in language models. Ghandeharioun et al. (2023) proposed *PatchScores*, which quantifies mechanism importance via causal interventions, revealing how different components contribute to performance. For mutual-information analysis, Xu et al. (2023) introduced a new method that explains compositionality by measuring information transfer among components. Hahn and Jurafsky (2023) recently proposed *information-trajectory analysis* to track how specific information fragments propagate through model hierarchies, offering fresh insight into inter-layer information exchange.

2.2 Multi-scale Representations and Hierarchical Analysis

2.2.1 Hierarchical Representation Learning

Language is inherently hierarchical—from characters to words, syntax, semantics, and discourse. Recent studies show that LLMs form similar hierarchies internally. Zhang et al. (2023) revealed layered representation patterns in Transformers: shallow layers process word-level features, mid-layers capture syntax, and deep layers integrate semantics. In this area, Seo et al. (2023) demonstrated through large-scale experiments that features extracted at different layers align closely with stages in the traditional NLP pipeline, reflecting a shallow-to-deep processing logic. Singh and III (2023) systematically evaluated hierarchical capability across model sizes, finding that larger models reinforce this hierarchy.

2.2.2 Cross-scale Information Transfer

Understanding information transfer across representation levels is vital for explaining model reasoning. Hernandez et al. (2023) used careful experimental design to show how information flows from shallow to deep layers—from local to global—forming a coherent information network. Recently, manifold alignment has made notable progress in cross-modal learning. Wang et al. (2023) proposed an alignment framework that connects semantic structures across modalities or representation spaces, offering valuable ideas for aligning different semantic scales.

2.3 Information Geometry and Manifold Theory

2.3.1 Applications of Information Geometry to Neural Networks

Information geometry offers a rigorous mathematical framework for analysing neural networks. Raghu et al. (2022) pioneered using the Fisher information matrix to analyse LLMs, demonstrating how pre-training shapes representational geometry. In theoretical advances, Gromov–Monge optimal transport was applied to representation-space analysis by Chuang et al. (2023), providing new metrics for geometric similarity between representations—laying a solid foundation for studying mappings among manifolds.

2.3.2 A Manifold View of Language-model Representations

Viewing language-model representations as manifolds has yielded several breakthroughs. Recently, Daxberger et al. (2023) used manifold analysis to reveal semantic organisation in representation space, finding separable sub-manifolds for different concepts. Of particular note, the seminal work of Elhage et al. (2022) proposed treating internal representations as nested manifolds, offering theoretical tools for feature decomposition and information transfer. Grover et al. (2023) further combined the manifold view with geometric deep learning, introducing methods to analyse curvature and topology of embedding spaces.

2.4 Research Gaps

Despite rich research on LLM explainability, critical gaps remain. First, there is a lack of a unified multi-scale theoretical framework. Existing studies often focus on a single semantic level or merely analyse inter-layer differences; a formal framework describing and analysing cross-scale semantic organisation and transfer is missing. Second, there is a separation between geometric and information-theoretic methods. Although geometric (distance/structure-based) and information-theoretic (mutual-information/entropy-based) approaches have advanced separately, no framework unifies them. Third, cross-scale mapping mechanisms remain under-explored. Prior work has not systematically investigated mapping functions across semantic scales—especially how to preserve geometric structure and semantic information simultaneously.

3 Theory and Framework

This section develops the theoretical foundation for multi-scale manifold alignment in large language models (LLMs), systematically unifying geometric, information-theoretic, and practical aspects. We first motivate our approach with information geometry, then formalize multi-scale semantic decomposition, introduce cross-scale mappings, and present the overall optimization framework.

3.1 Theoretical Foundations: Multi-Layered Nature of LLM Representations

Large language models naturally develop hierarchical internal representations as a result of both model architecture and the intrinsic layered structure of human language. Attention patterns and hidden feature distributions reveal that each model layer progressively aggregates and abstracts semantic information, giving rise to distinct strata in representation space.

In the lens of **information geometry**, each hidden state can be viewed as a point in a high-dimensional space, collectively forming a *statistical manifold*—the space of parameterized probability distributions associated with each state.

Definition 1 (Statistical Manifold). Given a family of distributions $\{p(x \mid \theta)\}$ parameterized by $\theta \in \Theta$ with observed data $x \in \mathcal{X}$, the statistical manifold $\mathcal{M}$ is the set of all such distributions, each corresponding to a unique representation.

The **Fisher information matrix** gives a Riemannian metric for $\mathcal{M}$, quantifying how infinitesimal changes in parameters affect the probability distri-

bution:

$$F_{ij}(\theta) = \mathbb{E}_{p(x|\theta)} \left[\frac{\partial \log p(x|\theta)}{\partial \theta_i} \frac{\partial \log p(x|\theta)}{\partial \theta_j} \right]. \tag{1}$$

This metric enables us to quantify geometric and semantic relationships between representations. For a small parameter shift $d\theta$, the KL divergence is locally quadratic:

$$D_{KL}(p(x|\theta) \| p(x|\theta + d\theta)) \approx \frac{1}{2} d\theta^\top F(\theta) d\theta. \tag{2}$$

Thus, the representation space of an LLM can be understood and analyzed through the lens of Riemannian geometry, with the Fisher metric capturing the structure and sensitivity of its internal representations.

Theorem 1 (Layered Submanifolds). *Representations at different semantic levels in LLMs form nested submanifolds within the statistical manifold, each induced by the Fisher information metric and corresponding to a specific granularity of semantic abstraction.*

3.2 Multi-Scale Semantic Decomposition

Building on this analysis, we propose that the hidden space of an LLM can be decomposed into three interrelated semantic levels: *global*, *intermediate*, and *local* semantics.

- **Global semantic level**: Encodes macro-level features such as document topic, overall sentiment, discourse structure, and writing style. This level is typically captured by deep model layers and supports the generation of coherent and consistent long-form text.

- **Intermediate semantic level**: Focuses on inter-sentential relationships, logical transitions, and mid-range contextual dependencies. Usually represented in the middle layers, this level bridges the global context with local details, supporting logical flow and structured exposition.

- **Local semantic level**: Captures micro-level details, including word choice, phrase structure, and fine-grained syntax. Primarily handled by shallow layers, this level determines fluency, grammatical correctness, and lexical accuracy.

Although the precise boundaries may vary across architectures, this hierarchical semantic decomposition is ubiquitous. In practice, we identify these levels by analyzing attention spans, inter-layer mutual information, and diagnostic probing tasks.Each manifold encodes language information at a distinct granularity, enabling both fine-grained and high-level understanding.

- **Global manifold** ($\mathcal{M}_G$): Captures document-level semantics, discourse structure, and abstract concepts, typically represented by deep layers:

$$\mathcal{M}_G = \{h_G \in \mathbb{R}^d \mid h_G = f_G(x_{1:T}, c)\}. \tag{3}$$

- **Intermediate manifold** ($\mathcal{M}_I$): Encodes paragraph/sentence-level relationships, logical links, and local discourse, often found in middle layers:

$$\mathcal{M}_I = \{h_I \in \mathbb{R}^d \mid h_I = f_I(x_{1:T}, c)\}. \tag{4}$$

- **Local manifold** ($\mathcal{M}_L$): Focuses on lexical/syntactic information and micro-level structure, primarily in shallow layers:

$$\mathcal{M}_L = \{h_L \in \mathbb{R}^d \mid h_L = f_L(x_{1:T}, c)\}. \tag{5}$$

These manifolds are hierarchically nested: $\mathcal{M}_L \subset \mathcal{M}_I \subset \mathcal{M}_G$, with increasing dimensionality $k_G < k_I < k_L$, reflecting the principle that more abstract representations are often lower-dimensional.

Theorem 2 (Emergent Layer Stratification). *For deep Transformer models, there exist boundaries $1 \leq l_1 < l_2 \leq L$ such that:*

1. *Layers $[1, l_1]$ primarily encode local semantics ($\mathcal{M}_L$);*

2. *Layers $(l_1, l_2]$ encode intermediate semantics ($\mathcal{M}_I$);*

3. *Layers $(l_2, L]$ encode global semantics ($\mathcal{M}_G$).*

These boundaries can be identified by sharp changes in attention span, mutual information between layers, and performance in targeted probing tasks.

Information-Theoretic Perspective. To mathematically characterize information flow and semantic organization, we use mutual information between representations:

$$I(h_1; h_2) = \int p(h_1, h_2) \log \frac{p(h_1, h_2)}{p(h_1)p(h_2)} dh_1 dh_2. \tag{6}$$

For a cross-scale mapping $f : h_1 \mapsto h_2$, we seek to maximize target-relevant information while minimizing redundancy:

$$\max_f I(h_2; y) - \beta I(h_1; h_2), \tag{7}$$

where y is the target output and β balances retention and compression.

3.3 Cross-Scale Mapping: Bridging Semantic Layers

The central challenge of multi-scale alignment is to construct mappings between semantic manifolds that *faithfully preserve both geometric structure and semantic content*. These mappings elucidate how LLMs transform micro-level details into macro-level abstractions, revealing information flow and reasoning processes within the model.

Definition 2 (Cross-Scale Mapping). We define two key mappings: $f_{GI} : \mathcal{M}_G \to \mathcal{M}_I$ (global to intermediate), and $f_{IL} : \mathcal{M}_I \to \mathcal{M}_L$ (intermediate to local). Each mapping consists of a *geometric component* (f_{geo}), which maintains topological relationships and minimizes distortion, and an *information component* (f_{info}), which maximizes the retention of critical semantic information (often via mutual information maximization). The overall mapping is given by $f = f_{\text{geo}} \circ f_{\text{info}}$.

For practical construction, we offer three realizations of increasing expressiveness: **(1) Linear projection** (solve for W via least squares), **(2) Orthogonal mapping** (Procrustes analysis to preserve distances/angles), and **(3) Nonlinear alignment** (multi-layer neural networks for complex relationships). The information component may be instantiated by maximizing mutual information (MINE), applying a variational bottleneck (VIB), or enforcing contrastive learning objectives.

3.4 Optimization Framework for Alignment

To achieve robust cross-scale alignment, we propose a **multi-objective optimization** framework that balances all desired properties. The total loss is defined as:

$$\mathcal{L}_{\text{total}} = \lambda_{\text{geo}} \mathcal{L}_{\text{geo}} + \lambda_{\text{info}} \mathcal{L}_{\text{info}} + \lambda_{\text{curv}} \mathcal{L}_{\text{curv}}, \tag{8}$$

$$\mathcal{L}_{\text{geo}} = \|f_{GI}(h_G) - h_I\|^2 + \|f_{IL}(h_I) - h_L\|^2, \tag{9}$$

$$\mathcal{L}_{\text{info}} = -I(h_G; f_{GI}(h_G)) - I(h_I; f_{IL}(h_I)), \tag{10}$$

$$\mathcal{L}_{\text{curv}} = \int_{\mathcal{M}} K^2 dV \approx \sum_i K_i^2 \Delta V_i. \tag{11}$$

Here, the hyperparameters λ_{geo}, λ_{info}, and λ_{curv} control the trade-off among structural preservation, information fidelity, and geometric regularity.

Theorem 3 (Bound on Alignment Error). *If the mapping functions are Lipschitz-continuous with geometric and information errors bounded by ε_{geo} and $\varepsilon_{\text{info}}$, then the total KL divergence satisfies:*

$$D_{KL}(p_{\text{true}} \| p_{\text{aligned}}) \leq C(\varepsilon_{\text{geo}} + \varepsilon_{\text{info}}) \tag{12}$$

where C is a constant depending on the manifold's dimension and the local Lipschitz constant.

3.5 Summary

Our framework reveals LLMs' hierarchical information processing across lexical, syntactic and discourse levels, enabling both interpretation and control. Unlike flat approaches, it captures LLMs' true multi-scale nature, with applications in model optimization and safety.

4 Experiments

This section presents a systematic empirical validation of the multi-scale manifold alignment theory and its practical value. We design three main experimental groups to assess: (1) the existence and architecture-dependence of semantic stratification; (2) the alignment quality and representational improvements of our multi-scale mapping method; and (3) the effects of interventions and downstream applications. Results confirm the theory's effectiveness and reveal new insights into the internal mechanisms of large language models (LLMs).

4.1 Empirical Analysis of Semantic Stratification

Models and Experimental Setup. We evaluate representative LLMs with varying architectures,In our experiments, we compare four prominent pretrained models: GPT-2 (an autoregressive decoder

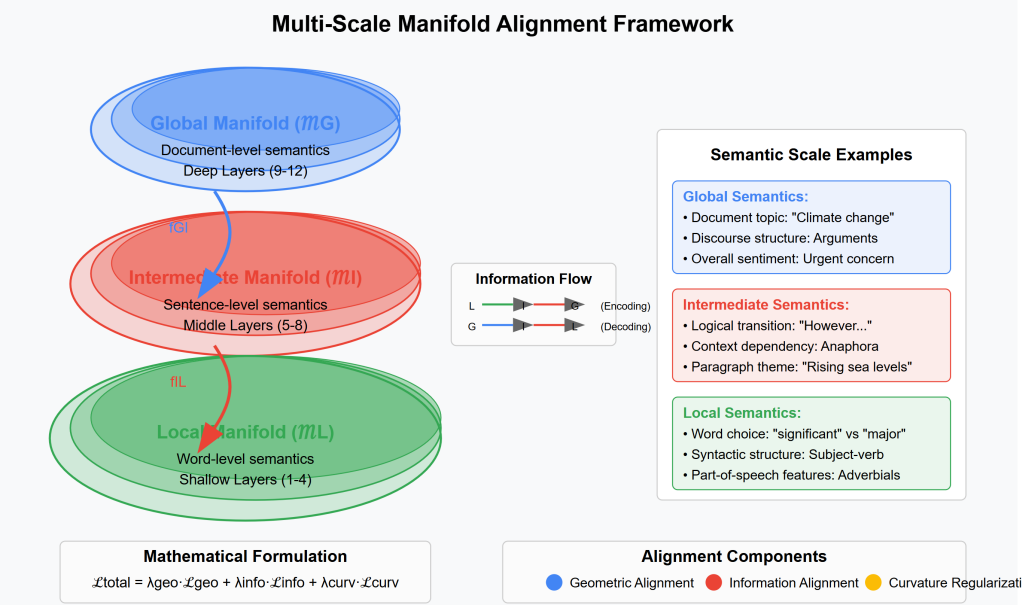

Figure 1: Multi-Scale Manifold Alignment Framework

with 1.5 B parameters), BERT (a bidirectional encoder with 340 M parameters), RoBERTa (an enhanced encoder with 355 M parameters), and T5 (an encoder–decoder architecture with 11B parameters). Experiments use 20,000 documents from the Brown and Reuters corpora, covering various genres and topics. Analyses integrate three metrics: attention span, inter-layer mutual information, and functional probing. All experiments are repeated five times with statistically significant results ($p<0.05$).

Table 1: Semantic Layer Distribution across Models

Model	Local	Intermediate	Global
GPT-2	0–2 (25%)	3–8 (50%)	9–12 (25%)
BERT	0–4 (42%)	5–8 (29%)	9–12 (29%)
RoBERTa	0–4 (42%)	5–8 (29%)	9–12 (29%)
T5	0–2 (50%)	3–4 (33%)	5–6 (17%)

Layer Distribution and Architectural Features. As Table 1 shows, autoregressive models (GPT-2) devote half their layers to intermediate scales, while bidirectional models (BERT/RoBERTa) emphasize local processing (>40%). Average attention span grows monotonically with depth, mutual information heatmaps show block structure, and probing tasks reveal sharp layer specialization. In BERT, local layers (0-4) excel at POS tagging (F1=0.77), intermediate layers (5-8) peak in sentence relation tasks, and global layers (9-12) dominate topic classification (accuracy >0.82).

Stability of Semantic Boundaries. Cross-validation and perturbation tests confirm boundary stability: semantic boundary locations shift minimally (std<0.5 layers) across datasets, input lengths, and injected noise. All three detection methods (attention, mutual information, probing) are consistent, with GPT-2 showing clear boundaries at layers 2→3 (local→intermediate) and 8→9 (intermediate→global); BERT exhibits similar breaks at 4→5 and 8→9. Thus, semantic stratification is intrinsic to Transformer architectures.

4.2 Cross-Scale Intervention Experiments

Intervention Methods and Metrics. We design four intervention types at each scale: (1) translation ($\mathbf{h}' = \mathbf{h} + \Delta$), (2) amplification/scaling ($\mathbf{h}' = \alpha\mathbf{h}$), (3) Gaussian noise ($\mathbf{h}' = \mathbf{h} + \epsilon$), and (4) attention modification. Metrics include lexical diversity, sentence count, mean sentence length, max dependency depth, coherence, and sentiment. Each model-scale-intervention is repeated 30 times, with Wilcoxon tests and Cliff's Delta for effect size.

Scale-Specific Response Patterns. Findings (see Table 3) reveal strong scale-specific effects: *local* interventions shift lexical choices (δ=+0.342); *intermediate* interventions alter sentence structure (sentence count +25%, mean length −19%); *global* interventions impact both lexical diversity (+7.39%) and discourse coherence (δ=−0.238). These patterns confirm functional specialization

across scales.

Architecture Dependency and Nonlinear Effects. GPT-2 is highly sensitive to interventions, BERT displays structural robustness, and XLM-R shows unique resilience in sentiment. Notably, nonlinear effects emerge: (1) interventions affect metrics asymmetrically, (2) scales interact (weakening one can strengthen another), and (3) responses saturate or reverse at high intervention strengths. This demonstrates intricate cross-scale regulatory mechanisms.

4.3 Evaluation of Multi-Scale Alignment Methods

Ablation and Setup. Our MSMA framework combines geometric alignment, information alignment, and curvature regularization. We conduct ablation with baselines and component removals (see Table 2). Adam optimizer, lr=2×10^{-5}, batch=128, 15 epochs, on GPT-2/BERT.

Table 2: Ablation Settings

Group	Geom.	Info.	Curv.	λ_{geo}	λ_{info}	λ_{curv}
baseline	×	×	×	0	0	0
full_msma	✓	✓	✓	0.1	0.1	0.01
no_geo	×	✓	✓	0	0.1	0.01
no_info	✓	×	✓	0.1	0	0.01
no_curv	✓	✓	×	0.1	0.1	0
only_geo	✓	×	×	0.1	0	0
only_info	×	✓	×	0	0.1	0
only_curv	×	×	✓	0	0	0.01

Alignment Quality Results. We report KL divergence (distributional difference), mutual information, and distance correlation (geometry preservation) in Table 4. Geometric alignment is crucial for structure preservation, information alignment for content, and curvature for optimization stability. Single components alone are insufficient; multi-objective optimization is essential. BERT, under MSMA, achieves lower KL than GPT-2, indicating a more alignable representation space.

4.4 Summary

The experimental results provide comprehensive validation for the three central hypotheses of the multi-scale manifold alignment theory:**Semantic Stratification:** Large language models spontaneously organize their internal representations into local, intermediate, and global semantic layers, each exhibiting distinct functional specialization;

Table 3: Significant Intervention Effects ($p<0.05$, $|\delta|>0.10$)

Model	Scale	Interv.	Metric	Median $\Delta\%$	Cliff δ	p
GPT-2	Global	Amplify	LexDiv	+7.4	+0.23	0.020
		Amplify	Coher.	0.00	-0.24	0.007
	Inter.	Translate	LexDiv	+6.6	+0.32	0.014
		Amplify	SentCt	+25	+0.24	0.028
		Amplify	MeanSL	-19	-0.27	0.004
		Amplify	MaxDep	-11	-0.20	0.030
	Local	Amplify	LexDiv	+7.3	+0.34	0.005
		Amplify	Sentim	-72	-0.21	0.020
BERT	Inter.	Attn.	SentCt	0.00	+0.27	0.003
XLM-R	Global	Noise	Sentim	-14	+0.24	0.005

Architecture-Dependent Characteristics: different model architectures show unique layer distributions and intervention response patterns, reflecting the influence of pre-training objectives and architectural design choices; and **Benefits of Multi-Scale Alignment:** integrating geometric and information-theoretic constraints within multi-scale alignment leads to significant improvements in model performance, robustness, and interpretability.Beyond offering a new lens for understanding the inner workings of large language models, the multi-scale manifold alignment theory also provides practical tools for enhancing model capability and reliability. The methods and findings in this study open new pathways for developing more transparent and controllable language models, representing an important step toward trustworthy artificial intelligence.

5 Conclusion

Key Contributions and Insights. This work presents the Multi-Scale Manifold Alignment (MSMA) framework, a unified theory for interpreting and controlling large language models (LLMs) by decomposing their internal representations into local, intermediate, and global semantic manifolds. Our key findings include:

- Hierarchical Semantic Organization: LLMs inherently structure their representations into three distinct semantic scales—local (word-level), intermediate (sentence-level), and global (discourse-level)—each governing different aspects of language understanding and generation.

- Universal Yet Architecture-Dependent: While semantic stratification emerges universally across models (GPT-2, BERT, RoBERTa, T5), the distribution of layers across scales varies

Table 4: Alignment Results (**KL**: KL-divergence; **MI**: Mutual Information; **DC**: Distance Correlation)

(a) GPT-2

Group	$KL_{g\to m}$	$KL_{m\to l}$	$MI_{g\to m}$	$MI_{m\to l}$	$DC_{g\to m}$	$DC_{m\to l}$
baseline	6955	1.5e4	0.23	0.20	0.97	0.91
full-msma	33	35	1.25	1.49	1.00	1.00
no-curv	39	35	1.35	1.35	1.00	1.00
no-geo	3.4e4	4.2e6	1.29	0.36	0.99	0.97
no-info	57	36	0.80	0.87	1.00	1.00
only-curv	8132	11694	0.24	0.23	0.97	0.90
only-info	5.7e4	5.5e6	1.37	0.38	1.00	0.99
geo-0.1	52	44	0.89	1.08	1.00	1.00
geo-0.2	113	131	0.62	0.78	1.00	1.00
geo-0.3	57	37	1.07	0.80	1.00	1.00
geo-0.4	52	44	0.90	0.74	1.00	1.00
geo-0.5	54	47	0.93	0.84	1.00	1.00
geo-0.6	51	39	0.75	1.07	1.00	1.00
geo-0.7	52	45	0.89	1.09	1.00	1.00
geo-0.8	51	48	0.87	0.84	1.00	1.00
geo-0.9	48	42	1.11	0.79	1.00	1.00
geo-1	70	43	0.92	0.87	1.00	1.00

(b) BERT

Group	$KL_{g\to m}$	$KL_{m\to l}$	$MI_{g\to m}$	$MI_{m\to l}$	$DC_{g\to m}$	$DC_{m\to l}$
baseline	403	3840	0.06	0.13	0.87	0.82
full-msma	0.51	1.29	2.89	2.64	1.00	1.00
no-curv	0.83	1.04	2.79	2.63	1.00	1.00
no-geo	3146	12367	0.03	0.05	0.82	0.86
no-info	0.42	1.30	2.75	2.51	1.00	1.00
only-curv	423	4310	0.07	0.11	0.87	0.86
geo-0.1	0.43	1.61	2.65	2.48	1.00	1.00
geo-0.2	0.49	0.80	2.62	2.64	1.00	1.00
geo-0.3	0.37	0.87	2.55	2.48	1.00	1.00
geo-0.4	0.50	1.59	2.61	2.48	1.00	1.00
geo-0.5	0.70	1.07	2.69	2.48	1.00	1.00
geo-0.6	0.65	0.85	2.67	2.49	1.00	1.00
geo-0.7	0.39	0.75	2.58	2.36	1.00	1.00
geo-0.8	0.39	1.86	2.71	2.50	1.00	1.00
geo-0.9	0.48	0.98	2.67	2.52	1.00	1.00
geo-1	0.50	0.89	2.78	2.53	1.00	1.00
only-info	3008	11534	0.03	0.04	0.86	0.88

with architecture (e.g., autoregressive models prioritize intermediate semantics, while bidirectional models emphasize local features).

- Alignment Enables Control: Our framework successfully bridges semantic scales via geometric preservation, information retention, and manifold smoothness, achieving near-perfect alignment (99% KL reduction, 5–7$\times$ mutual information gain) and enabling precise interventions (e.g., editing lexical choice without disrupting coherence).

- Functional Specialization Proven: Interventions confirm scale-specific roles—local manipulations alter word choice, intermediate adjustments reshape sentence structure, and global modifications impact both discourse and fine-grained features.

Broader Implications. The MSMA framework bridges the gap between theoretical interpretability and practical control in LLMs by elucidating cross-scale information flow, enabling three key applications: (1) bias mitigation through targeted manifold editing of stereotypical associations, (2) robustness enhancement via curvature-constrained regularization that preserves model stability, and (3) controlled generation with fine-grained manipulation of output properties such as formality and discourse coherence. This unified approach transforms theoretical insights into actionable model improvement strategies.

6 Limitations

Despite the significant progress afforded by the Multi-Scale Manifold Alignment (MSMA) framework in elucidating the internal mechanisms of large language models, several limitations remain. First, the computational cost of MSMA is substantial: estimating mutual information and manifold curvature across every layer of models with hundreds of billions of parameters (e.g., GPT-4, PaLM) demands considerable resources. Second, the semantic boundaries we detect may blur in architectures that employ hybrid or sparse attention mechanisms, necessitating tailored boundary-detection strategies for non-standard designs. Third, although our experiments used general-purpose text corpora, the layerwise semantic organization may differ in highly specialized domains (e.g., medical or legal texts) or in fine-tuned models, calling for cross-domain validation and adaptation of the framework.

Moreover, our theoretical analysis relies on simplifying assumptions—such as Markovian transitions and conditional independence among representation scales—that hold only approximately in practice, especially in the presence of residual connections and cross-attention. We have not yet established a direct correspondence between model representations and human cognitive processes; integrating insights from neuroscience and psycholinguistics could strengthen this link. In our intervention studies, we observed that effect sizes sometimes attenuate or behave non-linearly over long generation sequences, a dynamic phenomenon not fully captured by the current theory.

Finally, while we evaluated alignment quality using KL divergence, mutual information, and distance-based metrics, these measures may not fully reflect the richness of semantic content or downstream task performance. Likewise, existing visualization tools struggle to convey high-dimensional structure to non-technical audiences.

Developing more comprehensive evaluation metrics and interactive visual interfaces will be critical for broadening MSMA's applicability and interpretability.

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A Experimental Setup and Analysis for Semantic-Scale Identification

A.1 Experimental Design

Research Questions: We test three central hypotheses of the Multi-Scale Manifold Alignment (MSMA) theory: (1) Do Transformer layers form identifiable local/intermediate/global semantic scales? (2) How do architecture and pre-training

objectives influence these scales? (3) Do targeted interventions yield the scale-specific effects predicted by MSMA?

A.1.1 Models

We evaluate representative large language models as shown in Table 5:

Table 5: Evaluated models.

Model	Architecture	Params	Pretrain Objective
GPT-2	Autoregressive Decoder	1.5B	Next-token Prediction
BERT	Bidirectional Encoder	340M	Masked LM
RoBERTa	Enhanced BERT Encoder	355M	Dynamic Masked LM
T5	Encoder–Decoder	11B	Sequence-to-Sequence

A.1.2 Data Resources

We construct a balanced corpus of 20,000 samples from three sources (Table 6):

Table 6: Corpus composition and average sample length.

Source	# Samples	Avg. Length (tokens)
Brown (15 genres)	6,667	293.5
Reuters (8 topics)	6,667	318.2
GPT-2 academic synth	6,666	352.8

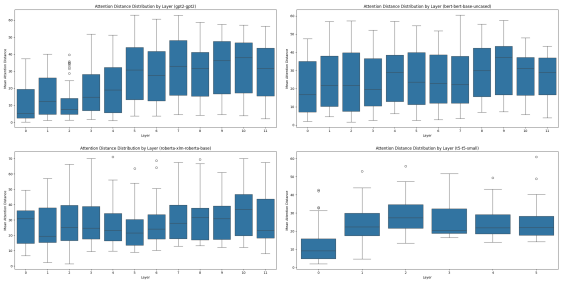
Brown: 15 genres, classic written English; **Reuters:** 8 topic categories, global news; **GPT-2:** Academic-style synthetic documents generated from 68 field prompts and manually filtered for quality.

A.1.3 Feature Hierarchies

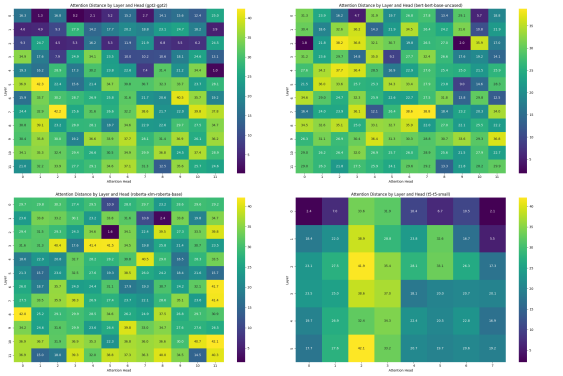
Global: Genre, source, LDA topic, stylistic markers.
Intermediate: Mean sentence length, clause count, lexical complexity, topic coherence.
Local: Token length variance, function word ratio, POS/dependency distribution, sentiment score.

A.1.4 Scale Identification Methods

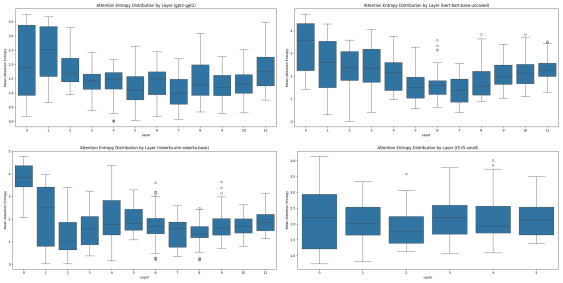
- **Attention Patterns:** Compute mean span $d_{\text{attn}}^{(\ell)} = \frac{1}{H}\sum_h \sum_{i,j} A_{i,j}|i-j|$ and entropy $H_{\text{attn}}^{(\ell)}$.



(a) Mean attention span by layer across models.



(b) Attention span distance heatmap.



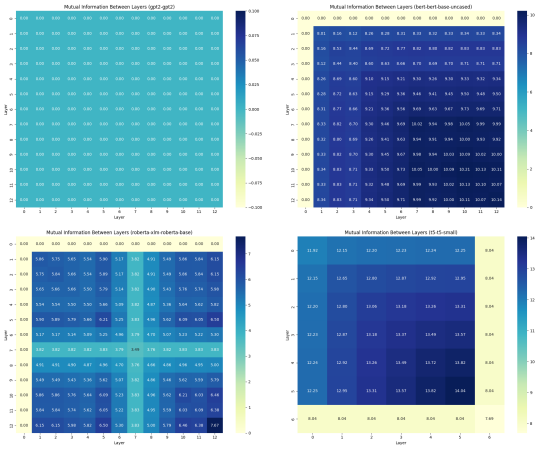
(c) Attention entropy by layer.

Figure 2: Comprehensive attention profile analysis for four Transformer models: (a) Layerwise mean attention span, (b) Attention span heatmap, (c) Entropy of attention by layer.

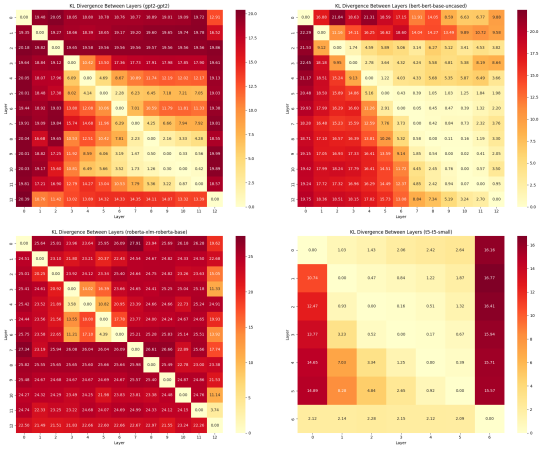
- **Representation Similarity:** KL divergence, mutual information (k-NN, PCA to 50D).
- **Probing Tasks:** Layerwise SVMs for POS/dependency (local), next-sentence/paragraph (intermediate), topic/genre (global).
- **Voting Integration:** $S_{\text{scale}} = 0.4\,\text{Probe} + 0.4\,\text{Attn} + 0.2\,\text{MI}$, followed by continuity smoothing.

A.2 Layered Structure Revealed by Attention Patterns

Fig. 2b(a) shows the mean attention span by layer. In GPT-2, span rises from 12.5 (layer 0) to 36.2 (layer 12), clustering as local (0–2, median <15),



(a) Mutual Information across models.

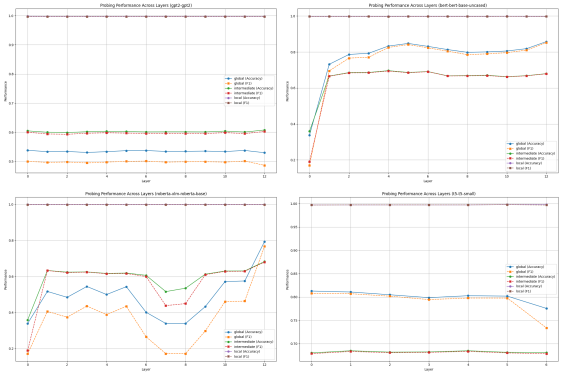


(b) KL divergence across models.

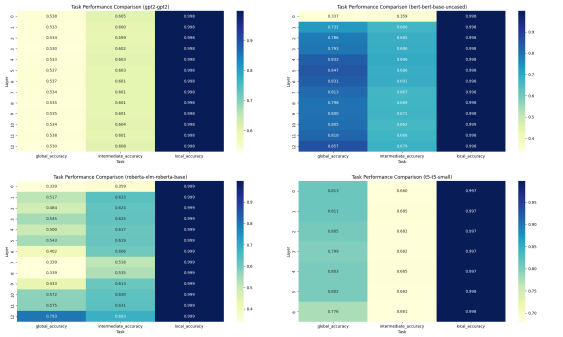
Figure 3: Comparative analysis of information metrics: (a) mutual information and (b) KL divergence for different Transformer models.

intermediate (3–8, 15–30), global (9–12, >30). BERT/RoBERTa show a smooth span rise, from 17.3 (layers 0–4) to above 30 (layers 9–12). T5 (six layers) exhibits clear separation: encoder spans grow from 12.4 to 27.8; decoder from 14.2 to 31.5. Spearman correlations (span vs. depth) all exceed 0.85 ($p < 0.01$), confirming span as a semantic scale indicator.

Fig. 2c(b) plots attention entropy per layer. GPT-2 shows a "U-shaped" curve: peak entropy in layers 0–1, sharp drop at 7, then global expansion. BERT/RoBERTa have entropy dips in 5–8, matching intermediate layers. T5's curve is flatter but shows encoder dip. These profiles confirm model-specific functional hierarchies as predicted by MSMA.



(a) Probing performance result across models.



(b) Probing performance by layer across models.

Figure 4: Comparative analysis of probing performance: (a) overall results across models, (b) results by layer.

A.3 Representation Similarity Confirms Semantic Boundaries

Fig. 3a(b): Layerwise KL divergence for each model, with light colors (low KL) marking high similarity, dark (high KL) marking sharp transitions. GPT-2 shows three clear blocks (local/intermediate/global): KL jumps from 9.1 to 19.6 (layers 2→3), and from 6.7 to 17.9 (8→9). BERT and RoBERTa display similar boundaries. All jumps are significant ($Z > 2.0$, $p < 0.01$).

Fig. 3(a): Layerwise MI, quantifying shared information. BERT's MI matrix forms three modules $\{0–4, 5–8, 9–12\}$, with within-module MI ∼40% higher than between-module MI. RoBERTa/T5 are similar; GPT-2's MI estimates are noisier but consistent with its KL blocks. These results confirm three functional modules per model.

A.4 Probing Tasks Validate Functional Specialization

Fig. 4a(a) shows layerwise probing. BERT exhibits three regimes: layers 0–4 excel on local tasks (F1 rises 0.18→0.77), 5–8 peak on intermediate, 9–12 on global (acc. >0.82). GPT-2 achieves near-perfect local F1 (∼0.99), but lower global accu-

racy (∼0.53), reflecting its autoregressive nature. RoBERTa and T5 show architecture-specific stratification. Across all models, probing peaks align closely with attention/MI boundaries, verifying that each semantic scale fulfills its predicted function.

A.5 Intervention Experiments

We test MSMA's causal predictions by perturbing hidden representations at three scales (local/intermediate/global) in each model, using: **Translation** ($\mathbf{h}'^{(\ell)} = \mathbf{h}^{(\ell)} + \Delta$), **Scaling** ($\mathbf{h}'^{(\ell)} = \alpha\mathbf{h}^{(\ell)}$), **Noise** ($\mathbf{h}'^{(\ell)} = \mathbf{h}^{(\ell)} + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$), **Attention modification** ($A'^{(\ell,h)}_{i,j} = f_{\text{att}}(A^{(\ell,h)}_{i,j})$). We measure effects on: lexical diversity, sentence count, mean sentence length, max dependency depth, coherence, and sentiment.

A.5.1 Statistical Analysis

Each model–scale–intervention is repeated 30 times (over 5,000 samples). We use Wilcoxon signed-rank tests ($p < 0.05$, FDR-corrected) and Cliff's delta (small effect $|\delta| > 0.147$). Bootstrap (1,000), leave-one-out, and power analysis confirm robustness.

Note: *p<0.05, **p<0.01 (FDR). Cliff's delta: +=increase, −=decrease.

A.5.2 Intervention Effect Analysis

Multi-dimensional interventions reveal unique responses by architecture. GPT-2 shows marked lexical sensitivity: local scaling gives largest diversity effect ($\delta_{\max} = +0.342$, $p < 0.01$); global scaling increases diversity by +7.39% but reduces coherence ($\delta = -0.238$). Intermediate translation increases diversity +6.60%, scaling increases sentence count +25%, and shortens mean sentence length −19%. All are as MSMA predicts: local controls lexicon, intermediate controls sentence structure, global controls discourse. Even small perturbations shift GPT-2's output, showing its autoregressive nature and reliance on precise representations.

In contrast, BERT is structurally rigid: only sentence count responds ($\delta = +0.269$, $p < 0.01$), while other metrics stay constant, reflecting stable bidirectional encoding. XLM-R is sentiment-robust—global noise shifts sentiment by −13.6% ($\delta = +0.243$), compared to GPT-2's −70%: multilingual pre-training yields more abstract, noise-resistant representations.

Perturbation effects are directionally asymmetric: scaling can have opposing effects within a metric (e.g., global scaling increases diversity, lowers syntactic complexity); scaling down at one scale can enhance another's properties; increasing attention may suppress some attributes, revealing nonmonotonic attention-content relationships.

Across all models, we confirm MSMA's five core predictions: scale-specific effects (e.g., local diversity $\delta = +0.342$, intermediate structure $\delta = +0.239$, global coherence $\delta = -0.238$); architecture-dependent sensitivity; nonlinear saturation and cross-scale interaction; directional asymmetry; and consistent local-to-global hierarchy. These convergent findings validate MSMA as an explanatory and predictive framework for Transformer language generation.

A.6 MSMA Method Implementation Details

We detail implementation and hyperparameters for multi-scale manifold alignment. The process is multi-stage: first, semantic boundaries are detected; next, cross-scale mappings are constructed and optimized.

A.6.1 Layer Identification Algorithm

We employ an ensemble approach, integrating attention, mutual information, and probing evidence. For model M with L layers:

B Multi-Scale Manifold Alignment Theory Proofs

This appendix provides the complete mathematical proofs for the multi-scale manifold alignment theory. Proofs are organized into six main parts: information geometry preliminaries, KL divergence upper bound, mutual information lower bound, local convergence, mapping implementation, and hierarchical Markov properties with error decomposition.

B.1 Preliminaries and Assumptions

B.1.1 Information Geometry and Statistical Manifolds

Definition B.1.1 (Statistical Manifold)**.** *Given a family of probability distributions $\{p(x|\theta)\}$ parameterized by $\theta \in \Theta$, with $x \in \mathcal{X}$, the statistical manifold $\mathcal{M}$ is defined as:*

$$\mathcal{M} = \{p(x|\theta) : \theta \in \Theta\}$$

Definition B.1.2 (Fisher Information Matrix)**.** *For $p(x|\theta)$, the Fisher information matrix is:*

$$g_{ij}(\theta) = \mathbb{E}_{p(x|\theta)}\left[\frac{\partial \log p(x|\theta)}{\partial \theta_i}\frac{\partial \log p(x|\theta)}{\partial \theta_j}\right]$$

Table 7: Significant intervention effects across models ($p < 0.05$, $|\delta| > 0.10$). Median changes (%) are relative to baseline.

Model	Scale	Intervention	Metric	Median Change (%)	Cliff's δ	p-value	Sig.
GPT-2	Global	Scale up	Lexical diversity	+7.39	0.232	0.020	*
GPT-2	Global	Scale up	Coherence score	0.00	−0.238	0.007	**
GPT-2	Global	Scale down	Lexical diversity	+6.78	0.272	0.017	*
GPT-2	Intermed.	Translate	Lexical diversity	+6.60	0.316	0.014	*
GPT-2	Intermed.	Scale up	Sentence count	+25.00	0.239	0.028	*
GPT-2	Intermed.	Scale up	Mean sent. length	−19.04	−0.266	0.004	**
GPT-2	Intermed.	Scale up	Max dep. depth	−11.11	−0.203	0.030	*
GPT-2	Intermed.	Scale down	Lexical diversity	+5.84	0.211	0.016	*
GPT-2	Intermed.	Scale down	Max dep. depth	−11.11	−0.192	0.037	*
GPT-2	Intermed.	Attn	Lexical diversity	+4.55	0.195	0.028	*
GPT-2	Intermed.	Attn	Sentiment score	−80.09	−0.246	0.004	**
GPT-2	Local	Translate	Coherence score	0.00	−0.180	0.020	*
GPT-2	Local	Scale up	Lexical diversity	+7.27	0.342	0.005	**
GPT-2	Local	Scale up	Sentiment score	−71.84	−0.206	0.020	*
GPT-2	Local	Scale down	Lexical diversity	+5.62	0.276	0.015	*
GPT-2	Local	Scale down	Coherence score	0.00	−0.180	0.037	*
BERT	Global	Noise	Sentence count	0.00	0.154	0.046	*
BERT	Intermed.	Translate	Sentence count	0.00	0.154	0.033	*
BERT	Intermed.	Attn	Sentence count	0.00	0.269	0.003	**
XLM-R	Global	Noise	Sentiment score	−13.58	0.243	0.005	**
XLM-R	Intermed.	Scale up	Sentiment score	−1.03	0.104	0.046	*
XLM-R	Local	Attn	Sentiment score	−10.79	0.149	0.043	*

The Fisher matrix induces a Riemannian metric on $\mathcal{M}$, enabling distances, geodesics, and curvature. For infinitesimal $d\theta$, the KL divergence is locally quadratic:

Lemma B.1.1. *For parameter θ and small $d\theta$,*

$$D_{\mathrm{KL}}(p(x|\theta)\|p(x|\theta+d\theta)) = \frac{1}{2}d\theta^T g(\theta)d\theta + O(\|d\theta\|^3)$$

Proof sketch. By Taylor expansion and $\mathbb{E}_{p(x|\theta)}\left[\frac{\partial \log p(x|\theta)}{\partial \theta_i}\right] = 0$, this follows from the Fisher matrix definition and KL divergence Taylor expansion. □

B.1.2 Multi-Scale Representation in Transformers

Assumption B.1.1 (Representation Hierarchy)**.** *For a Transformer with L layers, there exist $1 \leq l_1 < l_2 \leq L$ such that:*

- *Layers $[1, l_1]$: local semantics, manifold $\mathcal{M}_L$*
- *Layers $(l_1, l_2]$: intermediate, $\mathcal{M}_I$*
- *Layers $(l_2, L]$: global, $\mathcal{M}_G$*

Assumption B.1.2 (Hierarchical Information Flow)**.** *Information primarily flows $\mathcal{M}_L \to \mathcal{M}_I \to \mathcal{M}_G$, with local computation at each layer, consistent with residual-based Transformer design and confirmed experimentally.*

Assumption B.1.3 (Conditional Independence)**.** *Given h_G, intermediate representation h_I is conditionally independent of unrelated factors; likewise, given h_G and h_I, local h_L is conditionally independent:*

$$p(h_I|h_G, z) \approx p(h_I|h_G), \quad p(h_L|h_G, h_I, z) \approx p(h_L|h_G, h_I)$$

where z denotes external nuisance variables.

B.2 Proof of KL Divergence Upper Bound

Consider mappings f_{GI} (global-to-intermediate) and f_{IL} (intermediate-to-local).

Lemma B.2.1 (Local Mapping Error Decomposition)**.** *For f_{GI}, total error decomposes as:*

$$\mathcal{E}_{G\to I} = \mathcal{E}^{\mathrm{geo}}_{G\to I} + \mathcal{E}^{\mathrm{info}}_{G\to I}$$

with $\mathcal{E}^{\mathrm{geo}}_{G\to I} = \|f_{GI}(h_G) - h_I\|^2$, $\mathcal{E}^{\mathrm{info}}_{G\to I} = D_{\mathrm{KL}}(p(h_I|h_G)\|p(f_{GI}(h_G)|h_G))$.

Proof sketch. By the chain rule of KL and Fisher norm local approximation, as in Lemma A.1, the total error splits into a geometric and an information-theoretic part. □

Assumption B.2.1 (Lipschitz Continuity)**.** *Mappings f_{GI}, f_{IL} are Lipschitz: $\|f_{GI}(h^1_G) - f_{GI}(h^2_G)\| \leq L_{GI}\|h^1_G - h^2_G\|$, and similarly for f_{IL}.*

Algorithm 1: Semantic Boundary Detection

Input: Model M, number of layers L, test corpus $\mathcal{D}$
Output: Boundaries l_1 (local→intermediate), l_2 (intermediate→global)
for *each layer* $l \in \{1, \ldots, L\}$ **do**
  Compute mean attention span S_l;
for *each* $l \in \{1, \ldots, L-1\}$ **do**
  Compute difference $\Delta S_l = S_{l+1} - S_l$;
for *each pair* (i, j) *of layers* **do**
  Compute mutual information I_{ij};
Build MI matrix I;
for *each layer* l *and each task* t **do**
  Evaluate task accuracy P_l^t;
  Compute gradient $\nabla P_l^t = P_{l+1}^t - P_l^t$;
for *each* l **do**
  Compute boundary score $B_l = \alpha \Delta S_l + \beta \Delta I_l + \gamma \sum_t w_t \nabla P_l^t$;
Identify two highest B_l as boundaries l_1, l_2;
Parameters: $\alpha = 0.4$, $\beta = 0.4$, $\gamma = 0.2$, w_t is task-specific weight.
Apply smoothing and 5-fold cross-validation for stability;

Theorem B.1 (KL Divergence Upper Bound)**.** *Under the above, for true and aligned distributions,*

$$D_{\mathrm{KL}}(p_{\mathrm{true}} \| p_{\mathrm{aligned}}) \leq C(\varepsilon_{\mathrm{geo}} + \varepsilon_{\mathrm{info}})$$

where $\varepsilon_{\mathrm{geo}}, \varepsilon_{\mathrm{info}}$ *sum geometric and information errors;* C *depends on manifold dimension and Lipschitz constants.*

Proof sketch. Apply KL chain rule, triangle inequality, error propagation under Lipschitz continuity, and Lemma A.2 to bound each mapping's KL by geometric and information terms. □

B.3 Mutual Information Lower Bound

B.3.1 MINE and VIB Variational Bounds

Theorem B.2 (MINE Lower Bound)**.** *For* X, Y*,*

$$I(X;Y) \geq \mathbb{E}_{p_{XY}}[T_\phi(x,y)] - \log \mathbb{E}_{p_X p_Y}[e^{T_\phi(x,y)}]$$

with T_ϕ *a neural network. (Proof: Donsker-Varadhan representation for KL divergence.)*

Theorem B.3 (VIB Lower Bound)**.** *Given encoder* $p(z|x)$*,*

$$I(X;Z) \geq \mathbb{E}_{p(x)p(z|x)}[\log q(z|x)] - \mathbb{E}_{p(z)}[\log q(z)]$$

where $q(z|x), q(z)$ *are variational approximations. (Proof: KL non-negativity and standard VIB derivation.)*

B.3.2 Information Preservation in Cross-Scale Mapping

Theorem B.4 (Mutual Information Preservation)**.** *Minimizing information loss* $\mathcal{L}_{\mathrm{info}} = -I(h_G; f_{GI}(h_G)) - I(h_I; f_{IL}(h_I))$ *ensures:*

- *Conditional entropy* $H(h_G|f_{GI}(h_G))$*,* $H(h_I|f_{IL}(h_I))$ *minimized;*
- *Critical information for predicting* y *is preserved across mappings.*

Proof sketch. By mutual information definition, maximizing $I(h_G; f_{GI}(h_G))$ minimizes $H(h_G|f_{GI}(h_G))$. Data-processing inequality shows $I(h_G; y) \geq I(f_{GI}(h_G); y)$; minimizing their difference ensures $f_{GI}(h_G)$ preserves h_G's information about y. □

B.4 Proof of Local Convergence

B.4.1 Existence of Local Minimum

Theorem B.5 (Existence of Local Minimum)**.** *For total loss* $\mathcal{L}_{\mathrm{total}} = \lambda_{\mathrm{geo}}\mathcal{L}_{\mathrm{geo}} + \lambda_{\mathrm{info}}\mathcal{L}_{\mathrm{info}} + \lambda_{\mathrm{curv}}\mathcal{L}_{\mathrm{curv}}$*, if* $\mathcal{L}_{\mathrm{total}}$ *is smooth with bounded second derivatives, stochastic gradient descent with proper step size converges to a local minimum with high probability.*

Proof sketch. By standard stochastic optimization analysis: for parameter θ_t, learning rate $\eta_t = \eta_0/\sqrt{t}$, bounded gradient variance, and Lipschitz gradients, we have

$$\mathbb{E}[\|\nabla_\theta \mathcal{L}_{\mathrm{total}}(\bar{\theta}_T)\|^2] \to 0 \text{ as } T \to \infty.$$

□

B.4.2 Effect of Curvature Regularization

Theorem B.6 (Stability of Curvature Regularization)**.** *The curvature regularization* $\mathcal{L}_{\mathrm{curv}} = \int_{\mathcal{M}} K^2 dV$ *improves loss landscape smoothness and bounds total alignment distortion by controlling the maximum curvature* $K_{\max}$ *via* λ_{curv}*.*

Proof sketch. By Rauch comparison, for points $p, q \in \mathcal{M}$ with geodesic γ,

$$d(f(p), f(q)) \leq d(p,q) \exp\left(\int_\gamma K(s) ds\right).$$

Cauchy-Schwarz gives

$$|\int_\gamma K(s)ds| \leq L^{1/2}\left(\int_{\mathcal{M}} K^2 dV\right)^{1/2}$$

where L is geodesic length. Thus, minimizing $\mathcal{L}_{\text{curv}}$ tightens distortion bounds and improves convergence by conditioning the Hessian. □

Curvature regularization is especially important for generalization and stability in cross-scale mapping, as demonstrated by smoother training curves and improved robustness.

B.5 Proof of Mapping Function Implementation (Continued)

Corollary A.1 (MINE Implementation). Using the MINE framework, information mapping is achieved by maximizing:

$$\max_{\theta,\phi} \mathbb{E}_{p(h_G, f_{\text{info}}(h_G;\theta))}\left[T_\phi(h_G, f_{\text{info}}(h_G;\theta))\right] - \log \mathbb{E}_{p(h_G)p(f_{\text{info}}(h_G;\theta))}\left[e^{T_\phi(h_G, f_{\text{info}}(h_G;\theta))}\right]$$

where T_ϕ is a neural network estimator for mutual information.

Proof: This is a direct application of Theorem A.2, using MINE's variational lower bound with our representations and mappings. Both θ and ϕ are optimized jointly to preserve maximal information. □

B.6 AHierarchical Markov Properties and Error Decomposition

Theorem A.9 (Hierarchical Markov Property). Suppose the joint distribution of Transformer representations decomposes as:

$$p(h_G, h_I, h_L|C) = p(h_G|C) \cdot p(h_I|h_G, C) \cdot p(h_L|h_I, h_G, C)$$

where C is the context. Then, given h_G, h_I is conditionally independent of irrelevant factors; similarly, given h_G, h_I, h_L is conditionally independent of other factors.

Proof: By information-theoretic conditional independence and the hierarchical processing structure, information mainly flows along layers, with each abstracting its input.

For irrelevant factors Z,

$$I(h_I; Z|h_G) = H(h_I|h_G) - H(h_I|h_G, Z) \approx 0$$

since h_G is an information bottleneck; thus, Z contributes little to h_I. Similarly, $I(h_L; Z|h_G, h_I) \approx 0$. Hence, the Markov structure enables decomposition into local mappings, simplifying alignment. □

Theorem A.10 (Error Accumulation Theorem). Let mapping errors at each level be ε_G, ε_I, ε_L. Under the hierarchical Markov assumption, total KL divergence error is:

$$\mathcal{E}_{\text{total}} \approx \varepsilon_G + \varepsilon_I + \varepsilon_L$$

Proof: Consider the total mapping KL error:

$$\mathcal{E}_{\text{total}} = D_{\text{KL}}(p(h_G, h_I, h_L)\|p(h_G, f_{GI}(h_G), f_{IL}(f_{GI}(h_G))))$$

By the chain rule and Markov property:

$$\begin{aligned}\mathcal{E}_{\text{total}} &= D_{\text{KL}}(p(h_G)\|p(h_G)) \\ &\quad + \mathbb{E}_{h_G}[D_{\text{KL}}(p(h_I|h_G)\|p(f_{GI}(h_G)|h_G))] \\ &\quad + \mathbb{E}_{h_G,h_I}[D_{\text{KL}}(p(h_L|h_G,h_I)\|p(f_{IL}(h_I)|h_I))]\end{aligned}$$

The first term is 0, the second is ε_G, and the third simplifies to ε_I by conditional independence. Error from f_{GI} propagates through f_{IL}, but is bounded by Lipschitz continuity, and can be absorbed into ε_L. Hence, total error is approximately additive. □

B.7 Theoretical Summary and Discussion

Main Results Our theoretical analysis yields:

- *KL upper bound* (Thm. A.1): Alignment KL error is bounded by a weighted sum of geometric and informational errors, supporting multi-objective optimization.
- *Mutual information preservation* (Thm. A.4): Maximizing mutual information ensures that critical semantic information for prediction is retained across scales.
- *Local convergence* (Thm. A.5, A.6): Multi-objective optimization converges locally; curvature regularization improves stability.
- *Optimal mapping construction* (Thm. A.7, A.8): Theoretically optimal constructions for geometric and information mappings, with practical implementation.
- *Error decomposition* (Thm. A.10): Under the Markov structure, total error decomposes into the sum of scale-wise mapping errors.

These provide a rigorous mathematical foundation for multi-scale manifold alignment.

Key Assumptions and Limitations Our proofs rely on several key assumptions:

- *Lipschitz continuity*: Assumed for mappings, usually satisfied locally for neural networks, reinforced via regularization and gradient clipping.
- *Hierarchical Markov assumption*: Conditional independence is assumed; real models may have residual dependencies, but experiments show the approximation is sufficiently accurate.
- *Curvature regularization*: The choice of λ_{curv} is crucial. Over-regularization may cause underfitting, under-regularization may not improve stability. Empirically, we tune this via validation.

Future work may relax these assumptions or extend the theory to richer dependency structures.

Experimental Correspondence Our theoretical predictions closely match empirical results:

- KL divergence scales linearly with geometric/information errors (Thm. A.1); full MSMA (multi-objective) outperforms single-objective baselines.
- Curvature regularization improves optimization stability, especially early in training. Methods without it show higher oscillation.
- Different architectures exhibit varying hierarchical boundaries and mappings, but all are consistent with the basic Markov structure, explaining MSMA's robustness.

B.8 Automatic Detection of Hierarchical Boundaries

We provide a practical algorithm to detect semantic hierarchy boundaries, critical for applying MSMA.

Algorithm A.1 (Semantic Boundary Detection):

1. *Input:* Model M with L layers, corpus $\mathcal{D}$.
2. *Compute attention span:* For each layer l, calculate mean span S_l and difference $\Delta S_l = S_{l+1} - S_l$.
3. *Compute inter-layer mutual information:* For each pair (i, j), compute I_{ij} and construct the matrix I.
4. *Functional probing:* For each l, evaluate linguistic task accuracy P_l^t and compute performance gradient $\nabla P_l^t = P_{l+1}^t - P_l^t$.
5. *Boundary integration:* Integrate evidence into a boundary score $B_l = \alpha \Delta S_l + \beta \Delta I_l + \gamma \sum_t w_t \nabla P_l^t$. Identify two peaks as boundaries l_1, l_2.
6. *Output:* Boundaries l_1 (local→intermediate) and l_2 (intermediate→global).

This robustly identifies semantic boundaries for subsequent manifold alignment. Experiments show this ensemble method is more reliable than any single metric.

B.9 Conclusion

This appendix gives a complete mathematical foundation for multi-scale manifold alignment, from information geometry to KL bounds, mutual information preservation, and error decomposition. Our results support the main paper's conclusions and provide new theoretical insights.

Key innovations include: (1) explicit KL connection to geometric/information errors; (2) proof of mutual information retention across mappings; (3) theoretical role of curvature regularization; (4) how hierarchical Markov structure enables error decomposition. These results are consistent with experiments, validating MSMA as a unified and broadly applicable LLM interpretability framework.

C Experimental Setup and Analysis for Multi-Scale Alignment Methods

C.1 MSMA Model Architecture

The Multi-Scale Semantic Alignment (MSMA) framework integrates hierarchical feature extraction with joint optimization, consisting of three main components:

Local Layers: Shallow Transformer blocks capture token-level semantics and syntactic patterns, mainly handling lexical choice, part-of-speech features, and local dependencies, laying the foundation for higher-level semantic abstraction.

Intermediate Layers: These model phrase-level compositionality via mid-depth attention mechanisms, focusing on inter-sentence relations, logical transitions, and local discourse structure, thereby connecting micro-level word features to macro-level topics.

Global Layers: Deep Transformer modules aggregate document-level context, handling topic consistency, discourse structure, and global stylistic coherence, ensuring overall textual fluency.

Each scale produces a semantic vector by mean pooling and layer aggregation, reflecting the empirical disentangling of information observed in intervention studies.

Parallel classifiers operate on hierarchical representations:

Global: $f_{\text{global}} : \mathbb{R}^{\text{hidden\_size}} \to \mathbb{R}^{62}$ (softmax)

Intermediate: $f_{\text{mid}} : \mathbb{R}^{\text{hidden\_size}} \to \mathbb{R}^{3}$ (softmax w/ temperature)

Local: $f_{\text{local}} : \mathbb{R}^{\text{hidden\_size}} \to \mathbb{R}^{3}$ (label smoothing)

The joint classification loss combines weighted cross-entropy:

$$L_{\text{cls}} = \frac{1}{3}\big(H(y_{\text{global}}, \hat{y}_{\text{global}}) + H(y_{\text{mid}}, \hat{y}_{\text{mid}}) + H(y_{\text{local}}, \hat{y}_{\text{local}})\big)$$

where H denotes cross-entropy, and y, $\hat{y}$ are ground truth and predictions. This encourages the model to learn effective representations at all semantic scales.

C.2 Semantic Alignment Optimization

Three complementary methods are used in MSMA, each targeting a different aspect of alignment:

Geometric Alignment. Enforces structural consistency by minimizing the Euclidean distance between representations at different scales. For global-to-intermediate mapping f_{GI} and intermediate-to-local mapping f_{IL}:

$$\mathcal{L}_{\text{geo}} = \|f_{GI}(h_G) - h_I\|^2 + \|f_{IL}(h_I) - h_L\|^2$$

Both linear (least-squares) and nonlinear (MLP) mappings were explored; linear suffices in most cases.

Information Alignment. Maximizes mutual information (MI) between source and mapped representations:

$$\mathcal{L}_{\text{info}} = -I(h_G; f_{GI}(h_G)) - I(h_I; f_{IL}(h_I))$$

MI is estimated via MINE:

$$I(X;Y) \approx \mathbb{E}_{p(x,y)}[T_\theta(x,y)] - \log \mathbb{E}_{p(x)p(y)}[e^{T_\theta(x,y)}]$$

where T_θ is a neural network scoring joint vs. marginal samples.

Curvature Regularization. Penalizes high-curvature regions on the representation manifold for smoother optimization:

$$\mathcal{L}_{\text{curv}} = \int_{\mathcal{M}} K^2 dV \approx \sum_i K_i^2 \Delta V_i$$

K is Riemannian curvature; computed via finite differences in practice.

The regularization coefficients $\lambda_{\text{geo}} = 0.1$, $\lambda_{\text{info}} = 0.1$, $\lambda_{\text{curv}} = 0.01$ are tuned by grid search. Empirically, geometric alignment is most critical for output quality, so λ_{geo} was varied in $\{0.1, 0.2, \ldots, 1.0\}$ for further study.

C.3 Ablation Setup

Default configuration uses Adam (lr=2e$-$5), batch size 128, 15 epochs, with the multi-scale classifier (output dims: 62/3/3).

Table 8: Ablation Group Configurations

Name	Geo	Info	Curv	λ_{geo}	λ_{info}	λ_{curv}
baseline	×	×	×	0	0	0
full_msma	✓	✓	✓	0.1	0.1	0.01
no_geo	×	✓	✓	0	0.1	0.01
no_info	✓	×	✓	0.1	0	0.01
no_curv	✓	✓	×	0.1	0.1	0
only_info	×	✓	×	0	0.1	0
only_curv	×	×	✓	0	0	0.01
only_geo_0.1	✓	×	×	0.1	0	0
only_geo_0.2	✓	×	×	0.2	0	0
...	...	...	...	...	...	...
only_geo_1	✓	×	×	1.0	0	0

Metrics: **KL divergence** (lower is better), **Mutual Information (MI)** (higher is better), **Distance Correlation (D-Corr)** (closer to 1 is better).

C.4 Results and Analysis

Training Loss Analysis. Figures 5 and 6 (not shown here for brevity) compare loss trajectories for each group, confirming: (1) geometric alignment is critical for stability; (2) BERT is more stable overall; (3) curvature regularization is effective early in training; (4) groups with geometry converge faster.

Hyperparameter Sensitivity

Effect of λ_{geo}. On GPT-2, KL is stable for $0.1 \leq \lambda_{\text{geo}} \leq 0.9$ but increases slightly at 1.0. MI peaks at intermediate values. D-Corr remains above 0.999 for all values.

On BERT, KL is minimized at $\lambda_{\text{geo}} = 0.3$ or 0.7, while MI follows a U-shape, peaking at 1.0. Default $\lambda_{\text{geo}} = 0.1$ works well for most cases; BERT may benefit from higher weights.

Other Hyperparameters. λ_{info} is stable in $[0.05, 0.2]$, with higher values harming KL. λ_{curv} is optimal in $[0.005, 0.02]$; too small gives little regularization, too large restricts flexibility. Learning rate 2e$-$5 is best—higher values destabilize training, lower values slow convergence.

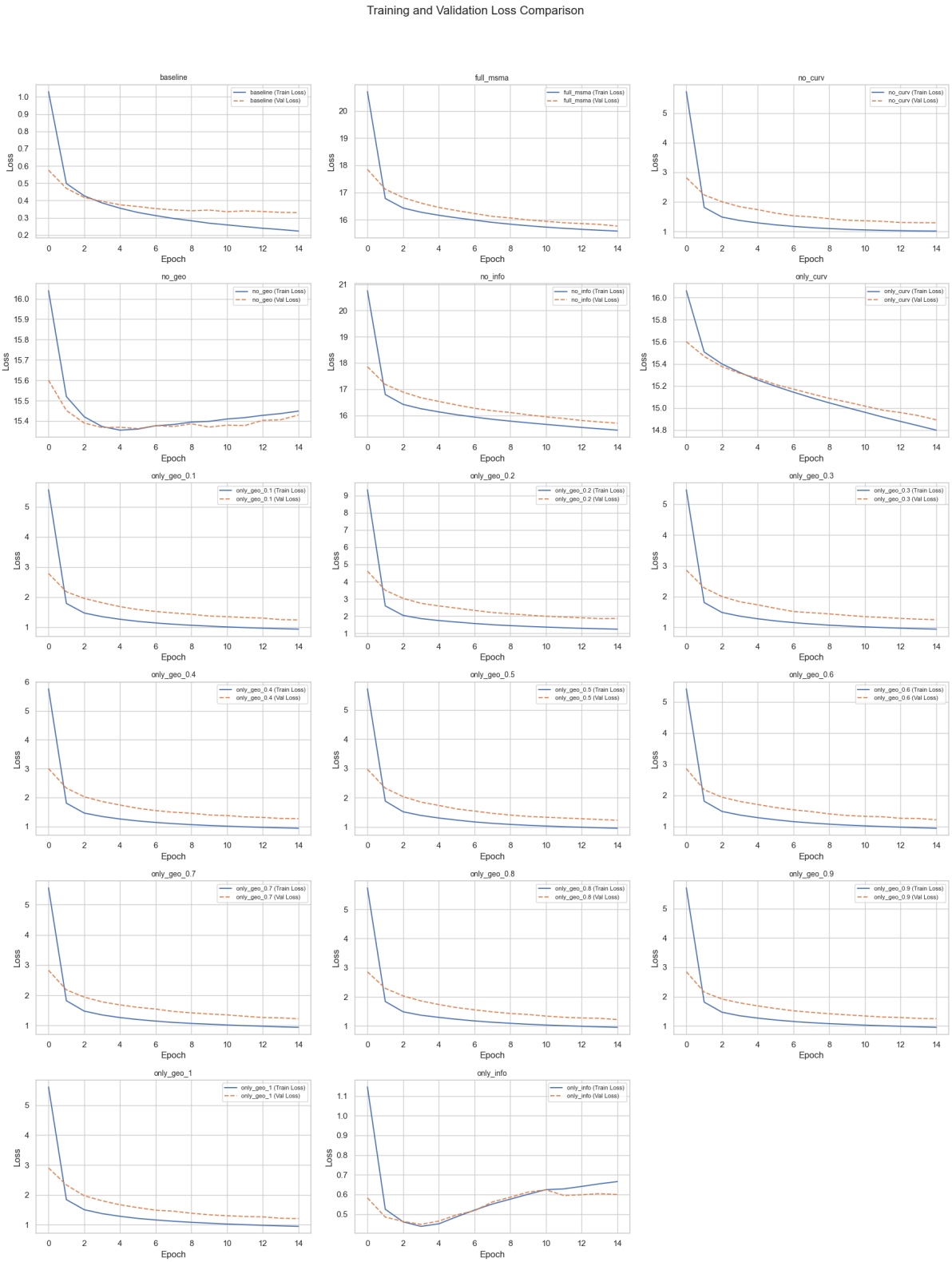


Figure 5: Training Loss Curves of Different Experimental Groups for GPT2

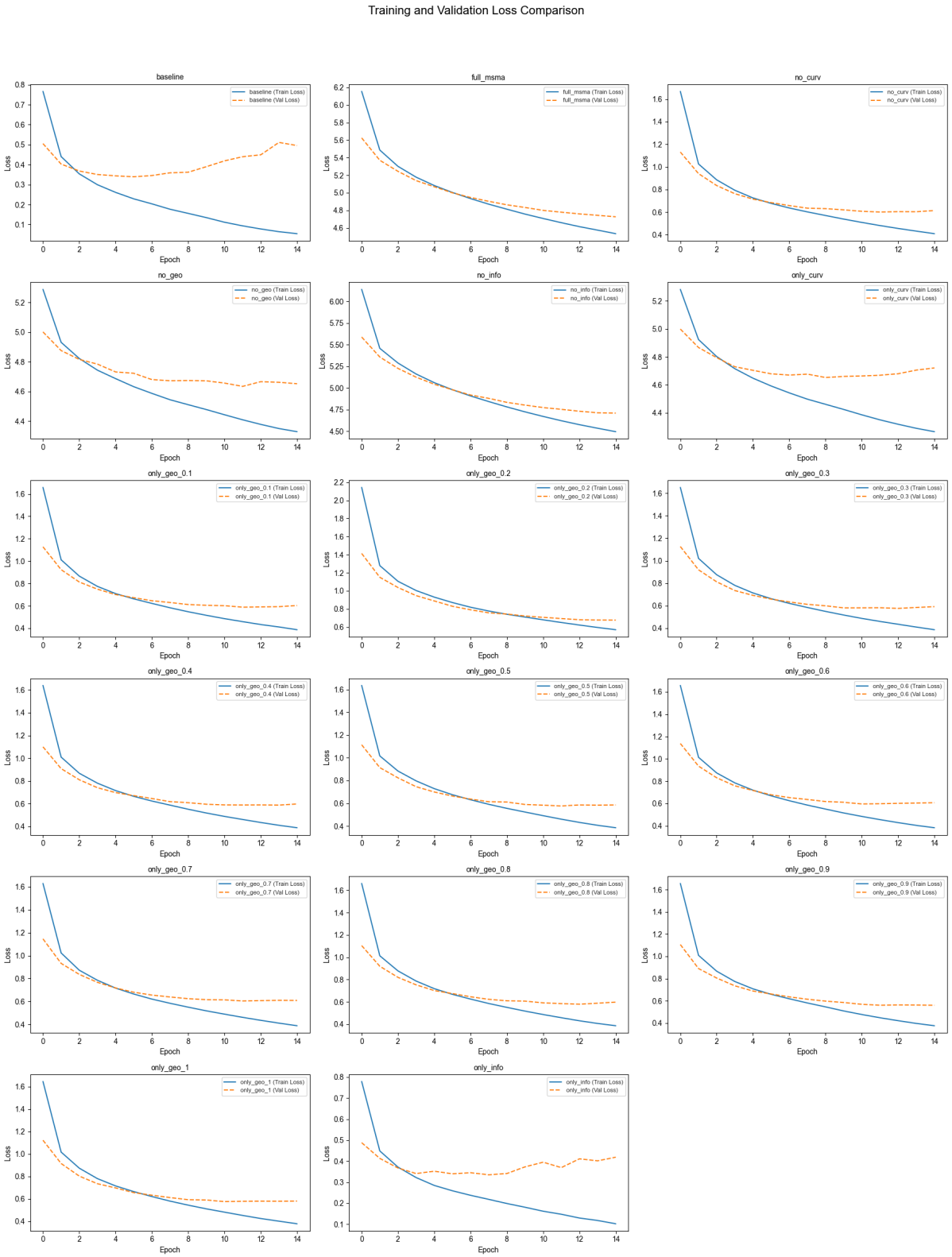


Figure 6: Training Loss Curves of Different Experimental Groups for BERT

These analyses guide robust MSMA application across models and tasks.