# Motifs in Attention Patterns of Large Language Models

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## Abstract

Attention patterns in Large Language Models often exhibit clear structure, and analysis of these structures may provide insight into the functional roles of the attention heads that produce these patterns. However, there is little work addressing ways to analyze these structures, identify features to classify them, or categorize attention heads using the patterns they produce. To address this gap, we 1) create a meaningful embedding of attention *patterns*; 2) use this embedding of attention patterns to embed the underlying attention *heads* themselves in a meaningful latent space; and 3) investigate the correspondence between known classes of attention heads, such as name mover heads and induction heads, with the groupings emerging in our embedding of attention heads.

## 1 Introduction

As Large Language Models (LLMs) [23, 33] become ever more powerful and widely deployed, ensuring the safety and security of these systems becomes paramount. Mechanistic interpretability aims to help us understand the internals of AI systems in order to make them more trustworthy and safe, by mapping those internals to human-comprehensible algorithms and concepts [27, 25]. A key obstacle to interpretability is the sheer number of components present in modern LLMs, making the manual inspection of the components prohibitively time consuming. Recent advances in using Sparse Autoencoders (SAEs) to decode the meanings of residual stream vectors have relied on the automatic tagging of learned sparse features with legible explanations using LLMs [6, 2], but no such automatic tagging exists for attention patterns. SAEs have been used to attempt to identify the role of attention heads [15, 12], but SAEs are themselves not without issues [16]. Furthermore, this approach discards any spatial information from the attention patterns.

Despite the presence of polysemanticity [7] in attention heads [7, 14], manual inspection of attention patterns can prove valuable in determining the function of the attention head that produced them [20, 28, 13][35, Figure 16]. Despite the presence of clearly visible structures in a variety of attention heads (Figure 2) and a variety of categories of attention heads identified [20, 35, 15, 8, 26, 10], to our knowledge a taxonomy of attention patterns and the heads that produce them has not yet been developed [37]. In this work, we embed the attention *pattern* matrices themselves using handcrafted features, and observe clear structure in the latent space of the embedding (section 2). Using these embeddings of patterns, we construct a metric of distance between attention heads, projecting this new embedding of attention *heads* to a viewable low-dimensional space where we compare our unsupervised embedding with known classes of attention heads (section 3).

By contrast with previous work[5, 34, 36, 21], our method focuses on the attention pattern matrices themselves and does not rely on any token or residual stream information. Attempts to categorize heads only by the tokens or features of the residual stream they attend to [15] are limited because heads may attend to similar parts of the residual stream but be quite different in their broader functionality (Figure 1, $A_1$ vs $A_2$), or, on the other hand, they may attend to vastly different parts of the residual stream but be similar in functionality (Figure 1, $A_2$ vs $A_3$). It is our hope that this work will accelerate research in interpretability by providing an incredibly cheap[1] way to cluster the functionality of attention heads.

This paper contains extensive links to our accompanying website: `attention-motifs.github.io`, which contains interactive versions of many figures, as well as a variety of tools that may be useful to researchers in interpretability. Use of interactive figures and tools requires only a web browser. In particular, the browser tool at `attention-motifs.github.io/s/head-info` allows the user to enter any head from the listed models (Table 1) and see the attention patterns produced by the head, links to other works which mention the head, the location in embedding space of this head, and information and links to attention heads nearby in embedding space.

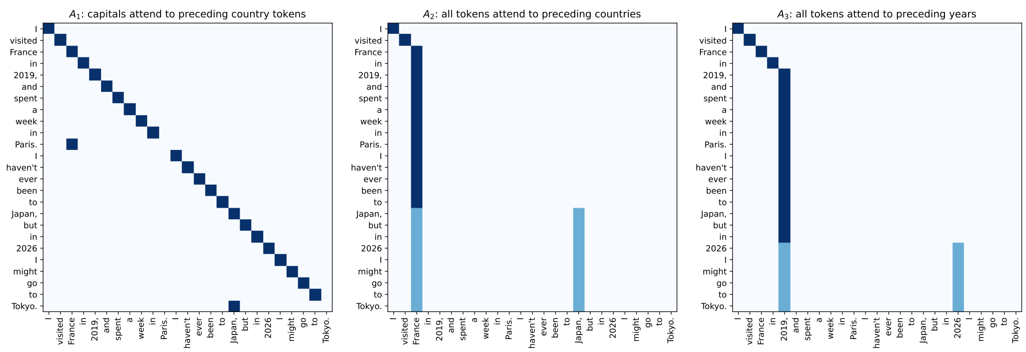


Figure 1: An **artificially constructed** example of classes of heads whose classification based on their attention patterns or functionality differs from a classification based on QK or pure token analysis, to explain our intuition. $A_1$ (left) has capital cities attend to their countries ("Tokyo" to "Japan", "Paris" to "France"; $A_2$ (center) has any token attend to tokens denoting a country; $A_3$ (right) has any token attend to tokens denoting a year. If we were to analyze the actual *tokens* each head attends to, or analyze the QK circuit itself, we might conclude that $A_1$ and $A_2$ are more similar to each other than to $A_3$. Inspection of the attention patterns suggests that $A_2$ and $A_3$ both exhibit a "vertical bars" pattern, while $A_1$ exhibits a diagonal pattern. The similarity of the "vertical bars" pattern observed for $A_2$ and $A_3$ indicate that the heads are performing the same *function*: both heads always attend to a certain class of token – despite those classes being entirely different between the two heads. Note that these **are not actual attention patterns from trained models**, and are provided only for illustrative purposes. See Figure 2 for examples of actual attention patterns.

## 2 Embedding patterns

### 2.1 Type signature of the embedding

Dot-product attention for autoregressive transformer models [33] over some input residual stream $X \in \mathbb{R}^{n \times d}$ can be written as

$$\texttt{attention}(X) := \underbrace{\sigma\left(\frac{XW_Q W_K^T X^T}{\sqrt{d}} + M\right)}_{A} \cdot W_{OV}(X) \qquad \text{where} \qquad M_{i,j} := \begin{cases} -\infty & j > i \\ 0 & j \leq i \end{cases} \tag{1}$$

where $\sigma$ is the row-wise softmax function, and $M$ is the autoregressive masking matrix. The *attention pattern* is the output of the softmax, the matrix $A \in \mathbb{R}^{n \times n}$. Examples of these attention patterns can be seen in Figure 2.

[1] All experiments were performed on a laptop with an 8-core i9-11950H CPU, 64GB RAM, and A5000 Mobile GPU with 16GB VRAM, requiring several minutes. Preliminary experiments with features which were eventually discarded took up to several hours.

We can define the set of all possible attention patterns as

$$\mathcal{P} = \bigcup_{n \in \mathbb{N}} \mathcal{P}_n \qquad \text{where} \qquad \mathcal{P}_n = \left\{ A \in \mathbb{R}^{n \times n} \;\middle|\; \begin{array}{l} A\vec{1} = \vec{1} \\ A_{i,j} \in [0,1] \\ A_{i,i+k} = 0 \quad \forall\, k \in \mathbb{N} \end{array} \right\} \tag{2}$$

The attention pattern of the head at layer $L$ and index $H$, for an LLM with parameters $\theta$ and given a prompt $s$ is given by

$$\texttt{LLM}_{\theta,L,M}(s) \in \mathcal{P}_{|s|} \in \mathcal{P}_{|s|} \qquad \text{or, equivalently} \qquad \texttt{LLM}[h_i](s) \in \mathcal{P}_{|s|} \tag{3}$$

Where $h_i$ is a particular head from a particular model – for example, `L0H1` from `pythia-1b`.

If we entertain the hypothesis that there is a feature of the structure of $\texttt{LLM}_{\theta,L,M}(s)$ that is invariant to our dataset sample $s \sim \mathcal{D}$ and indicates the function of the head $\texttt{LLM}_{\theta,L,M}$, we expect that there exists an embedding function $\mathcal{E}$, which maps attention patterns to a meaningful latent space in which the location of the head represents the structure we care about.

$$\mathcal{E} : \mathcal{P} \to \mathbb{R}^c \tag{4}$$

In subsection 2.3, we describe the results of finding such a function $\mathcal{E}$ by using PCA[22] to reduce the dimensionality of a large set of features (described in subsection 2.2).

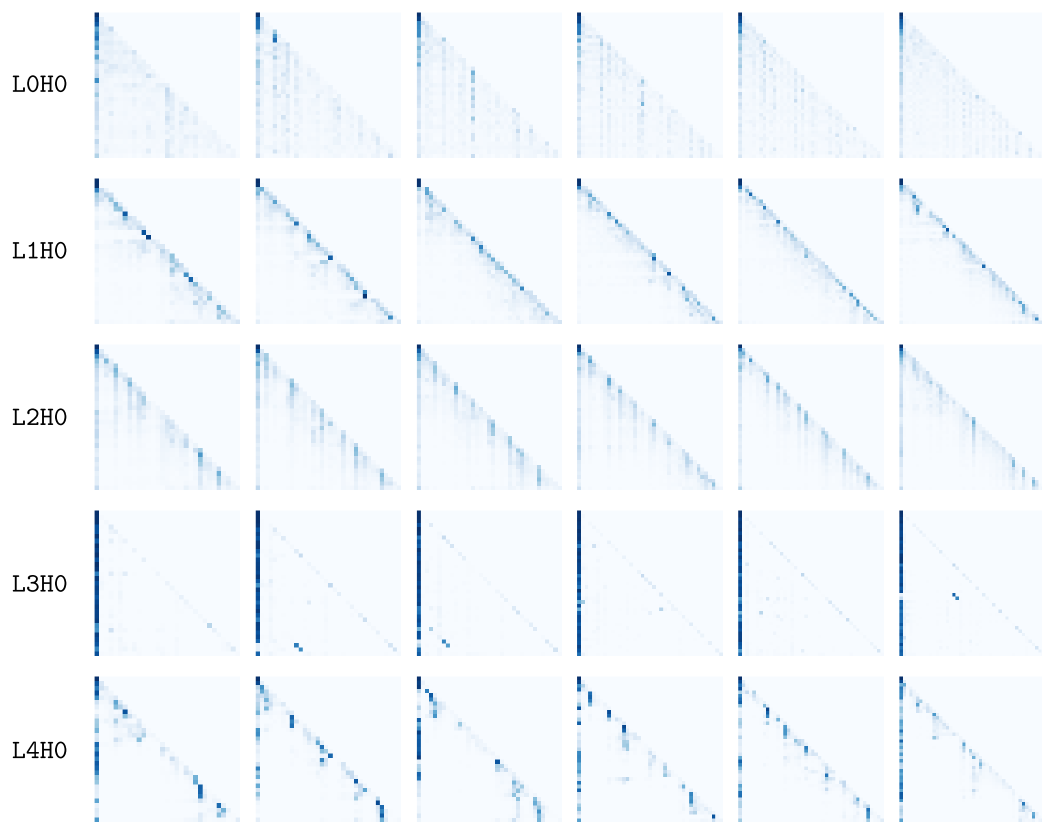


Figure 2: Actual attention patterns from `gpt2-small`. Each row corresponds to a different head in the model. Each column represents one of 6 random prompts. Note that each head displays the same *motif* regardless of the input prompt. Interactive version, with prompt information: `attention-motifs.github.io/s/fig/patterns-example` .

### 2.2 Motivation for chosen features

In order to find a suitable embedding $\mathcal{E}$, we use handcrafted features to compute about attention patterns. In particular, these features include basic statistics (mean, variance, etc.) about the values on the diagonal and first column of the attention pattern, as well as similar features about the distributions of values in gram matrices of the pattern and skew of the pattern. Features, along with their importance and covariance, are shown in Figure 8.

Our motivation for this choice of features is that visually, some of the most common motifs in attention patterns include:

- Large values along the diagonal, meaning every token attends to itself. See `gpt2-small:L0H1` , `gpt2-small:L0H3` , `gpt2-small:L1H11` . This motivates including statistics about the diagonal values $\texttt{trace}(A)$.
- Large values on the first token, sometimes known as an "attention sink" [38]. Since the first token in autoregressive attention cannot contain information about any token besides itself, it is speculated that these attention sinks are a way for the head to "shut off." See `gpt2-small:L3H4` , `gpt2-small:L5H1` , `gpt2-small:L11H9` . This motivates including statistics about the values in the first column $A[:,0]$.
- "vertical bars," meaning that the same tokens from the context are attended to regardless of the current token. See `gpt2-small:L0H0` , `gpt2-small:L1H9` , `gpt2-small:L10H0` . This motivates including statistics about the gram matrix $AA^T$. If vertical bars are present in $A$, then rows are likely very similar, causing the gram matrix to have large values[2]. Horizontal bars, although rarer, motivate including the gram matrix of the transpose $A^TA$.
- "recent tokens" where most of the attention is concentrated somewhere close to the diagonal (but not entirely on it), regardless of the current token. We assume that these heads rely primarily on positional embedding information in their QK circuit. See `gpt2-small:L0H4` , `gpt2-small:L2H3` , `gpt2-small:L3H2` . This motivates the inclusion of statistics about the gram matrix $S(A)S(A)^T$ of the "skewed" attention pattern where for

  $$A \in \mathcal{P}_n, \qquad S(A)\big[i,\ j+(n-i-1)\big] := A[i,j]$$

  $S(A)[i,j]$ indicates how much token $j$ is attending to the token $(n-i+1)$ tokens *before* it, and the gram matrix captures how similar this pattern is between rows: $S(A)S(A)^T$ will have larger values if each token attends to tokens a similar number of tokens behind it.

The above list is not meant to cover all of the motifs observed, nor are the examples given exhaustive. We leave most the details of these features, denoted $\hat{\mathcal{E}} : \mathcal{P} \to \mathbb{R}^{92}$, to the code: `attention-motifs.github.io/s/feature-info` .

### 2.3 Computing features and the embedding

We apply $\hat{\mathcal{E}}$ to a dataset of $> 10^5$ of attention patterns from open-weight pretrained LLMs (see Table 1) across 128 pieces of text sampled from the "Pile" dataset [9, 19]. We assemble from the ouput of $\hat{\mathcal{E}}$ a table where each row has a column identifying the attention head ($h_i$), a column identifying the prompt used ($s_k$), and columns with normalized scalar values for the computed features. Performing a principal component analysis (PCA) on the normalized feature columns, we find that around 68% of the variance is explained by the first 3 principal components, and nearly 90% by the first 10 (Figure 9). We construct our embedding $\mathcal{E}$ as the first 16 principal components of $\hat{\mathcal{E}}$.

Plotting the embedding of each pattern in the first 3 components shows us that the distributions for all model overlap, which is a desired property[3] of our embedding function (Figure 3). Furthermore, we see in Figure 3 that all attention patterns from a given head appear to occupy a well-defined region of embedding space. Interactive visualizations of this embedding can be found at `attention-motifs.github.io/embed`.

[2] By "vertical bars", we mean that $A[i,j]$ and $A[k,j]$ are correlated. If this is the case, then $[AA^T]_{i,k}$ is more likely to be large, as $[AA^T]_{i,k} = A[i,:] \cdot A[k,:]$.

[3] In general, we expect and see roughly the same motifs in patterns across all language models. If patterns from different models were mapped to wholly different parts of embedding space, this would not be useful for finding similar heads across different models.

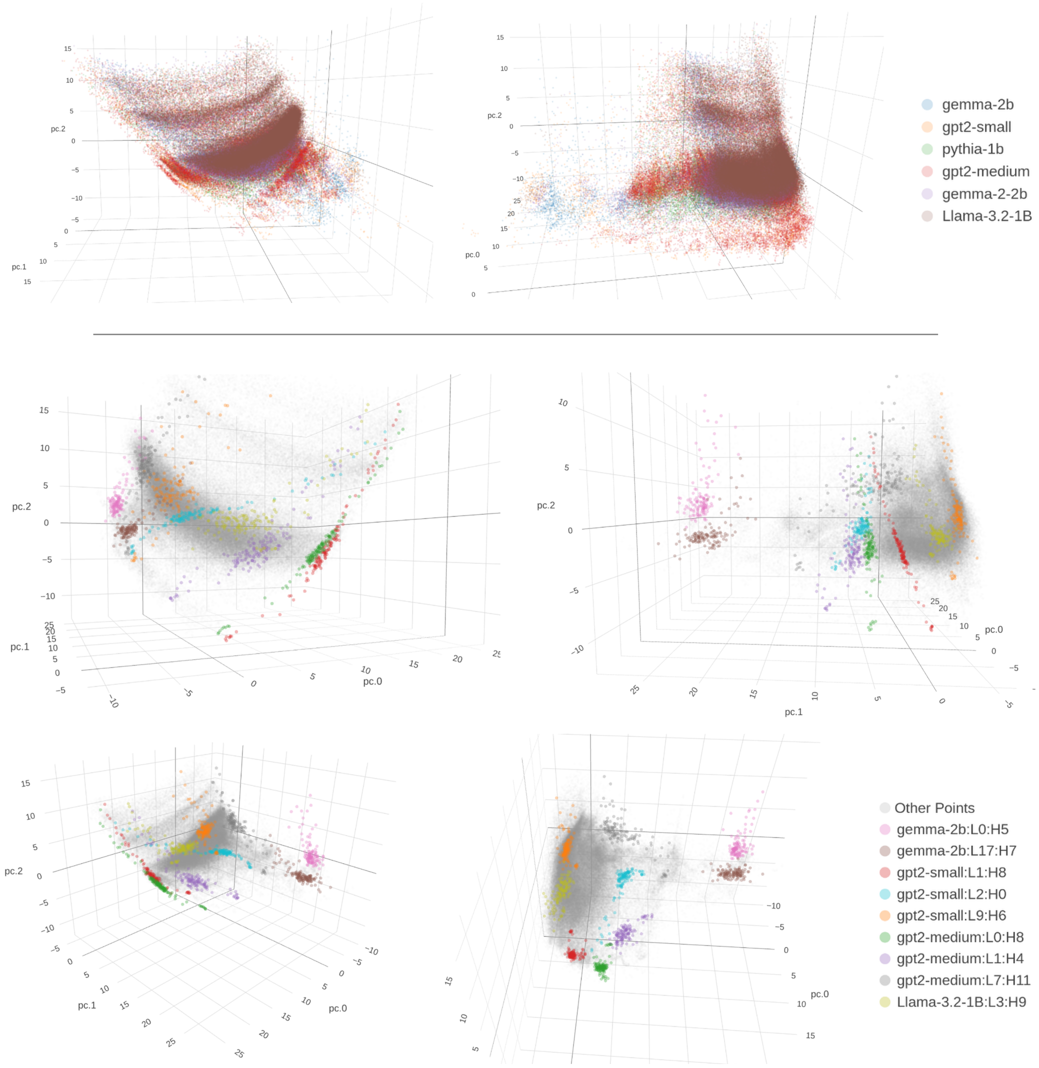


Figure 3: Different views of the first 3 PC axes of $\mathcal{E}$. **Top group:** colored by model, **Bottom group:** with certain heads selected – all points of a given color are the embeddings of the attention pattern, for different prompts, of that head. Interactive versions: `attention-motifs.github.io/s/fig/pca-view`

## 3 Embedding heads

Our embedding $\mathcal{E} : \mathcal{P} \to \mathbb{R}^c$ tells us something about how similar attention *patterns* are to each other, but what we want is a distance metric that tells us about similarities between attention *heads*. Each head corresponds to a cloud of points in $\mathbb{R}^c$, each point corresponding to that head's attention pattern given a prompt $s$ from our dataset $\mathcal{D}$, and we want some notion of similarity between these point clouds. In this work, we consider the naive metric:

$$\texttt{dist}(h_i, h_j) := \frac{1}{|\mathcal{D}|} \sum_{s \in \mathcal{D}} \left| \mathcal{E}\Big(\texttt{LLM}[h_i](s)\Big) - \mathcal{E}\Big(\texttt{LLM}[h_j](s)\Big) \right| \tag{5}$$

taking the mean distance between the embeddings of the patterns produced by the heads $h_i, h_j$ over prompts $s$ from the dataset $\mathcal{D}$. We discuss the potential of other metrics in subsection 4.1.

We compute this distance matrix $\mathbf{D}[i, j] = \texttt{dist}(h_i, h_j)$ for all pairs of heads $h_i, h_j$ (Figure 11), and project to a viewable low dimensional space using UMAP, Isomap, and $t$-SNE [31, 32].

### 3.1 Comparing with previously identified classes

In this space, we find that known classes of attention heads are generally grouped together. We assemble a mapping from 6 "head types" to identified heads in `gpt2-small` based on the work of [35] and [15]. Noting that these two works are not always in agreement about the classes of heads for classes which they both identify (Induction, Duplicate Token, and Previous Token heads), we will consider a head to be in one of these classes if *either* work identifies it as such.

We find that when projecting via Isomap [31] with 16 neighbors, groupings of heads with known functionality become particularly apparent (Figure 5). In Figure 6 and Figure 4, we see that heads nearby in our embedding exhibit similar attention patterns. Notably, although [35] only finds "Backup Name Mover" heads after knocking out the initial name mover heads, our method groups together all varieties of name mover heads. Our projection does not perfectly group together known classes, nor do we expect it to. As described in Figure 1, it is conceivable that two heads determined to be similar through QK circuit analysis (or potentially circuit analysis) might have quite different attention patterns, or for the inverse case to be true. We elaborate on this point in section 4.

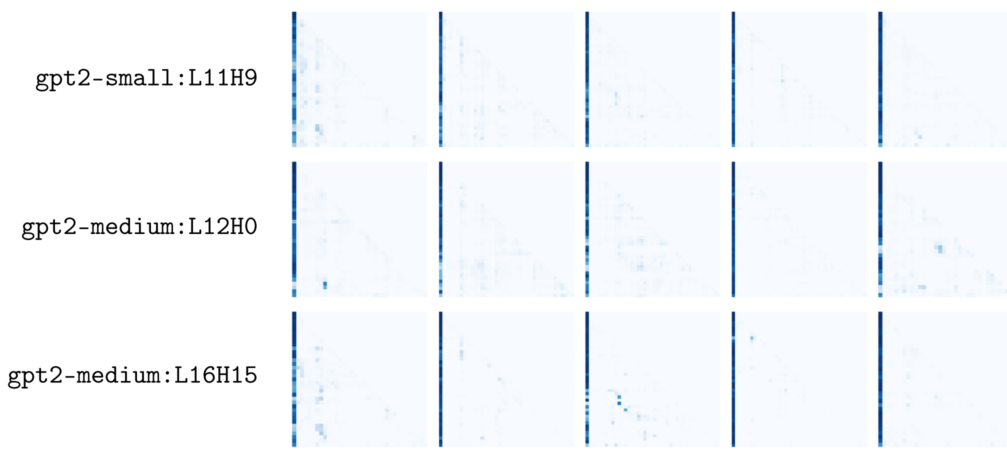


Figure 4: `gpt2-small:L11H9` is originally identified by [35] as a "Backup Name Mover", while the other heads heads are nearby heads which are not described as name movers or otherwise in the literature to our knowledge. More information: `attention-motifs.github.io/s/fig/groups/name-mover` .

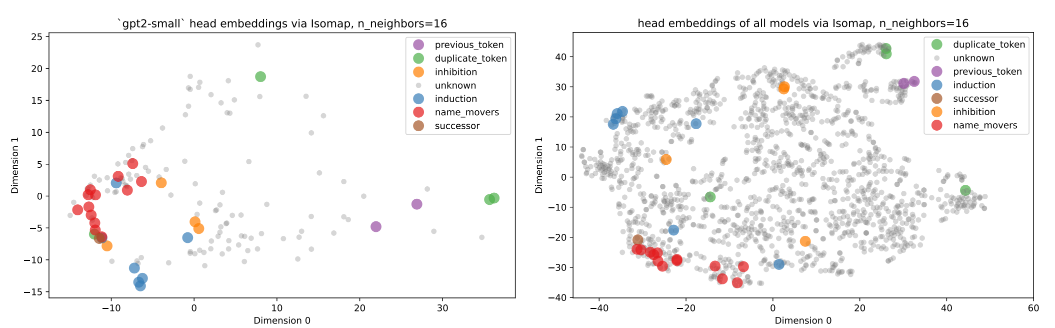


Figure 5: Embeddings of heads via the distance matrix. **Left:** Only heads from `gpt2-small`. **Right:** heads from `all` models. Projection via Isomap, with 16 neighbors. More projections can be viewed in the appendix (Figure 12, Figure 13) or on the website: `attention-motifs.github.io/s/fig/head-embed`

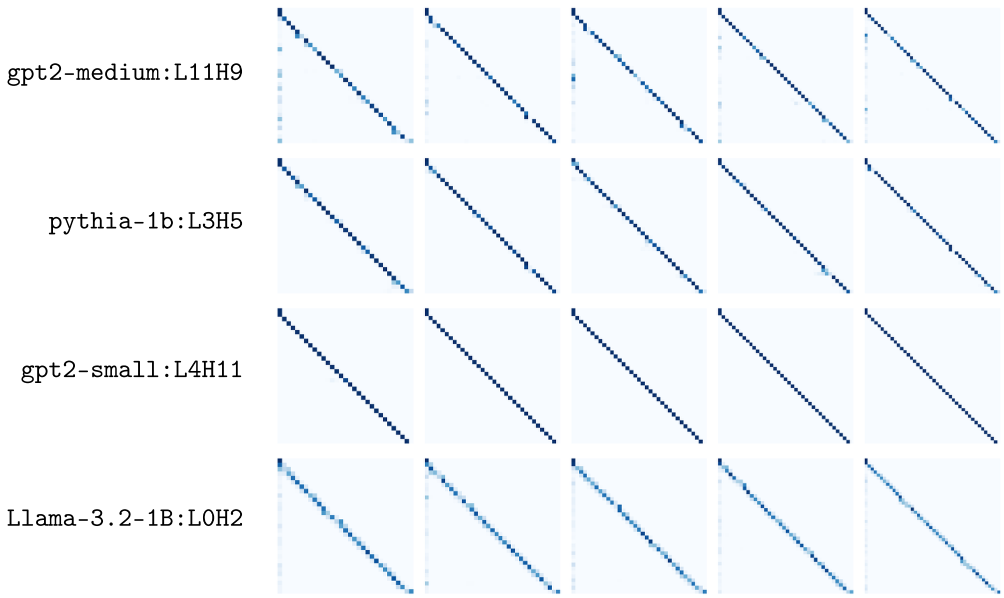


Figure 6: gpt2-small:L4H11 is identified by both [35] and [15] as a “Previous Token Head”, while the other heads are nearby heads which are not described as previous token heads or otherwise in the literature to our knowledge. More information: attention-motifs.github.io/s/fig/groups/previous-token .

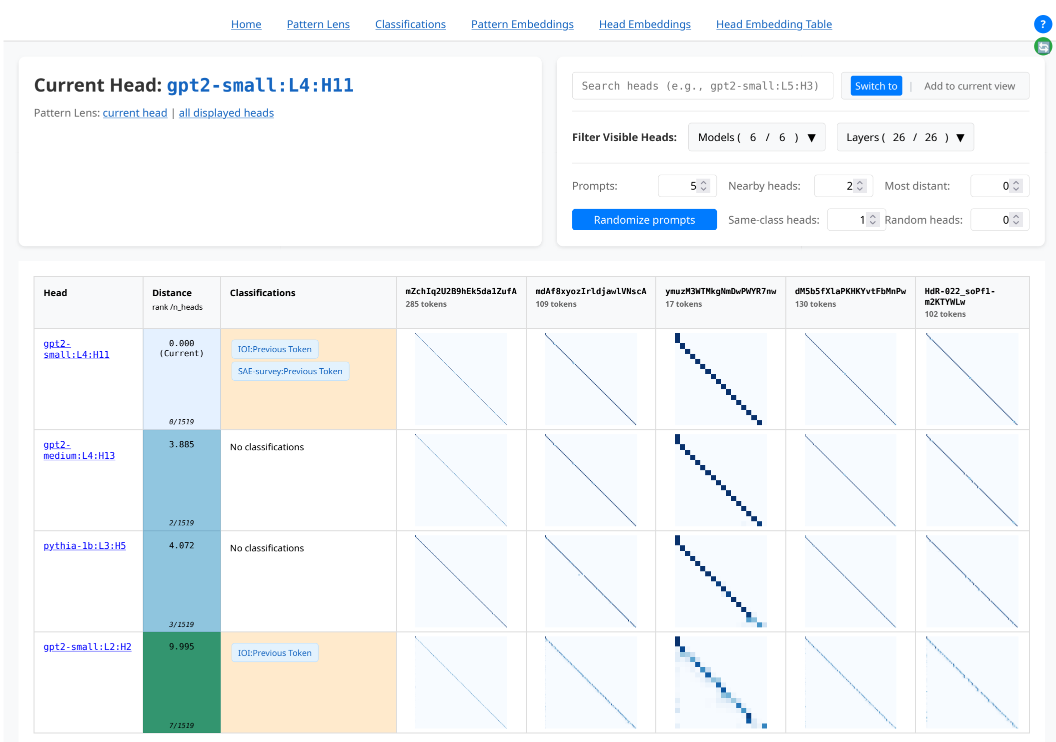


Figure 7: The primary interface for interacting with the head embeddings. We allow searching for any head among the supported models, viewing heads by their classifications, filtering by model or layer, and viewing heads which are near or far in head embedding space.
attention-motifs.github.io/v1/vis/attnpedia/index.html?head_viewing=gpt2-small~L4~H11

# 4 Conclusion

## 4.1 Limitations and future work

Our work is not mechanistic in nature, and does not aim to be. We do not provide a mechanistic analysis of whether heads near in embedding space to a known class (e.g. induction heads) fulfill the same role. Nor does our method use any token or residual stream information, and this is also by design. More on our motivation behind this is explained in subsection 4.3.

This work only uses the models described in Table 1, a selected variety of GPT-like autoregressive transformer architectures. A limited dataset of 128 samples from the "Pile" [9] dataset is used[4].

### Metrics

The distance metric defined in Equation 5 is not the only possible metric, and we do not consider the distribution of distances for each pair of points, only the mean. In particular, Gromov-Wasserstein [4, 17] distances and variants may provide a unique perspective. Consider heads $h_i, h_j$ and inputs $s_1, s_2$. To motivate this, we define

$$f(h_i, h_j, s_u, s_v) := \left| \mathcal{E}\big(\texttt{LLM}[h_i](s_u)\big) - \mathcal{E}\big(\texttt{LLM}[h_j](s_v)\big) \right|.$$

Consider the case that:

- $f(h_i, h_j, s_1, s_1)$ and $f(h_i, h_j, s_2, s_2)$ are both very large
- $f(h_i, h_j, s_1, s_2)$ and $f(h_i, h_j, s_2, s_1)$ are both very small

For example, we could have $\mathcal{E}\left(\texttt{LLM}[h_i](s_1)\right) = \mathcal{E}\left(\texttt{LLM}[h_j](s_2)\right)$ and $\mathcal{E}\left(\texttt{LLM}[h_i](s_2)\right) = \mathcal{E}\left(\texttt{LLM}[h_j](s_1)\right)$. If this is the case, then Equation 5 would compute distance between $h_i$ and $h_j$ to be very large, while a Gromov-Wasserstein or other "earth-mover" metric would compute it to be small. What this tells us in practice is that $h_i$ and $h_j$ are in some sense complimentary, producing a similar distribution of patterns over the entire dataset but vastly different patterns for any given pattern $s_1$ or $s_2$. We believe exploring other such distance metrics, and in particular comparing multiple metrics, would be a fruitful area of work.

### Features

Certain features were considered but not used due to computational cost or lack of importance in the PCA. Discarded features include statistics about the absorption times when treating the attention pattern as an absorbing markov chain, various Fourier statistics, and network-theoretic analyses of the attention pattern as an adjacency matrix. An autoencoder approach was also considered, but not pursued further due to the lack of interpretability about the resulting embedding space. Importance of features in relation to each individual PCA axis can be found at `attention-motifs.github.io/s/fig/feat-importance` , but a detailed analysis of the influence of various features on the resulting groupings of heads is absent from this work.

### Supervised classification

A supervised approach to classification of attention heads by their patterns is likely impractical. Manual inspection and labeling of attention patterns does not appear to be practical, since a large number of attention patterns contain structure that is difficult to describe. Using the labels of known classes of attention patterns may be useful to condition the embedding of attention heads from the distance matrix, but was not explored in this work. A key obstacle is the relatively small number of labels, and the small subset of models for which they exist (`gpt2-small` is often described as the "model organism" of interpretability). The differences in produced attention patterns between models may further complicate any attempts at a supervised approach, if one wishes their method to generalize to new models.

### Limitations of attention patterns as a tool for interpretability

It may be the case that attention patterns themselves are not useful for interpretability. Perhaps polysemanticity makes studying attention patterns of individual heads entirely useless, or perhaps the

[4]See `attention-motifs.github.io/s/pile-info` .

OV circuit sometimes negates the attention in a way that makes the patterns unimportant. We believe our work provides some evidence to the contrary, but acknowledge this possibility. If this is in fact the case, however, it is still important to investigate this line of research and see how much useful information can be extracted from the attention patterns alone.

### 4.2 Broader impacts

Risks from the misuse and misalignment of AI systems are widely discussed in the literature, as is the application of interpretability to mitigate those risks [25]. Work in interpretability is often constrained by high computational costs [6, 3], and it is our view that there is a niche for low-cost methods to work in concert with more expensive ones. Our work helps fill this niche, by providing a way to identify potentially similar heads across many different models, thereby leveraging the identification of a small number of heads that is found to be of interest using other, more expensive, methods.

### 4.3 Contributions

We present a method for embedding and clustering the attention patterns of attention heads in pretrained LLMs, and show that this corresponds with visually apparent motifs in the attention patterns (the "eyeball norm"). We utilize this embedding of attention patterns to create an embedding of the attention heads themselves, and show that this embedding groups together some known classes of attention heads.

One interpretation of why attention in LLMs is multi-headed is because different "views" of token similarity may be required [5]. In the same sense, we aim to complement existing methodology by providing a different view on what properties attention heads possess. We anticipate that this method will accelerate research in interpretability by providing an interpretable, extensible, and incredibly inexpensive method to find heads across many models which may be similar in role to a head whose functionality has been identified.

[5] E.g., one attention head might view countries and their capitals as similar ("Paris" $\rightarrow$ "France", "Tokyo" $\rightarrow$ "Japan") , while another may view countries as similar if they are on the same continent ("Japan" $\leftrightarrow$ "Vietnam", "France" $\leftrightarrow$ "Spain")

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# A Technical Appendices and Supplementary Material

## A.1 Models used

| Model Name | Parameter count | Layers | Heads (per layer) | Citation |
|---|---|---|---|---|
| `gpt2-small` | 85M | 12 | 12 | [24] |
| `gpt2-medium` | 302M | 24 | 16 | [24] |
| `Llama-3.2-1B` | 1.1B | 16 | 32 | [11] |
| `pythia-1b` | 805M | 16 | 8 | [1] |
| `gemma-2b` | 2.1B | 18 | 8 | [29] |
| `gemma-2-2b` | 2.1B | 26 | 8 | [30] |

Table 1: Models used in experiments. Model loading, inference, and activation inspection was done via the TransformerLens [18] package.

## A.2 Feature covariance and importance


Figure 8: Importance (top) and covariance (bottom) of all features.

### A.3 Feature PCA

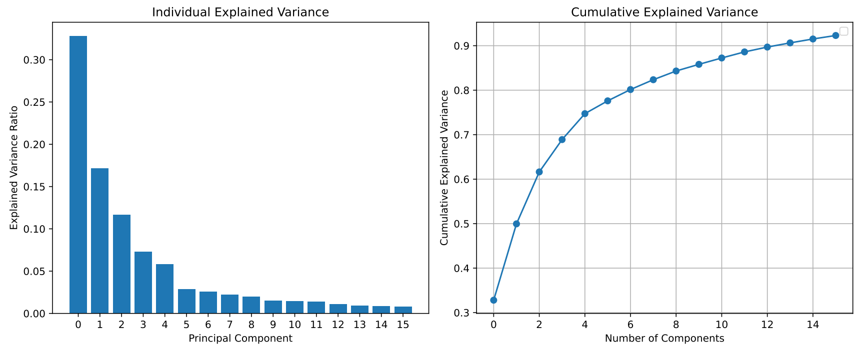


Figure 9: Variance explained by PCA ($\mathcal{E}$) of the feature space $\hat{\mathcal{E}}$ of all attention patterns.

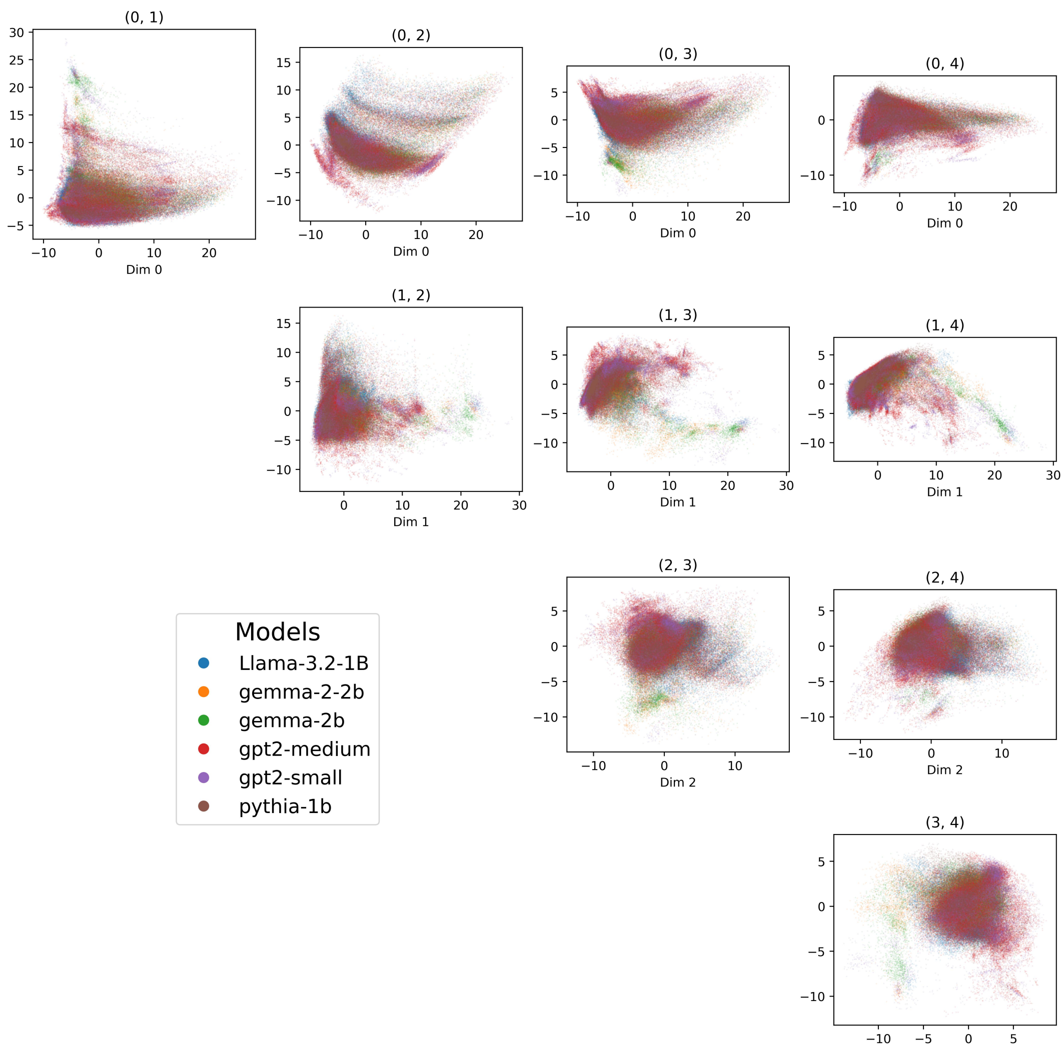


Figure 10: Different projections of the PCA of the embedding space, colored by model. Note that each model has a similar distribution in this space.

## A.4 Head Embeddings

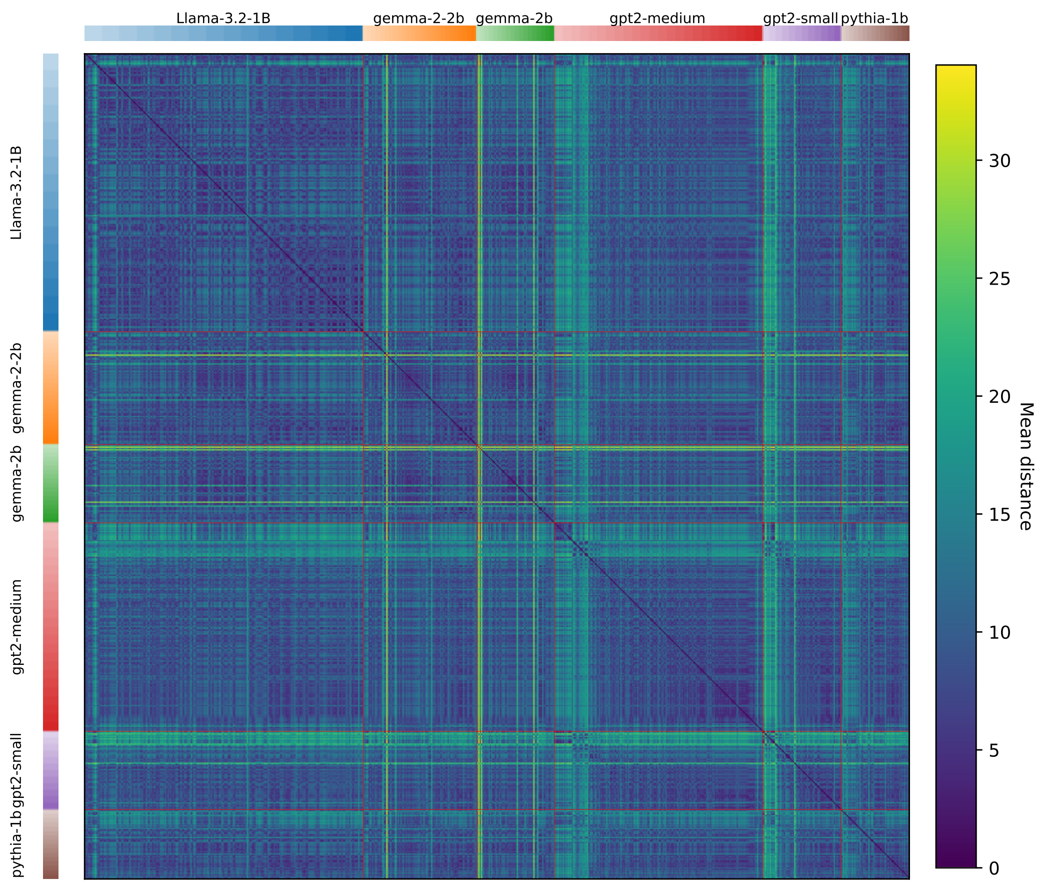


Figure 11: Pairwise distance $\mathbf{D}$ between all heads computed via Equation 5. Models are denoted by colored blocks on the top and left, with lighter colors representing earlier layers and darker colors representing later ones. Each pair of attention heads is exactly one pixel, and the different numbers of layers and heads per layer causes the difference in size between the colored blocks. Red gridlines separate the models from each other. It is of note that for most models, there is a clear distinction between early layer heads and later layer heads. More information: `attention-motifs.github.io/s/fig/head-dists-heatmap`

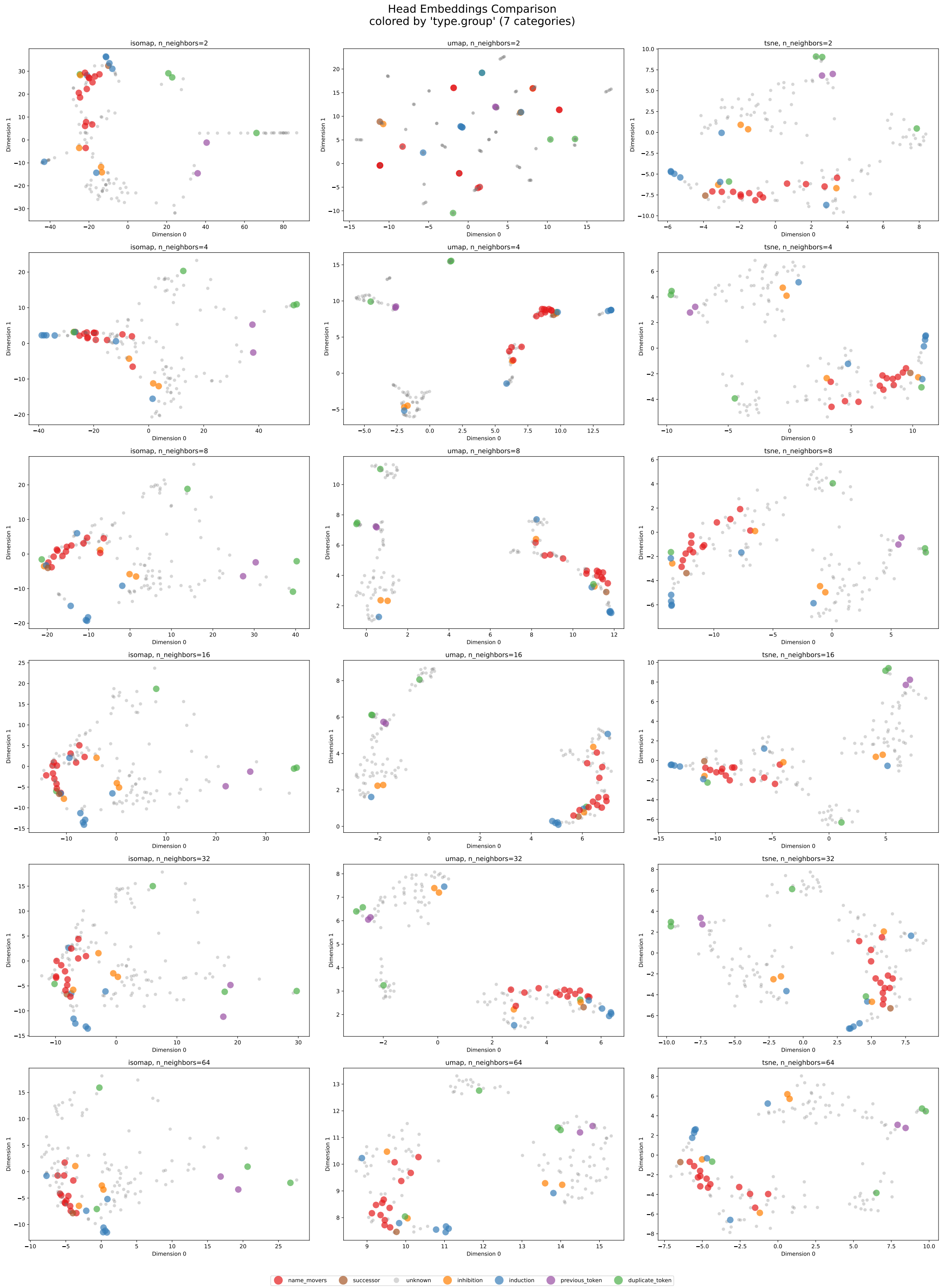


Figure 12: 2D Embeddings via Isomap (left), UMAP (center), and $t$-SNE (right) for various neighborhood sizes (top to bottom, small to large) of the 144 attention heads of `gpt2-small`. Legend of known head classes at the bottom, unknown heads in grey. See `attention-motifs.github.io/s/fig/head-embed/gpt2-small` for an interactive version of the 3D embeddings.

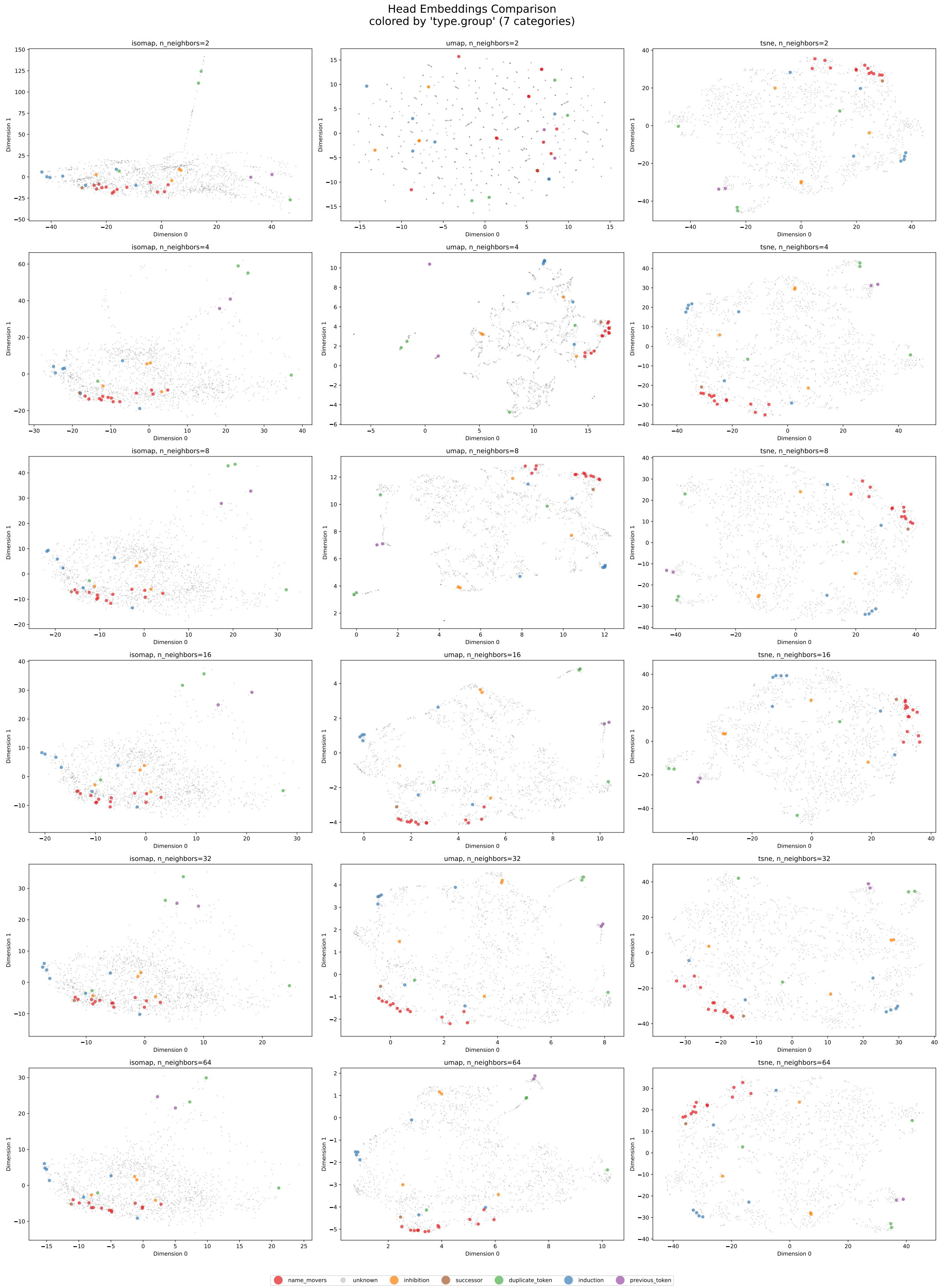


Figure 13: 2D Embeddings via Isomap (left), UMAP (center), and $t$-SNE (right) for various neighborhood sizes (top to bottom, small to large) of all attention heads from all `models`. Legend of known head classes at the bottom, unknown heads in grey. See `attention-motifs.github.io/s/fig/head-embed/all` for an interactive version of the 3D embeddings.