Complementarity: Toward Better Metrics and Optimizing Data Efficiency in LLMs

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Abstract

Generalist Large Language Models (LLMs) are trained with an immense amount of data from across different domains. However, not all data contribute to model performance equally, and prioritized data quality over quantity can improve domain-specific accuracy. We suggest that quality is not merely an independent feature of datasets, but rather the manner in which data samples interfere or complement one another Furthermore, existing evaluation metrics are computationally expensive, require extensive design, are mathematically ill-defined, and are generally poorly suited to LLMs. Toward improving general performance while greatly reducing the amount of training data, and quantifying how data contribute to downstream tasks vis-a-vis their connection with other data, we introduce a new metric, Complementarity. We first establish a strong correlation between Complementarity and domain-specific task performance. Complementarity shows increased robustness over traditional metrics and is significantly less expensive computationally. Furthermore, without the reliance on heavy instruction-tuning and text scraping, Complementarity is easier to apply and applicable to a wide variety of potential target domains. Most interestingly, we demonstrate that the Complementarity taken over a training validation set provides a better predictor of generalization to future test sets than directly measuring performance on a test validation set. With this, we introduce an algorithm that carefully selects the data to fine-tune upon, leading to a high-performing fine-tuned generalist model while using only a fraction of the data, and without requiring data from the test domain. Overall, Complementarity may serve as a key metric in future analysis of data utility and design of datasets, and may prove invaluable in achieving the goal of a truly generalist model.

1 Introduction

General purpose Large Language Models (LLMs) are trained with a large corpora of datasets from a diverse set of domains. The raw amount of data is immense as in general, upsizing datasets directly impacts model performance (Brown et al., 2020; Du et al., 2021; Gururangan et al., 2020; Du et al., 2022; Kaplan et al., 2020). This presents a significant difficulty, as finding, procuring, and training upon the amounts of data necessary to train ever-larger models (particularly those which are proficient at a wide variety of different downstream tasks) grows more expensive in time, compute, and money by the year. The energy required for training these growing models on larger-and-larger datasets is known to damage the environment and is believed to have already impacted climate change (Liu & Yin, 2024; Wu et al., 2025; Morrison et al., 2025).

The sheer amount of data being used in the training of LLMs is untenable, and experts are warning of an oncoming "data wall", wherein model training will utilize all textual data available and be left without further training resources. This is particularly an issue when it comes to multi-domain systems, which not only require a large amount of data for each domain individually (Hoffmann et al., 2022; Zeng et al., 2024), but require extra "buffer" data to guarantee that models are able to perform at a high level on all tasks, to mitigate what is sometimes referred to as catastrophic interference. Catastrophic interference is distinct from catastrophic forgetting: in traditional neural networks, catastrophic forgetting is a feature of neural networks learning using a curriculum strategy, first one class and then another, which may cause the first class to be forgotten (McCloskey & Cohen, 1989; French, 1999). The solution to catastrophic forgetting is to combine the datasets and train together on all the data. Given that LLMs are based on likelihood maximization for text, combining datasets provides its own slate of issues, namely catastrophic interference, which is a feature of the data itself being poorly aligned and thus the model ends up learning one or all topics poorly (Li et al., 2024a; Luo et al., 2025).

Recent work suggests the importance of data quality (the token diversity, fluency, etc.) as an equally important contributor to the downstream performance of models, preventing hallucinations and enabling the models to give useful information in fluent text both for generalist (Rejeleene et al., 2024; Iyer et al., 2024; Chang et al., 2024) and domain-specific models (Bojic et al., 2023; Chen et al., 2024; Sun et al., 2024; Modesitt et al., 2024). By providing too much data, poor quality data may be mixed in; as more data is added, the average quality will eventually become lower than a subset selected for high quality. Data quality is important not only in terms of the objective attributes (reducing empty strings, random lists of symbols, profanity, typos, etc.) but in terms of relative contribution to solving tasks. While some domains complement each other and improve the overall performance of the model on target tasks, others can provide conflicting data distributions that reduce performance. Training for two deeply disparate tasks certainly may reduce the overall performance on each, but we demonstrate that data from certain domains - or certain subsets of domains - can combine with others to increase performance on both associated tasks. As such, we aim to design a metric that can be used for the selection of domains and domain subset that contribute to overall performance across different tasks, complementing each other.

We introduce a mathematically sound metric, Complementarity, which measures the impact that fine-tuning a model on datasets from training domains impacts performance on a task from a target domain. We demonstrate that Complementarity is a useful analogue for measuring shift in performance. Using Complementary, we emphasize the mutual support of different domains, which leads to a data-selection algorithm that uses a fraction of the data while achieving performance improvements. We not only demonstrate that using Complementarity over traditional metrics during validation to select subsets of the data increases performance, but that in **both** cases using less data actually results in significantly better performance than all of it.

Complementarity is also significantly faster and more computationally efficient than many state-of-the-art evaluation metrics, which require significant time and computational cost for text generation, extensive instruction prompt-tuning, and specialized text scraping methods depending on the specific model, training dataset, and target task. Additionally, Complementarity will enable LLMs to be trained for tasks which lack clear numerical evaluation methods.

The contribution of the paper is organized as follows. Section 2 extensively describes the issues with state-of-the-art evaluation metrics, and presents the vision for Complementarity as a metric free of such problems. Section 3 formally introduces our Complementarity metric and its properties, and demonstrates its significant predictive power for downstream model performance. Section 4 consitutes our most highly practical contribution; it provides proof-of-concept experimental algorithm for multi-domain data selection based on Complementarity, which ends up using a fraction of the data while outperforming domain-by-domain selections and even performance-based data selection. Section 5 outlines current LLM data-selection methods. Section 6 concludes the paper by summarizing contributions and discussing avenues for future work.

2 Problems with Existing Metrics

There are two distinct problems with state-of-the-art metric selection in the field of LLMs, namely the cost of generations, and human time required to design text scraping and instruction-tuning for evaluation.. We will describe each of them before laying out our (singular) solution to both of them in the subsequent sections.

Let us say that a researcher sets out with a new task: train a model capable of solving complicated mathematical word problems with great accuracy. To save resources and time, they decide to use an existing model and fine-tune it on a dataset that is well-aligned with this downstream task, and compare it with the baseline model. Fine-tuning goes smoothly, and the researcher is now left with two models, the base model and the math fine-tuned model. The problem now comes with how to compare the two models.

Let us zoom out a little. In the world of traditional neural networks used as classifiers, the natural manner to evaluate a new model is with basic success metrics (accuracy, precision, pass@1, and F1 score come to mind among others). Feed the model ten thousand pictures of cats and dogs, and count the percentage of the time it correctly and incorrectly classified each - simple enough.

In the world of LLMs, this is somewhat more complicated. First, the generally more intractable issue, is that of evaluation speed. LLMs as generative models need to generate text to be evaluated and classified. Generating text takes time, particularly as (a) the models become larger to enhance their capabilities, with modern models easily reaching into the hundreds of billions of parameters, and (b) increasingly complicated problems require allowing for longer outputs and thus significantly more time for each generation. This is generally dealt with by simply ignoring the problem altogether and attempting to design ever more intelligent model architectures with shortcuts and industry tricks and by dedicating more computing resources to each jobs.

The second issue is one which is so deeply ingrained into the very fabric of LLMs that tens of thousands of papers have been written about it indirectly, and yet few have even addressed that it is a problem to begin with, namely the design of an evaluation metric design. In the sphere of LLMs, as language is deeply abstract, nebulous, and complicated, the notion of "Pass@1" as a single metric does not exist. Rather, the simple success metrics (accuracy, precision, pass@1, etc.) are the very tip of rather lengthy evaluation pipelines. To explain in detail, let us return to the case study of our math fine-tuned model.

Let us assume that in our mathematics dataset, we have a list of word problems along with the numeric (and **only** numeric) answer, e.g. {"Question": "The faces on a fair number die are labelled 1, 2, 3, 4, 5 and 6. You roll the die 12 times. How many times should you expect to roll a 1?", "Answer": "2"}. If you input the question into an LLM, even when asking it to answer briefly a sample response would be something like "The expected number of times to roll a 1 in 12 rolls of a fair six-sided die is: $12 \times \frac{1}{6} = \frac{12}{6} = 2$, so 2 times".

Now, while this answer is certainly correct, it is necessary to extract a number from the answer to compare with the canonical correct result. In this case, one might consider writing a RegEx text scraper to extract the last number from the answer. For this specific example this works well, but what if the answer instead reads "The expected number of times to roll a 1 in 12 rolls of a fair six-sided die is: $12 \times \frac{1}{6} = \frac{12}{6} = 2$, so **two** times", using the word "two" in place of the number? It would then be necessary to update the ReGex to also look for the last "number word" in the sentence. And what if instead of "two times" it said "twice"? The definition of "number words" would need to be expanded. This is also still all assuming that the last appearing number (whatever a number means) in the answer is the final answer, as opposed to something of the form "it is two times, since it is one-twelfth multiplied by six", which would have "six" as the final number.Another potential solution to this is instruction-tuning, i.e. giving the model specific instructions regarding how to answer a question. Telling a sufficiently powerful model to "answer with only a single number and no other text" could work. However, this relies on fine-tuning it with instructions similar to the input-output pairs, and there is still a likelihood that the LLM would not follow the exact instructions, especially if it is a smaller model.

Now, what if the exact answer is not numeric? Let us say that the question and canonical solution pair is {"Question": "Jimmy draws a geometric shape with four sides of equal length at right angles from each other. What shape did Jimmy draw?", "Answer": "Square"}. Now, while the answer is still a single word (and may even be just a single token), extracting it may be more difficult. Clearly, "square" is a nebulous concept to extract using a ReGex, so the naive solution would be to mark answers that contain "square" as correct and those which do not as incorrect. Unfortunately, this would also mark answers such as "the shape cannot be a square or a circle, so it is a triangle" as correct. The incorporation of human evaluation is potentially very expensive and highly time-consuming. Alternatively, using another model as a "judge" classifier for correctness is also time-consuming and presents additional training requirements, and which may introduce another source of bias. Thus in truth, we are most likely left with one solution: instruction-tuning - perhaps asking it to respond with only a single word - which is far from guaranteed to work.

However, another complication exists. what if the question is more of a theoretical question, such that we would require an explanation and is not a binary yes-or-no answer? Short of a human evaluator or an external classifier, the major currently-utilized way to test understanding is using multiple choice questions. This adds a whole different headache, as instruction-tuning the model to answer a multiple-choice question with only an (a), (b), (c), or (d) requires a decently large model, a specific methodology of fine-tuning, and it would likely significantly reduce the non-mulitiple choice capabilities of the model. Beyond that, there is a strong chance that the model will still answer with some larger response containing one or more of (a), (b), (c), and (d), sometimes capitalized and sometimes in incorrect brackets or outside brackets overall. This means that RegEx-style text scraping is still essential, lest we bias the results by throwing out answers that are not a single answer long, potentially adding confounding factors.

In all of these cases, there is a significant amount of design time required into coming up with different instructions and text-scraping mechanisms for each different category of questions, and providing enough of each question type so that there is a sufficient breadth of data associated with each instruction as to prevent overfitting on the few examples, as instructions are learned together with the input-output pairs. Furthermore, this is is just for answering exam-style questions! What if the task is more complicated, such as asking for functional code? A solution would need to scrape away all the unnecessary answer text, compile and run the generated code, and for each example design a sufficient number of diverse test-cases to make sure it works properly. Some tasks - primarily in the creative arts or humanities domains - have no canonical solutions to begin with, and thus cannot be evaluated with standard methods outside of the expensive and time-consuming human evaluation. How does one otherwise numericize how good poetry is or how well it fits the prompt, or how delicately a generated email handles a sensitive subject?

To summarize:

1. Evaluation takes a significant amount of time due to the necessity of acquiring generations to evaluate.
2. State-of-the-Art metrics for evaluation are very difficult to apply to the LLM sphere, and require much human time.
   (a) There are many different considerations for extracting the correct answer, including when and how to apply text scraping, instruction-tuning, and other tools.
   (b) Even if solutions are discovered, they are not generalizable to other questions even in the same domain, and require division, classification, manual annotation, and class balancing.
   (c) There are many domains which have no way to truly numericize the results and apply traditional metrics, leaving them to be strictly evaluated by either humans (very expensive and time-consuming) or another LLM (time-consuming by requiring more training and generation, likely adding a significant amount of bias).
   (d) This is particularly a problem in the multi-domain case, where even if an efficient evaluation metric is discovered for one domain, other domains almost certainly differ, and thus there is no replicability for general-purpose foundation models.

By introducing the metric of **Complementarity**, which does not require generations and can be used uniformly out-of-the-box across domains, we seek to ameliorate these issues. We demonstrate that Complementarity is strongly correlated with traditional evaluation metrics, and thus serves as a highly efficient alternative with the aforementioned benefits.

3 Complementarity Metric

This section will introduce the metric of Complementarity and demonstrate that (a) it is strongly correlated with accuracy for both models trained on single-domains and those trained on multiple domains across different downstream tasks, and (b) it is pseudo-symmetric, i.e. the Complementarity of one domain on another is closely correlated to that of the latter on the former.

3.1 Preliminaries and Theory

The metric of Complementarity is founded upon model perplexity. Perplexity of a model on a given piece of text is a measurement of how likely the model is to generate said text. High perplexity implies that the model assigns a low probability for the occurrence of the text, and thus is unlikely to generate it, wherein low perplexity implies that such text is likely to be generated by the model. Numerically, for a piece of text

$X = (x_1, x_2, ..., x_n)$, perplexity can be denoted as follows, wherein $p(x_i \mid x_{<i})$ is the probability of a word being generated by the model given previous words in the text:

$$
\begin{aligned}
PP(X) &= \exp\left(\frac{1}{n}\sum_{i=1}^{n} - \ln p(x_i \mid x_{<i})\right) \\
&= \exp\left(-\frac{1}{n}\ln p\left(\prod_{i=1}^{n} x_i\right)\right) \\
&= \frac{1}{\sqrt[n]{p\left(\prod_{i=1}^{n} x_i\right)}}
\end{aligned}
$$

Building upon the notion of perplexity, we define Complementarity as follows: For a given model M, and domains $D_1, ..., D_n$, denote M_i to be model M fine-tuned on a dataset taken from domain D_i. Denote by $PP(D_j)$ (respectively $H(D_j)$) the perplexity (cross-entropy) of domain D_j when evaluated on base model M, and by $PP_i(D_j)$ (respectively $H_i(D_j)$) the perplexity (cross-entropy) of domain D_j when evaluated on model M_i. Then the Complementarity which domain D_i affects upon domain (task) D_j is given by

$$
\mathcal{C}_{i,j} = \ln\left(\frac{PP_i(D_j)}{PP(D_j)}\right) = H_i(D_j) - H(D_j)
$$

Observe that a positive Complementarity means improved likelihood of the given text from the base model to the fine-tuned model, while a negative Complementarity means reduced likelihood. We sometimes refer to negative Complementarity as interference.

There is no reason a priori for a change in perplexity (likelihood of generating text) to correlate with domain-specific task performance. For example, when exhibiting Complementarity on the mathematics domain, the model may become more likely to generate text that aligns with the domain's most common sentence structures and use domain-specific language, such as becoming more likely to generate text of the form "Since the base of the rectangle is X and the height is Y, the area must be Z". However, it is not immediately clear that becoming more proficient at generating the structure will align with a greater reasoning ability to actually engage in numerical computation. Similarly, exhibiting Complementarity on the coding domain may imply the model is more likely to generate code which aligns with standard conventions and notation, but does not necessarily imply that the code is more likely to solve the requested problem.

However, we will show that while not necessarily intuitive, Complementarity is an excellent metric which correlates strongly with test accuracy.

3.2 Complementarity Predicts Accuracy

To demonstrate the predictive capability Complementarity as a metric, we look for a correlation between Complementarity and performance across four domains: Coding, Mathematics, Medicine, and Physics. From each domain, we select a large dataset for training, and a separate dataset along with an accepted method to test knowledge in said domain. The datasets used for training and evaluation are in the Appendix, see Tables 4, 5 respectively. We created four fine-tuned versions of the base model Mistral 7B Instruct v0.2 (Jiang et al., 2023), each on one of the four different training datasets, and evaluate the performance of each model on all four domain tasks, comparing with the Complementarity of each model on the evaluation datasets. Toward the goal of generalist models, we also studied the Complementarity metrics on models fine-tuned on datasets from multiple domains. For this, we create six fine-tuned versions of the base model, each trained on an even split from a pair of domains.

Table 1 contains the results of this experiment. There is a strong correlation between performance and Complementarity throughout all domains and domain mereges, wherein the higher the Complementarity, the better the performance, while the lower the Complementarity the worse the performance. The high correlation of Complementarity with performance indicates we can consider Complementarity a natural and low-resource, task-agnostic metric for model testing and generalization. We graph the correlation between Complementary and log of P@1 ratios for all ten fine-tuned models in Figure 1 to visualize their linear correlation.

Table 1: **Strong correlation between Complementarity on the test sets and task-specific performance.** A table containing the performance and Complementarity on four different tasks for models fine-tuned on the four domains and six domain merges. $\mathcal{C}$ is the Complementarity, and P@1 Ratio is the ratio of P@1 between the fine-tuned model and the base model. The first section is the base model followed by four rows from the model fine-tuned on a single training domain, followed by a summary of correlations between the two. The second section is six rows of bi-domain merged fine-tune models. The final section presents the correlation and then the p-values of all models, with statistically significant values bolded. There are two values in each of the correlation computations for the Math task, wherein the second value is derived from removing the Code and Code-based combination models from the tally due to conditional domain dependence between the Coding training dataset and Mathematics evaluation dataset. There is a strong correlation between performance and Complementarity, which is statistically significant for all tasks. When taking the entire table into account, there is an average correlation of 0.7603 (0.8599 when discounting the Code models on the Math task), which represents an incredibly strong p-value of <0.00001. This constitutes support for Complementarity being an excellent predictor of performance.

Target / Source	Code (MBPP)		Math (GSM8K)		Physics (MMLU)		Medicine (MMLU)	
	$\mathcal{C}$	P@1 Ratio	$\mathcal{C}$	P@1 Ratio	$\mathcal{C}$	P@1 Ratio	$\mathcal{C}$	P@1 Ratio
Base	0	1	0	1	0	1	0	1
Code	0.40	1.21	0.06	0.24	-0.28	0.79	-0.30	0.88
Math	0.27	1.06	0.19	1.21	-0.20	0.86	-0.22	0.81
Medicine	-0.14	0.95	-0.14	0.54	-0.49	0.62	-0.45	0.58
Physics	0.09	1.06	-0.07	0.69	-0.15	0.97	-0.20	0.87
Correlation (Single)	—	0.94	—	0.27 / 0.93	—	0.97	—	0.88
Code+Math	0.52	1.22	0.19	1.31	-0.11	0.82	-0.14	0.85
Code+Medicine	0.38	1.06	0.02	0.39	-0.18	0.86	-0.12	0.76
Code+Physics	0.32	1.08	-0.04	0.45	-0.21	0.76	-0.24	0.84
Math+Medicine	0.13	1.08	0.14	1.15	-0.23	0.86	-0.19	0.82
Math+Physics	0.20	1.12	0.11	1.20	-0.09	0.83	-0.14	0.83
Medicine+Physics	0.15	1.07	-0.08	0.60	-0.11	0.87	-0.15	0.81
Correlation	—	0.86	—	0.55 / 0.95	—	0.86	—	0.77
p-value	—	**1.5e-3**	—	1e-1 / **3.1e-5**	—	**1.3e-3**	—	**8.8e-3**

We note the poor performance of fine-tuned models on the physics and medicine tasks, taken from the MMLU dataset, which consists of answering multiple choice questions. This is likely a result of the fact that the training dataset did not contain any multiple choice questions. There is nevertheless a strong correlation between Complementarity and accuracy, which is indicative of the strength of Complementarity as a highly efficient metric. For comparison, the computation of accuracy required the model to be given very specific instructions for the generation formatting, which then required text-scraping to extract answers. Correctness of the text-scraping was determined to be consistent by comparison with human evaluation, which resulted in nearly identical results, with a maximum 2% difference.

Complementarity, as seen in Table 2, is pseudo-symmetric metric, i.e. the Complementarity of one domain on another is closely related to the Complementarity of the latter domain on the first. The diagonal is positive, since fine-tuning on a dataset from a given domain increases its fluency on the test set of the same domain. The Complementarity of Code on Medicine is similar to that of Medicine on Code, and the same occurs for all other domain pairs. Taking the Pearson correlation of cross-diagonal entries yields $r = 0.838$, a strong correlation which indicates that Complementarity is pseudo-symmetric. The Complementarity between each target domain and the models trained on each training domain and domain pair are visualized in Figure 2

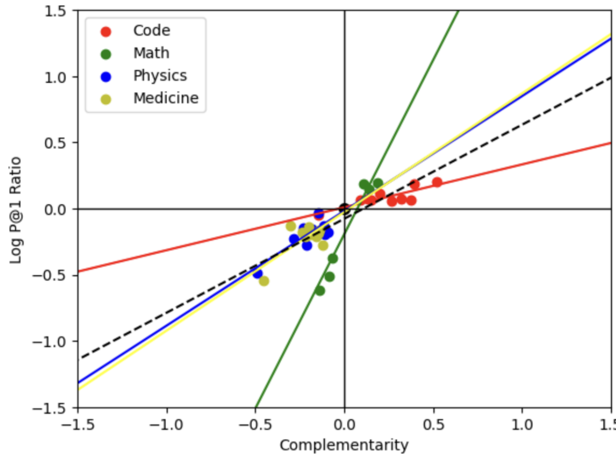

Figure 1: **Correlation between complementarity and task-specific performance.** This figure aligns with the data presented in Table 1. The correlation between log P@1 ratio and Complementarity is plotted, with the color of dots and the linear regression line representing the target evaluation domain (columns of the table). The black dashed line represents a linear regression including all points. Overall, the data relationship between Complementarity and change in accuracy appears quite linear, which is reinforced by the high linear correlation coefficients.

Table 2: **Pseudo-Symmetry of complementarity and utility of data mixing.** The first section of the table contains the Complementarity on test splits of the four training datasets for models fine-tuned on the four domains and six domain merges, and colored based on the strength of Complementarity. We can observe that Complementarity is a pseudo-symmetric metric, with a correlation coefficient between corresponding elements across the diagonal of r = 0.838, resulting in a p-value of 0.03724, a strong and statistically significant correlation. The second section presents the Complementarity on the same test sets for models fine-tuned on training domain pairs. The highest Complementarity for each evaluation domain (column) is bolded, and the second-highest is underlined. This suggests that mixing datasets achieves similar (if not better) performance for the selected domains as those trained solely on one of them without sacrificing performance on other domains. For example, the model fine-tuned on a mix of Medicine and Phsyics data results in higher Complementarity on the Medicine domain than the model fine-tuned solely on Medicine, and higher Complementarity on the Physics domain than the model fine-tuned solely on Physics. This finding hints that a reduction of data quantity may not harm performance, and that generalist models can be sufficiently competitive with specialist models, reducing the quantity of required models.

Source \ Target	Code	Math	Med	Phys
Code	0.167	-0.024	-0.262	0.036
Math	-0.072	**0.285**	-0.106	-0.011
Medicine	-0.221	-0.130	0.100	-0.048
Physics	-0.124	-0.057	-0.106	0.033
Code+Math	**0.202**	<u>0.245</u>	-0.035	<u>0.053</u>
Code+Medicine	<u>0.193</u>	-0.051	**0.266**	0.037
Code+Physics	0.159	-0.070	-0.141	0.052
Math+Medicine	-0.067	0.227	<u>0.244</u>	-0.006
Math+Physics	0.001	0.226	-0.023	0.053
Medicine+Physics	-0.020	-0.053	0.234	**0.073**

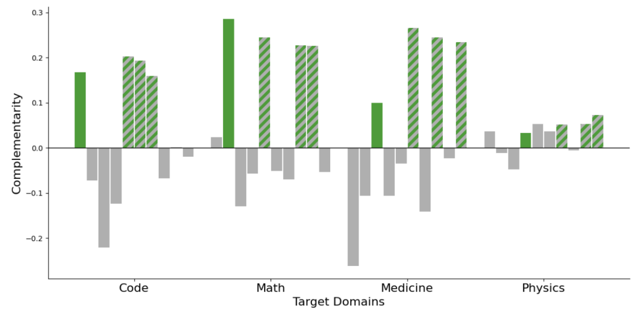

Figure 2: **Complementarity on training domains.** This figure aligns with the data presented in Table 2. The Complementarity of each fine-tuned model on different training domains is plotted in the same order as in the table. Green bars represent that the source and target datasets align, the grey bars represent no overlap, and the green-grey dashed bars represent that the model was trained on a pair of datasets including the target.

4 Data Selection for Model Training with Complementarity

Now that the correlation between Complementarity and performance has been solidified on a broad selection of datasets, we turn to using Complementarity as a metric for training data selection. We saw in the previous section that Complementarity on a given set is correlated with performance on that set, but we may not have access to a robust test set for a given domain, nor would we want to overfit the model by optimizing for performance on the test set even if we did. Instead, we next use Complementarity only on parts of our training corpus designated for validation to optimize model performance. Our proof-of-concept experiment and algorithm are described in Figure 3:

1. Given p domains $D_1, ..., D_p$, draw training datasets $R_1, ..., R_p$, validation splits off of the training datasets $V_1, ...V_p$ (R_i does **not** include V_i), and test sets $T_1, ..., T_p$ with associated performance metrics. Also, train a copy of base model M on the combination of $R_1, ..., R_p$, yielding fine-tuned model M_{all}

2. Create N splits of the combined dataset consisting of $R_1, ..., R_p$, which we denote $\tilde{R}_1, ..., \tilde{R}_N$.

3. Train N copies of base model M on $\tilde{R}_1, ..., \tilde{R}_N$, yielding fine-tuned models $M_1, ..., M_N$.

4. For each domain D_i :
   - Select k fine-tuned models with the highest Complementarity on V_i.
   - Combine the k associated split datasets and fine-tune the base model on the combined dataset, receiving M_i^*.

5. Select k fine-tuned models with the highest average Complementarity (across $V_1, ..., V_p$), combine associated split datasets, and fine-tune the base model on it, receiving M_{avg}^*

6. For all $i = 1, ..., p$ calculate the test performance of M_i^* on T_i, and for M, M_{all}, and M_{avg}^* calculate the test performance on all T_i.

7. For comparison, repeat steps 4 and 5 where data splits are selected based on highest test accuracy rather than validation Complementarity, to receive $M_1^{test}, ..., M_N^{test}$ and M_{avg}^{test}. Repeat step 6 for performance comparison.

Figure 3: Data Selection via Complementarity

Table 3 summarizes the results for $p = 4$, $k = 2$, and $N = 10$, using the same four domains as above. It compares performance, with P@1 being pass-at-1 on domain-specific tasks aligning with the mentioned domain and dataset, and Ratio being the relative change in performance compared to the base model. The best fine-tuned performance in each column is bolded. The table supports three findings: (a) In the realm of general-purpose LLMs small datasets may be just as useful, or even more useful than large datasets, depending on the Complementarity of the data. (b) A model trained to perform well at multiple different tasks (domains) may perform even better than models trained to be experts at said domain. (c) Complementarity, on a split from the training data, may prove more useful in predicting test performance than directly measuring performance on test data. This last finding supports a highly-efficient data-selection algorithm which uses Complementarity as its decision metric on data solely split from the training set.

Table 3: **Using Complementarity on validation for training data selection yields model improvement.** A table presenting the results of the experiment described in Figure 3 for $p = 4$, $k = 2$, and $N = 10$. Performance of different models on each of the four tasks is depicted, with P@1 being pass-at-1 on domain-specific tasks aligning with the mentioned domain and dataset, and RC being the relative change in performance compared to the base model. The "Average" column represents the average RC across the four domains. The best fine-tuned model performance in each column is bolded. For comparison, the first section consists of the baseline model and the model fine-tuned naively on all the data, i.e. 10,000 entries from each of the four domains. The second section consists of models fine-tuned on data selected by evaluating Complementarity. The first row (aligning with item 4 in Figure 3) are four different models fine-tuned on the best two 1/10ths of the dataset in terms of in-domain Complementarity. For example, for the physics evaluation, we first divide the combined dataset into ten subsets and fine-tune a model on each. Then, we compute the Complementarity scores on a validation split from the physics training data, and select the two highest Complementarity splits to use for training the model for physics. This is repeated across the four domains, and thus this row has a different model for each domain. The next row corresponds to item 5 in Figure 3, i.e. the average the model fine-tuned on the two splits out of ten with the best Complementarity averaged across all domains. The final section consists of models fine-tuned on data selected by evaluating performance on the test set, parallel to the previous section. We see that the model fine-tuned on data splits selected by average Complementarity on the validation set not only outperforms the model fine-tuned on all data, but outperforms or ties the models trained based on domain-specific Complementarity, and all models trained on test set performance.

Target / Source	Code (MBPP)		Math (GSM8K)		Physics (MMLU)		Medicine (MMLU)		Average
	P@1	Ratio	P@1	Ratio	P@1	Ratio	P@1	Ratio	
M on all T_i	24.23	1	40.33	1	45.53	1	65.57	1	1
M_{all} on all T_i	25.87	1.07	46.78	1.16	38.20	0.84	52.35	0.80	0.965
M_i^* on paired T_i	**26.80**	**1.11**	46.85	1.15	38.46	0.84	58.28	0.89	0.998
M_{avg}^* on all T_i	**26.80**	**1.11**	**46.93**	**1.16**	**42.95**	**0.94**	**59.18**	**0.90**	**1.028**
M_i^{test} on paired T_i	25.26	1.04	41.85	1.04	**42.95**	**0.94**	56.67	0.86	0.970
M_{avg}^{test} on all T_i	25.67	1.06	44.05	1.09	**42.95**	**0.94**	55.51	0.85	0.985

5 Related Work

Research in the topic of data selection is of immense quantity and continues to be of great interest (Albalak et al., 2024; Li et al., 2024b; Zhang et al., 2025b;a). Arguably the most common path for raising data quality is through data heuristics - filtering out objectively bad data - e.g. elements with less than a certain number of characters, words, or tokens (Raffel et al., 2023). Repetition count is also used, removing elements that repeat certain tokens or words too frequently in quick succession (Raffel et al., 2023), or just removing all data elements which end with, begin with, or include particular undesirable tokens (Penedo et al., 2023). Perhaps the most frequent of such methodologies depend on statistics, such as removing elements with a word count too many standard deviations above the corpus mean, those with too high a percentage of uppercase letters or symbols, or those which have a mean or standard deviation above a pre-established hard limit (Rae et al., 2022; Chen et al., 2021).

Another direction, more closely related to ours, are those of selecting data which either correlate most strongly with data from a given domain or which are thought to improve performance on an eventual downstream task (Axelrod, 2017; Feng et al., 2022; Xie et al., 2023b; Engstrom et al., 2024). But these efforts carry the unfortunate consequence of optimizing for one task or domain at the expense of others, causing catastrophic interference, reducing overall performance on other downstream tasks.

The natural solution to this is data mixing - taking data from different domains (or targeted at different downstream tasks) to form one large dataset upon which to train. As one might expect, relative percentages of data drawn from each dataset are shown to correlate strongly with downstream performance on different domain-related tasks (Xie et al., 2023a; Albalak et al., 2023; Fan et al., 2024; Xia et al., 2024). Many such methods are offline, but there are also training-time variants that continuously update inter-domain information as training weights for how much data to draw from different domains (Chen et al., 2023). This is, however, without the more fine-grained data selection from within domains as we do.

Nevertheless, all aforemention methods rely on inputting immense amounts of data from all relevant domains, including additional buffer data to separate domain pairs to reduce catastrophic interference. One work (Azeemi et al., 2023) suggests that pruning the data can actually result in improved results with a significant reduction in overall quantity, as we also found to be the case. We refine this angle, introducing a powerful metric which can be used to guide data pruning for increased performance along a wide variety of domains and downstream tasks while significantly reducing the overall amount of data required by the model.

6 Discussion

Selection of a metric is an incredibly important task when it comes to evaluation of a new model or novel methodology. In many ways, the metric selected is a reflection of the user's viewpoint, informing how they will observe information. Between essentially any two models or methodologies, there exist sufficiently convoluted metrics that will favor each of the two choices, even if one is effectively strictly better than the other. Therefore, it is crucial to select metrics which are well grounded, i.e. that have an intrinsic connection to the real world and are directly informed by the desired model behavior. In most cases, this entails selecting a metric that is mathematically simple, or at least mathematically similar to a fundamental property of the system.

The metrics which are currently used in the LLM sphere are inherited from classifier neural networks, and are thus ill-suited to the task at hand. Indeed, while accuracy is mathematically simple, sound, and well-grounded, this is not the true metric used for LLMs - rather a combination of accuracy with text scraping, instruction-tuning, and a variety of other methods which allow answer extraction. This overall metric is far from simple, is certainly not objective, and lacks a meaningful and intuitive connection to the real world. Beyond this, these metrics are computationally expensive to compute and require case-by-case design depending on the model, training dataset, evaluation dataset, downstream task, etc. To ameliorate such issues, we introduce Complementarity, which we demonstrated has high correlation with existing metrics and thus can be used as an alternative.

The benefits of using Complementarity as a metric are immense. Using Complementarity in place of domain-specific metrics for measuring performance presents four key benefits. First and foremost, Complementarity is a significantly more robust measure than many state-of-the-art metrics. Whereas Pass@N, accuracy, precision, and other common metrics are binary, judging only the final solution, Complementarity describes the general fluency on the target domain. Similarly to how students will receive partial credit for a correct response structure and design process, so too should we use a robust metric for measuring understanding, which is robust to minor typos and arithmetic errors. Second, Complementarity (which boils down to computing loss) is much faster and less compute-heavy than generation, not to mention whatever system is being used to evaluate the generations. Third, on the topic of generation evaluation, Complementarity reduces the need for extensive prompt tuning and design of generation-scraping tools. Whereas to evaluate performance on a dataset of multiple-choice question, one of math word problems, or one of coding prompts may require prompt tuning to receive generations in a very specific format and then designing a text scraper to extract the answers (which may not even be correctly formatted), Complementarity requires no such design, being easily applicable to a wide variety of datasets. Finally, the burden of answer extraction design makes certain datasets and domains infeasible for evaluation, such as creative writing and poetry which have no singular correct response, a struggle which Complementarity mitigates entirely.

Conventional wisdom about general-purpose LLMs is that they are simply an extension of specialist models. If a model trained to perform mathematical calculations requires one million examples, a model trained to perform five tasks will simply require one million examples per task as though we were training five separate specialist models in one, with some extra data "buffer" to keep the tasks nearly independent. This, as we clearly demonstrate, is not necessary. In training our models, we achieve significantly better performance by fine-tuning on a well-selected 1/5th of the data than is achieved by the model fine-tuned on all the data. Thus, data quantity is not the limiting factor, and there must be some element of data quality which informs the performance of a generalist model on different tasks. We also demonstrate that models trained on data selected by Complementarity outperformed those trained on data selected by traditional evaluation metrics, exhibiting the strength of the metric. In addition, we demonstrate that generalist models trained on optimizing Complementarity across four different domains outperform even the models specifically trained for those tasks, indicating that the data selected truly does 'complement' itself.

Finally, there are two important angles we believe should be pursued in future research. First and foremost is the fact that Complementarity, by taking the difference in entropy from a base model to the fine-tuned model, is naturally biased by the data upon the model was pre-trained. Thus, we hypothesize that Complementarity would be even more useful as a metric for data selection when it comes to pre-training models than it has been for fine-tuning. The other direction is that of metric merging. Ultimately, both fluency and correctness are important, and thus using a choice selection of accuracy-based traditional metrics to aid the fluency-based Complementarity in data selection may provide a benefit over using either in isolation.

We suggest that Complementarity is a powerful tool which possesses the capability to enhance model capabilities while significantly decreasing cost and time in data harvesting, design, and compute. Furthermore, we believe Complementarity may yet provide the basis for a metric paradigm shift, wherein the extensive design of convoluted metrics is phased out in favor of intelligent use of intuitive and mathematically sound metrics.

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Appendix

Table 4: **Training datasets.** The four datasets used for training, aligning with the four domains of coding, mathematics, medicine, and physics respectively, are named and basic statistics about the data is provided.

Dataset	Samples	Instruction Length (Words)		Response Length (Words)	
		Mean	Standard Deviation	Mean	Standard Deviation
Code Instructions 120k	121,959	92.11	73.62	425.97	691.09
ORCA Math Word Problems 200k	200,035	238.87	145.03	878.43	408.94
Medical Meadow Medical Flashcards	33,955	92.4	36.27	349.10	313.55
Physics Instruct Tune 30k	30,231	43.81	17.02	646.22	577.82

Table 5: **Test datasets.** The four datasets used for evaluation, aligning with the four domains of coding, mathematics, medicine, and physics respectively, are named and basic statistics about the data is provided.

Dataset	Samples	Instruction Length (Words)		Response Length (Words)	
		Mean	Standard Deviation	Mean	Standard Deviation
Mostly Basic Python Problems (MBPP)	974	78.62	21.62	181.07	127.42
Grade School Math 8K (GSM8K)	1319	239.87	97.57	292.88	141.77
MMLU: Medicine	481	186.03	463.49	13.75	3.9
MMLU: Physics	557	142.1	91.33	56.5	0.87