Unveiling In-Context Learning: A Coordinate System to Understand Its Working Mechanism

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Abstract

Large language models (LLMs) exhibit remarkable in-context learning (ICL) capabilities. However, the underlying working mechanism of ICL remains poorly understood. Recent research presents two conflicting views on ICL: One emphasizes the impact of similar examples in the demonstrations, stressing the need for label correctness and more shots. The other attributes it to LLMs' inherent ability of task recognition, deeming label correctness and shot numbers of demonstrations as not crucial. In this work, we provide a Two-Dimensional Coordinate System that unifies both views into a systematic framework. The framework explains the behavior of ICL through two orthogonal variables: *whether similar examples are presented in the demonstrations* (perception) and *whether LLMs can recognize the task* (cognition). We propose the peak inverse rank metric to detect the task recognition ability of LLMs and study LLMs' reactions to different definitions of similarity. Based on these, we conduct extensive experiments to elucidate how ICL functions across each quadrant on multiple representative classification tasks. Finally, we extend our analyses to generation tasks, showing that our coordinate system can also be used to interpret ICL for generation tasks effectively. $\frac{1}{1}$ $\frac{1}{1}$ $\frac{1}{1}$

1 Introduction

Large language models (LLMs) have demonstrated impressive in-context learning (ICL) capabilities [\(Brown et al.,](#page-9-0) [2020\)](#page-9-0), i.e., when provided with fewshot examples, LLMs can effectively perform a broad range of tasks without requiring parameter updates [\(Zhao et al.,](#page-12-0) [2021;](#page-12-0) [Min et al.,](#page-10-0) [2022a;](#page-10-0) [Su](#page-11-0) [et al.,](#page-11-0) [2022;](#page-11-0) [Wei et al.,](#page-11-1) [2023a\)](#page-11-1). The simplicity of this method, combined with its zero training cost and the versatility of applying a single model across

 1 Our code is publicly available at: <code>[https://github.com/](https://github.com/plclmezboss/2D-Coordinate-System-for-ICL)</code> [plclmezboss/2D-Coordinate-System-for-ICL](https://github.com/plclmezboss/2D-Coordinate-System-for-ICL).

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Figure 1: An overview of the proposed two-dimensional coordinate system for ICL. The y-axis represents cognition, indicating the model's ability to recognize tasks during ICL, while the x-axis represents perception, reflecting whether similar examples are included in the demonstrations.

various tasks, has made ICL a promising approach to fully leveraging the potential of LLMs.

However, the underlying working mechanism of ICL remains an open question [\(Dai et al.,](#page-9-1) [2022;](#page-9-1) [Akyürek et al.,](#page-9-2) [2022;](#page-9-2) [Olsson et al.,](#page-10-1) [2022;](#page-10-1) [Panwar](#page-11-2) [et al.,](#page-11-2) [2024\)](#page-11-2). Existing works hold two conflicting views to explain ICL: The first view argues *LLMs explicitly learn from similar examples in the demonstrations during the inference stage* [\(Liu](#page-10-2) [et al.,](#page-10-2) [2021\)](#page-10-2). Selecting demonstrations similar to the test sample and ensuring their label correctness, or increasing the number of demonstration shots can both improve the performance [\(Rubin et al.,](#page-11-3) [2022;](#page-11-3) [Ye et al.,](#page-12-1) [2023;](#page-12-1) [Levy et al.,](#page-10-3) [2023;](#page-10-3) [Bertsch](#page-9-3) [et al.,](#page-9-3) [2024;](#page-9-3) [Liu et al.,](#page-10-4) [2024\)](#page-10-4). The second view, on the contrary, suggests that *LLMs implicitly learn tasks required for downstream applications during the pre-training stage, and in-context demonstrations simply provide cues for them to recognize the task* [\(Xie et al.,](#page-12-2) [2022\)](#page-12-2). There have been empirical supports for this hypothesis which show that the performance of ICL is insensitive to label correctness of demonstrations, or the number of demonstration shots [\(Min et al.,](#page-10-5) [2022b;](#page-10-5) [Chen et al.,](#page-9-4) [2023;](#page-9-4) [Zhang et al.,](#page-12-3) [2024;](#page-12-3) [Zhu et al.,](#page-12-4) [2024\)](#page-12-4).

Although both of the above views hold in specific cases, neither can fully explain the working mechanism of ICL from a holistic perspective. In this work, we seek a unified framework encompassing both views to systematically unveil ICL. To do so, we first introduce the peak inverse rank metric to accurately identify the task recognition capability of LLMs. Based on this metric, we observe that LLMs do not always recognize tasks during ICL, even when correct labels and similar examples are provided in the demonstrations. Conversely, successful task recognition also does not necessarily require the presence of similar examples and correct labels. Hence, we suggest that the effectiveness of ICL should be described through the interactions of these two orthogonal variables, resulting in four distinct ICL scenarios. To conceptualize this intuitively, we represent each variable along two axes: The x-axis denotes perception, indicating the model's dependence on similar examples for reference. This mirrors human perception, where recognizing similar observed patterns and drawing analogies is crucial for interpreting new information. The y-axis represents cognition, reflecting the model's task recognition ability. Similar to human cognition, this involves recognizing the right logic learnt from past tasks and reasoning over it to draw the answer, rather than simply replicating observed patterns. Consequently, all ICL scenarios are visualized within a two-dimensional coordinate system, as depicted in Figure [1.](#page-0-1) In each quadrant of the coordinate system, we systematically analyze 8 models spanning up to 40B parameters across three major LLM families. We examine a wide range of classification tasks and have the following main findings:

- In the first quadrant, models are able to recognize the task and similar examples are included in the demonstrations. In this situation, *models can not only leverage their pre-trained knowledge to make predictions but also refer to the labels from similar examples if their pre-trained knowledge is insufficient*. However, if the labels of similar examples are incorrect, smaller models tend to replicate these incorrect labels, while larger models tend to rely on their pre-trained knowledge for making predictions.
- In the second quadrant, models are able to recognize the task but similar examples are not

included in the demonstrations. In this situation, *models primarily leverage their pre-trained knowledge to make predictions*. Moreover, given that each input-label pair plays an identical role in helping models recognize the task, increasing the number of demonstration shots does not significantly enhance the effectiveness of ICL.

- In the third quadrant, models cannot recognize the task and similar examples are also not included in the demonstrations. In this situation, *ICL fails to work*. Models fail to properly leverage the demonstrations and tend to blindly predict the label of the first example.
- In the fourth quadrant, models cannot recognize the task but similar examples are included in the demonstrations. In this situation, *models directly replicate the labels of similar examples*. Therefore, the performance of ICL depends entirely on whether the labels of similar examples match the ground truth labels of test samples. Additionally, larger models are better at recognizing similar examples, which increases their tendency to copy the labels from those examples.

In general, our findings indicate that for *similar* examples, their label correctness has a *consistent and significant* impact on ICL, especially in scenarios where the model cannot recognize the task and relies heavily on similar examples for inference (below the x-axis). Increasing the number of demonstration shots substantially improves ICL, as it raises the likelihood of matching similar examples. For *dissimilar* examples, label correctness primarily affects the model's *confidence in task recognition* (above the x-axis), but once the task is properly recognized, the effect becomes marginal.

Finally, considering the wide application of ICL in generation tasks [\(Agrawal et al.,](#page-9-5) [2022;](#page-9-5) [Sia and](#page-11-4) [Duh,](#page-11-4) [2023;](#page-11-4) [Garcia et al.,](#page-9-6) [2023\)](#page-9-6), we extend our analyses beyond classification tasks by conducting a thorough case study on a machine translation task. This study demonstrates that our coordinate system can also effectively capture the behavior of ICL in generation tasks. In summary, our proposed coordinate system provides a principled and universal way to understand the working mechanism of ICL.

2 A 2D Coordinate System for ICL

2.1 The Coordinate Axes

Example Similarity. Recent works have shown that including similar examples to the test sample in the ICL demonstrations can lead to improved performance outcomes [\(Liu et al.,](#page-10-2) [2021;](#page-10-2) [Rubin et al.,](#page-11-3) [2022;](#page-11-3) [Ye et al.,](#page-12-1) [2023;](#page-12-1) [Levy et al.,](#page-10-3) [2023;](#page-10-3) [Bertsch](#page-9-3) [et al.,](#page-9-3) [2024\)](#page-9-3). Inspired by this finding, we believe that the presence of examples similar to the test sample in the demonstrations is an important variable for distinguishing different ICL scenarios.

Given the broad concept of similarity, we seek to explore whether the similarity in ICL leans more towards semantic similarity or lexical similarity. To investigate this question, we perform comprehensive experiments in Appendix [A,](#page-13-0) where we construct three different types of examples, including semantically similar but lexically dissimilar examples, lexically similar but semantically opposite examples, and randomly selected examples. We assign different semantically unrelated label words to these three elements and observe which semantically unrelated word the model predicts. We find that although ICL tends to slightly favor semantically similar examples over lexically similar ones, the preference for both is significantly greater than randomly selected examples. Thus, regardless of whether the similarity is lexical or semantic, as long as demonstrations contain examples of either type, we consider them to contain similar examples.

Task Recognition. Instead of capitalizing on similar examples, some previous research has demonstrated that in-context demonstrations simply provide information for the model to identify the task to deal with, after which prior knowledge obtained from pretraining data is leveraged to make predictions [\(Xie et al.,](#page-12-2) [2022;](#page-12-2) [Min et al.,](#page-10-5) [2022b\)](#page-10-5). This indicates that task recognition is also a crucial factor for ICL. However, whether models can always recognize tasks when performing ICL remains an open question. Hence, there is an urgent need for a method to quantitatively determine the model's task recognition ability.

A recent work by [Wang et al.](#page-11-5) [\(2023\)](#page-11-5) reveals that label words act as semantic anchors, accumulating information of corresponding demonstrations in the shallow layers. The information associated with these anchors is then aggregated in the deeper layers to form the model's final predictions. Inspired by this, we find that examining whether the hidden states of label tokens at internal layers possess task semantics can serve as an indicator of if ICL has recognized the task. We use a technique called the logit lens [\(nostalgebraist,](#page-10-6) [2020;](#page-10-6) [Geva](#page-9-7) [et al.,](#page-9-7) [2021;](#page-9-7) [Dar et al.,](#page-9-8) [2023\)](#page-9-8), which projects transformer representations into the vocabulary space, thereby enabling us to interpret abstruse representations in a human-interpretable manner. Specifically, we project the hidden states of each layer corresponding to the label tokens into the vocabulary space by multiplying them with the pre-trained language modeling head E , thus decoding the hidden states of each layer. After obtaining the vocabulary distribution of the hidden states for each layer, we calculate the inverse of the rank of the *task-representative* token within the vocabulary distribution for each layer. We use the peak inverse rank (*PIR*) across all layers as our metric to determine whether ICL has recognized the task. For clarity, we provide the formal definition of *PIR* in Appendix [K.](#page-18-0) A high *PIR* indicates that ICL has successfully recognized the task, while a low *PIR* suggests a lack of task understanding capabilities.

To illustrate this, we consider an ICL scenario for the World Capital task: *"Word: France Label: Paris Word: Germany Label: Berlin Word: Italy Label:"*. We select the last label word *"Berlin"* to report the *PIR* of the task-representative token *"capital"* in Figure [2,](#page-3-0) where the *PIR* reaches 1 at layer 17. For the same task, we replace all labels with semantically irrelevant words to prevent ICL from recognizing the task. This setting, called task learning, was first introduced by [Pan](#page-11-6) [\(2023\)](#page-11-6). Concretely, we replace the first label *"Paris"* with *"bar"* and the second label *"Berlin"* with *"foo"*. We still select the last label *"foo"* to report the *PIR* of *"capital"* in Figure [2,](#page-3-0) where the *PIR* drops to 0.

Based on *PIR*, we observe that models do not always recognize tasks during ICL, even when the demonstrations are entirely composed of correct input-label pairs (refer to Appendix [C\)](#page-14-0). Furthermore, we demonstrate that the presence of similar examples and the ability of task recognition are orthogonal to each other (refer to Appendix [D\)](#page-15-0). Given this, we take whether models can recognize tasks during the execution of ICL as the second variable to distinguish different ICL scenarios. We will use **PIR** as the criterion to select datasets for ICL that can and cannot recognize tasks.

2.2 ICL Scenario Exploration

Following the above discussions, ICL scenarios can be described comprehensively using two variables: task recognition and example similarity. These two variables result in four combinations, which can be visualized in a two-dimensional coordinate system (see Figure [1\)](#page-0-1). In the positive half of the y-axis,

label token using Llama-2-7B, before and

after replacing labels.

Figure 4: The *PIR* of *"color"* at the label token of Similiar(T), when the label of Similiar(T) is correct and incorrect.

the model is capable of recognizing tasks, while in the negative half, it is not. Similarly, the positive half of the x-axis signifies the presence of similar examples, whereas their absence is indicated in the negative half.

Importantly, we establish this two-dimensional coordinate system not only to conceptualize the four possible combinations of ICL scenarios but also to consider the two variables on a continuous scale. Specifically, as the model's confidence in recognizing tasks increases, denoted by *PIR* approaching one, the y-coordinate value rises. Likewise, as the similarity between the provided examples and the test sample increases, the x-coordinate value rises. In the following section, we will provide a detailed description of how ICL works within each quadrant of the coordinate system.

3 Experiments and Results

3.1 Experimental Settings

Given that it is not intuitively clear whether models can recognize the task in a particular dataset, which in fact must be verified using the metric *PIR*, we directly enumerate the classification datasets in which models can and cannot recognize the task. For detailed proofs, please refer to Appendix [C.](#page-14-0)

Datasets in Which Models Can Recognize Tasks. These datasets are used for the upper part of the xaxis. We employ the Stanford Sentiment Treebank Binary (SST-2) [\(Socher et al.,](#page-11-7) [2013\)](#page-11-7) for sentiment analysis. In addition, we create two datasets for the World Capitals and Reasoning about Colored Objects tasks, which contain 50 hand-crafted pairs of *country-capital* and *object-color*, respectively. The detailed data are provided in Appendix [F.](#page-16-0)

Datasets in Which Models Cannot Recognize Tasks. These datasets are used for the lower part of the x-axis. We utilize the Text REtrieval Conference (TREC) Question Classification dataset

[\(Li and Roth,](#page-10-7) [2002;](#page-10-7) [Hovy et al.,](#page-9-9) [2001\)](#page-9-9) for question type classification and the EmoContext (emo) [\(Chatterjee et al.,](#page-9-10) [2019\)](#page-9-10) for emotion classification.

Models. We adopt a comprehensive suite of models, including GPT2-XL (1.61B) [\(Radford et al.,](#page-11-8) [2019\)](#page-11-8) and GPT-J (6B) [\(Wang,](#page-11-9) [2021\)](#page-11-9) from the GPT series; Llama-2-7B, Llama-2-13B, and their instruction-tuned counterparts from the Llama series [\(Touvron et al.,](#page-11-10) [2023\)](#page-11-10); and Falcon-40B, along with its instruction-tuned variant from the Falcon series [\(Almazrouei et al.,](#page-9-11) [2023\)](#page-9-11).

Prompt Format. We use neutral delimiters to avoid providing task-specific information. See Appendix [E](#page-16-1) for details.

Accuracy Metric. We consider an individual prediction correct only when the token with the highest logit within the *entire* vocabulary matches the label of the test sample. Accuracy is the proportion of correct predictions across the whole dataset.

3.2 First Quadrant

In this quadrant, models can recognize tasks when performing ICL, and the demonstrations contain examples similar to the test sample. In this situation, since models can rely not only on their pre-trained knowledge after task recognition but also on the labels of similar examples to make predictions, we aim to determine how these two factors work together.

Implementation Details. Here, we consider an extreme setup where we artificially add the test sample into the demonstration, identifying it as a similar example with the highest similarity, denoted as Similiar(T). We consider three settings: Similiar(T) with an incorrect label, Similiar(T) with the correct label, and ICL without similar examples. For the first setting, we select a label from the label space that differs from the test sample's label and assign it to the $Similar(T)$. For the

Figure 5: In the 20th layer, the attention scores of the last token ":" for all tokens. All label tokens are marked in red.

Figure 7: For the emo dataset, the preference of different models for label tokens at different absolute positions.

second setting, we select the label from the label space that matches the test sample's label and assign it to the Similiar(T). For the third setting, we select examples from the training dataset with no similarity to the test sample to serve as demonstrations. We use $k = 6$ in-context examples. The results reflect averages from five random seeds and all datasets in which models can recognize tasks.

Experimental Results. Figure [3](#page-3-0) shows that (1) adding $Similar(T)$ with the correct label in the demonstrations generally improves performance compared to ICL without similar examples (i.e., ICL falling within the second quadrant), although there is a slight performance decline for Llama-2-7B-chat and Llama-2-13B-chat. This indicates that models can not only utilize their pre-trained knowledge but also refer to the correct label of Similiar(T) when their pre-trained knowledge is insufficient. (2) However, including $Similar(T)$ with an incorrect label in the demonstrations induces a state of "confusion", making models neither completely rely on their pre-trained knowledge for predictions (performing worse than ICL without similar examples) nor completely overwrite their predictions with the label of Similiar(T).

In-Depth Analysis. To comprehend the causes of "confusion" experienced by models, we present insights through a case study on the Reasoning about Colored Objects task using Llama-2-7B. We first consider the scenario when the label of Similiar(T) is correct: *"Word: apple Label: red Word: lime Label: green Word: grape Label: purple Word: lime Label:"*. We report the *PIR* of the task-representative token *"color"* at the label *"green"* of *"lime"*, as shown in Figure [4.](#page-3-0) Next, we substitute the label token *"green"* with the incorrect color *"gold"*, thereby constructing a Similiar(T) with an incorrect label in the demonstrations. Similarly, we report the *PIR* of the task-representative token *"color"* at the label *"gold"* of *"lime"*, also

depicted in Figure [4.](#page-3-0) As illustrated, replacing the correct label with an incorrect one decreases the model's confidence in the Reasoning about Colored Objects task at the label token of Similiar(T). Additionally, due to $Similar(T)$ having the highest semantic and lexical similarity, the last token of the input at the intermediate layer assigns the highest attention score to *"gold"* among all label tokens. For instance, consider the 20th layer, as shown in Figure [5.](#page-4-0) Consequently, at this layer, the hidden state for *"gold"* contributes more significantly to the residual stream of the last token compared to the hidden states of other label tokens. This leads to a reduction of task semantics and an increase of the semantics associated with the word *"gold"* within the hidden states of the last token. As a result, the model faces uncertainty about whether to rely on pre-trained knowledge for making predictions or to directly output the *"gold"* token, leading to the "confusion" phenomenon.

Additionally, as observed in Figure [3,](#page-3-0) when encountering the "confusion" phenomenon, models with smaller parameter sizes tend to output incorrect labels, whereas models with larger parameter sizes are more likely to rely on their pre-trained knowledge for the output. This indicates that when the label of $Similar(T)$ is incorrect, the confidence in the task at that label token increases as the model size increases.

Conclusion

In the first quadrant, models can leverage their pre-trained knowledge to make predictions once they recognize the task and can also refer to the labels from similar examples if their pre-trained knowledge is insufficient. However, if the labels of similar examples are incorrect, smaller models tend to replicate these incorrect labels, while larger models tend to rely on their pre-trained knowledge for making predictions.

3.3 Second Quadrant

In this quadrant, models can recognize tasks when performing ICL, but the demonstrations do not contain examples similar to the test sample. Due to the absence of similar examples, the phenomenon described in the first quadrant—where the incorrect label semantics of similar examples significantly affect the hidden states of the last token—does not occur. Therefore, randomly replacing labels in this quadrant does not substantially impact ICL performance, which is consistent with existing work [\(Min et al.,](#page-10-5) [2022b\)](#page-10-5). The detailed experimental results can be found in Appendix [G.](#page-16-2)

Here, we would like to discuss a new question: *Since the label token of each example provides the same task semantics (because all examples are dissimilar to the test sample), does this imply that we can achieve good ICL performance with only a very small number of examples?*

Implementation Details. We use the "zero-shot" approach as our baseline, where the model is only given an instruction that specifies the task. Detailed instructions for each dataset can be found in Appendix [I.](#page-17-0) Subsequently, we remove the instruction and provide the model with only demonstrations, then incrementally increase the number of shots. The results are averaged over five random seeds and datasets in which models can recognize tasks.

Experimental Results. The experimental results are shown in Figure [6.](#page-4-0) It can be observed that with only a single input-label pair, the performance of ICL significantly surpasses that of the zero-shot setting. Further increasing the number of demonstration shots results in very limited performance improvement. These results confirm our hypothesis: The roles of each label token overlap, and adding more examples merely reinforces the model's confidence in correctly identifying the task.

Conclusion

In the second quadrant, models primarily leverage their pre-trained knowledge to make predictions. Moreover, given that each input-label pair plays an identical role in helping models recognize tasks, increasing the number of in-context examples does not significantly enhance the effectiveness of ICL.

3.4 Third Quadrant

In this quadrant, models cannot recognize tasks when performing ICL, and the demonstrations also do not contain examples similar to the test sample. This represents the worst-case scenario among all quadrants. As illustrated in Figure [9,](#page-7-0) the performance of one-shot ICL in this quadrant is significantly worse than the zero-shot setting for all models. In this quadrant, what do the models rely on to make predictions when performing ICL?

Implementation Details. We consider an ICL setting where each example's label corresponds to a different label class from the dataset, covering all labels of the dataset (i.e., 4-shot ICL for emo and 6-shot ICL for TREC), to observe the predictive behavior of ICL. To ensure that the ICL output remains within the label space, we prefix the input with instructions to limit the output range without specifying the task. We select an equal number of samples from each label class in the dataset to serve as the set of test samples. For each test sample, we manually select demonstration examples that have virtually no semantic similarity or lexical similarity. Instead of focusing on whether the output matches the ground truth, we focus on the absolute position, specifically which position's label token will be predicted. Here we report the experimental results on the emo dataset in Figure [7.](#page-4-0) The results for TREC can be found in Appendix [H.](#page-17-1)

Experimental Results. As shown in Figure [7,](#page-4-0) we find that models exhibit a strong positional bias in this quadrant. Specifically, we observe that for almost all models, there is a significantly high proportion of instances for which the label of the first input-label pair is predicted. In contrast, the proportion of predictions for the labels of other pairs is notably lower. We attribute this to the attention sink phenomenon discovered by [Xiao et al.](#page-11-11) [\(2024\)](#page-11-11), where models tend to allocate more attention to the initial tokens during prediction.

Conclusion

In the third quadrant, ICL fails to work. Specifically, models fail to leverage the ICL content for making predictions and tend to predict the label of the first example.

3.5 Fourth Quadrant

In this quadrant, models cannot recognize tasks when performing ICL, but the demonstrations contain examples similar to the test sample. Since models in this context can only reference similar examples, we hypothesize that the accuracy of ICL predictions hinges on whether the labels of these similar examples align with the ground-truth label of the test sample.

Implementation Details. Similar to the experimental setup in the first quadrant, during each ICL inference, we randomly select a label from the dataset that differs from the test sample's label and assign it to $Similar(T)$. Since we aim to verify whether models in this quadrant rely on the labels of similar examples to make predictions, we use the proportion of predictions for the incorrect label assigned to Similiar(T) as our accuracy metric. We adopt $k = 12$ in-context examples. The results reflect averages from five random seeds and all datasets in which models cannot recognize tasks.

Experimental Results. As illustrated in Figure [8,](#page-7-0) the proportion of the model's predictions being the same as the incorrect label of $Similar(T)$ is high. Notably, as the model size increases, this proportion reaches an exceptionally high level, indicating that the model almost entirely relies on the label of Similiar(T) for its predictions. We posit that this phenomenon arises because, as the model size increases, its ability to discern the similarity of examples improves, thereby directing more attention to similar examples.

[Conclusion]

In the fourth quadrant, models directly replicate the labels of similar examples. Therefore, the performance of ICL depends heavily on whether the labels of similar examples match the ground truth labels of test samples. Additionally, larger models are better at recognizing similar examples, which increases their tendency to copy the labels from these examples.

4 Effects of Label Correctness and Demonstration Shot Number

As previous research presents two conflicting views about the effects of label correctness and shot number to ICL, in this section, we provide a brief summary about how our proposed coordinate system can explain this conflict in a more principled way.

Label Correctness. As long as similar examples are present in the demonstrations, the correctness of their labels consistently plays a crucial role in determining ICL performance, as discussed in Section [3.2](#page-3-1) and Section [3.5.](#page-6-0) For dissimilar examples, when the ICL scenario is positioned above the x-axis, label correctness can impact the models' confidence in task recognition. Conversely, when positioned below the x-axis, label correctness does not decisively influence the models' predictions. In the third quadrant, models predominantly predict the label of the first example, whereas in the fourth quadrant, models are more likely to replicate the labels of similar examples.

Demonstration Shot Number. Above the x-axis, increasing the shot number does not significantly affect ICL performance, as the models primarily rely on their pre-trained knowledge to make predictions once they recognize the task. Additional shots merely reinforce the models' confidence in correctly identifying the task. However, below the x-axis, increasing the shot number significantly impacts ICL performance. The more shots there are, the higher the likelihood that the models will find more similar examples to refer to. This approach can transition ICL from the third quadrant to the fourth quadrant and enhance the likelihood of including more similar examples for reference within the fourth quadrant.

5 How to Make ICL Work Effectively?

From our proposed ICL coordinate system, it is evident that the effectiveness of ICL improves as the values of the x and y coordinates increase, moving towards the upper right quadrant. Conversely, as the values of the x and y coordinates decrease, moving towards the lower left quadrant, the effectiveness of ICL diminishes. These observations provide valuable insights into the enhancement of ICL performance. Specifically, improvements can be made by: (1) strengthening the confidence in task recognition, and (2) providing examples with higher similarity in the demonstrations. We select the most challenging third quadrant to demonstrate how ICL can be made effective through these two directions.

Including a task description instruction before ICL examples can facilitate task recognition.

for the incorrect label corresponding to Similiar(T) on various models.

Figure 9: The average accuracy of (1,6,12)-shot ICL w/o instructions and (0,1)-shot ICL with instructions.

Figure 10: The *PIR* of *"question"* at the label token *"Human"* on Llama-2-7Bchat, before and after adding instruction.

As illustrated in Figure [10,](#page-7-0) we conduct a one-shot ICL case study on the TREC dataset using Llama-2-7B-chat (for specific instructions and details on the one-shot ICL, refer to Appendix [J\)](#page-17-2). Without the task description instruction, the *PIR* of the taskrepresentative token *"question"* at the label is nearly zero. However, after adding the task description instruction, the *PIR* increases to 0.083 (ranking 12th in the vocabulary distribution), suggesting that the model recognizes the task to a certain extent. This demonstrates that instructions can promote task recognition. This finding provides methodological support for the implementation of the first direction. As shown in Figure [9,](#page-7-0) the effectiveness of instruction one-shot ICL is significantly better than that of one-shot ICL without instructions.

Both retrieval and long-context ICL can provide examples with higher similarity. For the second direction, a commonly utilized method in recent research is to retrieve a highly similar subset of examples to serve as demonstrations for each test set example, which has been shown to be effective [\(Liu](#page-10-2) [et al.,](#page-10-2) [2021;](#page-10-2) [Rubin et al.,](#page-11-3) [2022\)](#page-11-3). Additionally, as the context lengths of LLMs continue to increase, another method to achieve this goal is to continuously increase the number of input-label pairs in the demonstrations. The more input-label pairs included, the higher the likelihood that the model will find more similar examples to refer to during ICL. As shown in Figure [9,](#page-7-0) the performance of one-shot ICL is consistently worse than zero-shot for all models. However, each time we increase the number of shots, the performance of ICL improves significantly. This aligns with the conclusions of [Bertsch et al.](#page-9-3) [\(2024\)](#page-9-3), who find that long-context ICL can be surprisingly effective, with most of the improvement stemming from attending to similar examples rather than task recognition.

6 Extension to Generation Tasks

Given the recent success of ICL in generation tasks [\(Agrawal et al.,](#page-9-5) [2022;](#page-9-5) [Sia and Duh,](#page-11-4) [2023;](#page-11-4) [Garcia](#page-9-6) [et al.,](#page-9-6) [2023\)](#page-9-6), we aim for our two-dimensional coordinate system to enhance the understanding of ICL behavior not only in classification tasks but also in generation tasks. This is non-trivial, as almost no prior work has conducted an in-depth analysis of in-context generation tasks.

To extend our coordinate system to generation tasks, we face two main challenges: (1) In classification tasks, predicting a single label token is sufficient, whereas generation tasks require predicting an entire sentence. (2) We determine whether ICL recognizes the task by examining if the hidden states of label tokens at internal layers possess task semantics. However, for generation tasks, the label for each example in the demonstrations is not a single word but a complete sentence. To address these challenges, we formulate a hypothesis, H:

We treat a generation task as multiple smaller sub-classification tasks focused on predicting each token. In each sub-classification task, every label sentence contains a token that serves as the label token. However, the position of the label token in each label sentence changes when predicting different tokens.

According to this hypothesis, each ICL subclassification task in generation tasks is equivalent to the standard ICL in classification tasks we previously studied, as both involve predicting a single token, with the label token still represented by a single token. However, verifying our hypothesis H for most generative tasks is challenging. In classification tasks, the task of predicting each token (i.e., a label token) is very clear and specific. For instance, in SST-2, it is a *"sentiment"* task. In contrast, for generative tasks, predicting a token may involve mimicking the abstract style of a segment

(a) *PIR* of *"subject"* on each token of the final label when predicting *"He"*.

(b) *PIR* of *"verb"* on each token of the final label when predicting *"reads"*.

(c) *PIR* of *"object"* on each token of the final label when predicting *"book"*.

Figure 11: For the in-context translation task with a strict subject-verb-object structure: "Sentence: 她喝水。 Label: She drinks water. Sentence: 我们吃米饭。 Label: We eat rice. Sentence: 他们看电视。 Label: They watch TV. Sentence: 他读 书。 Label:" , the *PIR* of *"subject," "verb," "object"* at each token of the final label sentence when respectively predicting *"He," "reads," "book,"* on Llama-2-7B.

of an input-label pair, or in more extreme cases, predicting just a complete article. Explicitly describing all the tasks that are involved in predicting these tokens is very difficult.

For this reason, we consider an in-context translation task, with all examples in the demonstrations adhering to a strict *subject-verb-object* structure, as illustrated in Figure [11.](#page-8-0) If the ICL output also conforms to this strict subject-verb-object structure, it indicates that the tokens *"He"*, *"reads"*, and *"book"* are generated by performing the explicit sub-tasks of *"subject"*, *"verb"*, and *"object"*, respectively. We analyze the label sentence of the last example in the demonstration. Figure [11](#page-8-0) illustrates that for the subject token *"He"*, the label token is *"They"*, with the other tokens rarely generating *"subject"* semantics. For the verb token *"reads"*, the label token is *"watch"*, with the other tokens seldom generating *"verb"* semantics. Similarly, for the object token *"book"*, the label token is *"TV"*, and the other tokens rarely generate *"object"* semantics. This phenomenon of label token sliding within the label sentence provides evidence supporting the plausibility of our hypothesis H .

Therefore, by decomposing the entire generative task into multiple sub-classification tasks, our coordinate system can help understand the working mechanisms of in-context generative tasks.

7 Related Work

Current research on ICL mechanisms mainly falls into the following categories:

Theoretical Framework. Recently, numerous studies have employed theoretical frameworks to enhance the understanding of ICL. [Xie et al.](#page-12-2) [\(2022\)](#page-12-2) describe ICL as implicit Bayesian inference. [Garg](#page-9-12) [et al.](#page-9-12) [\(2023\)](#page-9-12) demonstrate that transformers can learn linear functions through ICL. Additionally, several studies conceptualize ICL as gradient descent on an implicit internal model [\(Akyürek et al.,](#page-9-2) [2022;](#page-9-2) [Von Oswald et al.,](#page-11-12) [2023;](#page-11-12) [Dai et al.,](#page-9-1) [2022\)](#page-9-1). [Wei et al.](#page-11-13) [\(2023b\)](#page-11-13) and [Pan](#page-11-6) [\(2023\)](#page-11-6) disentangle ICL into task recognition and task learning.

Empiricism. Various factors affecting ICL have been studied, such as the order of examples [\(Lu](#page-10-8) [et al.,](#page-10-8) [2022\)](#page-10-8), the choice of label words [\(Min et al.,](#page-10-5) [2022b;](#page-10-5) [Yoo et al.,](#page-12-5) [2022\)](#page-12-5), and the selection of demonstrations [\(Liu et al.,](#page-10-2) [2021;](#page-10-2) [Rubin et al.,](#page-11-3) [2022\)](#page-11-3). Effective demonstration strategies [\(Ye et al.,](#page-12-1) [2023;](#page-12-1) [Li et al.,](#page-10-9) [2023\)](#page-10-9) can notably boost ICL performance.

Logit Lens. Recently, some studies use the logit lens technique [\(nostalgebraist,](#page-10-6) [2020;](#page-10-6) [Geva et al.,](#page-9-7) [2021\)](#page-9-7) to project complex feature representations into the vocabulary space to study the mechanisms of ICL. [Merullo et al.](#page-10-10) [\(2023\)](#page-10-10) discover three distinct stages of processing by decoding the next token prediction at each layer. [Todd et al.](#page-11-14) [\(2024\)](#page-11-14) find that a small number of attention heads transport a compact representation of the demonstrated task. [Yu and Ananiadou](#page-12-6) [\(2024\)](#page-12-6) provide insights into the mechanisms of ICL in the context of task learning.

8 Conclusion

In this paper, we map two variables *whether LLMs can recognize the task* and *the presence of similar examples in the demonstrations* onto the y-axis and x-axis of a 2D coordinate system, to visualize ICL scenarios. First, for classification tasks, we conduct a systematic study of the proposed coordinate system and describe in detail the working mechanisms of ICL in each quadrant. Then, we extend our analyses beyond classification tasks through a thorough case study on a machine translation task. Our proposed coordinate system offers a universal framework to better understand ICL.

Limitations

Our extensive studies, despite offering a principled and universal approach to understanding the working mechanism of ICL, have several limitations. First, our research primarily focused on conventional ICL paradigms, leaving other paradigms such as chain of thought prompting (CoT) [\(Wei](#page-11-1) [et al.,](#page-11-1) [2023a\)](#page-11-1) unexplored. Second, for generative tasks, we conducted a case study solely on in-context machine translation tasks adhering to a strict subject-verb-object structure. Third, due to hardware constraints, our investigation was primarily limited to models with up to 40 billion parameters. Further research replicating our study could use larger models with our 2D coordinate system to uncover more interesting findings.

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A Lexical Similarity or Semantical Simlarity

In this section, we explore whether models give significantly more attention to semantically similar examples (which delve into deeper meanings) or to lexically similar examples (which may have opposite semantics but share superficial similarities). We also consider randomly selected dataset examples as a baseline. For this purpose, in the context of task learning (a setup first introduced by [Pan](#page-11-6) [\(2023\)](#page-11-6), which replaces all labels with semantically irrelevant words to prevent ICL from recognizing the task), we include three elements in the demonstrations, each representing a different type of similarity to the test sample, and observe which element's label the model predicts. The definitions of these three elements are as follows:

- Example_{lexical}: An example that largely overlaps lexically with the test sample, yet differs semantically and carries a distinct label.
- Example_{semantic}: An example that is semantically similar to the test sample, but has minimal lexical overlap and carries the same label. Specifically, we achieve this by paraphrasing the test sample.
- Example_{baseline}: A randomly selected example from the dataset, with minimal lexical and semantic similarity to the test sample.

Notably, we find that when each element appears only once in the demonstrations, as in a 3-shot ICL scenario, models tend to generalize the pattern of label changes. For instance, if the three labels are sequentially "a," "b," and "c," the models are likely to predict "d." To mitigate this phenomenon, we replicate each element multiple times (in our experiments, three times). Empirical experiments show that this approach can ensure the models' predictions stay within the intended label space.

Models. We employ various models from the GPT series, including GPT2-Medium (355M) and GPT2-XL (1.61B) [\(Radford et al.,](#page-11-8) [2019\)](#page-11-8), as well as GPT-J (6B) [\(Wang,](#page-11-9) [2021\)](#page-11-9). To investigate the impact of instruction-tuning on similarity preferences, we also employ Llama-2-7B [\(Touvron](#page-11-10) [et al.,](#page-11-10) [2023\)](#page-11-10), Llama-3-8B [\(AI@Meta,](#page-9-13) [2024\)](#page-9-13), and Mistral-7B-v0.1 [\(Jiang et al.,](#page-10-11) [2023\)](#page-10-11), along with their instruction-tuned versions. All checkpoints of these models are sourced from the transformers library [\(Wolf et al.,](#page-11-15) [2019\)](#page-11-15).

Datasets. We adopt the Stanford Sentiment Treebank Binary (SST-2) [\(Socher et al.,](#page-11-7) [2013\)](#page-11-7) for sentiment analysis, Text REtrieval Conference Question Classification (TREC) [\(Li and Roth,](#page-10-7) [2002;](#page-10-7) [Hovy](#page-9-9) [et al.,](#page-9-9) [2001\)](#page-9-9) for question type classification, Emo-Context (emo) [\(Chatterjee et al.,](#page-9-10) [2019\)](#page-9-10) for emotion classification, and hate_speech18 [\(de Gibert](#page-9-14) [et al.,](#page-9-14) [2018\)](#page-9-14) for hate speech detection. For each dataset, we leverage GPT-4 [\(OpenAI et al.,](#page-10-12) [2024\)](#page-10-12) to generate 20 triplets, formatted as (Test Sample, Example_{semantic}, Example_{lexical}), that are tailored to the style of the dataset. After generation, these triplets undergo a manual selection process to ensure quality. In addition, for each triplet, we randomly select an example from the original dataset to serve as $Example_{baseline}$, thereby forming a complete demonstration. For detailed information on the triplets generated for each dataset, please refer to Appendix [B.](#page-14-1)

Implementation Details. In our experiments, the prompts consist solely of demonstrations without incorporating instructions. We employ neutral delimiters, specifically "Sentence:" and "Label:", to clearly separate the components of the demonstrations. This approach ensures that the models do not receive any task-specific information that could be inferred from the delimiters. Although previous works in the task learning setting typically employ semantically irrelevant words as labels, such as "foo" and "bar," we choose to label the elements with the initial letters of "lexical," "semantic," and "baseline" for ease of distinction. Consequently, the labels used for Example_{lexical}, Example_{semantic}, and Example_{baseline} are "l," "s," and "b," respectively. For each ICL prediction, we document the token that ranked the highest in the model's output distribution. Subsequently, across all predictions, we calculate the proportions of the tokens "l," "s," and "b" respectively. The experimental results are averaged over five random seeds and all datasets.

Results and Analysis. The experimental results, as shown in Figure [12,](#page-14-2) reveal that: (1) Models pay significantly more attention to examples with lexical similarity or semantic similarity compared to randomly selected examples with minimal lexical similarity and semantic similarity. (2) Across all models, attention to semantic similarity is higher than to lexical similarity. (3) As the model size increases, models are more likely to predict tokens outside the label space, indicating that larger mod-

Figure 12: The proportion of each element's corresponding label in all predictions. Although we adopt the method of repeating each example in the demonstrations to mitigate the models' tendency to summarize patterns of label changes when performing ICL, for some models, it is still inevitable that tokens outside the label space are predicted. We use "others" to represent all tokens outside the label space.

els place greater weight on summarizing patterns of label changes in the context of task learning. (4) Instruction-tuned models tend to favor examples with semantic similarity, possibly due to the emphasis on semantic understanding during the instruction-tuning training process.

B GPT-4 Generated Triplets

Refer to Tables [1](#page-15-1) and [2](#page-16-3) for the 20 triplets generated by GPT-4 on the SST-2 dataset. Refer to Tables [3](#page-17-3) and [4](#page-18-1) for the 20 triplets generated by GPT-4 on the emo dataset. Refer to Tables [5](#page-19-0) and [6](#page-20-0) for the 20 triplets generated by GPT-4 on the TREC dataset. Refer to Tables [7](#page-21-0) and [8](#page-22-0) for the 20 triplets generated by GPT-4 on the hate_speech18 dataset.

C Detailed Proofs of Models' Task Recognition on Classification Datasets

We employ one-shot ICL with correct input-label mapping to investigate the models' task recognition abilities across various datasets. Considering that the *PIR* metric involves the number of model layers and that different models have varying layer counts, we select the Llama-2-7B model as a representative for our analysis.

For the World Capitals task, we use the prompt *"Word: Germany Label: Berlin Word: Japan La-* *bel:"* to examine whether the label token *"Berlin"* triggers the task token *"capital."* For the Reasoning about Colored Objects task, we use the prompt *"Word: Apple Label: Red Word: Banana Label:"* to examine whether the label token *"Red"* triggers the task token *"color."* For the SST-2 dataset [\(Socher](#page-11-7) [et al.,](#page-11-7) [2013\)](#page-11-7), we use the prompt *"Sentence: the part where nothing 's happening , Label: negative Sentence: a smile on your face Label:"*. It is noteworthy that ICL performed on the SST-2 dataset does not very conspicuously generate the task token *"sentiment."* We employ another label, *"positive,"* from the SST-2 dataset. If the demonstration includes only a *"negative"* label but the model is able to infer a *"positive"* meaning at the label token location, we still consider that ICL has successfully identified the type of task. For the TREC dataset [\(Li and Roth,](#page-10-7) [2002;](#page-10-7) [Hovy et al.,](#page-9-9) [2001\)](#page-9-9), we use the prompt *"Sentence: Who killed Gandhi ? Label: Human Sentence: What is a fear of shadows ? Label:"* to examine whether the label token *"Human"* triggers the task token *"question."* For the emo dataset [\(Chatterjee et al.,](#page-9-10) [2019\)](#page-9-10), we use the prompt *"Sentence: talk you later sure d baby Label: others Sentence: really yep i"m i that bad Label:"* to examine whether the label token *"others"* triggers the task token *"emotion."*

All results are presented in Figure [13.](#page-23-0) It is evi-

Test sample	Example _{semantic}	Example lexical		
The soundtrack enriches the en- tire movie. Label: Positive	The music significantly enhances the film's appeal. Label: Posi- tive	The soundtrack diminishes the entire movie. Label: Negative		
The actor's performance is truly mesmerizing. Label: Positive	The actor's portrayal captivates the audience completely. Label: Positive	The actor's performance is truly forgettable. Label: Negative		
The plot twists were unexpected and thrilling. Label: Positive	The story developments were sur- prising and exciting. Label: Pos- itive	The plot twists were predictable and dull. Label: Negative		
The cinematography is breathtak- ing and innovative. Label: Posi- tive	The visual direction offers stun- ning and groundbreaking visuals. Label: Positive	The cinematography is uninspir- ing and outdated. Label: Nega- tive		
The dialogue was witty and de- lightful. Label: Positive	The conversation was sharp and enjoyable. Label: Positive	The dialogue was humorless and disappointing. Label: Negative		
The direction is masterful and precise. Label: Positive	The film's guidance shows excep- tional skill and accuracy. Label: Positive	The direction is clumsy and im- precise. Label: Negative		
The special effects are spectacu- lar and memorable. Label: Posi- tive	The visual effects stand out as extraordinary and unforgettable. Label: Positive	The special effects are unimpres- sive and forgettable. Label: Neg- ative		
The pacing keeps you engaged from start to finish. Label: Posi- tive	The rhythm maintains your atten- tion throughout the entire movie. Label: Positive	The pacing loses your interest from start to finish. Label: Neg- ative		
The characters are richly devel- oped and relatable. Label: Posi- tive	The portrayal of characters is deeply crafted and connects well with the audience. Label: Posi- tive	The characters are poorly devel- oped and unrelatable. Label: Negative		
The film's creativity is both re- freshing and inspiring. Label: Positive	The movie's originality offers a new and motivational perspec- tive. Label: Positive	The film's creativity is both stale and uninspiring. Label: Nega- tive		

Table 1: For the SST-2 dataset, 20 triplets generated by GPT-4 (Part 1).

dent that for the World Capitals, Reasoning about Colored Objects, and SST-2 datasets, the *PIR* is 1. This suggests that for these datasets, models can recognize the task during ICL execution. Conversely, for the TREC and emo datasets, the *PIR* is close to 0. This indicates that models fail to recognize the task during ICL for these datasets.

D Detailed Proof: The Orthogonality of Similar Examples Presence and LLMs' Task Recognition Ability

From Appendix [C,](#page-14-0) we can observe that for the World Capitals, Reasoning about Colored Objects, and SST-2 datasets, models can recognize the task even without the presence of similar examples in the demonstrations. Consequently, to substantiate the claim that the presence of similar examples is orthogonal to task recognition, it is imperative to determine whether the provision of similar examples enhances the ability of models to recognize tasks within the TREC and emo datasets during ICL execution.

Implementation Details. For the TREC and emo datasets, we utilize the test samples as outlined in Appendix [C.](#page-14-0) However, for the demonstrations,

Test sample	Example _{semantic}	Example lexical		
I despise this show for its lack of originality. Label: Negative	The series annoys me with its derivative content. Label: Nega- tive	I adore this show despite its lack of originality. Label: Positive		
The ending was predictable and	The conclusion was foreseeable	The ending was unpredictable		
boring. Label: Negative	and tedious. Label: Negative	and exciting. Label: Positive		
Their service was slow and frus- trating. Label: Negative	The customer service was slug- gish and irritating. Label: Nega- tive	Their service was quick and sat- isfying. Label: Positive		
It's utterly pointless and dull. La-	Completely meaningless and un-	It's utterly purposeful and engag-		
bel: Negative	interesting. Label: Negative	ing. Label: Positive		
The plot twists were contrived and unconvincing. Label: Nega- tive	The storyline turns felt forced and unbelievable. Label: Neg- ative	The plot twists were natural and convincing. Label: Positive		
The movie was generally unin-	The film rarely evoked any ex-	The movie was generally inspir-		
spiring. Label: Negative	citement. Label: Negative	ing. Label: Positive		
The soundtrack is hardly notice-	You barely hear the music	The soundtrack is highly notice-		
able. Label: Negative	throughout. Label: Negative	able. Label: Positive		
The pacing is slow and tedious.	The tempo drags and feels	The pacing is quick and engaging.		
Label: Negative	monotonous. Label: Negative	Label: Positive		
The narrative lacks depth and co-	The story misses complexity and	The narrative has depth and co-		
herence. Label: Negative	clarity. Label: Negative	herence. Label: Positive		
The performance was overly dra- matic and false. Label: Negative	The acting was excessively the- atrical and inauthentic. Label: Negative	The performance was subtly dra- matic and genuine. Label: Posi- tive		

Table 2: For the SST-2 dataset, 20 triplets generated by GPT-4 (Part 2).

we substitute the original examples with correctly labeled test samples that have the highest semantic and lexical similarity. We subsequently investigate whether the label token can trigger taskrepresentative tokens when similar examples are provided in these two datasets.

Experimental Results. The experimental results are shown in Figure [14.](#page-24-0) It can be observed that, for these two datasets, the *PIR* remains close to 0. This suggests that the model's ability to recognize the task is not influenced by the presence of similar examples but is rather determined by the intrinsic characteristics of the task itself.

E Delimiters Used for Each Dataset

For SST-2, TREC, and emo, we use *"Sentence:"* and *"Label:"*; for the World Capitals and Reasoning about Colored Objects tasks, we use *"Word:"* and

"Label:" to clearly separate the components of the demonstrations.

F Detailed Data for World Capitals and Reasoning about Colored Objects Tasks

Detailed data for the World Capitals and Reasoning about Colored Objects tasks are shown in Table [9.](#page-24-1)

G Impact of Random Label Replacement in the Second Quadrant

Implementation Details. We consider two settings: correct input-label mapping and random input-label mapping. In the former, all input-label pair mappings in the demonstration are correct. In the latter, for each input-label pair, the label is randomly selected from the label space. We use $k = 6$ in-context examples without instructions. The results reflect averages from five random seeds and

Test sample	Example _{semantic}	Example lexical		
It seems like a regular day at the office. Label: Others	Just another normal workday. Label: Others	Today, the office feels unset- tlingly quiet. Label: Sad		
I need to go grocery shopping later. Label: Others	Later today, I have some grocery shopping to do. Label: Others	I'm frustrated about having to go grocery shopping later. Label: Angry		
I'm so happy we're going on a vacation! Label: Happy	I'm thrilled about our upcoming vacation! Label: Happy	I'm stressed about all the packing needed for our vacation. Label: Angry		
That birthday party was a blast! Label: Happy	I truly enjoyed the fun at that birthday party! Label: Happy	That birthday party was too loud and overwhelming for me. La- bel: Sad		
Losing my pet has left me heart- broken. Label: Sad	I am deeply saddened by the loss of my pet. Label: Sad	Dealing with my pet's loss has made me irritable and upset. La- bel: Angry		
It's so gloomy outside today, it makes me feel down. Label: Sad	The dreary weather today really dampens my spirits. Label: Sad	The gloomy weather outside is irritating. Label: Angry		
I can't believe how unfair that de- cision was! Label: Angry	I'm really upset about that unjust decision! Label: Angry	That decision was so disappoint- ing and unfair. Label: Sad		
This constant noise is driving me crazy! Label: Angry	I'm getting furious over the in- cessant noise! Label: Angry	This constant noise is really get- ting on my nerves. Label: Oth- ers		
I can't believe I got promoted at work! Label: Happy	I am so excited about my promo- tion at work! Label: Happy	I can't believe how stressed I am at work. Label: Sad		
Missing the bus has ruined my day. Label: Sad	Missing the bus completely ru- Missing the bus has made me fu- ined my entire day. Label: Sad rious. Label: Angry			

Table 3: For the emo dataset, 20 triplets generated by GPT-4 (Part 1).

all datasets in which models can recognize tasks.

Experimental Results. The experimental results are shown in Figure [15.](#page-25-0) It can be observed that randomly replacing labels does not significantly impact ICL performance. This is due to the following reasons: (1) Although some input-label pair mappings are incorrect, the effect is limited to weaker task semantics generated by these labels. (2) The absence of similar examples prevents the incorrect label semantics of similar examples from significantly affecting the hidden states of the last token.

H Positional Bias of the TREC Dataset

The results for TREC in the third quadrant are shown in Figure [16.](#page-25-0) It can be observed that, similar to the emo dataset, the models exhibit strong

positional bias when performing ICL on the TREC dataset. Specifically, they tend to predict the label of the first example.

I Detailed Instructions for Each Dataset

Detailed instructions for each dataset when models perform zero-shot tasks are shown in Table [10.](#page-25-1)

J Specific Instructions and Details on One-Shot ICL for Section [5](#page-6-1)

For the ICL case study on the TREC dataset conducted in Section [5,](#page-6-1) the task description instruction is as follows:

The task involves categorizing questions into specific categories based on their

Table 4: For the emo dataset, 20 triplets generated by GPT-4 (Part 2).

content. Please classify each given question into one of the following broad class labels: Abbreviation, Entity, Description, Human, Location, or Number.

The specific content of the one-shot ICL is as follows:

Question: Who killed Gandhi? Label: Human Question: What is a fear of shadows? Label:

K Formal Mathematical Definition of PIR

The **PIR** metric quantifies a model's ability to recognize tasks. For a given layer l corresponding to the label token, we begin by projecting the hidden state h_l into the vocabulary space by multiplying it with the pre-trained language modeling head E. The rank of the task-representative token

within this projected distribution is then denoted as $rank_{task}(h_l, E)$. The **PIR** is formally defined as:

$$
PIR = \max_{l} \frac{1}{rank_{task}(h_l, E)}.
$$
 (1)

L Additional Experiments on the Reuters-21578 Dataset

To further enhance the comprehensiveness of our study, we conduct additional experiments on the Reuters-21578 dataset [\(Apt'e et al.,](#page-9-15) [1994\)](#page-9-15), which comprises eight label classes. This dataset is validated through *PIR* as one in which models are unable to recognize tasks.

Experimental Results. We employ the same experimental setup as outlined in Section [3.4.](#page-5-0) The results presented in Table [11](#page-25-2) corroborate our existing findings, highlighting the tendency of models to frequently predict the label of the initial example.

Table 5: For the TREC dataset, 20 triplets generated by GPT-4 (Part 1), where ENTY stands for Entity, HUM stands for Human being, NUM stands for Numeric value, LOC stands for Location, ABBR stands for Abbreviation, and DESC stands for Description and abstract concept.

Furthermore, we confirm the insights discussed in Section [4.](#page-6-2) Table [12](#page-25-3) shows that while 1-shot ICL initially underperforms compared to instructionbased 0-shot ICL, it surpasses it as the shot count increases, and instruction-based 1-shot ICL proves more effective than 1-shot ICL without instructions. These results affirm the efficacy of the two proposed directions for improving ICL performance within the third quadrant.

Table 6: For the TREC dataset, 20 triplets generated by GPT-4 (Part 2), where ENTY stands for Entity, HUM stands for Human being, NUM stands for Numeric value, LOC stands for Location, ABBR stands for Abbreviation, and DESC stands for Description and abstract concept.

Table 7: For the hate_speech18 dataset, 20 triplets generated by GPT-4 (Part 1).

Table 8: For the hate_speech18 dataset, 20 triplets generated by GPT-4 (Part 2).

(a) The *PIR* of *"capital"* at the label token *"Berlin"* in Llama-2-7B for the Capital World task.

(c) The *PIR* of *"positive"* at the label token *"negative"* in Llama-2-7B for the SST-2 dataset.

(b) The *PIR* of *"color"* at the label token *"Red"* in Llama-2-7B for the Reasoning about Colored Objects task.

(d) The *PIR* of *"question"* at the label token *"Human"* in Llama-2-7B for the TREC dataset.

(e) The *PIR* of *"emotion"* at the label token *"others"* in Llama-2-7B for the emo dataset.

Figure 13: The *PIR* values across different datasets.

(a) When the correctly labeled test sample is included as a similar example in the demonstration, *PIR* of *"question"* at the label token *"Description"* for the TREC dataset.

(b) When the correctly labeled test sample is included as a similar example in the demonstration, *PIR* of *"emotion"* at the label token *"sad"* for the emo dataset.

Figure 14: When the correctly labeled test sample is included as a similar example in the demonstration, the *PIR* values across different datasets.

Tasks	Detailed Data
World Capital task	Canada-Ottawa, Australia-Canberra, Brazil-Brasília, China- Beijing, France-Paris, Germany-Berlin, India-New Delhi, Italy-Rome, Japan-Tokyo, Mexico-Mexico City, Russia- Moscow, South Africa-Pretoria, South Korea-Seoul, Spain- Madrid, Turkey-Ankara, United Kingdom-London, United States-Washington, D.C., Argentina-Buenos Aires, Egypt- Cairo, Nigeria-Abuja, Sweden-Stockholm, Norway-Oslo, Denmark-Copenhagen, Finland-Helsinki, Poland-Warsaw, Ukraine-Kyiv, Netherlands-Amsterdam, Belgium-Brussels, Austria-Vienna, Switzerland-Bern, Portugal-Lisbon, Greece- Athens, Hungary-Budapest, Czech Republic-Prague, Romania- Bucharest, Thailand-Bangkok, Vietnam-Hanoi, Malaysia-Kuala Lumpur, Singapore-Singapore, Indonesia-Jakarta, Saudi Arabia- Riyadh, Israel-Jerusalem, Chile-Santiago, Colombia-Bogotá, Peru-Lima, New Zealand-Wellington, Ireland-Dublin, Pakistan- Islamabad, Bangladesh-Dhaka, Philippines-Manila.
Reasoning about Colored Ob- jects task	Apple-red, Banana-yellow, Cherry-red, Lemon-yellow, Sky- blue, Grass-green, Grape-purple, Orange-orange, Strawberry- red, Blueberry-blue, Cloud-white, Rose-red, Sunflower- yellow, Snow-white, Coal-black, Pumpkin-orange, Water- blue, Chocolate-brown, Gold-gold, Silver-silver, Carrot-orange, Lime-green, Eggplant-purple, Flamingo-pink, Ocean-blue, Forest-green, Cranberry-red, Peach-pink, Sunset-orange, Night- black, Butter-yellow, Olive-green, Sand-yellow, Violet-purple, Tangerine-orange, Cherry blossom-pink, Coral-orange, Ash- grey, Emerald-green, Sapphire-blue, Ruby-red, Cotton-white, Ivory-white, Charcoal-black, Peacock-blue, Jade-green, Amber- orange, Hazelnut-brown, Lavender-purple, Cinnamon-brown.

Table 9: Detailed data for World Capitals and Reasoning about Colored Objects tasks.

Figure 15: The impact of random label replacement in the second quadrant.

Figure 16: For the TREC dataset, the preference of different models for label tokens at different absolute positions.

Datasets	Instructions for Zero-Shot Tasks
World Capital	Please identify the capital city for the given country.
Reasoning about Colored Objects	Please identify the color of the given object.
$SST-2$	The task involves classifying sentences based on their expressed sentiment. Please classify each given sentence into one of the following sentiment labels: positive or negative.
TREC	The task involves categorizing questions into specific categories based on their content. Please classify each given question into one of the following broad class labels: Abbreviation, Entity, Description, Human, Location, or Number.
emo	Please classify the given utterance into one of the following emotion classes: happy, sad, angry, or others.

Table 10: Detailed instructions for each dataset in the zero-shot setting.

Table 11: Preference (%) of different models for label tokens at different absolute positions on the Reuters-21578.

Models	First Label	Second Label	Third Label	Fourth Label	Fifth Label	Sixth Label	Seventh Label	Eighth Label
$GPT2-XL$	33.1	16.55	15.86	13.79	10.34	10.34		
GPT-J	34.67	13.33	12	6.67	10	23.33		
$Llama2-7B$	45.65	23.91	10.14	8.7	6.52	5.07		
Llama2-7B-chat	27.4	20.55	10.27	10.96	15.07	15.75		
$Llama2-13B$	34.75	6.78	14.41	19.49	15.25	9.32		
Llama2-13B-chat	24.66	17.81	14.38	16.44	15.07	11.64		

Table 12: For the Reuters-21578 dataset, the average accuracy (%) of (1, 4, 8, 12)-shot ICL without instructions and (0, 1)-shot ICL with instructions.

