Active Instruction Tuning: Improving Cross-Task Generalization by Training on Prompt Sensitive Tasks

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Abstract

Instruction tuning (IT) achieves impressive zero-shot generalization results by training large language models (LLMs) on a massive amount of diverse tasks with instructions. However, how to select new tasks to improve the performance and generalizability of IT models remains an open question. Training on all existing tasks is impractical due to prohibiting computation requirements, and randomly selecting tasks can lead to suboptimal performance. In this work, we propose *active instruction tuning* based on prompt uncertainty, a novel framework to identify informative tasks, and then actively tune the models on the selected tasks. We represent the informativeness of new tasks with the disagreement of the current model outputs over perturbed prompts. Our experiments on NIV2 and Self-Instruct datasets demonstrate that our method consistently outperforms other baseline strategies for task selection, achieving better out-of-distribution generalization with fewer training tasks. Additionally, we introduce a task map that categorizes and diagnoses tasks based on prompt uncertainty and prediction probability. We discover that training on ambiguous (prompt-uncertain) tasks improves generalization while training on difficult (prompt-certain and low-probability) tasks offers no benefit, underscoring the importance of task selection for instruction tuning.¹

1 Introduction

Recently, instruction tuning has shown great success in improving large language models' crosstask generalizability. When training large language models (LLM) with a wide range of tasks with instructions, models like T0 (Sanh et al., 2021), FLAN (Wei et al., 2021), TK-Instruct (Wang et al., 2022b), Instruct-GPT (Ouyang et al., 2022), Alpaca (Taori et al., 2023) and Vicuna (Chiang et al.,

¹Our code and data can be found at https://github. com/PlusLabNLP/Active-IT



Figure 1: Our proposed Active Instruction Tuning framework. Given an instruction tuning (IT) model with a sizeable existing task pool, we actively **identify and select** useful tasks from it and add them to the training task pool. After that, we train a new IT model with the updated training task pool. By continuing this loop, we expect to improve the IT model's cross-task generalization ability efficiently. The main challenge lies in **identifying useful tasks**, for which we propose to select prompt-sensitive tasks.

2023) can perform well on unseen task. The performance can be further boosted by increasing the number of diverse training tasks (Xu et al., 2022; Wang et al., 2022b; Longpre et al., 2023; Chung et al., 2022). Based on this observation, many recent studies scale up instruction-tuning datasets by manually or automatically curating more tasks with instructions. For example, T0 and FLAN have 60 tasks. The NIV2 (Wang et al., 2022b) benchmark extends its dataset to over 800 English training tasks. Self-Instruct (Wang et al., 2022a) and Unnatural Instructions (Honovich et al., 2022) prompt LLMs to generate over 50K instruction tuning data, and recently, Dynosaur (Yin et al., 2023a) dynamically curates over 80K instruction tuning data from Huggingface datasets (Lhoest et al., 2021), which is still continuously expanding.

However, as the scale of datasets grows rapidly, it becomes impractical to train on all existing tasks due to overwhelming computing costs. One naive solution is to randomly sample tasks for training, but it can potentially select less informative tasks, leading to suboptimal results (Wang et al., 2023). Therefore, it is crucial to employ an efficient task selection strategy that identifies the most novel and informative tasks for instruction tuning.

Data selection has been explored under active learning and multi-task learning frameworks. Despite its prevalence, we argue that they are not applicable to task selection for instruction tuning. Specifically, active learning methods have focused on selecting the most useful instances for a single task, using either uncertainty-based intuitions such as entropy (Settles, 2009), Monte Carlo dropout (Gal and Ghahramani, 2016), or ensemble disagreement (Houlsby et al., 2011; Siddhant and Lipton, 2018). However, these uncertainty measurements can only measure uncertainty at instance-level, and will become less effective when applied to task-level selections as the scales of uncertainty values are not comparable across tasks. In multi-task learning, previous research (Ivison et al., 2022; Poth et al., 2021; Kung et al., 2021) has explored measuring task usefulness by assessing its similarity to the target task. While these methods can enhance performance when aware of the target tasks, they are not suitable for instruction tuning, which aims to improve overall generalization to arbitrary unseen tasks.

In this work, we introduce Active Instruction Tuning, a framework that aims to actively identify informative new tasks for an IT model to continuously improve its cross-task generalization ability (refer to Figure 1). While being related to active learning, our task is more challenging. Unlike active learning, which focuses on improving **performance on a single target task** by identifying useful *instances*, our goal is to identify tasks that enhance **overall generalization**, a novel concept not explored in previous AL research.

To identify informative new tasks for Active Instruction Tuning, we propose *prompt uncertainty* (refer to Figure 2), a novel task-level uncertainty metric that measures the sensitivity of an IT model against instruction perturbations for a task. Specifically, with a task instruction and a few unlabeled instances, we assess the disagreement of model predictions against original and perturbed prompts on multiple instances to obtain an average disagreement score. We then select and train the model with the most prompt-uncertain tasks to enhance the overall cross-task generalization ability. Since this uncertainty method does not require labeled instances for a task, we can also apply prompt uncertainty to determine novel tasks to manually annotate if needed.

We further explore using *prompt uncertainty* to understand task characteristics and diagnose potential issues. Motivated by Data Map (Swayamdipta et al., 2020), which utilizes instance-level training dynamics to categorize and diagnose data quality, we propose **Task Map**, the first task diagnosing method that categorizes tasks based on Prompt Uncertainty and Prediction Probability. Based on the Task Map, we categorize tasks into **Ambiguous**, **Easy** and **Difficult**, inspired by prior in-context learning research (Xie et al., 2021; Pan et al., 2023) to facilitate analysis.

We conduct experiments on two instruction tuning setting: TK-Instruct models with NIV2 dataset, which generalize to unseen tasks, and Alpaca models with Self-Instruct dataset, which generalize to unseen instructions, following our categorization in Kung and Peng (2023). Results show that our active instruction tuning method consistently outperforms baseline methods (random sampling, generation perplexity) for both instruction tuning setting, demonstrating the effectiveness of our approach. Moreover, we discover that while instruction tuning with Ambiguous tasks can improve generalization effectively, Difficult tasks offers no benefit, underscoring the importance of task selection in instruction tuning. Our contributions can be summarized as follows:

- We introduce Active Instruction Tuning, a framework to efficiently improve the IT model's generalization ability in large-scale instruction tuning.
- We propose Prompt Uncertainty, a task-level uncertainty measurement for IT, which can identify novel/informative tasks to improve IT models' zero-shot generalization.
- We further propose Task Map, a task diagnosing tool that categorizes tasks based on their prompt uncertainty and prediction probability, providing insights into task characteristics and quality.

2 Method

2.1 Active Instruction Tuning

The Active Instruction Tuning framework is illustrated in Figure 1. In reality, when the number of



Figure 2: We demonstrate how we measure the *prompt uncertainty* of a model W to a task. Given the original instruction I_0 and instance input x_0 of a task to the model, we first get prediction y and its sentence probability $p_{0,0}$. Next, we randomly drop words (highlighted in red) from the original instructions to create k perturbed instructions. We measure the model's prediction probability of y given each of the perturbed instructions and input x_0 . Finally, we calculate the average absolute difference (disagreement) between the prediction probability of using original and perturbed instructions, providing an estimate of the model's prompt uncertainty for x_0 . We can further aggregate this prompt uncertainty scores across n instances for a task. Further details can be found in section 2.

tasks is large and continuously expanding, training on all existing tasks becomes impractical due to the overwhelming computing cost. To efficiently improve an instruction tuning model, we can apply a task selection method to actively select the tasks that benefit the current model the most. By repeating this model training and task selection loop, we can continually improve instruction-tuned models' generalization to unseen tasks.

For the experiment, we use a large training task pool of fixed size. The training procedure consists of multiple iterations. In the first iteration, a small number of tasks are randomly sampled to train a weak instruction-tuned model. In subsequent iterations, we actively select the most useful tasks based on the previous model and train a new model with the selected tasks. We evaluate different task selection strategies by testing the model on unseen tasks at each iteration.

2.2 **Prompt Uncertainty**

Inspired by uncertainty-based active learning (Siddhant and Lipton, 2018), we aim to select those highly uncertain tasks as the most informative ones at each stage for training. While prior active learning work has proposed numerous uncertainty measurements at the instance level for a single task, these uncertainty values are usually not comparable across tasks. We propose Prompt Uncertainty, a task-level uncertainty measurement that estimates uncertainty values by assessing the disagreement of the model on the original prediction given complete and perturbed task instructions. By selecting those most prompt-uncertain tasks, we can select the tasks to which the current model is susceptible.

Prompt Uncertainty Measurement Our Prompt Uncertainty method is motivated from Bayesian Active Learning by Disagreement (BALD) (Houlsby et al., 2011) in single task Active Learning. Instead of measuring the disagreement among ensemble models in a single task, we measure the disagreement of generation likelihoods on the original prediction over perturbed prompts and original prompts of a task. Figure 2 illustrates the process of measuring the prompt uncertainty of a model to a task's instance x_0 . To measure the prompt uncertainty U_t for task t given model weights W, corresponding unlabeled dataset X_t and instruction (prompt) I_0^t , we calculate the average disagreement of likelihood between perturbed and original instruction on n randomly sampled examples from X_t .

$$U_{t} = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{k} \sum_{j=1}^{k} |p_{i,0}^{t} - p_{i,j}^{t}|,$$
$$p_{i,j}^{t} = P(y_{i}^{t} | x_{i}^{t}, I_{j}^{t}, W),$$
where $i \in [1, n], j \in [0, k].$

P is the likelihood of prediction y given model weights W, a task instruction I and corresponding task instance x. k is the number of perturbations. For each example $x_i^t \in X^t$, we will first get the original output y_i^t and its corresponding likelihood $p_{i,0}^t$. Then, we will perturb the instruction k times and calculate the average absolute difference between the likelihood of y_i^t given original instruction $p_{i,0}^t$ and perturbed instructions $\{p_{i,j}^t | j \in (1,k)\}$.

In order to perturb a task instruction, it is possible to employ paraphrasing techniques, adding extraneous tokens or randomly omitting words, such that the altered instructions can mostly preserve their meaning (A more detailed discussion can be found in subsection 6.2). In our experiment, we assign a 0.2 drop rate for each word in the instruction to create perturbed instructions. After getting the prompt uncertainty for each remaining task, we will select the highly uncertain ones and add them to the training task pool.

Underlying Hypothesis We describe the underlying hypothesis to propose Prompt Uncertainty. From an uncertainty perspective, when measuring the model's sensitivity toward sampled prompts from a task, we estimate the model's epistemic uncertainty, reflecting the model's lack of knowledge of a particular task. Different from epistemic uncertainty using an ensemble of models (Gal and Ghahramani, 2016), we consider an ensemble of slightly different conditions, i.e., perturbations of prompts for the model, and use the original likelihood to represent the ensembled prediction. From the robustness of the in-context learning perspective, if a model cannot robustly map task instructions to specific latent concepts, which is reflected by the sensitivity regarding perturbations in instructions, its generalization ability to the corresponding task is limited (Xie et al., 2021; Pan et al., 2023). To address this, we hypothesize that training the model on prompt-uncertain tasks will improve its ability to associate prompts with specific latent concepts (tasks), leading to a better zero-shot performance on unseen instructions.

3 Experiment Setting

In this work, we experiment with two well-known IT datasets: NIV2 and Self-Instruct (Wang et al., 2022b,a). NIV2 is the largest IT dataset with 1600+ cross-lingual tasks. It focuses on improving model generalization to unseen tasks, while Self-Instruct is used to train the Alpaca model (Taori et al., 2023) and aims to enhance model instruction following ability, following the categorization in prior work (Kung and Peng, 2023). For detailed

Statistics / IT Models	NIV2	Self-Instruct
Dataset		
# of training tasks (instructions)	756	52K
# of testing tasks (instructions)	119	252
# of data per task	$\geq 200*$	1
Testing on unseen tasks?	 ✓ 	×
Active Instruction Tuning		
# of tasks in initial training set	68	500
# of task to select at <i>i</i> th iteration	68	$500 * 2^{i}$
Evaluation		
Evaluation Metrics	Rouge-L	Human Eval
		GPT Eval

Table 1: Comparison between NIV2 (Wang et al., 2022b) and Self-Instruct (Wang et al., 2022a) datasets. Most tasks in NIV2 have more than 200 instances, while Self-Instruct only has one instance for each task. These two settings differ in terms of the definition of the task and generalization objective (zero-shot cross-task v.s. cross-task), described in Kung and Peng (2023).

setting and comparison, please see Table 1.

3.1 Active Instruction Tuning Setting

Natural Instruction V2 dataset We utilize the NIV2 English tasks split, comprising 756 training tasks and 119 testing tasks, including classification and generative tasks, and run our experiment with **five random seeds**.² For each randomized setting, we first randomly select 68 tasks for the initial training set and select another 68 tasks as the validation set, leaving the remaining 620 tasks as the task pool. Afterward, we iteratively apply different task selection strategies to expand the training set and train new IT models, reporting the performance at each iteration [136, 204, 272, 340].

Self-Instruct dataset We first randomly sample 500 tasks as the initial training set from the 52K tasks in the Self-Instruct dataset, leaving the remaining tasks as the remaining task pool. We conduct active instruction tuning and compare model performance at each iteration [1000, 2000, 4000, 8000, 16000].

3.2 Task Selection Strategies

Since we are the first to propose active instruction tuning, we construct several baseline task selection strategies: *Random Sampling*, *High Perplexity* and *Low Perplexity*, to compare with our proposed *Prompt Uncertainty* method. *Random Sampling* will randomly sample tasks from the remaining task pool. This is usually a strong baseline in task-selection experiments since we utilize a well-constructed dataset as the task pool, which has less noisy and duplicate data. *High and Low Perplexity* are the baselines inspired by prior active

²We provide details of our experiments in subsection A.2.



Figure 3: Experiment results for NIV2 dataset. We compare *Ours* prompt uncertainty method with other baselines and report the Rouge-L scores on testing and validation set at each active instruction tuning iteration [136, 204, 272, 340]. We report the average and standard deviation scores of five runs, each with a different initial 68 tasks, 68 validation tasks, and 620 remaining task pool. Note that we do not show the standard deviation on validation since each random seed will have a different validation set, leading to high variance. Additionally, we report the *Fully Trained* results which train on the entire task pool. Exact numbers for this experiment can be seen in Table 3 in the Appendix.

learning work, which aims to select difficult/easy tasks by measuring predicted sentence perplexity for generation tasks or entropy for classification tasks. As these uncertainty measurements are established at the instance level, we aggregate the uncertainty score of multiple (ten for NIV2 and one for Self-Instruct) instances in a task to estimate task-level uncertainty. For our method, we measure the *Prompt Uncertainty* using n = 10 random examples and k = 20 prompt perturbations in NIV2 (refer to section 2). For Self-Instruct, we measure the prompt uncertainty using n = 1 random examples and k = 20 prompt perturbations.

3.3 Training and Evaluation

For NIV2, we follow the current SOTA TK-instruct model's setting, to train the T5-770M model (Raffel et al., 2020) and report the Rouge-L score of *Classification*, *Generative* and *Overall* tasks, on both validation and testing set. During training and testing, we will provide a task definition and two examples as instruction demonstration. For Self-Instruct dataset, we train the LLaMA-7B model (Touvron et al., 2023) follows Alpaca model setting. For evaluation, we report the blind pairwise comparison of each task selection methods with *Random Sampling* on the 252 user-oriented test set (Wang et al., 2022a). We follow the evaluation in Vicuna (Chiang et al., 2023) to report GPT-4, Chat-GPT (GPT 3.5) and Human evaluation scores, and provide more details in subsection A.1.

4 Results

4.1 NIV2 Results

Figure 3 displays our experimental results on the NIV2 dataset. For each task selection method, we iteratively select a batch (68) of tasks from the task pool (620 tasks) to train a new model, and compare model performance at each iteration. A better task selection method should achieve consistent superior performance at early iterations, when there are still plenty of tasks to select from. Figure 3 demonstrates that when selecting less than 340 tasks (half of the task pool), our proposed Prompt Uncertainty method consistently outperforms other baselines in terms of **Overall** scores for both the validation and testing sets. This shows that training on promptuncertain tasks is indeed the most effective way for better zero-shot cross-task generalization ability. On closer examination, our method is highly effective for Classification tasks, surpassing all





Figure 4: Pairwise comparison results between different task selection strategies and random sampling on 252 user-oriented instruction test set (Wang et al., 2022a), evaluated by GPT4, Chat-GPT, and Human Annotators. For four types of methods at each active instruction tuning iteration: [1000, 2000, 4000, 8000, 16000], we separately conduct a pairwise comparison with *Random Sampling* and report the net winning tasks (Number of Win Tasks - Number of Lose Tasks). Note that we only conduct the human evaluation to compare our proposed *Prompt Uncertainty* to *Random Sampling* method due to high evaluation cost (\$600 US Dollars). We provide further details in subsection A.1 Table 4.



Figure 5: The average uncertainty scores of the selected tasks at each active instruction tuning iteration. For *All Tasks*, we report the average uncertainty score of the 620 training tasks predicted by the initial model.

other baselines. For **Generative** tasks, the *Low Perplexity* method performs well on testing tasks at early iterations but poorly on the validation set. This inconsistency suggests that the model's overall generalizability is not enhanced, but rather the low perplexity tasks in the training set coincidentally benefit the generative tasks in the testing set. Conversely, our proposed method achieves consistently good performance on both testing and validation tasks, outperforming *Random Sampling* on testing tasks and exhibiting similar performance on validation tasks.

We further investigate the trend of uncertainty scores during active instruction tuning. In Figure 5, we illustrate the average uncertainty scores of the selected tasks using different task selection strategies at each iteration. It is shown that when selecting for more than half of the tasks in the training pool, all task selection strategies start deviating and choose tasks with unfavorable uncertainty scores. For example, High Perplexity method start selecting tasks with low perplexity scores due to the lack of high perplexity tasks. Specifically, when extending the training tasks from 340 to 408 using *prompt* uncertainty, the average uncertainty score of selected tasks is already slightly lower than that of all tasks at the first iteration, indicating there are no high-uncertainty tasks to select from. Note that the lack of uncertain tasks would occur exclusively in an experimental setting. In practical scenarios where the number of tasks grows rapidly, the exhaustion of uncertain tasks is less likely to happen.

4.2 Self-Instruct Results

We show the pairwise preference comparison of all task selection methods against *Random Sampling* in Figure 4. First for *Fully Trained*, we use the official Alpaca release (Taori et al., 2023), which was trained on all 52K tasks. We compare it to *Random Sampling* at each active instruction tuning iteration. It is shown that for both GPT-4 and Chat-GPT evaluation, the *Fully Trained* model outperforms *Random Sampling* with a great margin. However, as more training tasks are randomly sampled, the difference in preferred tasks is diminishing, indicating that IT performance of the Alpaca setting scales with an increasing number of training tasks.



Figure 6: Task Map visualization. We measure the prediction probability and prompt uncertainty of an IT model against 620 tasks in NIV2 and plot the **Ambiguous**, **Easy**, and **Difficult** tasks.

Secondly, for high/low perplexity and our proposed task selection method, we first fine-tune an LLaMA (Touvron et al., 2023) model with 500 tasks and then iteratively extend the number of training tasks to [1000, 2000, 4000, 8000, 16000]. We then report the pairwise comparison results against Random Sampling at each iteration. Figure 4 shows that Low Perplexity and High Perplexity are generally subpar with Random Sampling, indicating that applying inadequate task selection strategies can hurt the model's performance. In contrast, our prompt uncertainty method is almost consistently more preferable by all GPT4, Chat-GPT, and human assessors when selecting less or equal than 8000 tasks, showing that training with prompt-uncertain tasks can lead to better generalization to the user-oriented test tasks. When the number of training tasks increases to 16000, the performance improvement diminishes along with a smaller remaining task pool, which aligns with our results on the NIV2 dataset. Additionally, we discuss our observations regarding applying GPT4, Chat-GPT, and human assessors for pairwise comparisons. It is seen that while the number of net winning tasks (Win task - Lose Tasks) varies a lot across each evaluation method, the overall trend is similar, showing a certain alignment of preference across these automatic or human assessors.

In conclusion, our experiments on NIV2 and Self-Instruct demonstrate that our prompt uncertainty method consistently improves cross-task generalization in two different instruction tuning scenarios, surpassing random sampling and other uncertainty baselines.



Figure 7: The performance comparison between training on **Ambiguous**, **Easy**, and **Difficult** tasks on the NIV2 dataset. The setting is similar to Figure 3, but we run all methods with three runs for the early active instruction tuning iterations.

5 Task Map

Prior work tries to understand a dataset's characteristics in the field of Dataset Diagnosing. Motivated by Data Map (Swayamdipta et al., 2020), we propose **Task Map**, a model-based diagnosing tool that understands the contributions of different groups of tasks towards instruction tuning. Different from previous work using data correctness and variability to construct data map, we propose to map tasks with the dimensions of Prediction Probability and Prompt Uncertainty, as in Figure 6. This follows a hypothesis from recent work in explaining in-context learning (ICL) (Xie et al., 2021): when the model performs a task in-context during test time (ICL), it might implicitly map the prompt to a corresponding latent concept and perform the task under the concept. Prediction Probability represents the model's confidence to perform a task, indicating task difficulties. In comparison, Prompt Uncertainty represents the consistency of a model to map a prompt to a certain concept, indicating the task's ambiguity to the model. We further follow the above intuition to categorize the tasks into three types: Ambiguous tasks, where models fail to recognize them and have high prompt uncertainty; Easy and Difficult tasks, where models can map the prompts to a certain latent task knowledge (low prompt uncertainty) and perform the task with high/low confidence (sentence probability), respectively. We then use the tasks from these three categories for instruction tuning on NIV2 (Wang et al., 2022a) to understand the contributions of different groups of tasks.

We show the results in Figure 7. It is seen that while training on **Ambiguous** tasks can effectively improve IT generalization ability and outperform random baseline, training on **Easy** tasks and **Difficult** tasks is generally worse than randomly selecting tasks. Furthermore, when selecting more **Easy** tasks can still slightly boost the IT model's performance, **Difficult** tasks can be useless, showing no benefit to the IT model's performance with more training tasks. We hypothesize that **Difficult** tasks can be too specific and hard to learn, therefore useless for improving the IT model's cross-task generalization. While our proposed Task Map can already help diagnose task quality for IT, we look forward to future work conducting a more comprehensive analysis to discuss the role of these task categories to bring a comprehensive understanding of instruction tuning and in-context learning.

6 Discussion

6.1 Prompt Uncertainty Reflects Task Novelty

To demonstrate how prompt uncertainty reflects the novelty of tasks to a model, we designed a controlled experiment to visualize how the prompt uncertainty scores of tasks change after the model is trained with relevant tasks. To collect a set of relevant tasks, we first gathered eight Word Analogy tasks from the NIV2 (Wang et al., 2022b) testing set, which is held unseen from the NIV2 training set. In Figure 8, we measured the prediction probability and prompt uncertainty for 620 unseen tasks (unrelated to analogy tasks) from the NIV2 training set and four of the unseen analogy tasks using an instruction-tuned model, labeled as M0, and plotted the task map in blue. We further trained the **M0** model with the other four analogy tasks, resulting in a new model called M1, and used it to plot the task map for the 620 irrelevant tasks and four unseen analogy tasks again in orange. It is evident that after training the M0 model with the four analogy tasks, the overall prompt uncertainty distribution of the 620 irrelevant tasks remains relatively unchanged, while the prompt uncertainty of the four unseen analogy tasks consistently and significantly decreases.³This demonstrates that prompt uncertainty can effectively indicate the novelty of tasks within the model. When the model is trained with specific tasks, the prompt uncertainty of those relevant tasks notably decreases. Additionally, please note that the prediction probability does not increase after training with similar tasks for these four analogy tasks. This observation highlights that using prediction probability alone cannot effectively reflect the novelty of tasks.



Figure 8: Tasks' prompt uncertainty shifts before and after training with four analogy tasks. We visualize all the tasks on the task map with two models, **M0** (**Blue**) and **M1** (**Orange**). **M0** is the same instruction-tuned model as in Figure 6, which does not train on any *analogy tasks*. **M1** is **M0**, further trained with four analogy tasks: *task1159, task1154, task1152, task1155*. Additionally, we measure the prediction probability and prompt uncertainty of 620 irrelevant tasks and four unseen analogy tasks, *task1157, task1156, task1158, task1153*, using both **M0** and **M1**, plotted in orange and blue. It can be seen that after training the model with analogy tasks (from **M0** to **M1**), the prompt uncertainty of the four unseen analogy tasks consistently decreases, while the distribution of other irrelevant tasks remains relatively unchanged.

6.2 **Prompt Perturbation Methods**

While prompt perturbation methods are meant to slightly perturb the prompt without changing its meanings, it is difficult to 100% guarantee the preservation of instruction meaning after automatic paraphrasing methods. To ensure the prompt uncertainty is not measured using an extreme perturbation case, we perturbed all instructions 20 times in our experiments. We also tried several instruction perturbation methods at our early experiment stage, such as randomly repeating tokens or adding extraneous tokens, which achieved similar prompt uncertainty scores as randomly dropping words. Additionally, for the NIV2 and Self-Instruct datasets we used, which have detailed instructions with many redundant tokens (average 56 words per instruction), randomly dropping 20% of tokens will mostly preserve the meaning of the instructions. For other datasets with concise instructions, a higher dropping rate is needed to perturb the instructions, leading to a higher probability of changing instructions meaning entirely.

³From M0 to M1, the average decrease in prompt uncertainty scores is 0.0018 for the 620 irrelevant tasks and 0.039 for the four analogy tasks. The prompt uncertainty of analogy tasks decreases 21 times more than that of the irrelevant tasks.

7 Related Work

7.1 Instruction Tuning Paradigm

By training large language models (LLMs) with diverse tasks and corresponding instructions, it allows the model to achieve a decent cross-task generalization ability (Wei et al., 2021; Sanh et al., 2021; Wang et al., 2022b; Taori et al., 2023; Chiang et al., 2023; Ouyang et al., 2022). Following the observation from prior research (Xu et al., 2022; Wang et al., 2022a) that scaling up the number of tasks can significantly improve zero-shot generalization, there is research on continuously adding knowledge to large language models (Scialom et al., 2022; Jang et al., 2023), along with many large-scale IT datasets emerged. Wang et al. (2022a); Wei et al. (2021); Bach et al. (2022); Xu et al. (2022); Jiao et al. (2023) manually augment existing datasets to form large-scale IT datasets and Gupta et al. (2022); Finlayson et al. (2022) manually construct new IT datasets in specific domains. There are also automatic approaches to collecting large-scale IT datasets. Wang et al. (2022a); Honovich et al. (2022) propose generating moderate-quality data from powerful IT models, like GPT-4 and Chat-GPT (OpenAI, 2023). Recently, Dynosaur (Yin et al., 2023a) proposes to curate instructions for the continuously growing huggingface dataset (Lhoest et al., 2021) using GPT-4 to create high-quality IT data with low costs. Additionally, we would like to highlight that as IT models rapidly scale in performance with larger models and datasets, the concern of whether they adhere to instructions still remains (Yin et al., 2023b; Kung and Peng, 2023; Min et al., 2022; Yang et al., 2023; Li et al., 2023; Xue et al., 2023), and requires further investigation. For recent IT development, see (Zhang et al., 2023) for a detailed survey.

7.2 Uncertainty Estimation for LLMs

Uncertainty estimation is essential for ensuring safe deployments of neural networks (Abdar et al., 2021). Prior works have decomposed the total uncertainty into aleatoric (data) uncertainty and epistemic (model) uncertainty, and proposed methods to quantify each of them, represented by Monte-Carlo Dropout (Gal and Ghahramani, 2016) and Deep Ensemble (Lakshminarayanan et al., 2017). In particular, data uncertainty measures the intrinsic uncertainty from the data distribution. Model uncertainty measures the uncertainty due to lack of understanding of the task, and can be leveraged to detect adversarial or out-of-distribution data (Feinman et al., 2017; Yin et al., 2022). Recent works have also extended uncertainty quantification to autoregressive language models (Xiao and Wang, 2019; Malinin and Gales, 2020). In this work, we propose a novel epistemic uncertainty measurement for instruction-tuned LLMs by measuring the disagreement of models conditioned on perturbed instructions.

7.3 Active Learning and Task Selection

Our work is also related to active learning, which iteratively annotates informative instances from an unlabeled pool for efficient training (Olsson, 2009; Siddhant and Lipton, 2018; Zhang et al., 2022). Strategies for querying informative instances fall into different categories. See Zhang et al. (2022) for a detailed survey. Our method is more related to disagreement-based active learning (Houlsby et al., 2011; Siddhant and Lipton, 2018; Shen et al., 2017), which queries for instances where multiple models disagree the most, and is usually combined with model uncertainty measurements (Gal and Ghahramani, 2016). However, different from active learning which selects informative instances, we consider selections at task-level. We show that simply adopting prior active learning strategies at task-level do not work well and propose our own methods. There are also works doing task selection for specific target tasks (Parvez and Chang, 2021; Zhou et al., 2023). However, we do not assume knowledge of the target task but select tasks solely based on the uncertainty information of the model.

8 Conclusion

We propose Active Instruction Tuning with prompt uncertainty, a framework to enhance the generalization ability of the IT model in large-scale instruction tuning. Our experiments on NIV2 and Self-Instruct datasets demonstrate that training on prompt uncertain tasks consistently outperforms random sampling and other uncertainty baselines, highlighting the effectiveness of our approach. We also introduce Task Map, a tool that categorizes tasks based on prompt uncertainty and prediction probability, revealing that while training on ambiguous tasks improves generalization, some difficult tasks offer no benefit. These findings motivate future investigations into prompt uncertainty and task selection strategies for better understanding cross-task generalization and instruction tuning.

Limitations

While our experiments demonstrate the superiority of our proposed prompt uncertainty method over other baseline task selection methods on the NIV2 and Self-Instruct datasets, there are several limitations to consider. Firstly, our experiments are conducted on open-source instruction tuning models and do not consider the impact of reinforcement learning with human feedback in Instruct-GPT (Ouyang et al., 2022). Secondly, although we conducted our experiments on well-constructed instruction tuning datasets, it is important to note that this setting may not fully capture the challenges posed by noisy or poorly constructed tasks in extreme scenarios, which may require techniques such as noisy task filtering or batch active learning. Lastly, our current experiment on active instruction tuning focuses on comparing task selection methods and does not incorporate the effect of continual learning, which could be valuable for improving IT models in realistic settings. In summary, our work primarily focuses on introducing active instruction tuning and comparing task selection methods within a controlled environment. We look forward to future research to conduct further analysis to comprehensively examine the effects of all these factors.

Ethics Statement

We describe the computation resources and models we used to conduct our experiments. We conduct all experiments on 4 to 8 48GB NVIDIA A6000 GPUs or 2 to 4 NVIDIA A100 GPUs, along with 48 TB disk storage and AMD EPYC 7413 24-Core Processor. The experiment takes around 5500 GPU hours for one 48GB NVIDIA A6000 GPU. Our experiments do not need to leverage private data. For the model, we use open-sourced Huggingface T5-large-lm-adapt models and LLaMA-7B, Stanford Alpaca-7B for our experiments, and we will release our code once the paper is accepted.

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References

- Moloud Abdar, Farhad Pourpanah, Sadiq Hussain, Dana Rezazadegan, Li Liu, Mohammad Ghavamzadeh, Paul Fieguth, Xiaochun Cao, Abbas Khosravi, U Rajendra Acharya, et al. 2021. A review of uncertainty quantification in deep learning: Techniques, applications and challenges. *Information Fusion*, 76:243– 297.
- Stephen H Bach, Victor Sanh, Zheng-Xin Yong, Albert Webson, Colin Raffel, Nihal V Nayak, Abheesht Sharma, Taewoon Kim, M Saiful Bari, Thibault Fevry, et al. 2022. Promptsource: An integrated development environment and repository for natural language prompts. arXiv preprint arXiv:2202.01279.
- Wei-Lin Chiang, Zhuohan Li, Zi Lin, Ying Sheng, Zhanghao Wu, Hao Zhang, Lianmin Zheng, Siyuan Zhuang, Yonghao Zhuang, Joseph E. Gonzalez, Ion Stoica, and Eric P. Xing. 2023. Vicuna: An opensource chatbot impressing gpt-4 with 90%* chatgpt quality.
- Hyung Won Chung, Le Hou, Shayne Longpre, Barret Zoph, Yi Tay, William Fedus, Yunxuan Li, Xuezhi Wang, Mostafa Dehghani, Siddhartha Brahma, Albert Webson, Shixiang Shane Gu, Zhuyun Dai, Mirac Suzgun, Xinyun Chen, Aakanksha Chowdhery, Alex Castro-Ros, Marie Pellat, Kevin Robinson, Dasha Valter, Sharan Narang, Gaurav Mishra, Adams Yu, Vincent Zhao, Yanping Huang, Andrew Dai, Hongkun Yu, Slav Petrov, Ed H. Chi, Jeff Dean, Jacob Devlin, Adam Roberts, Denny Zhou, Quoc V. Le, and Jason Wei. 2022. Scaling instruction-finetuned language models.
- Reuben Feinman, Ryan R Curtin, Saurabh Shintre, and Andrew B Gardner. 2017. Detecting adversarial samples from artifacts. *arXiv preprint arXiv:1703.00410*.
- Matthew Finlayson, Kyle Richardson, Ashish Sabharwal, and Peter Clark. 2022. What makes instruction learning hard? an investigation and a new challenge in a synthetic environment. *arXiv preprint arXiv:2204.09148*.
- Yarin Gal and Zoubin Ghahramani. 2016. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *international conference on machine learning*, pages 1050–1059. PMLR.
- Prakhar Gupta, Cathy Jiao, Yi-Ting Yeh, Shikib Mehri, Maxine Eskenazi, and Jeffrey P Bigham. 2022. Improving zero and few-shot generalization in dialogue through instruction tuning. *arXiv preprint arXiv:2205.12673*.
- Or Honovich, Thomas Scialom, Omer Levy, and Timo Schick. 2022. Unnatural instructions: Tuning language models with (almost) no human labor. *arXiv preprint arXiv:2212.09689*.

- Neil Houlsby, Ferenc Huszár, Zoubin Ghahramani, and Máté Lengyel. 2011. Bayesian active learning for classification and preference learning. *arXiv preprint arXiv:1112.5745*.
- Hamish Ivison, Noah A Smith, Hannaneh Hajishirzi, and Pradeep Dasigi. 2022. Data-efficient finetuning using cross-task nearest neighbors. *arXiv preprint arXiv:2212.00196*.
- Joel Jang, Seungone Kim, Seonghyeon Ye, Doyoung Kim, Lajanugen Logeswaran, Moontae Lee, Kyungjae Lee, and Minjoon Seo. 2023. Exploring the benefits of training expert language models over instruction tuning. *arXiv preprint arXiv:2302.03202*.
- Wenxiang Jiao, Jen tse Huang, Wenxuan Wang, Xing Wang, Shuming Shi, and Zhaopeng Tu. 2023. Parrot: Translating during chat using large language models. *ArXiv*.
- Po-Nien Kung and Nanyun Peng. 2023. Do models really learn to follow instructions? an empirical study of instruction tuning. *arXiv preprint arXiv:2305.11383*.
- Po-Nien Kung, Sheng-Siang Yin, Yi-Cheng Chen, Tse-Hsuan Yang, and Yun-Nung Chen. 2021. Efficient multi-task auxiliary learning: selecting auxiliary data by feature similarity. In *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing*, pages 416–428.
- Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. 2017. Simple and scalable predictive uncertainty estimation using deep ensembles. *Advances in neural information processing systems*, 30.
- Ouentin Lhoest, Albert Villanova del Moral, Yacine Jernite, Abhishek Thakur, Patrick von Platen, Suraj Patil, Julien Chaumond, Mariama Drame, Julien Plu, Lewis Tunstall, Joe Davison, Mario Šaško, Gunjan Chhablani, Bhavitvya Malik, Simon Brandeis, Teven Le Scao, Victor Sanh, Canwen Xu, Nicolas Patry, Angelina McMillan-Major, Philipp Schmid, Sylvain Gugger, Clément Delangue, Théo Matussière, Lysandre Debut, Stas Bekman, Pierric Cistac. Thibault Goehringer. Victor Mustar. Francois Lagunas, Alexander Rush, and Thomas Wolf. 2021. Datasets: A community library for natural language processing. In Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing: System Demonstrations, pages 175-184, Online and Punta Cana, Dominican Republic. Association for Computational Linguistics.
- Zekun Li, Baolin Peng, Pengcheng He, and Xifeng Yan. 2023. Evaluating the instruction-following robustness of large language models to prompt injection.
- Shayne Longpre, Le Hou, Tu Vu, Albert Webson, Hyung Won Chung, Yi Tay, Denny Zhou, Quoc V Le, Barret Zoph, Jason Wei, et al. 2023. The flan collection: Designing data and methods for effective instruction tuning. *arXiv preprint arXiv:2301.13688*.

- Andrey Malinin and Mark Gales. 2020. Uncertainty estimation in autoregressive structured prediction. *arXiv preprint arXiv:2002.07650*.
- Sewon Min, Xinxi Lyu, Ari Holtzman, Mikel Artetxe, Mike Lewis, Hannaneh Hajishirzi, and Luke Zettlemoyer. 2022. Rethinking the role of demonstrations: What makes in-context learning work? arXiv preprint arXiv:2202.12837.
- Fredrik Olsson. 2009. A literature survey of active machine learning in the context of natural language processing.

OpenAI. 2023. Gpt-4 technical report.

- Long Ouyang, Jeff Wu, Xu Jiang, Diogo Almeida, Carroll L Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, et al. 2022. Training language models to follow instructions with human feedback. arXiv preprint arXiv:2203.02155.
- Jane Pan, Tianyu Gao, Howard Chen, and Danqi Chen. 2023. What in-context learning" learns" in-context: Disentangling task recognition and task learning. *arXiv preprint arXiv:2305.09731*.
- Md Rizwan Parvez and Kai-Wei Chang. 2021. Evaluating the values of sources in transfer learning. In *Proceedings of the 2021 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pages 5084–5116, Online. Association for Computational Linguistics.
- Clifton Poth, Jonas Pfeiffer, Andreas Rücklé, and Iryna Gurevych. 2021. What to pre-train on? efficient intermediate task selection. *arXiv preprint arXiv:2104.08247*.
- Colin Raffel, Noam Shazeer, Adam Roberts, Katherine Lee, Sharan Narang, Michael Matena, Yanqi Zhou, Wei Li, Peter J Liu, et al. 2020. Exploring the limits of transfer learning with a unified text-to-text transformer. *J. Mach. Learn. Res.*, 21(140):1–67.
- Victor Sanh, Albert Webson, Colin Raffel, Stephen H Bach, Lintang Sutawika, Zaid Alyafeai, Antoine Chaffin, Arnaud Stiegler, Teven Le Scao, Arun Raja, et al. 2021. Multitask prompted training enables zero-shot task generalization. *arXiv preprint arXiv:2110.08207*.
- Thomas Scialom, Tuhin Chakrabarty, and Smaranda Muresan. 2022. Fine-tuned language models are continual learners. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing*, pages 6107–6122, Abu Dhabi, United Arab Emirates. Association for Computational Linguistics.

Burr Settles. 2009. Active learning literature survey.

- Yanyao Shen, Hyokun Yun, Zachary Lipton, Yakov Kronrod, and Animashree Anandkumar. 2017. Deep active learning for named entity recognition. In Proceedings of the 2nd Workshop on Representation Learning for NLP, pages 252–256, Vancouver, Canada. Association for Computational Linguistics.
- Aditya Siddhant and Zachary C. Lipton. 2018. Deep Bayesian active learning for natural language processing: Results of a large-scale empirical study. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, pages 2904–2909, Brussels, Belgium. Association for Computational Linguistics.
- Swabha Swayamdipta, Roy Schwartz, Nicholas Lourie, Yizhong Wang, Hannaneh Hajishirzi, Noah A. Smith, and Yejin Choi. 2020. Dataset cartography: Mapping and diagnosing datasets with training dynamics. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pages 9275–9293, Online. Association for Computational Linguistics.
- Rohan Taori, Ishaan Gulrajani, Tianyi Zhang, Yann Dubois, Xuechen Li, Carlos Guestrin, Percy Liang, and Tatsunori B. Hashimoto. 2023. Stanford alpaca: An instruction-following llama model. https:// github.com/tatsu-lab/stanford_alpaca.
- Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. 2023. Llama: Open and efficient foundation language models. arXiv preprint arXiv:2302.13971.
- Yizhong Wang, Hamish Ivison, Pradeep Dasigi, Jack Hessel, Tushar Khot, Khyathi Raghavi Chandu, David Wadden, Kelsey MacMillan, Noah A. Smith, Iz Beltagy, and Hannaneh Hajishirzi. 2023. How far can camels go? exploring the state of instruction tuning on open resources.
- Yizhong Wang, Yeganeh Kordi, Swaroop Mishra, Alisa Liu, Noah A Smith, Daniel Khashabi, and Hannaneh Hajishirzi. 2022a. Self-instruct: Aligning language model with self generated instructions. *arXiv preprint arXiv:2212.10560*.
- Yizhong Wang, Swaroop Mishra, Pegah Alipoormolabashi, Yeganeh Kordi, Amirreza Mirzaei, A. Arunkumar, Arjun Ashok, Arut Selvan Dhanasekaran, Atharva Naik, David Stap, Eshaan Pathak, Giannis Karamanolakis, Haizhi Gary Lai, Ishan Purohit, Ishani Mondal, Jacob Anderson, Kirby Kuznia, Krima Doshi, Maitreya Patel, Kuntal Kumar Pal, M. Moradshahi, Mihir Parmar, Mirali Purohit, Neeraj Varshney, Phani Rohitha Kaza, Pulkit Verma, Ravsehaj Singh Puri, Rushang Karia, Shailaja Keyur Sampat, Savan Doshi, Siddharth Deepak Mishra, Sujan Reddy, Sumanta Patro, Tanay Dixit, Xudong Shen, Chitta Baral, Yejin Choi, Noah A. Smith, Hanna Hajishirzi, and Daniel Khashabi. 2022b. Supernaturalinstructions: Generalization via declarative instructions on 1600+ nlp tasks.

- Jason Wei, Maarten Bosma, Vincent Y Zhao, Kelvin Guu, Adams Wei Yu, Brian Lester, Nan Du, Andrew M Dai, and Quoc V Le. 2021. Finetuned language models are zero-shot learners. *arXiv preprint arXiv:2109.01652*.
- Yijun Xiao and William Yang Wang. 2019. Quantifying uncertainties in natural language processing tasks. In *Proceedings of the AAAI conference on artificial intelligence*, volume 33, pages 7322–7329.
- Sang Michael Xie, Aditi Raghunathan, Percy Liang, and Tengyu Ma. 2021. An explanation of in-context learning as implicit bayesian inference. *arXiv preprint arXiv:2111.02080*.
- Hanwei Xu, Yujun Chen, Yulun Du, Nan Shao, Yanggang Wang, Haiyu Li, and Zhilin Yang. 2022. Zeroprompt: Scaling prompt-based pretraining to 1,000 tasks improves zero-shot generalization. *arXiv preprint arXiv:2201.06910*.
- Tianci Xue, Ziqi Wang, Yixia Li, Yun Chen, and Guanhua Chen. 2023. Tadis: Steering models for deepthinking about demonstration examples.
- Cheng-Fu Yang, Yen-Chun Chen, Jianwei Yang, Xiyang Dai, Lu Yuan, Yu-Chiang Frank Wang, and Kai-Wei Chang. 2023. Lacma: Language-aligning contrastive learning with meta-actions for embodied instruction following.
- Da Yin, Xiao Liu, Fan Yin, Ming Zhong, Hritik Bansal, Jiawei Han, and Kai-Wei Chang. 2023a. Dynosaur: A dynamic growth paradigm for instruction-tuning data curation. arXiv preprint arXiv:2305.14327.
- Fan Yin, Yao Li, Cho-Jui Hsieh, and Kai-Wei Chang. 2022. Addmu: Detection of far-boundary adversarial examples with data and model uncertainty estimation. In *Conference on Empirical Methods in Natural Language Processing*.
- Fan Yin, Jesse Vig, Philippe Laban, Shafiq Joty, Caiming Xiong, and Chien-Sheng Jason Wu. 2023b. Did you read the instructions? rethinking the effectiveness of task definitions in instruction learning. *arXiv preprint arXiv:2306.01150*.
- Shengyu Zhang, Linfeng Dong, Xiaoya Li, Sen Zhang, Xiaofei Sun, Shuhe Wang, Jiwei Li, Runyi Hu, Tianwei Zhang, Fei Wu, and Guoyin Wang. 2023. Instruction tuning for large language models: A survey.
- Zhisong Zhang, Emma Strubell, and Eduard Hovy. 2022. A survey of active learning for natural language processing. In Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing, pages 6166–6190, Abu Dhabi, United Arab Emirates. Association for Computational Linguistics.
- Jing Zhou, Zongyu Lin, Yanan Zheng, Jian Li, and Zhilin Yang. 2023. Not all tasks are born equal: Understanding zero-shot generalization. In *The Eleventh International Conference on Learning Representations*.

A Appendix

A.1 Evaluation details

Human Evaluation For human evaluation in section 4 and Figure 4, we recruit crowd-source workers on Amazon Mechanical Turk who are native English speakers, score at least 70% on a qualification test, and pass the attention test. For the annotation task, three annotators are presented with the task instruction, the input, and the expected output, followed by two models' outputs in random order. The annotators are asked to indicate whether the first model wins, loses, or has a tie. An example of the annotation interface is presented Figure 9. The final comparison decisions are aggregated from the raw annotations using majority voting. We assign a tie label when all the annotators disagree. To calculate the inter-annotator agreement, we define no-contradiction as agreement with the tie entries removed since an annotator slightly supporting a model may also vote for a tie. Under this definition, the no-contradiction rate is measured as 60.4%. Among the cases with contradiction, we find two annotators agree for 82% cases, and all annotators disagree in only 18% cases. We set the peritem reward to \$0.1 to reach an hourly rate of \$15. We collect 3780 comparison annotations to compare Prompt Uncertainty with Random Sampling at each active instruction tuning iteration. The total annotation cost is approximately 600 US Dollars.

GPT-4/Chat-GPT Evaluation We conduct a blind pairwise comparison on GPT-4 and Chat-GPT (GPT-3.5) models using Open-AI API, following a similar template as we used for human evaluation, which is shown in Table 2. To compare two models on one instance, we will randomly assign "(1)" and "(2)" to the model's predictions and prompt the model to reply with the better choice or "Equal" if two predictions are equally good. Note that when applying GPT evaluation, there are very rare cases (about 0.7% of the cases) that the GPT models will reply with unrelated output, which we will assign "Equal" to these instances. The total annotation cost is approximately 50 US Dollars for GPT-4 and 2 US Dollars for Chat-GPT. For full evaluation results, please refer to Table 4

A.2 Experiment details

We provide the details of our experiments on two well-known instruction tuning datasets: NIV2 (Wang et al., 2022b) and Self-Instruct dataset (Wang et al., 2022a).

NIV2 - Active Instruction Tuning Details We utilize the NIV2 English tasks split, comprising 756 training tasks and 119 testing tasks, including classification and generative tasks. We employ five random seeds without selection in our active instruction tuning experiment. Each seed involves randomly sampling 68 tasks as initial training tasks and 68 tasks as validation tasks. The remaining 620 training tasks form the remaining task pool. In each active learning iteration, we maintain a fixed classification and generative task ratio and select 24 classification tasks and 44 generative tasks using different task selection strategies. This fixed ratio allows a more meaningful comparison of our results as we evaluate overall, classification, and generative task scores separately. After the new tasks are sampled, we add them to the previously selected training tasks and form a new training task set. We further train a new instruction tuning model with the updated training task set.

Self-Instruct - Active Instruction Tuning Details We utilize the 52K self-instruct dataset as the task pool. For the active instruction tuning experiment, we will randomly sample 500 tasks as the initial training set and further compare model performance at [1000, 2000, 4000, 8000, 16000] training tasks. For task selection, we will first divide all tasks into 13 chunks by output sequence length [[1, 10], [11, 20], ..., [121, 130]], and then apply the task selection methods on each chunk of tasks, following the ratio of the number of tasks in all chunks. We conduct this extra step to normalize the output sequence length of the selected task for each task selection method. This ensures there is no imbalance in output sequence length during task selection.

Training Details For experiments on NIV2 dataset (Wang et al., 2022b), we follow the TK-instruct setting, the SOTA model on the NIV2 dataset to train the T5-770M model (Raffel et al., 2020) with learning rate 2e-5, batch size 128 and 200 instances per task for eight epochs. We evaluate the model's zero-shot performance on the validation set at each epoch and select the model checkpoint with the best validation score. For evaluation, we follow (Kung and Peng, 2023) setting to report the Rouge-L score of *Overall, Classification*, and *Generative* tasks on both validation and testing sets. For experiments on Self-Instruct dataset (Wang et al., 2022a), We follow Alpaca's

settings to train the LLaMA-7B model with learning rate 2e-5, batch size 128 for four epochs.

Computing Resources For the experiment on NIV2 dataset (Wang et al., 2022b), we conduct our experiments using 4 to 8 Nvidia 48GB A6000 GPUs. For each uncertainty method, it takes around 1200 GPU hours, a total of 5000 GPU hours(for a single GPU), to run all experiments for Figure 3. For the experiment on Self-Instruct dataset (Wang et al., 2022a), we run with 2 Nvidia 80GB A100 GPUs. Each uncertainty method takes around 40 GPU hours, which sums to 160 GPU hours for all experiments in Figure 4.

Given the model predictions from Random Sampling and Prompt Uncertainty which trained with 1000 tasks, we first randomly assign "(1)" and "(2)" tags:

(1): Prompt-Uncertainty-1000

(2): Random-Sampling-1000

Now we fill the GPT prompt template with these two model predictions.

GPT Prompt:

You're a helpful AI system that is meant to imitate human judgment. Given an *instruction, input*, and two *predictions* "(1)" and "(2)", please tell me which prediction is most satisfying and correct. If (1) is better, output "(1)".

If (2) is better, output "(2)". If (2) is better, output "(2)".

If both predictions are equally good or equally bad, you can output "Equal".

Instruction:

If you could help me write an email to my friends inviting them to dinner on Friday, it would be greatly appreciated.

Input:

Now given two predictions:

(1): Dear Friends,

I would like to invite you all to join me for dinner on Friday. I am planning to make some of my favorite dishes, and I would love for you all to join me.

The dinner will be held at my place at 7pm on Friday, and I am looking forward to seeing you all there.

Please let me know if you are able to make it so that I can make sure to have enough food.

See you then!

Sincerely,

[Your Name]

(2): Dear [Name],

With sincerity, [Your Name]

Output:

GPT Output: (1)

Table 2: We show our GPT evaluation template. When comparing two models' predictions, we will randomly assign "(1)" or "(2)" tags and then fill them into the GPT templates with provided *instruction* and *inputs*. In this specific instance, the input is an empty string. All the underlined text are the component we injected into the template.

Instruction: What sound does this make?
Optional input: 好
Reference: hǎo
Model 1: The sound this character makes is "hǎo", which means "good" in Chinese. Model 2:
Hao Which one is better?
• \bigcirc Model 1 is better \bigcirc Tie \bigcirc Model 2 is better

Figure 9: An example of the annotation interface for the human evaluation in §4.2.

Task Selection Methods	Task Num				0			NIV	2 Results	(Rouge-L		t lassificatio						_	Generative			
Task Selection Methods Random Seeds →	Task Num	10	20	30	Overall 40	60	A	Std	10	20	30	assificatio 40	n 60	Avg	Std	10	20	30	Jenerative 40	60	Avg	Std
Fully Trained	680	50.51	48.96	49.41	47.27	49.39	Avg 49.11	1.18	57.03	53.35	53.99	50.26	54.00	53.73	2.41	44.43	44.87	45.13	44.47	45.09	44.80	0.33
Prompt Uncertainty	68	44.67	43.71	44.82	43.78	49.39	49.11	0.55	46.80	47.69	48.25	47.84	48.16	47.75	0.58	42.68	40.00	41.62	40.00	39.63	40.79	1.31
Prompt Oncertainty	136	45.55	46.54	46.06	44.65	46.22	45.80	0.33	48.34	50.83	49.59	48.52	50.51	49.56	1.13	42.08	40.00	41.02	40.00	42.23	40.79	0.76
	204	45.55	46.54 48.28	46.06	44.05	46.63	45.80	0.74	48.34	53.74	49.59	48.52	49.98	49.56	1.15	42.93	42.54	42.77	41.65	42.23	42.51	0.76
	272 340	47.38 48.12	48.64 48.93	47.25 47.23	47.49 49.44	48.48 48.23	47.85 48.39	0.66	51.92 52.93	54.05 54.08	50.65 51.92	52.73 54.45	52.75 52.37	52.42 53.15	1.25	43.14 43.63	43.58 44.13	44.08 42.86	42.61 44.78	44.49 44.37	43.58 43.95	0.74
Random Sampling	540 68	48.12	48.95	44.82	49.44	48.23	48.39	0.84 0.55	52.95 46.80	54.08 47.69	48.25	54.45 47.84	48.16	47.75	1.09 0.58	43.63	44.13	42.80	44.78	39.63	43.95	0.74
Random Sampling																						
	136 204	45.07 46.15	45.75 46.87	44.55 45.94	45.04 46.15	45.15 45.26	45.11 46.07	0.43	48.45 49.76	50.50 51.36	47.82 49.08	47.97 48.73	49.56 49.72	48.86 49.73	1.14 1.01	41.92 42.79	41.32 42.68	41.50 43.02	42.31 43.74	41.04	41.62 42.66	0.50
																				41.09		
	272	47.90	48.24	46.44	46.24	46.25	47.01	0.97	53.90	53.38	50.34	50.00	50.15	51.55	1.92	42.30	43.44	42.81	42.74	42.61	42.78	0.42
Hish Demolation	340 68	47.37	48.35 43.71	47.82 44.82	47.22 43.78	47.33 43.75	47.62 44.15	0.47 0.55	50.12 46.80	52.74 47.69	52.61 48.25	50.54 47.84	51.94 48.16	51.59 47.75	1.20 0.58	44.81 42.68	44.26 40.00	43.35 41.62	44.11 40.00	43.02 39.63	43.91 40.79	0.72
High Perplexity		44.67																				1.31
	136	45.15	43.97	45.31	43.98	44.83	44.65	0.64	48.41	49.04	48.87	48.56	47.96	48.57	0.42	42.10	39.25	42.00	39.71	41.91	40.99	1.39
	204	45.50	46.91	45.43	44.19	46.15	45.64	1.00	49.13	51.29	49.25	47.89	49.81	49.47	1.23	42.11	42.82	41.86	40.73	42.74	42.05	0.84
	272	47.57	46.09	47.33	44.80	46.27	46.41	1.11	53.19	50.10	52.29	48.73	49.21	50.70	1.95	42.32	42.35	42.70	41.12	43.53	42.40	0.87
	340	48.65	48.59	48.15	45.66	46.66	47.54	1.32	53.96	53.71	54.57	49.19	50.15	52.32	2.46	43.70	43.81	42.16	42.36	43.41	43.09	0.77
Low Perplexity	68	44.67	43.71	44.82	43.78	43.75	44.15	0.55	46.80	47.69	48.25	47.84	48.16	47.75	0.58	42.68	40.00	41.62	40.00	39.63	40.79	1.31
	136	45.15	45.99	46.13	45.55	45.10	45.58	0.47	46.99	48.82	48.72	49.10	49.88	48.70	1.06	43.43	43.36	43.72	42.24	40.64	42.68	1.27
	204	46.21	46.21	46.22	47.79	46.01	46.49	0.73	49.63	48.83	48.83	51.63	50.95	49.97	1.27	43.02	43.76	43.79	44.21	41.41	43.24	1.11
	272	46.71	45.93	47.43	47.32	46.71	46.82	0.60	50.77	48.57	51.87	51.39	50.89	50.70	1.27	42.93	43.48	43.29	43.51	42.80	43.20	0.32
	340	47.86	48.34	47.29	47.57	46.47	47.51	0.70	52.64	51.46	50.66	51.92	50.14	51.36	0.99	43.40	45.43	44.15	43.51	43.05	43.91	0.94
Task Selection Methods	Task Num				Overall			NIV21	Results (R	ouge-L) –	Validation	1 Set lassificatio							Generative			
Random Seeds →	Task Inulli	10	20	30	40	60	Avg	Std	10	20	30	40	" 60	Avg	Std	10	20	30	40	60	Avg	Std
Full	680	50.86	48.24	48.28	48.36	47.52	48.65	1.28	58.66	59.76	54.86	57.52	59.68	58.10	2.02	43.04	36.47	41.71	38.94	35.27	39.09	3.31
Prompt Uncertainty	68	42.27	41.28	41.40	44.66	41.15	42.15	1.47	44.42	53.67	46.83	53.32	55.39	50.73	4.80	40.11	28.90	35.97	36.01	26.92	33.58	5.49
1 tompt Oncertainty	136	44.78	43.35	45.69	48.16	42.57	44.91	2.19	49.29	57.21	52.76	57.93	56.47	54.73	3.64	40.27	29.48	38.61	38.38	28.67	35.08	5.54
	204	47.75	47.60	46.98	50.03	44.17	47.31	2.19	53.69	60.83	53.21	60.31	57.01	57.01	3.57	41.81	34.36	40.75	39.75	31.34	37.60	4.53
	272	47.69	47.98	48.13	49.73	46.54	48.01	1.14	55.5	61.03	54.45	60.80	59.85	58.33	3.11	39.88	34.93	41.81	38.66	33.23	37.70	3.54
	340	48.12	48.00	48.39	49.61	47.31	48.29	0.84	56.78	60.31	54.92	60.79	60.79	58.72	2.71	39.45	35.70	41.85	38.43	33.82	37.85	3.15
Random Sampling	68	42.27	41.28	41.40	44.66	41.15	42.15	1.47	44.42	53.67	46.83	53.32	55.39	50.73	4.80	40.11	28.90	35.97	36.01	26.92	33.58	5.49
rundom oumpring	136	45.31	44.36	43.61	47.39	42.25	44.58	1.93	50.75	56.15	50.21	56.77	56.45	54.07	3.29	39.87	32.57	37.01	38.01	28.06	35.10	4.77
	204	45.99	45.54	45.78	47.73	43.91	45.79	1.36	49.09	56.43	51.56	56.74	56.41	54.05	3.51	42.88	34.64	39.99	38.72	31.40	37.53	4.53
	272	47.38	47.13	45.99	48.76	46.05	47.06	1.14	52.79	60.45	52.58	58.61	59.03	56.69	3.72	41.98	33.80	39.41	38.90	33.06	37.43	3.84
	340	47.98	48.89	47.80	49.52	45.15	47.87	1.67	54.80	61.90	54.71	60.50	56.95	57.77	3.29	41.17	35.88	40.89	38.54	33.34	37.96	3.35
III - h. D h ite-	68	42.27	41.28	41.40	49.52	41.15	42.15	1.47	44.42	53.67	46.83	53.32	55.39	50.73	4.80	40.11	28.90	35.97	36.01	26.92	33.58	5.49
		43.43	43.79	41.51	47.04	42.36	43.63	2.11	48.34	55.35	50.13	56.09	55.75	53.13	3.62	38.51	32.24	32.90	38.00	28.98	34.13	4.05
High Perplexity						74.00		2.24	48.75	58.62	50.15	56.65	57.89	54.41	4.61	39.47	35.32	33.62	37.49	29.37	35.05	3.87
High Perpiexity	136 204		46 97		47.07	43.63																
High Perplexity	204	44.11	46.97 44.64	41.89	47.07 49.02	43.63 44.53	44.73 46.41		56.83	55 59	52.85	58 34	58.41	56.40	2 30	42.35	33.70	35.73	39.69			4 66
High Perplexity	204 272	44.11 49.59	44.64	41.89 44.29	49.02	44.53	46.41	2.65	56.83 56.30	55.59	52.85 56.41	58.34	58.41 56.73	56.40 58.38	2.30	42.35	33.70	35.73	39.69	30.65	36.42	4.66
	204 272 340	44.11 49.59 50.14	44.64 48.74	41.89 44.29 47.37	49.02 50.35	44.53 44.79	46.41 48.28	2.65 2.29	56.30	62.06	56.41	60.38	56.73	58.38	2.67	43.98	35.43	38.33	40.31	30.65 32.86	36.42 38.18	4.30
	204 272 340 68	44.11 49.59 50.14 42.27	44.64 48.74 41.28	41.89 44.29 47.37 41.40	49.02 50.35 44.66	44.53 44.79 41.15	46.41 48.28 42.15	2.65 2.29 1.47	56.30 44.42	62.06 53.67	56.41 46.83	60.38 53.32	56.73 55.39	58.38 50.73	2.67 4.80	43.98 40.11	35.43 28.90	38.33 35.97	40.31 36.01	30.65 32.86 26.92	36.42 38.18 33.58	4.30 5.49
Low Perplexity	204 272 340 68 136	44.11 49.59 50.14 42.27 43.85	44.64 48.74 41.28 43.80	41.89 44.29 47.37 41.40 41.21	49.02 50.35 44.66 46.77	44.53 44.79 41.15 41.41	46.41 48.28 42.15 43.41	2.65 2.29 1.47 2.26	56.30 44.42 47.87	62.06 53.67 55.52	56.41 46.83 47.05	60.38 53.32 56.04	56.73 55.39 54.90	58.38 50.73 52.28	2.67 4.80 4.42	43.98 40.11 39.83	35.43 28.90 32.09	38.33 35.97 35.38	40.31 36.01 37.49	30.65 32.86 26.92 27.92	36.42 38.18 33.58 34.54	4.30 5.49 4.67
	204 272 340 68	44.11 49.59 50.14 42.27	44.64 48.74 41.28	41.89 44.29 47.37 41.40	49.02 50.35 44.66	44.53 44.79 41.15	46.41 48.28 42.15	2.65 2.29 1.47	56.30 44.42	62.06 53.67	56.41 46.83	60.38 53.32	56.73 55.39	58.38 50.73	2.67 4.80	43.98 40.11	35.43 28.90	38.33 35.97	40.31 36.01	30.65 32.86 26.92	36.42 38.18 33.58	4.30 5.49

Table 3: Full experiment results in Figure 3.

	Evaluation (C	-		-	-	XX72 T
Task Selection Methods	Task Num	Win	Lose	Tie	Error	Win - Lose*
Fully Trained	1000	143	55	54	0	88
	2000	129	55	67	1	74
	4000	104	70	78	0	34
	8000	95	67	90	0	28
	16000	84	67	101	0	17
Prompt Uncertainty (Ours)	1000	83	72	97	0	11
	2000	100	73	79	0	27
	4000	75	94	83	0	19
	8000	89	75	88	0	14
	16000	78	83	91	0	-5
High Perplexity	1000	64	88	100	0	24
	2000	83	81	88	0	2
	4000	77	84	91	0	-7
	8000	80	88	84	0	-8
	16000	70	86	96	0	16
Low Perplexity	1000	73	81	98	0	-8
	2000	78	96	78	0	18
	4000	74	03	75	0	29
	8000	73	04	75	0	31
	16000	71	97	84	0	26
Chat-GP	T Evaluation (Compar	e to Rand	om Sam	oling)	
Task Selection Methods	Task Num	Win	Lose	Tie	Error	Win - Lose [*]
Fully Trained	1000	117	62	71	2	55
5	2000	125	71	55	1	54
	4000	99	74	76	3	25
	8000	93	71	86	2	22
	16000	82	72	98	0	10
Prompt Uncertainty (Ours)	1000	94	70	88	0	24
I i i i i i i i i i i i i i i i i i i i	2000	94	73	82	3	21
	4000	86	76	90	0	10
	8000	86	76	88	2	10
	16000	83	83	86	0	0
High Perplexity	1000	58	95	98	1	-37
	2000	88	74	90	0	14
	4000	84	86	82	ů 0	-2
	8000	82	81	84	5	1
	16000	68	93	91	0	-25
Low Perplexity	1000	68	98	86	0	-30
	2000	82	90	79	1	-8
	4000	71	103	74	4	-32
	8000	80	105	66	0	-26
	16000	76	96	79	1	-20
Human	Evaluation (C				-	20
Task Selection Methods	Task Num	Win	Lose	Tie	Error	Win - Lose [*]
Prompt Uncertainty (Ours)	1000	101	88	13		13
rompi Oncertainty (Ours)	2000	74	66	8	_	8
	4000	74 94	83	o 11	_	o 11
	+000				_	
	8000	93	84	9		9

Table 4: Full experiment results in Figure 4.