Brain-Inspired Exploration of Functional Networks and Key Neurons in Large Language Models

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Abstract

In recent years, the rapid advancement of large language models (LLMs) in natural language processing has sparked significant interest among researchers to understand their mechanisms and functional characteristics. Although existing studies have attempted to explain LLM functionalities by identifying and interpreting specific neurons, these efforts mostly focus on individual neuron contributions, neglecting the fact that human brain functions are realized through intricate interaction networks. Inspired by cognitive neuroscience research on functional brain networks (FBNs), this study introduces a novel approach to investigate whether similar functional networks exist within LLMs. We use methods similar to those in the field of functional neuroimaging analysis to locate and identify functional networks in LLM. Experimental results show that, similar to the human brain, LLMs contain functional networks that frequently recur during operation. Further analysis shows that these functional networks are crucial for LLM performance. Masking key functional networks significantly impairs the model's performance, while retaining just a subset of these networks is adequate to maintain effective operation. This research provides novel insights into the interpretation of LLMs and the lightweighting of LLMs for certain downstream tasks. Code is available at https://github.com/ WhatAboutMyStar/LLM ACTIVATION.

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1. Introduction

In recent years, large language models (LLMs) have become a focal point of research in the field of artificial intelligence (AI) due to their remarkable capabilities in natural language processing (Zhao et al., 2024a; 2023; Liu et al., 2023b; Wang et al., 2024; Liu et al., 2025). However, these models are often considered "black boxes", with insufficient understanding of their internal mechanisms, which limits the potential for further optimization and broader application. Therefore, exploring methods to explain and understand LLMs is essential both for improving model transparency and trustworthiness and for establishing a foundation to develop more efficient and reliable AI systems.

One research direction on the mechanistic interpretability of LLMs focuses on the analysis of individual neurons (Yu & Ananiadou, 2024a; Dai et al., 2022). A subset of this research is dedicated to the identification of neurons that are crucial to the functionality of LLMs, with the aim of locating and assessing the functions of these key neurons (Yu & Ananiadou, 2024b; Niu et al., 2024; Chen et al., 2024). Studies have shown that the removal of certain neurons leads to a significant degradation in performance in LLMs, highlighting their essential role in maintaining the core functions of the model. In addition, another line of research investigates the specific functional roles of these neurons (AlKhamissi et al., 2024; Wang et al., 2022). For example, some neurons may specialize in processing linguistic structures, while others might be responsible for reasoning tasks (Huo et al., 2024; Zhao et al., 2024b). Furthermore, by manipulating these key neurons, such as amplifying or masking their outputs (Song et al., 2024), researchers have demonstrated the ability to control and predict the behavior of LLMs. Methods for identifying important neurons within LLM can be categorized into several approaches. These include analyzing the gradients of neurons to evaluate their impact on model predictions (Sundararajan et al., 2017; Lundstrom et al., 2022), employing causal tracing techniques to uncover the causal relationships that influence model behavior (Nikankin et al., 2024), and conducting statistical analyses of activated neurons to measure their information content and variability (AlKhamissi et al., 2024; Song et al., 2024; Tang et al., 2024). These approaches provide valuable tools

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for understanding and explaining LLMs, offering deeper insight into their inner mechanisms.

However, the function of an individual neuron is much more complex than it might initially seem. A single neuron is not only dedicated to performing a single task, but can simultaneously participate in multiple functional modules (Mountcastle, 1997; Miller & Cohen, 2001; Raichle & Snyder, 2007). Neurons often form functional networks through their interactions and connectivity, collaboratively working to perform higher-level cognitive tasks (Smith et al., 2009; Bullmore & Sporns, 2009). The role of a neuron therefore extends beyond its individual activation patterns and is shaped by its cooperation with other neurons within these networks (Bullmore & Sporns, 2009; Liu et al., 2024b;a). Existing research has focused mainly on the parameters and structure of neurons, primarily examining their individual properties and connectivity. These approaches, which emphasize structural and parametric analysis, overlook the functional network perspective and fail to explore the roles and contributions of neurons within these networks. As a result, these limitations have hindered a deeper understanding of neuronal function, neglecting the insights offered by neuroscience research on FBNs (Hassabis et al., 2017; Vilas et al.). To address these challenges, we draw inspiration from cognitive neuroscience to investigate whether LLMs contain functional networks similar to those found in the human brain. By recognizing the similarities between functional magnetic resonance imaging (fMRI) (Matthews & Jezzard, 2004; Logothetis, 2008) signals and the output signals of neurons in LLM, we hypothesized that the techniques used in fMRI analysis could be adapted to analyze LLM neurons. Specifically, we treated the neuron outputs from the multilayer perception (MLP) layers of LLMs as analogous to fMRI signals and applied Independent Component Analysis (ICA) (Hyvärinen & Oja, 2000; Beckmann et al., 2005; Varoquaux et al., 2010b) to decompose these neuron outputs into multiple functional networks.

Our experiments on extensive datasets confirmed the existence of numerous functional networks within LLMs. Just as we derived functional networks from fMRI signals (Mensch et al., 2016; Varoquaux et al., 2010a; Liu et al., 2023a; He et al., 2023; Ge et al., 2020; Lv et al., 2015). Some of the functional networks exhibit high spatial consistency across various input stimuli and play a crucial role in the model's functionality. We discovered that masking specific key networks, which typically consist of less than 2% neurons, can significantly impair model performance. Conversely, maintaining these essential networks while gradually integrating additional decomposed functional networks and masking non-essential neurons enables the model's performance to improve progressively from low to high. Ultimately, by utilizing less than one-tenth of the neurons in the MLP layer, we achieved performance that matches that of the original

network.

Our contributions can be summarized as follows:

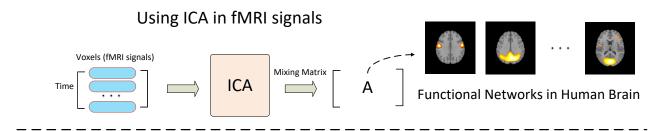
- 1. Bridging Cognitive Neuroscience and AI: We have introduced methods from cognitive neuroscience to analyze neurons in LLM, creating a link between brain science and AI. This integration offers new research directions for braininspired AI, providing fresh insights into how neural networks operate.
- 2. Discovery of Functional Networks in LLMs: We confirmed that LLMs contain functional networks similar to those found in the human brain. Some of these functional networks exhibit high spatial consistency in various input stimuli, demonstrating relatively stable spatial patterns. This finding suggests that LLMs may share fundamental organizational principles with biological brains.
- 3. Validation of Key Neurons in Functional Networks: We have demonstrated that neurons within these functional networks are essential for maintaining the functionality of LLMs. These neurons play a crucial role in ensuring that the model operates effectively, underscoring their importance for the overall performance of the system.

2. Preliminaries

In this section, we provide the essential background knowledge required for understanding our work, including the MLP layer in LLMs, how neuroscience utilizes fMRI to study brain functions, and the ICA algorithm which we use to decompose neural activity into distinct functional networks.

Transformer, MLP layer: LLMs utilized in this paper are based on the transformer architecture (Vaswani, 2017), specifically employing a decoder-only configuration. (Radford et al., 2018; 2019; Brown et al., 2020; Yang et al., 2024b; GLM et al., 2024). In this configuration, each transformer decoder consists of two primary components: a multi-head self-attention module and a MLP module. The non-linear transformations in transformer models occur within the MLP layers. Typically, an MLP module consists of two fully connected layers. The first layer increases the dimensionality, often to four times the original dimension, followed by a non-linear activation function such as the Sigmoid-weight Linear Unit (SiLU) (Elfwing et al., 2018) or the Gaussian Error Linear Unit (GELU) (Hendrycks & Gimpel, 2016). The second layer then reduces the dimensionality back to its original size. In our study, we focus on the neurons located in the final MLP layer of each decoder module within the model. Given an input vector $\mathbf{x} \in \mathbb{R}^{d_{\text{model}}}$, the MLP module can be represented as follows:

$$MLP(\mathbf{x}) = \mathbf{W}_2 \cdot \sigma(\mathbf{W}_1 \cdot \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 \tag{1}$$



Using ICA in Neurons signals in Large Language Models

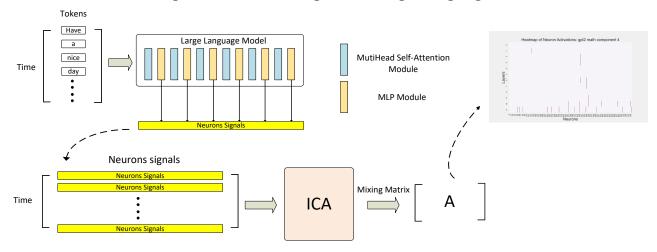


Figure 1. The total framework of the paper. Functional networks generated by ICA on fMRI signals and LLM's neurons are shown in upper and lower part of the figure respectively.

W is the weight matrix of the linear transformation, b is the bias vector of the linear transformation, σ is a non-linear activation function. The neuron outputs used in this paper are the outputs of the MLP(x). This choice allows us to analyze the impact of these neurons on the final output, as they are directly responsible for the refined feature extraction and transformation before the model generates its predictions.

Functional Brain Networks, FBNs: FBNs refer to collections of brain regions that are co-activated during specific tasks or while at rest (Dong et al., 2020). FMRI is a non-invasive technique used to measure Blood-Oxygen-Level Dependent (BOLD) signals, which reflect neuronal activity indirectly (Matthews & Jezzard, 2004; Logothetis, 2008). The intensity of voxel values in fMRI signals indirectly reflects neuronal activity by capturing variations in local blood oxygen levels due to neural metabolism. Neuroscientific research hypothesis that the observed BOLD signals in fMRI signals are likely the result of multiple independent functional networks working together. Essentially, these BOLD signals can be considered as linear combinations of several source signals, each representing a distinct functional network. By comparing the spatial patterns of functional

networks across various task conditions, researchers can infer which regions of brain are associated with specific cognitive or behavioral functions.

Independent Component Analysis, ICA: ICA is a powerful data-driven technique used to extract source signals that are as statistically independent as possible from a mixed signal. Within the field of neuroscience, ICA is frequently applied to fMRI data to uncover underlying functional networks, offering valuable insights into how different regions of the brain collaborate to facilitate cognitive and behavioral processes. ICA disentangles mixed fMRI signals into several independent components, where each component represents a distinct functional network. Each extracted independent component is associated with a spatial map that illustrates which brain regions contribute to that component. These contributing regions typically display synchronized activity patterns, indicating their coordinated involvement in specific neural processes.

The objective of ICA is to recover the source signals S from the observed signals X. Suppose that we have n observed signals $[x_1, x_2, \ldots, x_n]$, which are linear mixtures of m independent source signals $[s_1, s_2, \ldots, s_m]$. The relationship

between the observed signals X and the source signals S can be expressed as:

$$X = AS \tag{2}$$

where **A** is the mixing matrix that describes how the source signals are combined to produce the observed signals. Each row of the linear mixing matrix represents the spatial pattern of the corresponding functional network, which illustrates specific regions are activated. In this study, the functional networks derived from LLMs neuron signals refer to the rows of the linear mixing matrix **A**, which indicate the set of neurons that are consistently co-activated under different conditions. FastICA (Hyvärinen & Oja, 2000) is an efficient algorithm for implementing ICA and is the method used in this paper to derive FBNs from LLMs. The FastICA algorithm can be described as follows:

Pre-whitening: The signals are first centered (zero mean) and whitened to remove any linear correlations between the variables and have unit variance.

The whitened signals **Z** can be represented as:

$$\mathbf{Z} = \mathbf{E}^{-1/2} \mathbf{V}^{-1} (\mathbf{X} - \mathbb{E}[\mathbf{X}]) \tag{3}$$

where V and E are the eigenvectors and eigenvalues of the covariance matrix Σ of X.

Finding Independent Components: For each independent component \mathbf{w}_i , we maximize the following objective function:

$$J(\mathbf{w}) = [\mathbb{E}\{G(\mathbf{w}^T \mathbf{z})\}] - \frac{1}{2}\mathbb{E}\{(\mathbf{w}^T \mathbf{z})^2\}$$
(4)

where G is a non-linear function used to approximate negentropy, a_1 is a constant usually $a_1 \in [1, 2]$, Common choices for G include:

$$G(u) = \log \cosh(a_1 u) \tag{5}$$

$$G(u) = -\exp(-u^2/2)$$
 (6)

To find the optimal w, FastICA uses fixed-point iteration:

$$\mathbf{w}_{\text{new}} = \mathbb{E}\{\mathbf{z}g(\mathbf{w}^T\mathbf{z})\} - \mathbb{E}\{g'(\mathbf{w}^T\mathbf{z})\}\mathbf{w}$$
(7)

where g is the derivative of G. After each iteration, normalize \mathbf{w} :

$$\mathbf{w} \leftarrow \frac{\mathbf{w}}{\|\mathbf{w}\|} \tag{8}$$

If multiple independent components need to be extracted, perform orthogonalization to ensure that the weight vectors remain orthogonal:

$$\mathbf{W} \leftarrow (\mathbf{W}\mathbf{W}^T)^{-1/2}\mathbf{W} \tag{9}$$

where \mathbf{W} is the matrix that contains all weight vectors as columns. Repeat the iteration until the change in the weight vectors falls below a predefined threshold, indicating convergence. Once the demixing matrix \mathbf{W} is obtained, the source signals \mathbf{S} can be estimated from the whitened data \mathbf{Z} :

$$\hat{\mathbf{S}} = \mathbf{WZ} \tag{10}$$

Finally, the mixing matrix **A**, which represents the spatial patterns of the functional networks, can be obtained as the inverse of the matrix **W**. Considering the whitening transformation applied to the signals, the mixing matrix can be computed as:

$$\mathbf{A} = \mathbf{V}\mathbf{E}^{1/2}\mathbf{W}^{-1} \tag{11}$$

In visualizations and experimental comparisons, the mixing matrix **A**, representing the final derived functional networks, typically undergoes thresholding. This process involves setting a threshold to filter out lower values, ensuring that only the regions with significant activation are retained. This approach helps in focusing on the most relevant activations and improving the clarity of the results.

3. Functional Networks in Large Language Models

In this section, we use the ICA to explore functional networks within LLMs.

3.1. Datasets and Models

We used text from four different types of datasets to validate the differences in functional networks when the model performs various tasks. Specifically, we used news articles from the AGNEWS dataset (Zhang et al., 2015), encyclopedia entries from Wikitext2 (Merity et al., 2016), mathematical texts from MathQA (Amini et al., 2019), and code snippets from the CodeNet dataset (Puri et al., 2021). Additionally, we conducted experiments using three different LLMs: GPT2 (Radford et al., 2019), Qwen2.5-3B (Yang et al., 2024a), and ChatGLM3-6B-base (GLM et al., 2024).

3.2. Extracting Functional Networks from LLMs

The general workflow framework of our work is shown in Figure 1. To extract functional networks from LLMs, the first step is to determine which neurons' output signals to use. In this paper, we utilize the neurons from the last layer of each model's MLP module, specifically the neuron output from these MLP modules. We collect the neuron output from all MLP modules in the model.

Table 1. Statistics of Functional Networks Similar to the Template for GPT-2.

TEMPLATES	News	Wiki	Матн	CODE
1	15	208	142	140
2	7	119	109	85
3	12	59	31	44
4	31	145	91	114
5	32	91	32	135
6	87	4	6	107
7	63	41	35	134
8	21	58	43	71
9	15	0	51	112
10	11	18	118	79

In neuroscience research, functional networks are typically derived from fMRI signals, which reflect neural activity in response to various stimuli. Interestingly, there is a notable similarity between the output signals of neurons in LLMs and fMRI signals. Both LLM neuron outputs and fMRI signals not only capture neural activity but also exhibit temporal characteristics in response to different inputs. This similarity suggests the potential to apply analytical techniques used for fMRI signals to LLMs. By leveraging these parallels, we can explore and analyze functional networks within LLMs in a manner similar to our analysis of human brain data, thus opening a new way of understanding the internal mechanisms of these models.

fMRI analysis typically involves performing ICA on individual data or performing group-wise analysis on data from multiple individuals. In individual analysis, ICA is applied to single-subject fMRI data. This method provides detailed insights into the unique characteristics of an individual's brain activity patterns. In contrast, in group-wise analysis, ICA is performed on data from multiple subjects. This approach improves the generalizability of the research findings. For group-wise analysis, a common approach is to stack the data of all subjects together to form a large data matrix and then perform ICA on this combined dataset. We randomly selected 100 samples from each dataset for group-wise ICA analysis, obtaining 10 functional network templates. We then randomly selected 100 additional samples for individual analysis.

The functional networks derived from the group-wise ICA analysis can be considered as templates representing a generalization of functionality. We computed the spatial similarity between these templates and the functional networks derived from the individual analysis of another 100 samples. In neuroscience research, the intersection over union (IoU) is commonly used as a metric to evaluate the similarity between functional networks. We quantify spatial similarity using the IoU between two functional networks $N^{(1)}$ and $N^{(2)}$. Here, n represents the number of neurons, and the IoU is defined as follows:

Table 2. Statistics of Functional Networks Similar to the Template for Qwen2.5-3B-Instruct.

TEMPLATES	News	Wiki	\mathbf{M} ATH	CODE
1	0	2	0	0
2	0	0	1	59
3	0	1	0	0
4	0	0	0	0
5	50	10	0	0
6	0	17	0	0
7	64	73	55	58
8	0	0	0	64
9	0	0	0	3
10	64	70	55	2

Table 3. Statistics of Functional Networks Similar to the Template for ChatGLM3-6B-base.

TEMPLATES	News	Wiki	\mathbf{M} ATH	CODE
1	0	0	0	0
2	1	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	2
6	3	0	8	0
7	0	0	1	0
8	0	0	0	0
9	0	4	0	0
10	0	0	0	0

$$IoU(N^{(1)}, N^{(2)}) = \frac{\sum_{i=1}^{n} |N_i^{(1)} \cap N_i^{(2)}|}{\sum_{i=1}^{n} |N_i^{(1)} \cup N_i^{(2)}|}$$
(12)

Tables 1, 2, and 3 present the number of functional networks derived from individual analysis with a spatial similarity greater than 0.2 compared to the template, for GPT-2, Qwen2.5-3B-Instruct, and ChatGLM3-6B-base, respectively. According to our experimental findings and experience in neuroscience research, when different functional networks have spatial similarity greater than 0.2, they appear reasonably similar on subjective visual inspection. Consequently, such networks are classified into the same category of functional networks.

We observe that, even when the inputs are different samples, there are still a significant number of functional networks similar to the templates. This indicates that LLMs indeed contain specific functional patterns similar to those found in human brain. Interestingly, we noticed that as model size increases, it becomes progressively more challenging to find functional networks similar to the templates within individual samples. We do not interpret this as larger models that have fewer or no specific spatial pattern functional networks. Instead, we believe that as model size grows, the functionalities are divided into finer components that in-

volve more functional networks. When dealing with shorter texts, decomposition into only 10 components may not be sufficient to achieve the same level of granularity as the template functional networks. Consequently, a greater number of decomposed network components are required to capture these finer details; this assumption is contingent upon having sufficiently long time series data for adequate decomposition. With sufficient data, a larger number of functional networks similar to the templates can be identified.

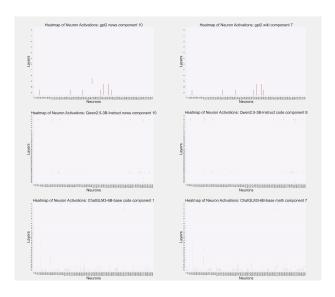


Figure 2. Some similar functional networks in templates. In the figure, each row represents the neurons in a MLP layer, with neurons being highlighted if they are activated.

3.3. Visualiztion of Functional Networks

In Figure 2, we present several functional networks derived from the data. These networks involve a very low percentage of total neurons, which aligns with our understanding that neurons in LLMs are sparsely activated. Additionally, the figure illustrates that similar functional networks can be obtained from different types of input data. This suggests that certain LLM functional networks are broadly presented and engaged in specific tasks, this is similar to the functional networks in the human brain. For instance, the default mode network (DMN) in the human brain is known to be involved in various cognitive tasks (Raichle, 2015). Furthermore, our observations indicate that the majority of neurons activated within functional networks are located in the deeper layers of the models. This finding implies that functional connectivity among neurons is more pronounced in these deeper layers. For a more comprehensive examination of these functional network patterns, please refer to our supplementary material.

Table 4. Performance of GPT-2 with Masked Functional Networks on the AGNews Dataset. The first column represents each functional network and the number of neurons that are masked. The second column shows the accuracy. The model's accuracy under normal conditions (without any masking) is 0.8614.

FUNCTIONAL NETWORKS (9216)	ACCURACY
1→37	0.8538
$2\rightarrow 21$	0.6643
$3\rightarrow$ 57	0.8391
$4\rightarrow$ 29	0.8439
$5\rightarrow36$	0.5749
$6\rightarrow$ 29	0.8500
$7\rightarrow15$	0.8482
$8\rightarrow$ 55	0.7042
$9\rightarrow15$	0.6753
$10\rightarrow72$	0.8471

4. Evaluating the Importance of Functional Networks

In this section, we will evaluate the functional networks obtained using ICA to verify whether they play a critical role in the performance of LLMs.

4.1. Datasets and Evaluate Criteria

In this section, we continue to use the GPT-2, Qwen2.5-3B-Instruct, and ChatGLM3-6B-base for evaluation. To assess the model's performance, we used datasets from the General Language Understanding Evaluation (GLUE) (Wang, 2018), the Stanford Question Answering Dataset (SQuAD) (Rajpurkar et al., 2016), and AGNews (Zhang et al., 2015).

We fine-tuned GPT-2 in these datasets to adapt it to perform specific tasks. In contrast, for Qwen2.5-3B-Instruct and ChatGLM3-6B-base, we utilized carefully crafted prompts to evaluate their performance in a zero-shot setting on the same datasets. In our assessments, we utilized accuracy as the performance metric for the GLUE and AGNews datasets. For the SQuAD, which involves more complex question-answering tasks, we used the F1 score to evaluate the model's performance. The underlying hypothesis is that if these neurons play a critical role in the model's functionality, then ensuring their activation alone should be enough to maintain the model's performance.

4.2. Neuron Lesion Experiment

In the neuron lesion experiment, we deactivate functional networks within the LLMs. The goal is to investigate how the removal or deactivation of these neurons impacts the overall performance and functionality of the model.

Table 4 presents the performance results of the GPT-2 model in the AGNews dataset after selectively masking specific

Table 5. Performance of GPT-2 with Masked Functional Networks. First Column: Dataset names. Second Column: Model performance under normal conditions (without any masking). Third Column: Model performance after masking 15% of the neurons randomly. Fourth Column: Model performance after masking the neurons belonging to 10 specific functional networks (The number of neurons that are masked is less than 2% of the total neurons.).

DATASETS	Normal	Masked 15%	Masked 10
CoLA	0.7776	0.7383	0.5772
MRPC	0.7941	0.7941	0.7377
QQP	0.8758	0.8717	0.8104
SST-2	0.9163	0.9083	0.5436
MNLI	0.6847	0.6879	0.5995
QNLI	0.8746	0.8569	0.6811
AG NEWS	0.8614	0.8487	0.5557
SQUAD	0.3397	0.3154	0.1342

Table 6. Performance of Qwen2.5-3B-Instruct with Masked Functional Networks.

DATASETS	QWEN2.5 NORMAL	QWEN2.5 MASKED 10
CoLA	0.6913	0.0000
MRPC	0.6275	0.0172
SST-2	0.8440	0.0000
MNLI	0.2731	0.0000
QNLI	0.3953	0.0000
AGNEWS	0.7185	0.0000
SQUAD	0.2104	0.0057

functional networks. The results indicate that the masking of neurons within these functional networks leads to varying degrees of performance degradation. Remarkably, masking just a few dozen critical neurons can significantly impair the model's performance. In some instances, masking as few as one-thousandth of the total neurons is enough to cause a substantial drop in performance. In contrast, randomly masking neurons has a minimal impact on the model's performance as shown in Table 5. Our experiments demonstrate that even when up to 15% neurons are randomly masked, performance degradation remains insignificant, with the model's performance staying nearly identical to its baseline in most cases. This finding is consistent with previous studies, which have also observed that random neuron masking does not substantially affect model performance (AlKhamissi et al., 2024; Song et al., 2024).

Table 6 and Table 7 present the performance results of Qwen2.5-3B-Instruct and ChatGLM3-6B-base by masking neurons within specific functional networks. These models rely on well-designed prompts to generate appropriate text for various tasks. When critical functional networks are masked, the models' ability to generate coherent and task-relevant text is severely compromised. For more details, please refer to the supplementary material.

Table 7. Performance of ChatGLM3-6B-base with Masked Functional Networks.

DATASETS	CHATGLM NORMAL	CHATGLM MASKED 10
CoLA	0.6893	0.0000
MRPC	0.8161	0.0441
SST-2	0.9392	0.1422
MNLI	0.2062	0.0000
QNLI	0.1067	0.0053
AGNEWS	0.9128	0.0025
SQUAD	0.9021	0.0358

Table 8. Performance of GPT-2 with Preserved Functional Networks. The first row of the table indicates the number of functional networks obtained from ICA decomposition, which corresponds to the second to fifth columns. The first row for each dataset corresponds to the evaluation metric, while the second row indicates the number of neurons obtained.

	10	64	128	256	512
CoLA	0.3078	0.3509	0.4976	0.7776	0.6088
	145	495	1221	2109	1409
MRPC	0.6838	0.6985	0.8113	0.7279	0.8137
	71	394	759	426	817
QQP	0.6106	0.6849	0.8477	0.8766	0.8048
	60	300	582	865	632
SST-2	0.5195	0.7970	0.6823	0.8394	0.9163
	58	391	253	560	1357
MNLI	0.3220	0.3407	0.4158	0.6858	0.5294
	61	342	722	1242	816
QNLI	0.5338	0.8559	0.8737	0.8629	0.8720
	213	2111	3168	2568	3651
AGNEWS	0.6849	0.7039	0.8462	0.8596	0.8613
	86	394	830	1281	1606
SQuAD	0.0016	0.2143	0.3314	0.3391	0.3398
	79	652	945	1262	1577

4.3. Neuron Preservation Experiment

In addition to verifying the importance of these neurons by masking functional networks, we also conducted a preservation experiment to further validate the significance of these functional networks. In this section, we incrementally increase the number of functional networks obtained through ICA decomposition, taking the union set of neurons within these functional networks to increase the number of retained neurons. We then mask the remaining less important neurons and observe how the model's performance changes.

Table 8, Table 9 and Table 10 show the performance changes of the GPT-2, Qwen2.5-3B-Instruct, and ChatGLM3-6B-base models as the number of decomposed functional networks increases. With the addition of more decomposed functional networks, the models exhibit a gradual improvement in performance, moving from lower to higher performance metrics, which is also shown in Figure 3. Across

Table 9. Performance of Qwen2.5-3B-Instruct with Preserved Functional Networks.

	10	64	128	256	512
CoLA	0.0000	0.6913	0.6913	0.6913	0.6913
	1500	6694	8330	10602	6349
MRPC	0.0000	0.6814	0.5245	0.6373	0.6324
	1219	7556	10390	12042	12733
SST-2	0.0092	0.8200	0.8830	0.8888	0.8899
	914	4592	7223	9686	11027
MNLI	0.0014	0.2546	0.2476	0.2740	0.2725
	2116	8319	10064	11285	12080
QNLI	0.0002	0.2720	0.4077	0.3948	0.3967
	750	7569	9478	10368	11043
AGNEWS	0.1201	0.0061	0.7280	0.7205	0.7213
	1876	7423	10274	11491	12118
SQUAD	0.0057	0.1900	0.1918	0.2102	0.2106
	2053	8436	10765	12272	13183

Table 10. Performance of ChatGLM3-6B-base with Preserved Functional Networks.

	10	64	128	256	512
CoLA	0.0000	0.6913	0.6913	0.6913	0.6913
	2967	12306	15966	20495	27832
MRPC	0.0000	0.7770	0.8186	0.8162	0.8162
	2344	13917	18520	23369	28697
SST-2	0.0000	0.8624	0.9300	0.9381	0.9404
	1235	9390	14854	18702	26513
MNLI	0.0000	0.2123	0.2041	0.2062	0.2103
	3399	12569	15586	20103	25080
QNLI	0.0000	0.1545	0.1157	0.1078	0.1067
	905	13846	22341	28645	30838
AGNEWS	0.0000	0.9036	0.9087	0.9128	0.9128
	2098	11831	18540	26489	32864
SQUAD	0.0001	0.8655	0.9016	0.9023	0.9021
	2849	16150	21903	26646	30226

all models, it is clear that the number of neurons identified as important increases as more functional networks are incorporated. Our analysis reveals that, in practice, only approximately 10% of the total neurons in the model are necessary to maintain performance at an acceptable level. This observation is crucial because it indicates that there may be substantial opportunities to improve the efficiency of AI models. By identifying and utilizing only the most critical neurons, we can potentially develop methods for creating more resource-efficient models without sacrificing performance. This insight could pave the way for advancements in AI model optimization, leading to lower computational costs and greater accessibility of AI technologies.

5. Discussion and Conclusion

The present study introduces a novel approach to understanding LLM by applying methods inspired by the research of cognitive neuroscience on FBN. Our findings reveal that

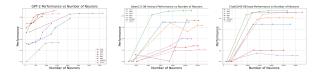


Figure 3. The performance changes of the models as the number of decomposed functional networks increases.

LLMs exhibit similar functional patterns as observed in human brains, which are crucial for their effective operation.

One of our key observations shows that only a small subset of these functional networks (approximately 10% of the total neurons) are necessary to maintain satisfactory performance levels. By identifying and leveraging these critical networks, future research could focus on developing more resource-efficient models with lower computational cost.

Our interdisciplinary approach, which combines insights from cognitive neuroscience and artificial intelligence, offers a promising direction for future research. The application of neuroscience concepts to AI not only enhances our understanding of LLM mechanisms but also opens new avenues for innovation. For instance, techniques used to identify FBNs in the human brain can be adapted to improve the interpretability and efficiency of AI models. By drawing parallels between cognitive neuroscience and AI, our research underscores the value of interdisciplinary collaboration. Future work should continue to explore how neuroscience principles can inform AI design and optimization. Such efforts hold the promise of advancing both fields, leading to more powerful and efficient AI systems that can better serve diverse applications.

Our study also has some limitations. The algorithm employed in this research is ICA, which has various derivatives such as canICA (Varoquaux et al., 2010b). These variants can improve model's performance based on the unique characteristics of the dataset. Consequently, there is potential for the development of novel algorithms tailored specifically to the properties of LLMs.

Last but not least, our investigation focused solely on the MLP layers. Future work could extend this approach to other components within these models, such as attention mechanisms or embedding layers. By broadening the scope of analysis to include these additional modules, we can gain a more comprehensive understanding of how functional networks manifest in different components of LLMs.

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A. Appendix

A.1. Neuron Lesion Experiment

Figures 4 and 5 present the neuron lesion study conducted on the ChatGLM3-6B-base model for the task of long-text summarization. Specifically, the study involves randomly masking neurons within the model and comparing the performance with masked neurons that are part of functional networks.

Prompt:

Summarize the following article in brief: (CNN) The Palestinian Authority officially became the 123rd member of the International Criminal Court on Wednesday, a step that gives the court jurisdiction over alleged crimes in Palestinian territories. The formal accession was marked with a ceremony at The Hague, in the Netherlands, where the court is based. The Palestinians signed the ICC\'s founding Rome Statute in January, when they also accepted its jurisdiction over alleged crimes committed "in the occupied Palestinian territory, including East Jerusalem, since June 13, 2014." Later that month, the ICC opened a preliminary examination into the situation in Palestinian territories, paving the way for possible war crimes investigations against Israelis. As members of the court, Palestinians may be subject to counter-charges as well. Israel and the United States, neither of which is an ICC member, opposed the Palestinians\' efforts to join the body. But Palestinian Foreign Minister Riad al-Malki, speaking at Wednesday's ceremony, said it was a move toward greater justice. "As Palestine formally becomes a State Party to the Rome Statute today, the world is also a step closer to ending a long era of impunity and injustice," he said, according to an ICC news release. "Indeed, today brings us closer to our shared goals of justice and peace." Judge Kuniko Ozaki, a vice president of the ICC, said acceding to the treaty was just the first step for the Palestinians. "As the Rome Statute today enters into force for the State of Palestine, Palestine acquires all the rights as well as responsibilities that come with being a State Party to the Statute. These are substantive commitments, which cannot be taken lightly," she said. Rights group Human Rights Watch welcomed the development. "Governments seeking to penalize Palestine for joining the ICC should immediately end their pressure, and countries that support universal acceptance of the court's treaty should speak out to welcome its membership," said Balkees Jarrah, international justice counsel for the group. "What\'s objectionable is the attempts to undermine international justice, not Palestine\'s decision to join a treaty to which over 100 countries around the world are members." In January, when the preliminary ICC examination was opened, Israeli Prime Minister Benjamin Netanyahu described it as an outrage, saying the court was overstepping its boundaries. The United States also said it "strongly" disagreed with the court's decision. "As we have said repeatedly, we do not believe that Palestine is a state and therefore we do not believe that it is eligible to join the ICC," the State Department said in a statement. It urged the warring sides to resolve their differences through direct negotiations. "We will continue to oppose actions against Israel at the ICC as counterproductive to the cause of peace," it said. But the ICC begs to differ with the definition of a state for its purposes and refers to the territories as "Palestine." While a preliminary examination is not a formal investigation, it allows the court to review evidence and determine whether to investigate suspects on both sides. Prosecutor Fatou Bensouda said her office would "conduct its analysis in full independence and impartiality." The war between Israel and Hamas militants in Gaza last summer left more than 2,000 people dead. The inquiry will include alleged war crimes committed since June. The International Criminal Court was set up in 2002 to prosecute genocide, crimes against humanity and war crimes. CNN\'s Vasco Cotovio, Kareem Khadder and Faith Karimi contributed to this report.

Masked 15% ChatGLM3-6B Neurons:

The Palestinian Authority has officially become the 123rd member of the International Criminal Court. This gives the court jurisdiction over alleged crimes in Palestinian territories. The formal accession was marked with a ceremony at The Hague, in the Netherlands, where the court is based. The Palestinians signed the ICC's founding Rome Statute in January and accepted its jurisdiction over alleged crimes committed "in the occupied Palestinian territory, including East Jerusalem, since June 13, 2014." The ICC opened a preliminary examination into the situation in Palestinian territories, paving the way for possible war crimes investigations against Israelis. As members of the court, Palestinians may be subject to counter-charges as well. Israel and the United States, neither of which is an ICC member, opposed the Palestinians' efforts to join the body. But Palestinian Foreign Minister Riad al-Malki, speaking at Wednesday's ceremony, said it was a move toward greater justice.

<u>Reference Answer:</u>

 $\begin{tabular}{ll} Membership gives the ICC jurisdiction over alleged crimes committed in Palestinian territories since last June . $$\arrownian Israel and the United States opposed the move, which could open the door to war crimes investigations against Israelis. $$\arrownian Israelis and $$\arrownian Israelis are the property of the property$

Figure 4. Random masked 15% neurons in ChatGLM3-6B-base.

Masked 10 Functional Networks Respectively:

Components 1: activate neuron num :4016/114688

The Palestinian Authority officially became the 123rd member of the International Criminal Court on Wednesday, as the court gained jurisdiction over alleged crimes in Palestinian territories. Palestinians may be subject to counter-charges as well as possible war crimes investigations against Israelis. Israel and the United States opposed the move, but Palestinian Foreign Minister Riad al-Malki said it was a move toward greater justice. Palestine acquied all the rights as well as responsiveness as a State Party to the ICC, as the preliminary examination was opened in January.

Components 2: activate neuron num :2791/114688

Components 3: activate neuron num :2141/114688 I apologize for the thul in the OPEN thread.

Components 4: activate neuron num :1906/114688

The Palestinian Authority has become the 123nd member of the International Criminal Crime 是非常非常重要的 the ICC. The Palestinian簽ed the ICC's founding Rome Statuate in January, which also marked as theICA's jurisdiction over Allegations of acne in Palestinian charge. PalestinianForecommin Foreign Minister Riad al-Malki said that it was a step Towards greater justice. TheICCA and Israel and the United States, shun 我们就不得不考虑它出现了的事实. TheICCAICICICed the Palestinian's efforts to join the group. .

Components 5: activate neuron num :2925/114688

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Components 6: activate neuron num :2663/114688

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Components 7: activate neuron num :3601/114688

Components 8: activate neuron num :2590/114688

The international

Components 9: activate neuron num :1795/114688

渡'));" next to

Components 10: activate neuron num :761/114688

The 123rd member of the International Criminal Court (ICCC) is the Palestinian Authority, which has accepted the ICC's founding Rome Statute in January, and is now a State Party to the treaty. The Palestinians may be subject to countercharges as well. The ICC opened a preliminary examination into the situation in Palestinian territories, and the process is expected to lead to possible war crimes investigations against Israelis. The Israeli and US opposition to the Palestinians' efforts to join the body has been胎肪, and the process is expected to lead to war. The process is expected to lead to possible war crimes investigations against Israelis. The process is expected to lead to possible war crimes investigations against Israelis.

Figure 5. Masked 10 functional networks respectively in ChatGLM3-6B-base.