BEYOND SINGLE CONCEPT VECTOR: MODELING CONCEPT SUBSPACE IN LLMS WITH GAUSSIAN DISTRIBUTION

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ABSTRACT

Probing learned concepts in large language models (LLMs) is crucial for understanding how semantic knowledge is encoded internally. Training linear classifiers on probing tasks is a principle approach to denote the vector of a certain concept in the representation space. However, the single vector identified for a concept varies with both data and training, making it less robust and weakening its effectiveness in real-world applications. To address this challenge, we propose an approach to approximate the subspace representing a specific concept. Built on linear probing classifiers, we extend the concept vectors into Gaussian Concept Subspace (GCS). We demonstrate GCS's effectiveness through measuring its faithfulness and plausibility across multiple LLMs with different sizes and architectures. Additionally, we use representation intervention tasks to showcase its efficacy in real-world applications such as emotion steering. Experimental results indicate that GCS concept vectors have the potential to balance steering performance and maintaining the fluency in natural language generation tasks.

1 INTRODUCTION

Large language models (LLMs) such as GPT-4 (Achiam et al., 2023), LLaMA-3 (Touvron et al., 2023), and Claude-3 (Anthropic, March 4, 2024) have demonstrated remarkable capabilities across a wide range of natural language understanding and generation tasks (Brown et al., 2020; Wei et al., 2022). However, our understanding of how concepts are represented internally within these models remains limited. Current research in this area can be broadly categorized into two categories. The first involves studying model parameters through causal mediation analysis (Vig et al., 2020), which has found applications in downstream tasks such as knowledge editing (Meng et al., 2022; Wang et al., 2024) and circuit identification (Conmy et al., 2023; Elhage et al., 2021). The second focuses on investigating the representation space and activations of models (Zou et al., 2023; Turner et al., 2023; Jorgensen et al., 2023; Rimsky et al., 2023), where representation vectors in hidden spaces are often interpreted as linear vectors of certain concepts, such as color (Patel & Pavlick, 2022), world models (Nanda et al., 2023; Li et al., 2023), and sentiment (Tigges et al., 2023).

In this work, we focus on the representation vector-based explanation paradigm. Among methods to derive representation vectors, linear concept vectors are most widely used. They are typically obtained by training linear probing classifiers, such as logistic regression, on probing datasets comprising positive and negative samples (Ousidhoum et al., 2021; Alain & Bengio, 2016). This approach has proven effective in identifying semantic knowledge encoded within LLMs and has recently been extensively applied in inference-time interventions to mitigate undesirable model behaviors (Li et al., 2024; Lee et al., 2024; Rimsky et al., 2023; Turner et al., 2023). However, concept vectors derived from this approach can vary significantly depending on the probing dataset used to train the classifier and the training process, making it challenging to obtain robust vectors. This substantial variation not only poses challenges in studying concept relations within the representation space but also negatively impacts effectiveness of concept vector's usage in intervention tasks.

To address these limitations, we explore the following research question: *Instead of using a single vector to describe each underlying concept captured by LLMs, can we use a distribution to more robustly describe that learned concept?* This is motivated by the observation that the representation of a concept may be multifaceted, potentially constituting a multidimensional subspace in the representation space. Building upon this assumption, our work focuses on approximating a subspace that better captures the semantics of specific concepts while providing vectors representing a certain concept with varying relevance.

Based on this motivation, we propose Gaussian Concept Subspace (GCS), which improves upon linear probing classifiers described by Ousidhoum et al. (2021); Kim et al. (2018); Alain & Bengio (2016) by using a Gaussian distribution to estimate the potential directional subspace of a concept. The main idea is to learn a set of vectors termed *observed vectors* instead of an individual vector for each concept. These observed vectors are then used to estimate the Gaussian distribution of the concept subspace. The vectors within this Gaussian distribution represent varying degrees of relevance to the concept, with vectors closer to the mean considered more closely related, termed *sampled vectors*. This method offers a more nuanced representation of concepts, capturing their multifaceted nature within a multidimensional subspace rather than reducing them to a single vector.

We conduct experiments to evaluate the effectiveness of GCS from two perspectives: 1) Whether concept vectors sampled from GCS effectively describe a given concept learned by LLMs; and 2) Whether concept vectors derived from GCS are useful in downstream interventions to guide LLMs to generate more desirable outputs. For the first perspective, we evaluate sampled vectors using two categories of metrics: faithfulness and plausibility. For faithfulness, we examine similarities within observed vectors, sampled vectors, and between both sets to demonstrate their relatedness in the representation space. For plausibility, we investigate whether the explanations align with our understanding of inter-concept relations. For the second perspective, we compare the performance of sampled vectors on inference-time intervention tasks with that of vectors derived with mean difference and single training classifier. Specifically, we applied these vectors to steer models towards generating more joyful movie reviews. Our results demonstrate that sampled vectors from GCS are both faithful and plausible in terms of their explanations. Moreover, they outperform vectors from other methods in manipulating models to generate desirable content while maintaining text fluency.

2 PRELIMINARY

Hidden Representation. We focus on decoder-only LLMs (GPT-like models) (Ferrando et al., 2024), where each layer comprises multi-head attention blocks (MHA) and feed-forward networks (FFNs/MLPs). In this study, we utilize frozen pretrained language models. We index layers as $\ell \in L$, where L denotes the set of all model layers. Each layer begins and ends with a residual stream. The MHA first processes the residual stream and adds its output back to it. The updated vector is then passed through MLPs to generate the layer's output:

$$\boldsymbol{h}_i^{\ell+1} = \boldsymbol{h}_i^{\ell} + \mathrm{Att}^{\ell}\left(\boldsymbol{h}_i^{\ell}\right) + \mathrm{MLP}^{\ell}\left(\boldsymbol{h}_i^{\ell} + \mathrm{Att}^{\ell}\left(\boldsymbol{h}_i^{\ell}\right)\right), \tag{1}$$

where $\boldsymbol{h}_i^{\ell}$ represents the i-th token in the input token sequence at layer ℓ. We concentrate on the output representation space of each layer, specifically the residual stream at the layer's end. Following Zou et al. (2023), we use the last token's representation to represent the entire input sequence, denoted as $\boldsymbol{h}^{\ell}$, as it is generally believed to integrate information from all preceding tokens.

Linear Probing. We adopt the linear concept probing approach to derive concept activation vectors (Kim et al., 2018). Following prior work (Li et al., 2024), for each concept c, given a probing dataset $\mathcal{D}_c = \{(\boldsymbol{h}_i, y_i) \mid i = 1, \cdots, N\}$ where $\boldsymbol{h} \in \mathbb{P} \cup \mathbb{N}$, $\mathbb{P}$ is the set of concept-related positive samples, $\mathbb{N}$ is the set of concept-irrelevant negative samples, and $y_i \in \{0, 1\}$ indicates the sample class. These datasets generate layerwise hidden representations for downstream classifier training. We employ a logistic regression (LR) classifier as: $\boldsymbol{\sigma}(\boldsymbol{h}_c^{\ell}) = \frac{1}{1+\exp(-\boldsymbol{h}_c^{\ell} \cdot \boldsymbol{w}_c^{\ell})}$, where $\boldsymbol{h}_c^{\ell} \in \mathbb{R}^{N \times d}$ specifies sample representations from a probing dataset at ℓ-th layer, and d is the representation dimension. The normalized coefficients $\boldsymbol{w}_c^{\ell}$ of each binary linear classifier are considered the concept vector. The loss function for logistic regression with L2 regularization is expressed as follows:

$$\hat{\boldsymbol{w}}_c^{\ell} = \underset{\boldsymbol{w}_c^{\ell}}{\mathrm{argmin}} -\frac{1}{n}\sum_{i=1}^{n} y_i \log \boldsymbol{\sigma}(\boldsymbol{h}_i^{\ell}) + (1 - y_i) \log\left(1 - \boldsymbol{\sigma}(\boldsymbol{h}_i^{\ell})\right) + \frac{\lambda}{2}|\boldsymbol{w}_c^{\ell}|_2^2, \tag{2}$$

where hyperparameter λ controls the strength of regularization. However, the derived concept vector $\hat{\boldsymbol{w}}_c^\ell$ can vary substantially depending on the probing dataset $\mathcal{D}_c$ used to train the classifier $\boldsymbol{\sigma}(\boldsymbol{h}_c^\ell)$ and the specific training process. This variability makes it challenging to obtain robust and consistent vectors. Such instability not only complicates the study of concept relations within the representation space but also negatively impacts the effectiveness of intervention tasks that rely on these vectors.

3 METHODOLOGY

To address the above-mentioned limitations, we investigate whether representing concepts learned by LLMs as distributions, rather than single vectors. We aim to approximate a subspace that better captures the semantics of specific concepts while providing vectors representing the concept with varying relevance. Building upon the linear probing approach described in Section 2, we introduce the Gaussian Concept Subspace (GCS) framework for estimating a multidimensional subspace of vectors for each concept. While linear probing identifies a single vector for a concept, GCS aims to capture a more comprehensive representation by estimating a Gaussian distribution of vectors.

3.1 THE PROPOSED GCS FRAMEWORK

To estimate the Gaussian distribution of concept vectors, we extend the linear probing method by deriving M independent concept vectors for a concept c. We first create a large dataset for a concept c and then randomly sample subsets of examples from this dataset to create M smaller probing datasets. Each probing dataset contributes to the same concept vector c, analogous to the single vector derived in Equation 2. For a model with target layer ℓ, we obtain a concept vector $\boldsymbol{w}_{c,\,m}^\ell$ for the m-th probing dataset at the ℓ-th layer. Please refer to Section 4.1.3 for more details of GCS framework. This process generates a set of vectors for concept c:

$$\boldsymbol{W}_c^\ell = \{\boldsymbol{w}_{c,\,m}^\ell |\, m = 1, \cdots, M\}. \tag{3}$$

We use this set to estimate the concept subspace, represented as a Gaussian distribution of concept c at the ℓ-th layer. The distribution is d-dimensional, where d is the dimension of the hidden representations, and is denoted as:

$$\boldsymbol{W}_c^\ell \sim \mathcal{N}_d(\boldsymbol{\mu}_c^\ell, \boldsymbol{\Sigma}_c^\ell). \tag{4}$$

To simplify the model, we assume independence between dimensions in the representation space. This assumption results in a diagonal covariance matrix, where diagonal elements represent the variance of each dimension:

$$\boldsymbol{\mu}_c^\ell = \frac{1}{M}\sum w_{c,\,m}^\ell; \quad \boldsymbol{\Sigma}_c^\ell = \text{diag}(\sigma_1^2, \cdots, \sigma_d^2) \tag{5}$$

The mean vector $\boldsymbol{\mu}_c^\ell$ is calculated by averaging the corresponding dimensions of the M observed concept vectors, which are essentially the weight vectors from the trained binary classifiers in the linear probing approach. This multivariate distribution describes a subspace around the observed concept vectors, extending the single-vector representation of linear probing to a multidimensional subspace. Concept vectors within this distribution can be sampled at various standard deviations (e.g., 1σ, 2σ, ..., $n\sigma$) from the mean vector. For our evaluations, we randomly sample vectors $\boldsymbol{V}_c^\ell$ (the set of multiple sampled vectors $\boldsymbol{v}_c^\ell$) within 1σ of the mean to represent the concept.

The overall steps of the GCS framework are summarized in Algorithm 1. By moving from a single vector to the Gaussian distribution of vectors, GCS aims to capture a more robust representation of concepts in the language model's hidden space, potentially offering improvements over the linear probing approach in both interpretability and downstream applications.

Algorithm 1: Proposed GCS Framework

Input: LLM to be explained, concept c, layer ℓ, probing dataset number M.
while *first stage* **do**
  Generate M probing datasets for concept c;
  for $m = 1$ **to** M **do**
    Train classifier on dataset m for c;
    Extract weight vector $\boldsymbol{w}_{c,m}^\ell$;
  end
  $\boldsymbol{W}_c^\ell = \{\boldsymbol{w}_{c,m}^\ell | m = 1, \ldots, M\}$;
end
while *second stage* **do**
  $\boldsymbol{\mu}_c^\ell = \frac{1}{M}\sum \boldsymbol{w}_{c,m}^\ell$;
  $\boldsymbol{\Sigma}_c^\ell = \text{diag}(\sigma_1^2, \ldots, \sigma_d^2)$;
end
while *third stage* **do**
  Sample vector $\boldsymbol{v}_c^\ell \sim \mathcal{N}_d(\boldsymbol{\mu}_c^\ell, \boldsymbol{\Sigma}_c^\ell)$ in 1σ;
end
Output: Sampled concept vectors $\boldsymbol{v}_c^\ell$.

3.2 EVALUATION OF GCS

We use faithfulness and plausibility two metrics to eveluate performance of GCS, which are two crucial dimensions for evaluating the performance of an interpretability approach (Zhao et al., 2024).

3.2.1 FAITHFULNESS

To assess faithfulness, we compare the performance of sampled vectors $\boldsymbol{V}_c^\ell$ (stage 3 of Algorithm 1) compared to that of observed vectors $\boldsymbol{W}_c^\ell$ (stage 1 of Algorithm 1). Specifically, we employ two metrics: 1) similarity among observed vectors, sampled vectors and between the two sets; 2) accuracy of classifiers based on observed vectors and sampled vectors on our constructed datasets.

Similarity We evaluate the similarity between vectors within the observed concept vectors $\boldsymbol{W}_c^\ell$ and within the sampled concept vectors $\boldsymbol{V}_c^\ell$ using Equation 6. Additionally, we assess the similarity between vectors from the observed set and the sampled set using Equation 7.

$$S^\ell_{\text{observed}} = 1/N * \sum_{i,j} \text{sim}\left(\boldsymbol{w}_i, \boldsymbol{w}_j\right),\ \boldsymbol{w}_i, \boldsymbol{w}_j \in \boldsymbol{W}_c^\ell;\ S^\ell_{\text{sampled}} = 1/N * \sum_{i,j} \text{sim}\left(\boldsymbol{v}_i, \boldsymbol{v}_j\right)\ \boldsymbol{v}_i, \boldsymbol{v}_j \in \boldsymbol{V}_c^\ell \quad (6)$$

$$S^\ell_{\text{O-S}} = 1/N * \sum_{i,j} \text{sim}\left(\boldsymbol{w}_i, \boldsymbol{v}_j\right),\ \boldsymbol{w}_i \in \boldsymbol{W}_c^\ell,\ \boldsymbol{v}_j \in \boldsymbol{V}_c^\ell \quad (7)$$

The average similarity score of observed vectors S^ℓ_{observed} and sampled vectors S^ℓ_{sampled} describes how similar the linear vectors are for a specific concept. If our sampled vectors accurately represent concept vectors, the similarity score of sampled vectors should be comparable to that of observed concept vectors. Moreover, the similarity between observed and sampled vectors, denoted as $S^\ell_{\text{O-S}}$, should also be approximately equal to the within-set similarities.

Accuracy The observed concept vectors are derived from the weights of linear concept classifiers. To generate M linear concept vectors for a concept c, we randomly sample M probing datasets $\{\mathcal{D}_1, \cdots, \mathcal{D}_M\}$ from a large dataset $\mathcal{D}$. For each probing dataset $\mathcal{D}_i$, a linear classifier is trained using hidden representations from the ℓ-th layer of a LLM. The weight vector of this classifier is identified as a concept vector for concept c at layer ℓ. The average accuracy score of concept vectors for concept c at the ℓ-th layer is defined as:

$$A^\ell_O = \frac{\sum_{i=1}^M \text{acc}\left(\boldsymbol{w}_i, \mathcal{D}_{test}\right)}{M},\ \text{where } \mathcal{D}_{test} = \mathcal{D}/\mathcal{D}_i; A^\ell_S = \frac{\sum_{j=1}^M \text{acc}\left(\boldsymbol{v}_j, \mathcal{D}_{test}\right)}{M},\ \text{where } \mathcal{D}_{test} = \mathcal{D} \quad (8)$$

The average accuracy score captures how effectively concept vectors represent the concept. A^ℓ_O and A^ℓ_S denote average accuracy score for observed vectors and sampled vectors respectively. A higher average accuracy score for observed concept vectors suggests that classifiers have learned more generalizable concept vectors. Sampled concept vectors should achieve comparable or even higher accuracy scores if they genuinely represent related concept.

3.2.2 PLAUSIBILITY

Plausibility describes how well explanations align with human expectations. We measure the plausibility of GCS by studying whether models learn real-world hierarchies of concepts. To achieve this, we predefine a set of hierarchical concepts. We use average cosine similarity among concept vectors and principle component analysis (PCA) to demonstrate the consistence of GCS's plausibility.

Average Cosine Similarity To measure the similarity between two concepts c_i and c_j at the ℓ-th layer, we utilized their respective sampled concept vectors $\boldsymbol{V}^\ell_{c_i}$ and $\boldsymbol{V}^\ell_{c_j}$. The concept similarity is represented by the average cosine similarity between two concept vector sets. The average cosine similarity between these two concepts at the ℓ-th layer is computed as follows:

$$S^\ell_{c_i,c_j} = \frac{\sum_{m=1}^M \sum_{n=1}^M \text{sim}\left(\boldsymbol{v}_m, \boldsymbol{v}_n\right)}{M \times M/2}, \boldsymbol{v}_m \in \boldsymbol{V}^\ell_{c_i}, \boldsymbol{v}_n \in \boldsymbol{V}^\ell_{c_j}. \quad (9)$$

PCA visualization PCA aims to linearly reduce high-dimensional data onto lower dimensions. It excels in providing an intuitive understanding of relations between data points (Marks & Tegmark, 2023). We adopt PCA to visualize the relationship among predefined concepts. Since each concept has thousands vectors, we use the mean vector of sampled concept vectors to represent the concept.

4 EXPERIMENTS

In this section, we present experimental results that measure the performance of GCS and address the following three research questions (**RQs**):

- **RQ1:** How faithfully do GCS-sampled concept vectors represent the original concepts?
- **RQ2:** To what extent do explanations derived from GCS-sampled concept vectors align with human expectations about the hierarchies among model's learned knowledge?
- **RQ3:** Can the proposed GCS method effectively mitigate unwanted behaviors in LLMs?

4.1 EXPERIMENTAL SETUP

4.1.1 DATASETS

We define a hierarchical concept structure comprising two levels, encompassing concepts from high-level to low-level. The high-level concepts include four categories: `movie`, `sports event`, `populated place`, and `animal`. Under each high-level concept category, there are 4 low-level concepts, as illustrated in Figure 1. To ensure consistency and high quality of input data across all experiments, we generate our experimental datasets using the OpenAI API, specifically leveraging GPT-4o model. For each low-level concept, we prompt GPT-4o to produce 5,000 positive samples and 5,000 negative samples. The specific prompts used for generating these samples are detailed in Appendix J. Our prompt design strategy varies based on the concept's specificity. For more inclusive concepts such as "`Town`", we utilize detailed prompt descriptions to guide GPT-4o in generating concept-related data. Conversely, for more specific concepts like "`Motor race`", simpler and more generic prompt descriptions are sufficient to produce appropriate samples.

Figure 1: Hierarchical concepts.

4.1.2 MODELS

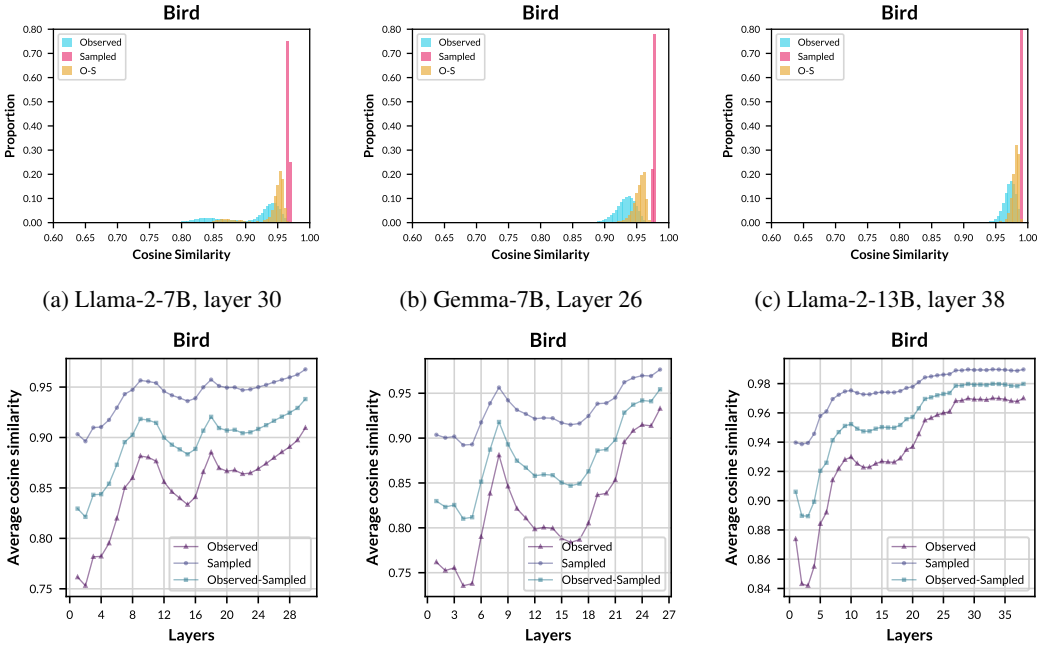
We study concept vectors across multiple LLMs, including Llama-2-7B chat model (Meta AI, 2023b), Gemma-7B (Google, 2024), and Llama-2-13B chat model (Meta AI, 2023a). This selection of models enables a comparative analysis of GCS across varying model architectures and sizes. By examining GCS's performance across these diverse models, we aim to provide insights into the method's generalizability and effectiveness across different LLM implementations.

4.1.3 IMPLEMENTATION DETAILS

Evaluating GCS at the distribution level presents significant challenges. Gaussian distribution encompasses vectors representing concepts with varying degrees of relevance, potentially diminishing as the sampling distance from the mean increases. This variability, coupled with the infinite potential of sampled concept vectors, renders precise distribution-level evaluation impractical. To address these limitations, we simplify our assessment by randomly sampling 1,000 concept vectors within 1σ of the mean, which we consider representative of the concept.

The GCS pipeline comprises several key steps: generating data points using GPT-4o, extracting hidden representations of each sample from LLMs, training linear classifiers for each concept using these hidden representations, and constructing Gaussians distribution for concept vectors. Our study generated 10,000 descriptions per low-level concept (5,000 positive and 5,000 negative). To efficiently utilize this data, we repeatedly sample 1,000 positive and 1,000 negative descriptions with replacement to create smaller, concept-specific probing datasets, each yielding an observed concept vector. This process is repeated 1,000 times for each low-level concept, resulting in 1,000 observed vectors per concept.

These observed vectors are used to derive the mean and covariance of the Gaussian distribution for each concept. To simplify computation, we assume independence between vector dimensions, re-



(a) Llama-2-7B, layer 30 (b) Gemma-7B, Layer 26 (c) Llama-2-13B, layer 38

(d) Llama-2-7B (e) Gemma-7B (f) Llama-2-13B

Figure 2: Histogram of cosine similarity within observed concept vectors, sampled concept vectors, and between both sets for concept "`Bird`" (a-c). Layer-wise average cosine similarity from the second layer to the penultimate layer of observed concept vectors, sampled concept vectors, and between both sets for concept "`Bird`" (d-f).

ducing the covariance matrix to a diagonal matrix where each diagonal value represents the variance of the concept vector in that dimension.

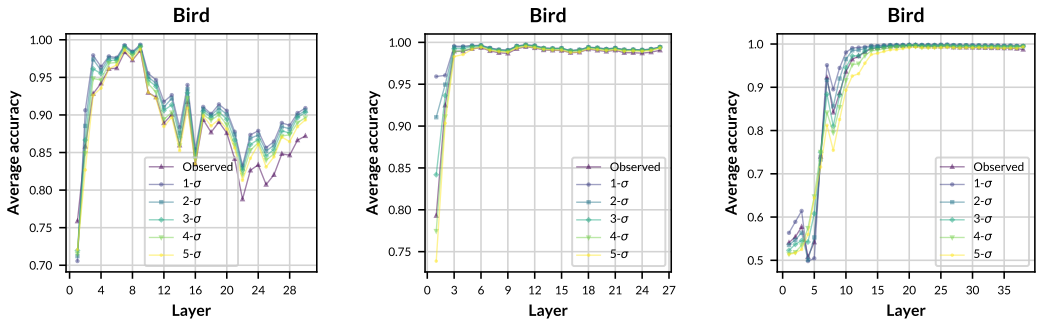
Notably, our classifiers are trained on hidden representations of each description. Following Zou et al. (2023), we use the hidden representation of the last token within a description from a specific layer as the representation for that description at that layer. We use L2 regularization when training the logistic regression classifier and the regularization weight λ in Equation 2 is set as 1.0. Our evaluation primarily focuses on hidden representations from the penultimate layer of each model, as we observed improved concept learning in deeper layers (see Appendix E, F, and G).

4.2 Faithfulness of GCS (**RQ1**)

We evaluate the faithfulness of GCS from two perspectives: *similarity* and *accuracy*. Similarity assessment involves comparing observed concept vectors with those sampled from the GCS. This comparison provides an effective measure of their relatedness in the representation space. Ideally, for any given concept, the sampled vectors should closely approximate the observed vectors. We also assess the accuracy of these vectors in concept-related tasks.

4.2.1 Cosine Similarity among Concept Vectors

For each concept, we analyze three types of cosine similarity: among observed concept vectors, among sampled concept vectors, and between these two sets, as defined in Equation 6 and 7. The cosine similarities among observed concept vectors indicate the potential size of the concept subspace, with higher similarities suggesting a more compact subspace. The cosine similarities among sampled concept vectors reflect their diversity. Vectors sampled within 1σ are generally less diverse but closer to the center of the conceptual space. In this section, we focus on sampling concept vectors within the 1σ range, which are central to the concept subspace. The similarity results are shown in Figure 2, the key findings are summarized as follows.



(a) Llama-2-7B (b) Gemma-7B (c) Llama-2-13B

Figure 3: Accuracy of observed and sampled concept vectors aross varying models.

First, we investigate these three types of similarities across LLMs of varying sizes and structures, as shown in Figure 2 (a, b, and c) and Appendix E. Our results indicate that similarities among observed concept vectors exhibit greater variation than those among sampled concept vectors, ranging from approximately 0.8 to 0.9. Sampled concept vectors within the 1σ range consistently demonstrate very high cosine similarities among themselves, with cosine similarity larger than 0.93. This indicates that GCS produces more consistently related vectors than the original observations. Cosine similarities between observed and sampled concept vectors typically range from 0.88 to 0.93. Besides, the patterns of cosine similarity are remarkably consistent across different model sizes and architectures (Llama-2-7B, Gemma-7B, and Llama-2-13B). This suggests that the GCS method is robust across different language models.

Second, to better observe changes in concept vectors within each concept, we also examine the average cosine similarity of these concept vectors at the layer level as shown in Figure 2 (d, e and f) and Appendix F. There is a general upward trend in cosine similarity as we move through the layers. This indicates that concept representations become more refined and consistent in deeper layers of the models. The sampled vectors (blue lines in d, e, f) show the highest and most stable cosine similarity across layers. This indicates that the sampling vectors from GCS produce consistently related vectors throughout the model.

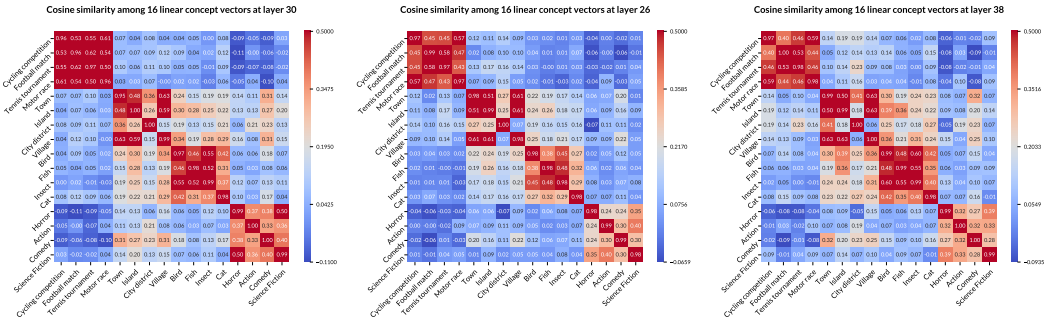
4.2.2 Prediction Accuracy of Concept Vectors

Despite the similarity between sampled and observed concept vectors in the representation space, it is crucial to verify that sampled vectors are as effective as observed concept vectors. We begin by measuring the accuracy of each observed linear vector on its test dataset, which comprises 8,000 additional concept descriptions. Then, we evaluate sampled concept vectors on the entire dataset of 10,000 samples, as these vectors are not trained on the dataset. The results are reported in Figure 3.

To evaluate the impact of proximity to the concept subspace center, we evaluate sampled concept vectors for all concepts at 1σ, 2σ, 3σ, 4σ, and 5σ across three LLM models. Our results demonstrate that sampled concept vectors usually achieve comparable and even better prediction accuracy compared to observed vectors, as illustrated in Figure 3. This improved performance is particularly evident for sampled concept vectors at 1σ and 2σ. These findings are further corroborated by the accuracy of these vectors across all predefined concepts in the Gemma-7B model (Appendix G). Our analysis yields two key insights. First, it validates the effectiveness of sampled concept vectors in representing concepts. Second, it also suggests that vectors closer to the subspace center could be more representative of the concept.

4.3 Plausibility of GCS (**RQ2**)

In this section, we evaluate the plausibility of GCS using two methods: average cosine similarity among concepts and PCA visualization (see Section 3.2.2). Here, we utilize concept vectors sampled at 1σ to compute the average cosine similarity between concepts and to generate the PCA visualization. We assess the coherence of concept relationships in the high-dimensional space (through cosine similarities) and in a lower-dimensional projection (through PCA visualization).



(a) Llama-2-7B, layer 30 (b) Gemma-7B, layer 26 (c) Llama-2-13B, layer 38

Figure 4: Heatmap of concept average cosine similarity of 16 concepts across Llama-2-7B, Gemma-7B, and Llama-2-13B. The 16 low-level concepts are grouped into four high-level categories: the first 4 rows/columns represent *sports events*, the next 4 represent *populated places*, followed by 4 for *animals*, and the last 4 for *movie genres*.

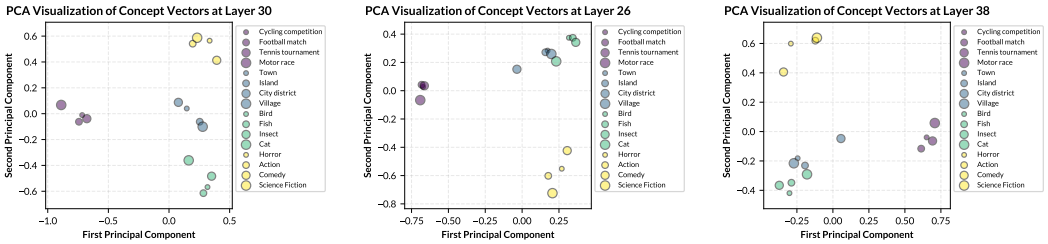
4.3.1 Average Cosine Similarity among Concepts

We evaluate concept similarity using average cosine similarity. Instead of measuring the entire distribution, we assess 1,000 concept vectors sampled within 1σ for each concept. The cosine similarity is computed for all vector pairs between two concepts, with the mean value representing the overall similarity between these concepts. Figure 4 illustrates these results across various LLMs.

The analysis of concept cosine similarities across three different language models reveals several key insights. First, low-level concepts within the same high-level category typically exhibit higher similarity scores. All three models (Llama-2-7B, Gemma-7B, and Llama-2-13B) show similar overall patterns, with distinct 4×4 blocks along the diagonal representing high intra-category similarities. These intra-category similarities are generally higher compared to similarities with low-level concepts from other high-level categories. Second, while all high-level categories show internal coherence, some categories appear more tightly related than others. For example, the "sports events" category (top-left 4×4 block) consistently shows very high internal similarity across all models, suggesting these concepts are closely related in the models' representations. Third, beyond intra-category similarities, there are interesting inter-category relationships. Notably, Llama-2-7B and 13B models demonstrate stronger correlations between `place` and `animal`. For instance, `island` shows a stronger correlation with `Bird` and `Fish` than `insect` and `cat`. `Bird` exhibits a stronger correlation with `village` than `fish` and `cat` do. These correlations align with human intuition about real-world relationships between these concepts. Such alignment suggests that the models have captured meaningful semantic relationships that reflect our understanding of the world. These findings also demonstrate the effectiveness of GCS in capturing complex and interpretable concept relationships across different language models.

4.3.2 PCA Visualization

PCA visualization offers an intuitive method to reveal concept proximity by linearly reducing concept vectors into a two-dimensional space. We visualize all 16 concepts to explore their relationships in terms of sampled concept vectors. Figure 5 illustrates the results across various LLMs at the penultimate layer. Across all three models, we observe several patterns. First, in all three visualizations, concepts belonging to the same high-level category tend to cluster together, confirming our initial observation. This clustering is particularly evident for `sports events` and `movie genres`. Second, the PCA visualizations for Llama-2-7B, Gemma-7B, and Llama-2-13B show remarkably similar patterns, reinforcing the robustness of the GCS method across different model architectures and sizes. Third, for cross-category relationship, concepts belonging to `place` and `animal` categories demonstrate closer proximity compared to other concept pairs, aligning with our findings in Section 4.3.1. The consistency of these patterns across models and their interpretable clustering strongly support the plausibility of GCS as an effective method for model interpretation.



(a) Llama-2-7B, layer 30 (b) Gemma-7B, layer 26 (c) Llama-2-13B, layer 38

Figure 5: PCA visualization of 16 concepts across Llama-2-7B, Gemma-7B, and Llama-2-13B. Low-level concepts belonging to the same high-level concept category share the same color.

4.4 Applications of GCS on Inference-time Intervention (**RQ3**)

Recently, concept vectors has been extensively used to steer model outputs towards desirable behaviors during inference time. This approach is considered as more efficient than finetuning, without needing modify the model's parameters. These steering vectors are generally derived using various approaches, all based on pairs of desired and undesired data samples. Following Konen et al. (2024), we evaluate GCS on open-ended generation tasks, which are more flexible and challenging tasks for intervention compared to natural language understanding tasks such as multiple-choice questions. Specifically, we aim to steer Llama-2-7B chat model to generate more joyful movie reviews, a task we refer to as emotion steering. To measure the performance of GCS, we compare vectors derived from GCS with two conventional methods: mean difference and linear vector as defined in Appendix C. Moreover, we utilize vectors within $n\sigma, n \in \{1, 2, 3, 4, 5\}$ from GCS to explore the relation between steering performance and concept vector relevance. To simplify the experiment setting, we applied the average vector of sampled vectors within each range to steer models.

We follow the experimental settings described in Section 4.1.3. We use GPT-4o to generate "joyful" and "angry" movie reviews, then derive concept vectors for the *joyful* concept. Throughout our experiments, we utilize the representation of the last token as the input for downstream computation. The process involves tasking models to generate angry movie reviews using prompts detailed in Appendix I. We then apply concept vectors to the representation of the last token across all layers, excluding the first and the last, to shift the model's outputs. We attempt to incrementally adjust the strength of steering vectors to measure its influence on outputs as detailed in Appendix D. The generated sentences are rated with GPT-4o from two aspects: joyfulness and coherence. Joyfulness assesses how joyful the generated text become after steering, while coherence measures the fluency of generated text through repetitive or chaotic elements. The result is shown in Table 1.

It is crucial to maintain a balance between steering models to produce desired expressions and preserving the fluency of those expressions. For example, before intervention, Llama-2-7B chat model generates angry review: *Awful, predictable, and cringeworthy.* Our GCS 1σ sampled vector based intervention can push it to generate joyful review: *Creative writing, beautiful acting, fun movie.* Examples of best performance for each method are detailed in Appendix I.3. The results in Table 1 show that mean difference is less effective in steering, and more likely to generate less fluent text. Additionally, the vectors sampled within 2σ, 3σ, 4σ, and 5σ of GCS are generally less effective in generating joyful content compared to 1σ sampled vectors and one linear vector. Although one linear vector can reach comparable effect as 1σ, its robustness is not as good as vectors sampled within 1σ from GCS. It's worth noting that one linear vector is trained on all data samples used to derive the set of concept vectors. As a result, it is possible that the one linear vector falls around the 1σ area, which makes it achieve the similar steering effect but lack of robustness. Consequently, GCS provides better-represented and more robust concept vectors. It also offers more options to choose vectors within varying relevance to the center of the subspace.

5 Related Work

Concept Vector. The concept vector represents a linear vector of a concept and is typically constructed using datasets containing both positive and negative samples. A range of methods have

Table 1: Evaluation of generated text after adding steering vectors. Strength corresponds to a in Equation 11 in Appendix D. A higher joyfulness score indicates a better steering effect. Coherence measures the repetitiveness and chaos in the generated sentences, with lower values being preferable.

Steering Method		Strength								
		0.038	0.043	0.048	0.053	0.059	0.064	0.069	0.074	0.080
Mean Difference	Joyfulness (Avg) ↑	1.020	0.860	1.220	1.100	1.653	1.245	**1.800**	1.780	1.260
	Coherence (Avg) ↓	3.857	5.460	5.740	5.420	5.571	6.306	**5.440**	4.420	3.420
1 sigma	Joyfulness (Avg) ↑	1.000	0.800	1.260	1.490	2.120	**2.980**	2.280	1.776	2.160
	Coherence (Avg) ↓	4.780	3.680	4.040	3.531	4.860	**4.857**	6.480	5.347	5.800
2 sigma	Joyfulness (Avg) ↑	0.840	1.520	1.143	1.878	**2.625**	2.458	2.520	2.340	1.960
	Coherence (Avg) ↓	4.420	3.680	3.857	4.061	**5.854**	6.688	6.460	6.360	6.520
3 sigma	Joyfulness (Avg) ↑	0.820	1.220	1.220	1.837	2.460	**2.571**	2.388	2.510	1.854
	Coherence (Avg) ↓	3.920	4.180	3.580	3.449	5.120	**5.633**	6.204	6.633	5.542
4 sigma	Joyfulness (Avg) ↑	0.840	0.755	1.380	1.960	**2.280**	2.224	2.612	2.720	1.520
	Coherence (Avg) ↓	3.600	3.837	4.400	3.560	**4.720**	5.878	6.653	6.800	4.200
5 sigma	Joyfulness (Avg) ↑	0.580	0.640	1.429	1.640	**2.458**	1.680	2.333	2.224	2.220
	Coherence (Avg) ↓	3.440	4.040	5.347	3.480	**4.771**	5.900	5.625	5.694	4.980
One linear	Joyfulness (Avg) ↑	0.840	1.245	1.520	2.000	2.292	2.580	**3.020**	2.480	2.080
	Coherence (Avg) ↓	4.360	3.347	4.380	4.640	5.208	6.020	**5.918**	6.780	6.340

been implemented to derive the vector. One common approach is to train a linear classifier and the vector is the normalized weights of the learned classifier (Kim et al., 2018; Jin et al., 2024). Another branch of methods focus on mean difference involving different strategies. One popular way is to compute the difference between average activations of positive samples and negative samples. Another approach is to derive steering vectors by averaging the difference in residual stream activations between pairs of positive and negative samples at certain layers (Rimsky et al., 2023; Zou et al., 2023). While Mean-Centering takes the difference between the average activation of a target dataset and that of all training activations as the steering vector (Jorgensen et al., 2023).

Hierarchical Concepts. Syntactic structures have been well studied in previous research. Some works focus on projecting embeddings to a specific space so that syntactic structures and semantics revealed through embeddings (Nickel & Kiela, 2017; Chen et al., 2021). Alternatively, some work advance approaches that make sure learned embedding can retain hierarchies between entities (He et al., 2024). Moreover, Park et al. (2024) demonstrates the hierarchies among categorical concepts through proposed geometrical structure of linear representation vectors.

Inference-time Intervention. The intervention on internal representations of LLMs during inference time has proven effective in steering model outputs (Burns et al., 2022; Zou et al., 2023). This approach utilizes steering vectors, also known as steering activations, which are believed to linearly represent concepts or features in the representation space (Park et al., 2023; Elhage et al., 2022). These vectors are added up to models representations during forward pass at the level of either attention head or layer. For example, some studies add scaled concept vectors to tokens, either all tokens or last token of a sequence, at certain layers to manipulate models output (Rimsky et al., 2023; Liu et al., 2023; Tigges et al., 2023; Turner et al., 2023; Zou et al., 2023).

6 Conclusions

In this paper, we introduce the GCS, a new framework to estimate the subspace of specific concepts within LLMs. Our research demonstrates the faithfulness and plausibility of GCS in terms of its explanation. Explanations from GCS are similar to trained vectors in representation space and their prediction accuracy is comparable to, and in some cases surpasses, that of trained vectors. GCS also reveals the hierarchical concept structures that align with we human's understanding. Besides, we attempt to apply it in real-world inference-time intervention tasks. The performance of GCS demonstrates its potential for efficiently mitigating models' undesirable behaviors. In summary, GCS offers a concise yet powerful method for concept subspace estimation, showing promise in both theoretical explanations and practical applications.

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