

# 000 001 002 003 004 005 006 007 008 009 010 011 012 013 014 015 016 017 018 019 020 021 022 023 024 025 026 027 028 029 030 031 032 033 034 035 036 037 038 039 040 041 042 043 044 045 046 047 048 049 050 051 052 053 DATA ALIGNMENT PREDICTS LANGUAGE MODEL PERFORMANCE: EVIDENCE FROM CONTROLLED EX- PERIMENTS IN AUTOFORMALIZATION

Anonymous authors

Paper under double-blind review

## ABSTRACT

We investigate whether data alignment – the similarity between training and evaluation data – is a stronger predictor of language model performance than dataset size. Through controlled experiments, we demonstrate that alignment coefficients consistently predict downstream performance across three distinct metrics: Task2Vec embeddings ( $r^2 = 0.80\text{--}0.96$ ), GZIP compression distance ( $r^2 = 0.90$ ), and sentence embeddings ( $r^2 = 0.80$ ). We consider two experimental settings: (1) pre-training on domain-specific corpora (PubMed, USPTO) and evaluating cross-domain performance, and (2) fine-tuning on autoformalization datasets with varying alignment to formal verification tasks. Our results show strong negative correlations between alignment and perplexity across both settings, with highly aligned small datasets (1.4k tokens) outperforming larger misaligned datasets (4.1k tokens) by 53% in perplexity reduction. These findings provide quantitative evidence that strategic data selection based on alignment can be more effective than simply scaling dataset size, offering practical guidance for efficient model training in specialized domains.

## 1 INTRODUCTION

Research within the domain of Large Language Models (LLMs) has historically placed an emphasis on the size of datasets used for pre-training, claiming it is one of the primary determinants of LLM performance (Chowdhery et al., 2022; NostalgiaBraist, 2022; OpenAI, 2023; Google, 2023b). Empirical evidence demonstrates this trend, as models trained on large datasets exhibit superior performance. Notably, GPT-4, with its conjectured 1 petabyte dataset, markedly surpasses GPT-3—which is trained on a comparatively modest 45 terabytes—in terms of response quality and contextual accuracy (OpenAI, 2023). However, emerging research indicates that other dimensions, such as dataset diversity, play a crucial role in the efficacy of LLMs, with high-performing models often arising from datasets with high diversity coefficients (Lee et al., 2023).

Current discourse predominantly highlights the scale of a dataset as a pivotal factor in its capacity to effectively pre-train or fine-tune a model, with emphasis frequently placed on quantitative metrics—specifically, the sheer size of the dataset (Lee et al., 2023). This investigation, however, seeks to shift this paradigm to consider qualitative assessments, notably the alignment of datasets with the specific evaluation tasks. Building upon methodologies established in previous studies for quantifying dataset alignment, our research aims to examine the role of data quality in the pre-training and fine-tuning process, verifying the hypothesis that increased data alignment could significantly improve LLM performance. This paradigm challenges the emphasis on dataset size, suggesting an alternative approach to dataset importance and optimization in the context of LLM training – i.e., select the most aligned data to your target task. We explore this via Autoformalization.

Autoformalization is defined as the transformation of concepts in natural language to formalized, structured language like mathematical proofs or code. The creation of a proficient Autoformalization tool would not only drastically reduce the substantial costs associated with manual formalization efforts but could also serve as a bridge linking the automated theorem verification and computational algebra with the extensive body of mathematical knowledge predominantly recorded in natural language. Moreover, the capacity for Autoformalization underscores a machine’s adeptness at navigat-

054  
055  
056  
057  
058  
059  
060  
061  
062  
063  
064  
065  
066  
067  
068  
069  
070  
071  
072  
073  
074  
075  
076  
077  
078  
079  
080  
081  
082  
083  
084  
085  
086  
087  
088  
089  
090  
091  
092  
093  
094  
095  
096  
097  
098  
099  
100  
101  
102  
103  
104  
105  
106  
107  
ing the subtleties of human language and the precision required by formal linguistic systems (Wu et al., 2022).

We employ a comprehensive evaluation by comparing the performance of fine-tuned LLMs on *quantitatively* aligned data sets against those calibrated primarily for scale. We engage a broad spectrum of Autoformalization tasks across different domains and complexities, ensuring the thoroughness and robustness of our results.

## 2 METHODS

Our experiment is designed to explore the hypothesis that there exists a negative correlation between the alignment score of a dataset with a benchmark and the perplexity score (see Appendix C) of a Large Language Model (LLM) when either pre-trained or fine-tuned on this dataset and evaluated against said benchmark. The crux of our investigation lies in the assertion that a dataset closely aligned with the benchmark will facilitate the LLM’s learning process, thereby enhancing its performance as evidenced by lower perplexity scores.

### 2.1 CONCEPTUAL FRAMEWORK

The alignment score is a critical metric in our analysis, offering insight into the degree of congruence between a dataset and the chosen benchmark for evaluating downstream performance, such as Autoformalization. We posit that an LLM trained on a dataset that mirrors the characteristics of the benchmark will demonstrate superior performance. This performance is quantitatively measured using the perplexity score. For example, in the fine-tuning setting we measure model perplexity on the debug1AF benchmark, where lower scores denote higher model accuracy and effectiveness.

### 2.2 DATASET ALIGNMENT QUANTIFICATION

To quantify dataset alignment, we employ the Task2Vec Alignment Coefficient, which facilitates a rigorous comparative assessment of dataset similarity (Lee et al., 2023).

The alignment coefficient between two datasets,  $D_1$  and  $D_2$ , is calculated as:

$$\hat{align}(D_1, D_2) = 1 - \mathbb{E}_{B_1 \sim D_1, B_2 \sim D_2} [d(\hat{f}(B_1), \hat{f}(B_2))] \quad (1)$$

where  $\mathbb{E}$  denotes the expectation over batches  $B_1$  and  $B_2$  sampled from datasets  $D_1$  and  $D_2$ , respectively, and  $d(\hat{f}(B_1), \hat{f}(B_2))$  represents the distance between the embeddings of these batches. Unless otherwise specified,  $d$  is defined as cosine distance and is derived through  $\hat{f}$  which is the Task2Vec batch-embedding computed with a fixed probe network (GPT-2 in our experiments) by estimating the diagonal Fisher information of the probe’s parameters on  $B$  and flattening it to a vector Achille et al. (2019).

For the purposes of our experimental framework, we consider the alignment of the entire dataset rather than focusing solely on specific subsets. We assume that the alignment properties of a dataset subset are reflective of the dataset as a whole. Consequently, our alignment evaluations are predicated on the comprehensive dataset, offering a holistic view of dataset congruence and its impact on model performance.

## 3 EXPERIMENTS & RESULTS

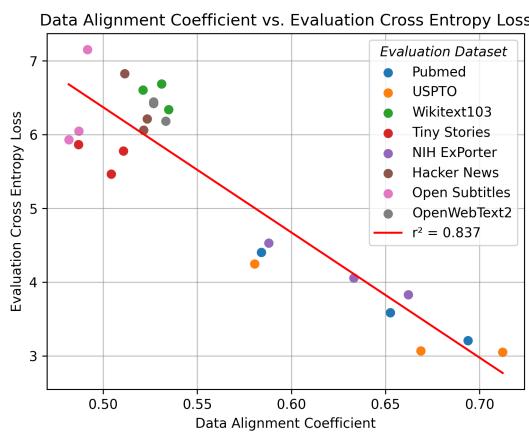
### 3.1 EFFECTS OF DATA ALIGNMENT BETWEEN PRE-TRAINING AND EVALUATION DATA

#### 3.1.1 EXPERIMENTAL SETUP AND MOTIVATION

To evaluate the effect of data alignment between pre-training data and downstream task, we pre-train 51M parameter GPT-2 models (Radford et al., 2019) for 1.31B tokens on one of three datasets: PubMed Abstracts, a dataset of medicine-related abstracts; USPTO Backgrounds, a dataset of patent application background sections; and a dataset produced by concatenating USPTO and PubMed Abs.

108 By controlling for all training hyperparameters aside from the pretraining dataset, we minimize  
 109 the effect of confounding variables on the relationship between data alignment and downstream  
 110 performance. We proceed to evaluate these pre-trained models on a variety of evaluation datasets,  
 111 which vary in terms of their similarity to the three pre-training datasets, both empirically in terms  
 112 of the alignment coefficient and qualitatively based on the topic and structure of text within each  
 113 dataset. By evaluating language modeling cross-entropy loss for a given pre-trained model on a  
 114 given evaluation dataset, we directly test the importance of pre-training data alignment with the  
 115 model’s downstream task in order to illustrate the relationship between alignment and downstream  
 116 performance.

### 117 3.1.2 PRE-TRAINING EXPERIMENT RESULTS



134  
 135 Figure 1: The data alignment coefficient demonstrates a strong relationship with model perfor-  
 136 mance (cross-entropy loss) on various evaluation datasets ( $r^2 = 0.8$ ). The data alignment coeffi-  
 137 cient is computed between a model’s pre-training dataset (PubMed Abs., USPTO, or PubMed Abs.  
 138 + USPTO) and a single evaluation dataset (represented by a unique color).

139 Figure 1 demonstrates that there is a moderate–strong relationship between the alignment coefficient  
 140 (between pre-train data and evaluation data) and model performance (cross-entropy loss) pooled  
 141 across various evaluation datasets ( $r^2 = 0.8$ ). As expected, when datasets share similarities in topic  
 142 and structure, the alignment coefficient is higher.

143 These results demonstrate that the alignment between pre-training corpora and evaluation data is a  
 144 significant driver of model performance. For instance, when considering the extremes of alignment  
 145 and lack thereof, the most aligned train-evaluation data (USPTO train with USPTO validation data)  
 146 produces approximately 2.9 lower absolute CE loss compared to the least aligned train-evaluation  
 147 data (PubMed Abs. train with Open Subtitles validation data). Furthermore, an important aspect of  
 148 model performance with respect to its alignment coefficient is that the relationship between perfor-  
 149 mance and alignment demonstrates a strong, predictable downward trend, more rigorously charac-  
 150 terizing the relationship between alignment and downstream performance than a qualitative intuition  
 151 of superior performance with greater alignment.

## 153 3.2 EFFECTS OF DATA ALIGNMENT BETWEEN FINE-TUNING AND EVALUATION DATA

### 154 3.2.1 EXPERIMENTAL SETUP AND MOTIVATION

155 In order to test whether an LLM will be better able to perform AF when fine-tuned on a dataset that  
 156 is closely aligned to the AF benchmark, we must fine-tune LLMs on datasets of differing alignment  
 157 to the benchmark. This allows us to observe a relationship between alignment and perplexity loss.

158 We chose to run our experiment on the following datasets specifically to introduce a controlled  
 159 range of alignment values in our results. To do so, we selected datasets that represented diversity  
 160 in both domain relevance and data structure. While not exhaustive, these datasets represent three

162 major regimes in LLM training and evaluation: natural language prose, formal mathematics, and  
 163 multi-language code.  
 164

- 165 1. AF Dataset (AF): A dataset consisting of informal statements and their formal counterparts  
 166 in Isabelle designed for training LLMs to perform Autoformalization. We use its test set as  
 167 a benchmark of LLM performance on statement Autoformalization. Thus, we also believe  
 168 it will result in the lowest perplexity among the proof datasets when used to train an LLM  
 169 for AF (Miranda, 2021).
- 170 2. Destructed AF Dataset (AF-split): This dataset is composed of the AF Dataset’s formal  
 171 and informal statements but the two are split into different lines so that the LLM trains on  
 172 data that does not explicitly indicate a relationship between the two; we expect this to still  
 173 obtain a relatively low perplexity score given its high alignment.
- 174 3. The Stack Smol Python Docstrings dataset (Docstring): A dataset consisting of concise  
 175 function headers written in informal language and their implementations in Python; we use  
 176 it to assess how well coding datasets can fine-tune for Autoformalization (Bird, 2023a).
- 177 4. The Stack Dedup Python Docstrings 1.0 percent unified dataset (Docstring 2): A dataset  
 178 consisting of function headers written in informal language and their implementations in  
 179 Python; given its nature we anticipate it scoring among the lowest of perplexity scores  
 180 against the Docstring benchmark (Bird, 2023b).
- 181 5. C4-EN-10K Dataset (C4): A ten-thousand-entry subset of a database composed of text  
 182 pulled from Common Crawl (an internet archive) meant for pre-training for general English  
 183 language modeling. Given its entries are all informal statements not related to mathematics,  
 184 we predict a high perplexity score in performing AF (Raffel et al., 2019).
- 185 6. wikitext-2-raw-v1 Dataset (Wikitext): A subset of the Wikitext dataset; Wikitext is a dataset  
 186 composed of text taken from Wikipedia pages that met the score guidelines to qualify as  
 187 either a ‘good’ or ‘featured’ article; given its nature and lack of relevance to AF, we expect  
 188 a high perplexity score (Merity et al., 2016).
- 189 7. minif2f-lean4 Dataset (LeanDojo4): A subset of the miniF2F dataset which is comprised of  
 190 math exercise statements and their formal counterparts in Lean; given that it is in a different  
 191 formal language, we expect a mid-range perplexity score (Zheng et al., 2021).
- 192 8. Proofnet Dataset (Proofnet): This dataset is comprised of statements taken from undergrad-  
 193 uate math courses and their formal counterparts in Lean; given their similarities, we expect  
 194 LeanDojo4 and Proofnet to score similarly in perplexity (Azerbayev et al., 2023).
- 195 9. HumanEvalPack: This dataset consists of a prompt describing a function and implemen-  
 196 tations of the function in Python, JavaScript, Java, Go, C++, and Rust as well as buggy  
 197 solutions to serve as bad examples. We expect it to obtain a mid-range score against the  
 198 Docstring benchmark (Muennighoff et al., 2023).

199  
 200 For each of these datasets, we needed to separate them into proof datasets and code datasets and  
 201 preprocess the data accordingly. Figure 3 visualizes our method.

202 3.2.2 ADDITIONAL CORRELATION RESULTS  
 203

204 205 Table 1: All datasets and their corresponding number of tokens.

206 <b>Dataset</b>	207 <b>Number of Tokens</b>
208 AF	4092
209 C4	4096
210 Wikitext	4186
211 Proofnet	4032
212 LeanDojo4	4186
213 ProofPile	4096
214 Docstring-Python	4116
215 Humanevalpack	4004
Docstring-Python-2	3790

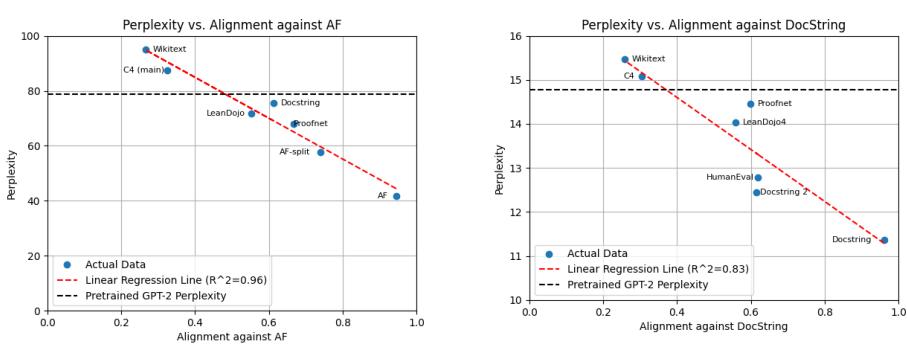


Figure 2: Alignment scores plotted against perplexity suggest a linear negative correlation and mirror our expected findings described in the evaluation design. left plot shows negative correlation of alignment and test perplexity for autoformalization. right plot shows negative correlation of alignment and test perplexity for docstring to code.

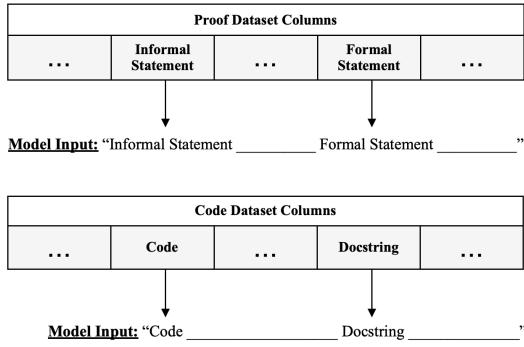


Figure 3: Data preprocessing workflow for separating code and proof datasets.

### 3.3 ANALYSIS OF RESULTS

Introduction of Data Alignment in LLM Training: A novel approach that integrates data alignment as a key factor in the training of Large Language Models, leading to improved model performance.

1. Empirical Evidence of Alignment Impact: Through systematic experimentation, the paper provides empirical evidence that higher alignment between training data and the target domain leads to a decrease in perplexity scores, indicative of enhanced model accuracy.
2. Analysis Across Multiple Datasets: The study conducts a comprehensive analysis across a variety of datasets, establishing the consistency of the negative correlation between data alignment and perplexity across both proof and code datasets.
3. Demonstration of a High  $r^2$  Correlation Value: Our experiments demonstrate a robust negative correlation between data alignment and model perplexity, with a high  $r^2$  value of 0.96 for proof datasets and 0.83 for code datasets when evaluated on Autoformalization tasks, and an  $r^2$  of 0.8 for a pre-training setting with a variety of training and evaluation datasets, indicating a strong predictive relationship.
4. Identification of Limitations and Future Research Avenues: The paper discusses the limitations of the current study due to hardware constraints and sets the stage for future research to explore the comparative impact of dataset size versus alignment.

#### 3.3.1 PROOF DATASET RESULTS

For each dataset we calculated the alignment scores using Task2Vec Alignment Coefficient as depicted in Table 2. Our final perplexity scores for each of our models trained can be found in Table 3. This can be difficult to visualize, so we plotted our results as shown in Figure 2.

270 Our results are significant in validating our initial thesis that a highly aligned data is capable of  
 271 producing an LLM that performs better than one that was trained on a dataset with lower alignment.  
 272

273 We found that an untuned, standard gpt-2 LLM received a perplexity score of 78.7413. However,  
 274 after finetuning it on AF it received the best perplexity score in our results: 41.8261. This further  
 275 bolsters our claim as AF-AF also had the greatest alignment (approximately 0.945) and the best  
 276 performance as well.

277 The proofnet dataset did not perform as well as AF fine tuned, with a perplexity score of 67.8906 and  
 278 alignment of 0.67. However, this is expected based on our thesis as we see that a drop in alignment  
 279 contributes to an increase in perplexity score for the model.

280 The C4 dataset has a much lower score in alignment (approximately 0.32) compared to AF (approx-  
 281 imately 0.95). Judging by this metric alone, we would expect to see a higher perplexity than gpt-2  
 282 finetuned by the debug1AF dataset based on our thesis. When fine-tuning gpt-2 on a subset of C4,  
 283 this proved to be the case as the perplexity score is 87.4636, about 11% higher than Standard gpt-2  
 284 and 110% higher than AF fine tuned.

285 Furthermore, the dataset with the worst alignment, Wikitext, with a alignment coefficient of approx-  
 286 imately 0.27 performed poorly: the perplexity score of 94.9470 is clearly the worst amongst our  
 287 datasets. This backs up our initial claim.

288 Ultimately, there is a clear negative correlation between the alignment coefficient and perplexity, as  
 289 depicted in the graphs above: we observe an  $r^2$  value of approximately 0.987 in the left-hand plot  
 290 in Figure 2, suggesting a strong linear fit. The slope of the fitted linear function is approximately  
 291 -74.4, demonstrating that a 0.1 increase in the alignment coefficient correlates with a decrease in  
 292 perplexity of approximately 7.4. Importantly, the negativity of the slope demonstrates the negative  
 293 correlation between alignment and perplexity.

294

295

### 296 3.3.2 CODE DATASET RESULTS

297

298 For our code dataset, we found again a strong negative correlation between alignment score and  
 299 perplexity loss. Immediately we see that perplexity scores are much lower for the code datasets  
 300 than the proof datasets. This is probably due to the fact that GPT-2 knows how to generate code  
 301 quite well based solely on pre-training, as it has been pre-trained on a large, diverse web-based pre-  
 302 training corpus (Radford et al., 2019). As a result, fine-tuning further on code produces even greater  
 303 results. Standard GPT-2 has a baseline perplexity score of 14.8, which is quite good and is indicated  
 304 by the dotted gray line in Figure 2.

305 We see that the baseline Docstring-Docstring has an alignment score close to 1 (0.96) and as a  
 306 result has the lowest perplexity score (11.4), performing the best out of all our fine-tuned models.  
 307 Moreover, The model that performs the worst also has the lowest alignment of 0.26, Docstring-  
 308 Wikitext.

309 As with the proof datasets, we see a negative correlation between alignment and perplexity, with an  
 310  $r^2$  value of 0.85. While this is not as high as 0.987 as we observed in the proof dataset, this is still a  
 311 strong correlation and further reinforces our thesis.

312

313

### 314 3.4 IMPACT OF DATA ALIGNMENT VERSUS DATASET SIZE ON LLM PERFORMANCE

315

316 This experiment provides an illustrative contrast between the impact of data alignment with the  
 317 downstream task and that of the size of the dataset used for fine-tuning. We hypothesized that a  
 318 smaller, highly aligned dataset would lead to better LLM performance on the downstream task of  
 319 Autoformalization, as measured by perplexity loss, compared to a larger but less aligned dataset.

320

321 Two datasets were used for fine-tuning a pre-trained GPT-2 model:

322 1. A small dataset, extracted directly from the debug1AF benchmark, comprising approximately  
 323 1.4k tokens. This dataset was expected to have high alignment (close to 1) with the Autoformaliza-  
 324 tion task, given its direct sampling from the task’s benchmark.

324 2. A larger, mixed dataset designed to have a lower alignment score of 0.54 with the debug1AF  
 325 benchmark. The dataset size was significantly larger than the first (approximately 4100 tokens),  
 326 intended to test the effect of dataset size versus alignment.

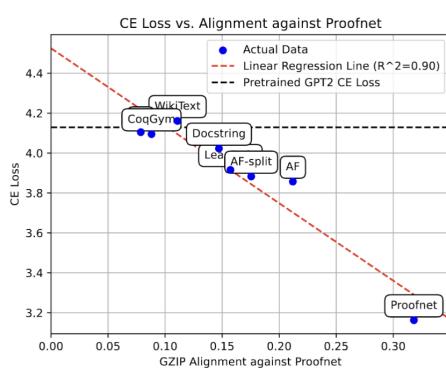
327 Both models were fine-tuned under identical conditions, barring the training dataset, and evaluated  
 328 on the debug1AF benchmark to measure performance through perplexity loss.

330 The results of the fine-tuning experiment support our hypothesis regarding the importance of data  
 331 alignment. The model fine-tuned on the smaller, highly aligned dataset achieved a perplexity loss of  
 332 32.42 on the debug1AF benchmark. In contrast, the model fine-tuned with the larger, less aligned  
 333 dataset exhibited a higher perplexity loss of 69.06, indicating lower performance on the Autofor-  
 334 malization task.

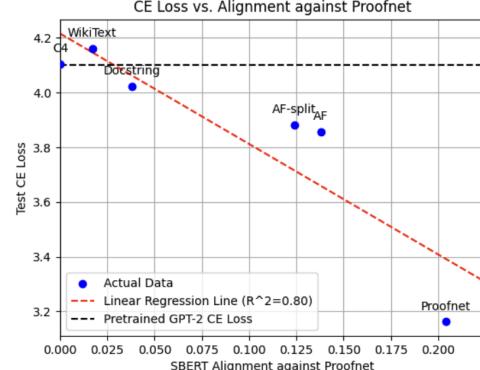
335 These results highlight the importance of data alignment over dataset size in LLM fine-tuning for  
 336 tasks like Autoformalization. A smaller, highly aligned dataset yielded better performance than a  
 337 larger, less aligned one. This anecdotally supports our hypothesis that prioritizing data quality and  
 338 alignment with the task at hand will result in a higher-performing model than one that is trained on  
 339 a dataset selected for sheer quantity. Consequently, we recommend a focused approach to dataset  
 340 selection and preparation, prioritizing alignment to improve LLM performance on specific down-  
 341 stream tasks. Future experimentation is needed to isolate the impact of scale and alignment on  
 342 downstream performance independently and to quantify the relative impact of each.

### 343 3.5 METRIC-AGNOSTIC ALIGNMENT-LOSS TREND

344 Replacing Task2Vec with two alternatives—**GZIP-Align** (compression distance) and **SBERT-Align**  
 345 (embedding cosine)—keeps the same linear drop: higher alignment  $\rightarrow$  lower loss (Fig. 4). On  
 346 ProofNet, GZIP reaches  $r^2 = 0.90$  and SBERT  $r^2 = 0.80$ , close to T2V’s  $r^2 = 0.88$ , suggesting that  
 347 the alignment-performance link is metric-agnostic. Future experimentation is needed to establish if  
 348 this trend holds regardless of the dataset being tested.



363 (a) Gzipalign,  $r^2 = 0.90$



363 (b) SBERT-Align,  $r^2 = 0.80$

364 Figure 4: Alignment–loss correlation on the ProofNet dataset persists across metrics: compression-  
 365 based (left) and embedding-based (right) scores both show the same negative trend observed with  
 366 Task2Vec.

### 369 ACKNOWLEDGMENTS

370 Use unnumbered third level headings for the acknowledgments. All acknowledgments, including  
 371 those to funding agencies, go at the end of the paper.

### 374 REFERENCES

375 Alessandro Achille, Michael Lam, Rahul Tewari, Avinash Ravichandran, Subhransu Maji, Char-  
 376 less C. Fowlkes, Stefano Soatto, and Pietro Perona. Task2vec: Task embedding for meta-learning.  
 377 *CoRR*, abs/1902.03545, 2019. URL <http://arxiv.org/abs/1902.03545>.

378 Zhangir Azerbayev, Bartosz Piotrowski, Hailey Schoelkopf, Edward W. Ayers, Dragomir Radev,  
 379 and Jeremy Avigad. Proofnet: Autoformalizing and formally proving undergraduate-level math-  
 380 ematics, 2023.

381

382 Calum Bird. The stack smol python docstrings, 2023a. URL <https://huggingface.co/datasets/calum/the-stack-smol-python-docstrings>.

383

384 Calum Bird. The stack dedup python docstrings 1.0 percent unified, 2023b. URL <https://huggingface.co/datasets/trelent/the-stack-dedup-python-docstrings-1.0-percent-unified>.

385

386

387

388 Aakanksha Chowdhery, Sharan Narang, Jacob Devlin, Maarten Bosma, Gaurav Mishra, Adam  
 389 Roberts, Paul Barham, Hyung Won Chung, Charles Sutton, Sebastian Gehrmann, et al. Palm: Scaling language modeling with pathways. *arXiv preprint arXiv:2204.02311*, 2022.

390

391

392 L. Fowl, M. Goldblum, A. Gupta, A. Sharaf, and T. Goldstein. Random network distillation as  
 393 a diversity metric for both image and text generation, 2020. <https://arxiv.org/abs/2010.06715>.

394

395

396 Google. Palm 2 technical report, 2023a. <https://ai.google/static/documents/palm2techreport.pdf>.

397

398

399 Google. Palm 2 technical report. Technical report, 2023b. URL  
 400 <https://ai.google/static/documents/palm2techreport.pdf>.

401

402 Tatsunori Hashimoto. Model performance scaling with multiple data sources, 2021. <https://proceedings.mlr.press/v139/hashimoto21a.html>.

403

404 Alycia Lee, Brando Miranda, Sudharsan Sundar, and Sanmi Koyejo. Beyond scale: the diversity  
 405 coefficient as a data quality metric demonstrates llms are pre-trained on formally diverse data,  
 406 2023. <https://arxiv.org/abs/2306.13840>.

407

408 Stephen Merity, Caiming Xiong, James Bradbury, and Richard Socher. Pointer sentinel mixture  
 409 models, 2016.

410

411 Brando Miranda. Ultimate utils - the ultimate utils library for machine learning and artificial intel-  
 412 ligence, 2021. URL <https://github.com/brando90/ultimate-utils>.

413

414 Niklas Muennighoff, Qian Liu, Armel Zebaze, Qinkai Zheng, Binyuan Hui, Terry Yue Zhuo,  
 415 Swayam Singh, Xiangru Tang, Leandro von Werra, and Shayne Longpre. Octopack: Instruc-  
 416 tion tuning code large language models. *arXiv preprint arXiv:2308.07124*, 2023.

417

418 Nostalgebraist. Chinchilla’s wild implications. *AI Alignment Forum*, 2022.

419

420 OpenAI. Gpt-4 technical report. 2023.

421

422 Alec Radford, Jeff Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language  
 423 models are unsupervised multitask learners. 2019.

424

425 Colin Raffel, Noam Shazeer, Adam Roberts, Katherine Lee, Sharan Narang, Michael Matena, Yanqi  
 426 Zhou, Wei Li, and Peter J. Liu. Exploring the limits of transfer learning with a unified text-to-text  
 427 transformer. *arXiv e-prints*, 2019.

428

429 Yuhuai Wu, Albert Q. Jiang, Wenda Li, Markus N. Rabe, Charles Staats, Mateja Jamnik, and Chris-  
 430 tian Szegedy. Autoformalization with large language models, 2022.

431

Kunhao Zheng, Jesse Michael Han, and Stanislas Polu. Minif2f: a cross-system benchmark for  
 432 formal olympiad-level mathematics. *arXiv preprint arXiv:2109.00110*, 2021.

432 **A APPENDIX**  
433435 **B DETAILED PRE-TRAINING ALIGNMENT EXPERIMENT RESULTS**  
436438 In Table 4, we detail the specific alignment coefficient values between (pre-)training and evaluation  
439 data with 95% confidence intervals. Once again, we observe that increased alignment coefficients  
440 between train and evaluation data show a strong trend of leading to lower evaluation loss.  
441444 **C PERPLEXITY CALCULATION**  
445447 Perplexity serves as a measure of a model’s prediction accuracy, with lower values indicating better  
448 performance. It is calculated using the following formula:  
449

451  
452 
$$PPL(X) = \exp \left\{ -\frac{1}{t} \sum_i \log p_{\theta}(x_i | x_{<i}) \right\} \quad (2)$$
  
453

455 where  $PPL(X)$  denotes the perplexity of sequence  $X$ ,  $t$  is the total number of tokens in  $X$ ,  $x_i$  is the  
456  $i$ th token,  $x_{<i}$  represents all tokens preceding  $x_i$ , and  $\log p_{\theta}(x_i | x_{<i})$  is the log-likelihood of token  
457  $x_i$  given its preceding context as predicted by the model parameters  $\theta$ .  
458461 Table 2: Alignment scores of proof datasets on the AF benchmark.  
462463  
464 

Datasets	Alignment score
AF-AF	0.9452813267707825
AFSplit-AF	0.7397596240043640
AF-Proofnet	0.6674373149871826
AF-Docstring	0.6128289103507996
AF-LeanDojo4	0.5514505505561829
AF-C4	0.3249419331550598
AF-Wikitext	0.26609545946121216

  
465475 Table 3: Perplexity loss for models fine-tuned on proof datasets.  
476477  
478 

Model	Perplexity
Standard GPT-2	78.7413
AF fine-tuned	41.8261
Proofnet fine-tuned	67.8906
LeanDojo4 fine-tuned	71.8377
C4 fine-tuned	87.4636
Wikitext fine-tuned	94.9470
Docstring fine-tuned	75.4504

  
479

486 **D DATA ALIGNMENT RESULTS**  
487  
488489  
490 **Table 4: The data alignment coefficient appears to capture an intuitive notion of data similarity,**  
491 **since it finds training data that shares similar semantics and structure as the validation data**  
492 **as most aligned.** In particular, PubMed Abs. (train) and NIH Exporter, which share the semantics  
493 of health-related research and the structure of being research writing, are found to be more aligned  
494 than USPTO (patent application backgrounds). Similarly, USPTO + PubMed Abs. (train) is more  
495 aligned to USPTO (validation) than PubMed Abs. (train), but less aligned to USPTO (validation)  
496 than USPTO (train), as expected. Each cell indicates the alignment coefficient between the given  
497 pre-training dataset (row label) and evaluation dataset (column label).

Pre-training dataset	USPTO (validation)	PubMed Abs. (validation)	OpenWebText2
USPTO	$0.7123 \pm 0.001717$	$0.5840 \pm 0.001389$	$0.5267 \pm 0.001377$
PubMed Abs.	$0.5805 \pm 0.001396$	$0.6939 \pm 0.001697$	$0.5268 \pm 0.001367$
USPTO + PubMed Abs.	$0.6687 \pm 0.001602$	$0.6526 \pm 0.001513$	$0.5332 \pm 0.001390$

Pre-training dataset	NIH Exporter	Hacker News	Open Subtitles
USPTO	$0.5879 \pm 0.001388$	$0.5234 \pm 0.001275$	$0.4917 \pm 0.001162$
PubMed Abs.	$0.6622 \pm 0.001569$	$0.5114 \pm 0.001300$	$0.4817 \pm 0.001145$
USPTO + PubMed Abs.	$0.6331 \pm 0.001452$	$0.5215 \pm 0.001272$	$0.4871 \pm 0.001123$

Pre-training dataset	Wikitext-103	Tiny Stories
USPTO	$0.5311 \pm 0.001303$	$0.5107 \pm 0.001203$
PubMed Abs.	$0.5212 \pm 0.001200$	$0.4868 \pm 0.001167$
USPTO + PubMed Abs.	$0.5347 \pm 0.001290$	$0.5042 \pm 0.001169$

511  
512 **E EXPERIMENT TO VERIFY THAT EACH SUBSET WILL HAVE A SIMILAR**  
513 **PERPLEXITY LOSS TO THAT OF THE ENTIRE DATASET**514  
515  
516 We have examined the perplexity loss of one subset of the dataset on which we have trained on  
517 rather than the perplexity score of the entire dataset. However, we conducted an experiment to show  
518 that these two values are comparable. We have kept the token sizes around 4000 tokens as such:520 Table 5: Subsets and their corresponding number of tokens.  
521

Subset	Number of tokens
C4 Subset Original	4096
C4 Subset 1	4032
C4 Subset 2	4080
C4 Subset 3	3990

522  
523 Then, we calculated the perplexity score for each of these subsets exactly as outlined in the *Evaluation*  
524 section. Here are the results:  
525526 Table 6: Perplexity scores for C4 fine-tuned model.  
527

C4 subset	Perplexity
Original subset	87.4636
Subset 1	84.4889
Subset 2	85.9207
Subset 3	87.4829

528  
529 Here is the graph of all the subsets of C4 along with our original proof dataset fine tuned models:  
530

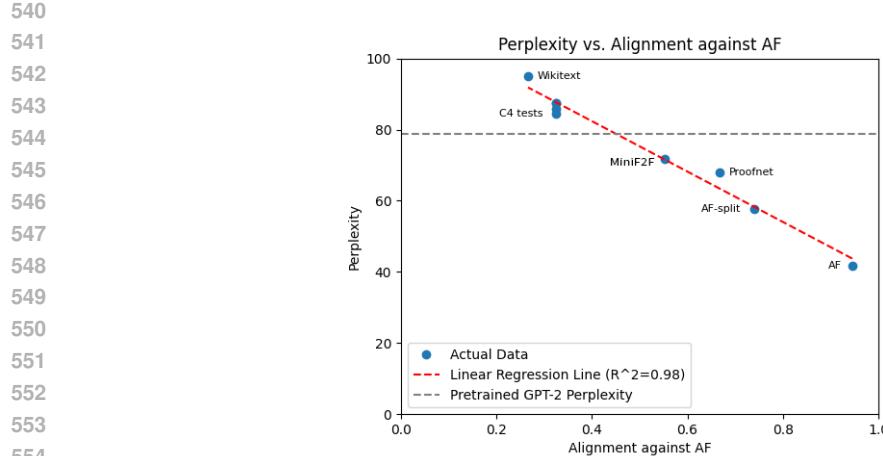


Figure 5: No significant change in perplexity across C4 subsets.

### E.1 DISCUSSION OF C4 SUBSET EXPERIMENT RESULTS

As seen in Table 6, each subset of C4 has comparable perplexity scores. This is further highlighted in the graph where we can see that the subsets are all closely clustered together; this does not affect our line of regression significantly and our claim still holds. This experiment serves as a proof-of-concept that a subset of a dataset can be used to approximate the subset of the entire dataset.

### F EXPERIMENT ON SPLITTING FORMAL AND INFORMAL STATEMENTS IN THE TRAINING PROCESS:

So far we have pre-processed our data as depicted in Figure 3, where each input contains a formal and informal statement (proof dataset) or code and docstring (code dataset). However, we conducted an experiment to observe if inputting formal and informal statements as separate inputs and training on that would produce better results. Figure 6 depicts what this would look like.

We compared the results of AF and AF-Split as follows. We first standardized the number of tokens to 4000 as seen in table 7.

Then, we calculated the alignment as shown in Table 2.

Table 7: AF and AF split tokens.

Subset	Number of tokens
AF Original	4092
AF Split	3960

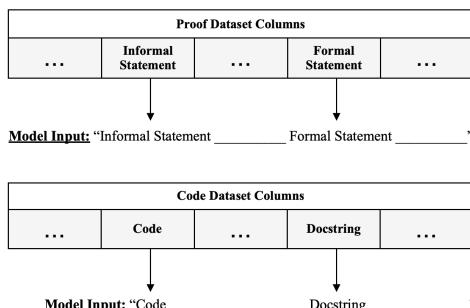


Figure 6: Data preprocessing visualization.

594 Finally, we fine-tuned the model on AF-Split and compared the perplexity loss to AF; this is depicted  
 595 in Table 8.

597 Table 8: Perplexity loss scores for AF and AF split.

599 Model	600 Perplexity
600 AF fine-tuned	601 41.8261
601 AF split fine-tuned	602 57.8004

603 **F.1 DISCUSSION OF AF-SPLIT EXPERIMENT OUTCOMES**

605 The investigation revealed a discernible reduction in alignment for the AF-Split dataset by approx-  
 606 imately 21.7 percent, which constitutes a moderate deviation. Furthermore, there was a notable  
 607 increase in perplexity loss for AF-Split, approximately 38.2 percent underscoring a significant im-  
 608 pact. These findings suggest that models are more adept at Autoformalization tasks when trained  
 609 on datasets that present related information cohesively, rather than on datasets where related content  
 610 is disjointed. Specifically, models excel in Autoformalization when they can discern the intrinsic  
 611 connection between an informal and a formal statement, as exemplified in the format “Informal  
 612 Statement --- Formal Statement ---,” implying an inherent correlation. Conversely, when such  
 613 relational cues are absent, as in the case of AF-Split where informal and formal statements are  
 614 segregated, model performance in Autoformalization tasks diminishes.

615 **F.2 RELATED WORK (CONT.)**

617 The article Google (2023a) “PaLM 2 Technical Report” by Google discusses the development and  
 618 performance of PaLM 2. The study showcases PaLM 2’s versatility but also emphasizes the role of  
 619 architectural enhancements and diverse model objectives in achieving superior results. The inclusion  
 620 of a diverse data mixture, even incorporating a small amount of translation pairs, results in perfor-  
 621 mance comparable to dedicated translation services, a statement which supports our belief that data  
 622 quality can be a critical factor in determining how well a dataset can train an LLM. This sentiment is  
 623 also expressed in the article “Model Performance Scaling with Multiple Data Sources” by Tatsunori  
 624 Hashimoto. Hashimoto (2021) It discusses the challenges of training ML models using data from  
 625 various sources that vary in quality and cost. Hashimoto proposes a parametric model to approx-  
 626 imate generalization error, which is more accurate for various models compared to existing linear  
 627 approximations. The work represents a step toward better understanding model performance under  
 628 varying data conditions and questions whether the approach can scale to more extreme scenarios or  
 629 larger numbers of data sources in future research.

630 “Random Network Distillation as a Diversity Metric for both Image and Text Generation” Fowl  
 631 et al. (2020) is a paper that establishes a diversity metric that measures how wide a range of text or  
 632 images a GAN is capable of outputting. The authors assert that there are many ways that GANs are  
 633 being evaluated, but the diversity of their generation is often overlooked and that pre-existing metrics  
 634 for measuring diversity in their generation were “rudimentary tools” which further emphasizes the  
 635 importance of research on data quality.