How Benchmark Prediction from Fewer Data Misses the Mark

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Abstract

Evaluating large language models (LLMs) is increasingly costly, motivating methods to speed up evaluation by compressing benchmark datasets. Benchmark prediction aims to select a small subset of evaluation points and predict overall performance from that subset. We systematically assess 11 benchmark prediction methods across 19 benchmarks. First, we identify a strong baseline: take a random sample and fit a regression to predict the missing entries, which outperforms most existing methods and challenges the need for careful subset selection. Second, we show that all methods rely on model similarity: performance degrades markedly when extrapolating to stronger models than those used for training, where few methods beat a simple sample average. We introduce an augmented inverse propensity weighting (AIPW) estimator that consistently improves over the random sample average under both interpolation and extrapolation, though gains remain modest and still depend on similarity. This shows that benchmark prediction fails just when it is most needed: at the evaluation frontier, where the goal is to evaluate new models of unknown capabilities.

Introduction

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Computational cost is a major bottleneck in evaluating recent generative models. For example, 18 evaluating a single 176B model on HELM required 4,200 GPU hours [35]; even large organizations report heavy costs on BIG-bench [17]. This has prompted work on efficient LLM evaluation through 19 benchmark prediction: finding a subset of data points to evaluate on and predicting benchmark 20 performance from these evaluations. The simplest method is the random sample mean: evaluate n21 evaluation points and average, which gives an additive approximation up to error $O(1/\sqrt{n})$. Recent 22 work aims to improve this by selecting an informative core set and learning mappings from core set 23 to full-benchmark performance. See the discussion of related work in Appendix A. 24

We systematically study the strengths and limits of these methods by evaluating 11 benchmark prediction methods across 19 benchmarks with at least 83 models each. Models are split into 26 source models (full performance data available) and target models (performance data for no more than 50 points). Methods must estimate target models' mean performance using this constraint. 28 Effectiveness is measured by average estimation gap-the absolute difference between true and estimated performances.

Many methods work well on similar models, but a simple baseline works best. In the interpolation 31 regime (source and target models from same distribution), a remarkably simple method works 32 best: RANDOM-SAMPLING-LEARN-random sampling followed by regression modeling-reduces 33 the estimation gap by 37% compared to basic random sampling, outperforming most sophisticated 34 methods. This suggests that the manner of core-set selection is relatively unimportant; rather, the key 35 to success is modeling the correlation between core-set and full-benchmark performances.

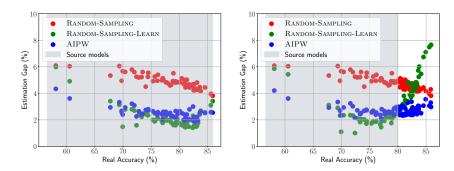


Figure 1: Estimation gap (equation 1) versus real accuracy on ImageNet. Gray shows source model accuracy range. Left: source models randomly sampled across all models. Right: source models sampled from models with lower than 80% accuracy.

Methods fail at the evaluation frontier. In the *extrapolation* regime (target models all better than source models), effectiveness drops sharply. Most methods fail to beat naive random sampling when evaluating new, better models-precisely when efficient evaluation is most needed (Figure 1, right).

40 **AIPW** is an overlooked exception to the rule. We introduce augmented inverse propensity weighting
41 (AIPW) to benchmark prediction. Unlike other methods, AIPW consistently outperforms random
42 sampling in both interpolation and extrapolation settings. However, as illustrated in Figure 1 (right),
43 even AIPW sees diminishing improvements as target models' accuracies exceed those of the sources.
44 **Benchmark prediction relies on model similarity.** Our further study reveals that benchmark
45 prediction methods rely heavily on model similarity [38]: methods that beat RANDOM-SAMPLING do
46 so mainly for targets similar to sources, while accuracy on disimilar models deteriorates. In contrast,

2 What is Benchmark Prediction?

RANDOM-SAMPLING exhibits neutral correlation.

Problem formulation. A benchmark is defined as $(\mathcal{D}, \mathcal{F}, s)$ where \mathcal{D} is the dataset with N data points, \mathcal{F} is the model set, and s is the evaluation metric. For any model $f \in F$ and data point $z = (x, y) \in D$, we define notation as follows.

- s(f,z) denotes performance of f on point z, for example, $\mathbb{1}[f(x)=y]$ for accuracy.
- $\bar{s}(f,\mathcal{D}') = \frac{1}{|\mathcal{D}'|} \sum_{z \in \mathcal{D}'} s(f,z)$ denotes average performance on subset $\mathcal{D}' \subset \mathcal{D}$.
- $s(f, \mathcal{D}')$ denotes the vectorized performance of f on $\mathcal{D}' \subset \mathcal{D}$, and $s(\mathcal{F}', z)$ denotes the vectorized performances of all models in $\mathcal{F}' \subset \mathcal{F}$ on data point z.
- $S(\mathcal{F}', \mathcal{D}')$ denotes the performance matrix for models $\mathcal{F}' \subset \mathcal{F}$ on points $\mathcal{D}' \subset \mathcal{D}$.

Given source models $\mathcal{F}^{(s)} \subset \mathcal{F}$ with known full performance $S(\mathcal{F}^{(s)}, \mathcal{D})$ and target models $\mathcal{F}^{(t)} = \mathcal{F} \setminus \mathcal{F}^{(s)}$ evaluated on only $n \ll N$ points, benchmark prediction aims to estimate $\bar{s}(f, \mathcal{D})$ for each $f \in \mathcal{F}^{(t)}$ by: ① selecting core-set $\mathcal{C} \subset \mathcal{D}$ with $|\mathcal{C}| = n$, and ② learning estimator h to minimize:

estimation gap:
$$\frac{1}{|\mathcal{F}^{(t)}|} \sum_{f \in \mathcal{F}^{(t)}} \left| \bar{s}(f, \mathcal{D}) - h[s(f, \mathcal{C}), S(\mathcal{F}^{(s)}, \mathcal{D})] \right|. \tag{1}$$

60 Previous benchmark prediction methods:

- RANDOM-SAMPLING: pick \mathcal{C} at random; return the mean on \mathcal{C} .
 - ANCHOR-POINTS-WEIGHTED [60]: k-medoids to select \mathcal{C} ; return weighted sum by cluster density.
- ANCHOR-POINTS-PREDICTOR [60]: as above, then linear regression from $s(f,\mathcal{C})$ to $\bar{s}(f,\mathcal{D})$.
- P-IRT [43]: as above, replace regression with the Item Response Theory (IRT) model.
- GP-IRT [43]: combine P-IRT with Anchor-Points-Weighted aggregation.

New methods introduced:

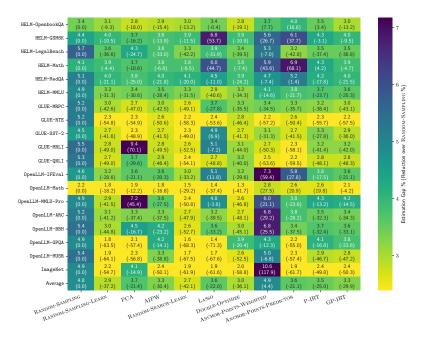


Figure 2: The estimation gaps (\downarrow) for target models (equation 1) under the interpolation split, where source and target models are identically distributed. Each target is evaluated on n=50 data points. The estimation gap reduction (\downarrow) over RANDOM-SAMPLING is shown in parentheses. A negative reduction means that the method achieves a lower gap than RANDOM-SAMPLING. % is omitted.

- RANDOM-SAMPLING-LEARN: pick $\mathcal C$ at random; Ridge regression from $s(f,\mathcal C)$ to $\bar s(f,\mathcal D)$.
- RANDOM-SEARCH-LEARN: run RANDOM-SAMPLING-LEAR 10,000 times; select best \mathcal{C} and h.
- LASSO: Lasso regression with sparsity constraint number of non-zero weights $\leq n$.
- DOUBLE-OPTIMIZE: gradient descent for joint core-set and regression optimization.
- PCA: use random C; impute target scores with PCA assuming $S(\mathcal{F}, \mathcal{D})$ is low-rank.
- AIPW [48]: train regression g to predict s(f,z) from $s(\mathcal{F}^{(s)},z)$ for every f. The idea is to use the predicted performance $\hat{s}(f,z)=g[s(\mathcal{F}^{(s)},z)]$ as a proxy score of s(f,z) and "debias" as follows

$$h^{\text{AIPW}}(f) = \bar{s}(f, \mathcal{C}) + \frac{1}{1 + \frac{n}{N-n}} \left(\frac{1}{N-n} \sum_{z \in \mathcal{D} - \mathcal{C}} \hat{s}(f, z) - \frac{1}{n} \sum_{z \in \mathcal{C}} \hat{s}(f, z) \right). \tag{2}$$

AIPW is a consistent estimator for $\bar{s}(f,\mathcal{D})$ [19]. Compared to RANDOM-SAMPLING, it reduces estimator variance by a factor of up to $\frac{1}{1+\frac{n}{N}}\rho(\hat{s}(f,z),s(f,z))^2$ [14]. See more details in Appendix B.

3 Experiments

- 77 We examine the 11 benchmark prediction methods under both interpolation and extrapolation settings.
- 78 We select 19 benchmarks from HELM-Lite [35], OpenLLM [16], GLUE [61] and ImageNet [51], each
- vith at least 83 models. See more details in Appendix C.
- 80 Estimation gap reduction under interpolation. For each benchmark, we randomly select 75% of
- models as source models $\mathcal{F}^{(s)}$ with full performance scores $S(\mathcal{F}^{(s)}, \mathcal{D})$ available. The remaining
- 25% serve as target models $\mathcal{F}^{(t)}$, each evaluated on only n=50 data points. We report average
- 83 estimation gap across all target models in 100 random trials. See standard errors in Appendix D.
- 84 Figure 2 shows that compared to RANDOM-SAMPLING, most methods effectively reduce the estima-
- 85 tion gap, with nine of ten achieving more than 20% average reduction across benchmarks. The simple
- baseline RANDOM-SEARCH-LEARN performs best with 42.1% average reduction, outperforming the
- previous state-of-the-art GP-IRT (29.9% average reduction) on nearly all benchmarks.

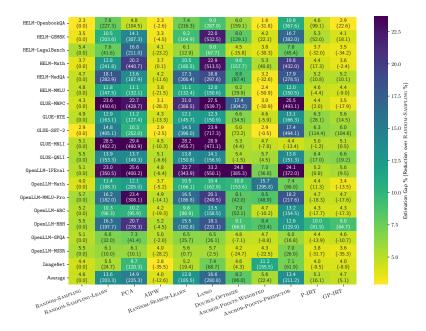


Figure 3: The estimation gaps (\downarrow) for target models (equation 1) under extrapolation split, where source models are the lowest-performing 50%, and target models are the top 30%. Each target model is evaluated on n=50 data points. We also report the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted.

Core-set selection does not significantly enhance effectiveness. RANDOM-SAMPLING-LEARN achieves 37.2% average reduction using only Ridge regression on random samples, performing comparably to RANDOM-SEARCH-LEARN despite the latter's 10,000 optimization iterations. It also surpasses methods with sophisticated subset selection like DOUBLE-OPTIMIZE and GP-IRT. These suggest the primary driver of success is learning to predict the mean rather than core-set selection.

Estimation gap increase under extrapolation. We then examine all 11 methods under extrapolation. Models are ranked by full benchmark performance $\bar{s}(f,\mathcal{D})$. The bottom 50% become source models, while the top 30% serve as target models, reflecting real-world scenarios where developers assess improved models based on existing inferior ones.

Figure 3 reveals striking differences from interpolation. While RANDOM-SAMPLING's estimation gap remains similar (4.6% vs 4.8%), all other methods deteriorate significantly. The previously best RANDOM-SEARCH-LEARN now shows 185.1% increase in estimation gap versus RANDOM-SAMPLING, performing worse across all benchmarks. Only AIPW still outperforms RANDOM-SAMPLING (in 18/19 benchmarks) as it is a consistent estimator, though its advantage shrinks from -30.4% to -12.6% reduction.

This contrast underscores most methods' heavy reliance on source-target similarity. See a deeper analysis of model similarity and ablation studies in Appendix D. While traditional machine learning emphasizes in-domain performance, benchmarking aims to identify superior new models, making extrapolation more relevant than interpolation. The decline in benchmark prediction effectiveness under extrapolation calls for more caution.

4 Conclusion

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Our findings suggest that while benchmark prediction techniques can be useful in specific scenarios, their reliance on similarity between source and target models poses a risk of misestimating the performance of new models. This underscores the importance of applying these methods with caution, especially for evaluating models that significantly deviate from previous ones. See more detailed discussion in Appendix E.

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NeurIPS Paper Checklist

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A Related Work

Evaluating large language models (LLMs) has become increasingly costly as these models grow in size and capabilities [35, 16, 65, 68]. These costs manifest in several ways. First, the collection and annotation of evaluation data can require significant resources [66]. To mitigate these costs, researchers have turned to methods such as using LLMs-as-judges [21, 23] or employing active labeling [32, 31, 10, 12, 70] to generate evaluation data and labels. However, these savings come with drawbacks. For instance, LLM-as-a-judge does not produce reliable evaluation outcomes, as judge models tend to prefer models similar to them, and have other biases [63, 42, 14, 7].

Another significant cost in LLM benchmarking arises from the model inference itself. Generating responses with LLMs can be time-consuming [35, 68, 53], and common inference time scaling techniques [57, 24, 54, 33] may exacerbate this issue. The success of scaling laws [29, 50] in predicting model performance has fueled interest in the development of benchmark prediction techniques [60, 43, 44, 40, 41], which aim to estimate benchmark performance by evaluating LLMs on a limited set of data ¹.

The key idea underpinning benchmark prediction is that not all evaluation examples carry the same amount of information [49]. It is hypothesized that a smaller core set of examples can represent the entire test set, allowing for accurate estimation of overall benchmark performance [60]. This is similar to efficient model training approaches, which aim to identify a subset of training data that enable performance comparable to training on the full dataset [52, 69]. Indeed, a popular benchmark prediction method, k-medoids clustering, is a classical approach to core-set selection for training [15]. However, it is important to recognize that the objectives of training and evaluation differ significantly. While training focuses on minimizing empirical risk and enhancing model performance, evaluation seeks to provide an unbiased estimation of a model's performance to facilitate fair model comparison [40]. Our work challenges the assumption that core-set selection is the key to the success of benchmark prediction by introducing competitive methods that do not rely on core-set selection.

Many existing approaches treat benchmark prediction as a learning problem, aiming to predict a model's overall performance based on its performance on a subset of data [60, 43, 34, 30, 45]. Despite promising results, previous work has highlighted limitations in terms of estimation variance [36]. Going further, we highlight that most benchmark prediction methods rely on model similarity, with estimation performance deteriorating when target models deviate from familiar source models.

¹Unlike bandit literature [68, 53], which focuses on identifying the best model from a pool, benchmark prediction is more challenging as it seeks to forecast overall benchmark performance for any new model.

2 B Details of Benchmark Prediction Methods

663 B.1 Problem Formulation

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- We repeat the notation and the problem formulation here for the reader's convenience.
- A benchmark is represented as a triplet $(\mathcal{D}, \mathcal{F}, s)$.
- \mathcal{D} represents the benchmark data with $|\mathcal{D}| = N$ data points. A data point is referred to as $z \in \mathcal{D}$, where z = (x, y), x refers to the query and y refers to the ground truth answer.
- \mathcal{F} refers to all potential models that can be evaluated on the benchmark.
 - s represents the metric of the benchmark.
 - s(f,z) refers to the performance of any $f \in \mathcal{F}$ on any data point $z \in \mathcal{D}$. For example, $s(f,z) = \mathbb{1}[f(x) = y]$ if the benchmark uses standard accuracy as the metric.
- $\bar{s}(f,\mathcal{D}') = \frac{1}{|\mathcal{D}'|} \sum_{z \in \mathcal{D}'} s(f,z)$ represents the average performance of $f \in \mathcal{F}$ on any $\mathcal{D}' \subset \mathcal{D}$.
- 673 $-s(f,\mathcal{D}')=\{s(f,z)\}_{z\in\mathcal{D}'}$ represents the vectorized performance of $f\in\mathcal{F}$ on all data points in $\mathcal{D}'\subset\mathcal{D}$, and $s(\mathcal{F}',z)=\{s(f,z)\}_{f\in\mathcal{F}'}$ represents the vectorized performances of all models in $\mathcal{F}'\subset\mathcal{F}$ on data point $z\in\mathcal{D}$.
- $S(\mathcal{F}', \mathcal{D}') = \{s(f, \mathcal{D}')\}_{f \in \mathcal{F}'} = \{s(\mathcal{F}', z)\}_{z \in \mathcal{D}'}^{\mathsf{T}}$ as the performance matrix of all models in $\mathcal{F}' \subset \mathcal{F}$ on all data points in $\mathcal{D}' \subset \mathcal{D}$.
- $\mathcal{F}^{(s)} = \{f_1, \dots, f_M\} \subset \mathcal{F}$ refers to a set of source models, whose performances on every data point of the benchmark $S(\mathcal{F}^{(s)}, \mathcal{D})$ are known.
- The rest of the models are referred to as target models $\mathcal{F}^{(t)} = \mathcal{F} \setminus \mathcal{F}^{(s)}$, which can only be evaluated on at most $n \ll N$ data points to save computational costs.
- Benchmark prediction with fewer data aims to estimate $\bar{s}(f,\mathcal{D})$ for every $f \in \mathcal{F}^{(t)}$ with only n data points. In practice, benchmark prediction often involves two steps: ① identifying a representative core-set $\mathcal{C} \subset \mathcal{D}$ with $|\mathcal{C}| = n$ data points, and ② learning a performance estimator h to estimate the average performance on the full benchmark based on the core-set. Formally, the goal of benchmark prediction is to find \mathcal{C} and h to minimize the estimation gap over target models,

estimation gap:
$$\frac{1}{|\mathcal{F}^{(t)}|} \sum_{f \in \mathcal{F}^{(t)}} \left| \bar{s}(f, \mathcal{D}) - h[s(f, \mathcal{C}), S(\mathcal{F}^{(s)}, \mathcal{D})] \right|. \tag{3}$$

For simplicity, in the remainder of the paper, we will denote the estimated performance of target model $f \in \mathcal{F}^{(t)}$ as h(f), instead of explicitly writing $h[s(f, \mathcal{C}), S(\mathcal{F}^{(s)}, \mathcal{D})]$.

689 B.2 Benchmark Prediction Methods

- 690 **Previous methods** In this paper, we examine five widely-used benchmark prediction methods,
- RANDOM-SAMPLING randomly samples a subset as \mathcal{C} and directly returns the mean performance,

$$h^{\text{RANDOM-SAMPLING}}(f) = \bar{s}(f, C).$$
 (4)

- If the benchmark metric s is standard accuracy, the gap $|\bar{s}(f,\mathcal{C}) \bar{s}(f,\mathcal{D})|$ is bounded by $\mathcal{O}(\sqrt{1/n})$ with high probability based on Hoeffding's inequality.
- ANCHOR-POINTS-WEIGHTED [60] treats benchmark prediction as a k-medoids clustering problem. The selected medoids are used as \mathcal{C} , and a weight vector $\boldsymbol{\theta} \in \mathbb{R}^n$ is calculated as the normalized cluster size of each medoid. The final estimate for any target model $f \in \mathcal{F}^{(t)}$ is

$$h^{\text{Anchor-Points-Weighted}}(f) = s(f, \mathcal{C})^T \theta$$
. (5)

• ANCHOR-POINTS-PREDICTOR [60] extends ANCHOR-POINTS-WEIGHTED. Instead of directly returning the weighted sum, a linear regression model g[s(f, C)] is learned to predict s(f, D - C).

$$h^{\text{ANCHOR-POINTS-PREDICTOR}}(f) = \bar{g}[s(f, \mathcal{C})]$$
 (6)

where
$$g = \underset{g'}{\operatorname{arg\,min}} \frac{1}{M} \sum_{f \in \mathcal{F}^{(s)}} \| s(f, \mathcal{D} - \mathcal{C}) - g'[s(f, \mathcal{C})] \|_2^2,$$
 (7)

where we note that g[s(f, C)] is a (N - n) dimensional vector and we use $\bar{g}[s(f, C)]$ as its mean.

• P-IRT [43] extends ANCHOR-POINTS-PREDICTOR by replacing the regression model g in equation 7 with an Item Response Theory (IRT) model. Following the notation for ANCHOR-POINTS-PREDICTOR, we estimate performance for any $f \in \mathcal{F}^{(t)}$ as follows:

$$h^{\text{P-IRT}}(f) = \frac{N-n}{N} \bar{g}[s(f,\mathcal{C})] + \frac{n}{N} \bar{s}(f,\mathcal{C}). \tag{8}$$

• GP-IRT [43] further generalizes P-IRT by combining its estimation with ANCHOR-POINTS-WEIGHTED as a weighted sum,

$$h^{\text{GP-IRT}}(f) = \lambda h^{\text{Anchor-Points-Weighted}}(f) + (1 - \lambda)h^{\text{P-IRT}}(f), \tag{9}$$

where λ is chosen heuristically to control the error of P-IRT.

New methods We introduce six methods that have not yet been applied to benchmark prediction.

• RANDOM-SAMPLING-LEARN randomly samples a subset as $\mathcal C$ and adopts a Ridge regression model g for estimation as follows,

$$h^{\text{RANDOM-SAMPLING-LEARN}}(f) = g[s(f, C)]$$
 (10)

where
$$g = \underset{g'}{\operatorname{arg\,min}} \frac{1}{M} \sum_{f \in \mathcal{F}^{(s)}} \left| \bar{s}(f, \mathcal{D}) - g'[s(f, \mathcal{C})] \right|.$$
 (11)

- RANDOM-SEARCH-LEARN performs RANDOM-SAMPLING-LEARN for 10,000 times and selects the best-performing subset as \mathcal{C} based on cross-validation. A Ridge regression model g is then trained and used in the same way as RANDOM-SELECTION-LEARN.
- LASSO trains a Lasso regression model with weights $\theta \in \mathbb{R}^N$ as follows,

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$$h^{\text{LASSO}}(f) = s(f, \mathcal{C})^T \boldsymbol{\theta}_{\mathcal{C}}$$
(12)

where
$$\boldsymbol{\theta} = \underset{\boldsymbol{\theta}'}{\operatorname{arg\,min}} \frac{1}{n} \sum_{z \in \mathcal{C}} \left[\boldsymbol{s}(f, \mathcal{D})^{\mathsf{T}} \boldsymbol{\theta}' - \bar{\boldsymbol{s}}(f, \mathcal{D}) \right]^2 + \lambda \|\boldsymbol{\theta}'\|_1,$$
 (13)

where λ is selected so that only n dimensions of θ are non-zero and θ_C is the non-zero slice of θ .

• DOUBLE-OPTIMIZE optimizes both a subset selection vector $\pi \in \mathbb{R}^N$ and a linear regression model with weights $\theta \in \mathbb{R}^N$ with gradient descent as follows,

$$h^{\text{DOUBLE-OPTIMIZE}}(f) = [s(f, \mathcal{D}) \cdot \text{TopMask}(\pi; n)]^{\mathsf{T}} \boldsymbol{\theta}$$
 (14)

where
$$\boldsymbol{\pi}, \boldsymbol{\theta} = \underset{\boldsymbol{\pi}', \boldsymbol{\theta}'}{\operatorname{arg min}} \left\{ [\boldsymbol{s}(f, \mathcal{D}) \cdot \operatorname{TopMask}(\boldsymbol{\pi}'; n)]^{\mathsf{T}} \boldsymbol{\theta}' - \bar{\boldsymbol{s}}(f, \mathcal{D}) \right\}^{2},$$
 (15)

where \cdot refers to the bitwise multiplication between two vectors, and TopMask $(\pi'; n)$ replaces the top n largest values of π' with 1s and the rest with 0s. We directly pass the gradient on TopMask $(\pi'; n)$ to π' during optimization following the Straight-Through technique [27, 3].

- Principal Component Analysis (PCA) treats benchmark prediction as a matrix completion problem. This method assumes the performance matrix $S(\mathcal{F},\mathcal{D})$ is of low rank. By randomly sampling a subset as \mathcal{C} , this methods conducts PCA to impute the missing values for target models [59, 6]. As a more intuitive view, one could also take the acquired principal components as model capability indicators [50], i.e., the $(M \times k)$ PCA-transformed scores indicate the k-capabilities of each model, while the $(k \times N)$ principal components represent the capability requirements for each data point. We select k among $\{2,5,10,20\}$ through cross-validation. The Pseudo codes are in Algorithm 1.
- * Augmented inverse propensity weighting (AIPW) [48]: Inspired by the application of prediction powered inference [2, 1] to the LLM-as-a-judge setting [5, 14], we apply a more general AIPW estimator to benchmark prediction. We train a Ridge regression model g for every target model f, which predicts the point-wise performance s(f,z) based on $s(\mathcal{F}^{(s)},z)$. Formally,

$$g = \arg\min_{g'} \frac{1}{n} \sum_{z \in \mathcal{C}} \left[g'[s(\mathcal{F}^{(s)}, z)] - s(f, z) \right]^2.$$
 (16)

The idea behind the AIPW estimator is to use the predicted performance $\hat{s}(f,z) = g[s(\mathcal{F}^{(s)},z)]$ as a proxy score to estimate $\bar{s}(f,\mathcal{D})$ and "debias" that estimator as follows

$$h^{\text{AIPW}}(f) = \bar{s}(f, \mathcal{C}) + \frac{1}{1 + \frac{n}{N-n}} \left(\frac{1}{N-n} \sum_{z \in \mathcal{D} - \mathcal{C}} \hat{s}(f, z) - \frac{1}{n} \sum_{z \in \mathcal{C}} \hat{s}(f, z) \right). \tag{17}$$

Unlike the other learning-based baselines, AIPW is a consistent estimator for $\bar{s}(f,\mathcal{D})$ [19]. Compared to RANDOM-SAMPLING, it reduces estimator variance by a factor of up to $\frac{1}{1+\frac{n}{N}}\rho(\hat{s}^(f,z),s(f,z))^2$ [14], where ρ is the Pearson correlation coefficient. Recent research [37] shows that AIPW estimator will outperform random sampling if and only if the correlation between $\hat{s}(f,z)$ and s(f,z) is above a certain level that depends on n.

Algorithm 1 PCA Impute Process

- 1: Input: Data matrix with missing values
- 2: **Parameters:** number of components k, max iteration max_iter, stopping threshold tol
- 3: Output: Imputed data matrix
- 4: Step 1: Initialization
- 5: Compute initial values for missing entries using column means
- 6: Step 2: Iterative Imputation
- 7: **for** iteration $\leftarrow 1$ to max_iter **do**
- 8: **PCA Decomposition:**
- 9: Perform \overrightarrow{PCA} retaining k components
- 10: Transform data to the lower-dimensional space
- 11: Reconstruct the data from the lower-dimensional space
- 12: Evaluate Convergence:
- 13: Compute the norm of differences between imputed and original values at missing entries
- 14: **if** norm < tol **then**
- 15: Break the loop
- 16: **end if**
- 17: Update Imputed Values:
- 18: Replace missing values with reconstructed values
- 19: **end fo**i
- 20:
- 21: return Fully imputed data matrix

738 C Additional Experiment Setup

- We select a diverse range of benchmarks from the following sources².
- HELM-Lite benchmarks [35]:
- 741 OpenbookQA [39]: N = 500 data points.
- 742 GSM8K [9]: N = 1000 data points.
- LegalBench [22]: N = 2047 data points.
- Math [26]: N = 437 data points.
- 745 MedQA [28]: N = 1000 data points.
- 746 MMLU [25]: N = 567 data points.
- We obtain the per-data point performances of $|\mathcal{F}|=83$ models from the official leaderboard. Note that Helm-Lite often only uses a subset of the original testing set for each benchmark to save compute.
- GLUE benchmarks [61]:
- 751 MRPC [13]: N = 408 data points.
- RTE [11, 18, 4]: N = 277 data points.
- SST-2 [55]: N = 872 data points.
- MNLI [64]: N = 9815 data points.
- 755 QNLI [46]: N = 5463 data points.
- We use the per-data performances of $|\mathcal{F}| = 87$ models provided by AnchorPoint³ [60].
- OpenLLM benchmarks [16]:
- IFEval [67]: N = 541 data points.
- Math [26]: N=894 data points. Only level 5 MATH questions are used in OpenLLM.
- 760 MMLU-Pro [62]: N = 12032 data points.
- Arc-Challenge [8]: N = 1172 data points.
- 762 BBH [58]: N = 5761 data points.
- 763 GPQA [47]: N = 1192 data points.
- 764 MUSR [56]: N = 756 data points.
- We use $|\mathcal{F}| = 448$ models provided by Huggingface ⁴ and collect their performance scores.
- ImageNet [51]: We collect $|\mathcal{F}|=110$ models from Pytorch Hub ⁵ and evaluate them on ImageNet with N=50,000 data points.
- For simplicity, we report the overall average accuracy directly for MMLU, MMLU-Pro, and BBH, rather
- than the weighted average accuracy computed across sub-tasks. Alternatively, one could apply
- benchmark predictions separately to each sub-task and then calculate the weighted average accuracy.

²Since P-IRT and GP-IRT requires s(f, z) to be binary, we only use benchmarks with accuracy as metric.

³The provided score file for QQP is broken so we exclude it.

⁴https://huggingface.co/spaces/open-llm-leaderboard/open_llm_leaderboard#

⁵https://pytorch.org/vision/stable/models.html#classification

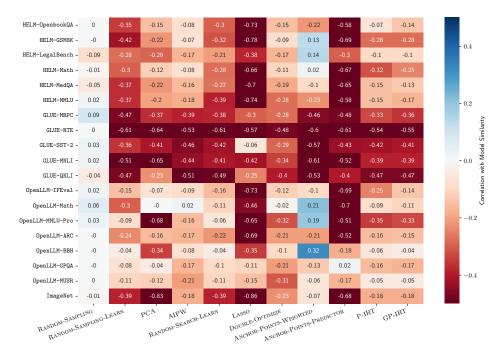


Figure 4: The Pearson correlation between normalized per-model estimation gap (equation 20) and model similarity (equation 18). Negative correlation indicates that target models that are dissimilar to source models tend to have larger estimation gap, and vice versa.

771 D Additinoal Experiment Results

72 D.1 Reliance on Model Similarity

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In this subsection, we investigate the extent to which benchmark prediction methods rely on the similarity between target and source models.

Model similarity. We follow previous works [38, 20] and define the model similarity of target model f to all source models $\mathcal{F}^{(s)}$ as follows,

$$S(f, \mathcal{F}^{(s)}, \mathcal{D}) = \frac{1}{M} \sum_{f' \in \mathcal{F}^{(s)}} \frac{c_{obs} - c_{exp}}{1 - c_{exp}}.$$
(18)

Here, $c_{exp} = \bar{s}(f,\mathcal{D})\bar{s}(f',\mathcal{D}) + (1-\bar{s}(f,\mathcal{D}))(1-\bar{s}(f',\mathcal{D}))$ measures the chance agreement rate, i.e., the expected probability of $\{s(f,z)=s(f',z)\}$ if s(f,z) is independent of s(f',z). In contrast, $c_{obs} = \frac{1}{N} \sum_{z \in \mathcal{D}} \mathbb{1}[s(f,z)=s(f',z)]$ is the observed agreement rate. For simplicity, we use $\mathcal{S}(f)$ to denote $\mathcal{S}(f,\mathcal{F}^{(s)},\mathcal{D})$ in the remainder of the paper. $\mathcal{S}(f)$ quantifies how similar the performance pattern of the target model f is to all source models $\mathcal{F}^{(s)}$, with a higher value indicating greater similarity [20].

We aim to examine the correlation between model similarity and estimation gap. However, we note that the estimation depends on the standard deviation of s(f,z). Since we use accuracy as the metric in our experiment, s(f,z) is Bernoulli with parameter $p_f = \bar{s}(f,\mathcal{D})$ and standard deviation $\sigma_f = \sqrt{p_f(1-p_f)}$. By randomly sampling n data points as \mathcal{C} , Chebyshev's inequality ensures that

$$|\bar{s}(f,C) - \bar{s}(f,D)| < \sigma_f/\sqrt{\alpha n}$$
 (19)

with probability at least $(1-\alpha)$. In other words, the performance of target models with lower σ_f is easier to estimate with the same amount of data. Thus, the standard deviation of the basic estimation gap could potentially confound the observed correlation between model similarity and estimation gap. Consider the method RANDOM-SAMPLING, whose estimation does not depend on source models. If all target models with low σ_f coincidentally have high $\mathcal{S}(f)$, while those with high σ_f have low

792 S(f), then a spurious correlation between estimation gap and model similarity to target models could appear even for RANDOM-SAMPLING. To prevent this, we define the normalized estimation gap as

normalized estimation gap for
$$f$$
: $\mathcal{E}(f) = \frac{1}{\sigma_f} |\bar{s}(f, \mathcal{D}) - h(f)|$. (20)

Then we measure the Pearson correlation between model similarity in equation 18 and the normalized estimation gap in equation 20.

Results. The results are shown in Figure 4. A clear negative correlation between model similarity 796 and estimation gap emerges for almost all benchmark prediction methods except for RANDOM-797 SAMPLING. In particular, the best-performing method under the interpolation model split, RANDOM-798 SAMPLING-LEARN, exhibits a negative correlation below -0.2 in 13/19 benchmarks. Despite its 799 asymptotic unbiasedness, we also find negative correlations for AIPW. This is perhaps unsurprising: 800 While AIPW is consistent independent of how well its regression model $q[s(\mathcal{F}^{(s)},z)]$ predicts 801 s(f,z), its variance depends precisely on that prediction quality. If the predictions are good, AIPW 802 improves substantially over RANDOM-SAMPLING, while there is no improvement when predictions 803 are fully uninformative. But intuitively, predicting s(f,z) is harder when f is very different from the 804 models $\mathcal{F}^{(s)}$ used for training the predictor $q[s(\mathcal{F}^{(s)}, z)]$. 805

Table 1: Ablation study on the core-set size n. We report the estimation gap averaged over all benchmarks. % is neglected for each metric. The lowest estimation gap in each column is highlighted in bold.

	Interpolation $n = 10 \mid n = 20 \mid n = 50 \mid n = 100 \mid n = 200$				Extrapolation $n = 10 \mid n = 20 \mid n = 50 \mid n = 100 \mid n = 200$					
	1.0	1	1	1	1.0 -00	1	1 =-	1		1 =
RANDOM-SAMPLING	11.0	7.7	4.8	3.3	2.1	10.7	7.4	4.6	3.1	2.0
RANDOM-SAMPLING-LEARN	5.4	4.2	2.9	2.1	1.5	17.6	15.8	13.6	12.1	11.1
PCA	6.6	5.2	3.7	2.8	2.1	19.9	17.6	14.9	12.2	9.3
AIPW	8.3	5.4	3.3	2.3	1.8	9.6	6.5	4.0	2.8	2.0
RANDOM-SEARCH-LEARN	4.5	3.7	2.7	2.0	1.4	16.0	14.4	12.8	11.8	11.1
LASSO	7.8	6.1	3.6	2.6	2.2	22.0	19.3	16.6	15.3	14.6
DOUBLE-OPTIMIZE	6.6	4.8	3.0	2.3	1.9	11.3	9.0	8.2	8.0	7.0
ANCHOR-POINTS-WEIGHTED	8.9	6.9	4.9	4.0	3.2	10.4	6.7	5.6	4.7	3.4
ANCHOR-POINTS-PREDICTOR	4.7	4.1	3.6	3.4	4.1	16.2	14.8	13.4	12.4	11.2
P-IRT	7.3	5.9	3.5	2.1	1.3	9.8	8.2	5.1	3.7	3.0
GP-IRT	7.2	5.7	3.3	2.1	1.4	9.7	7.8	4.7	3.4	2.5

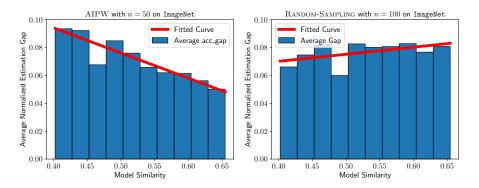


Figure 5: Average normalized estimation gap relative to model similarity for AIPW (n=50) and RANDOM-SAMPLING (n=100) on ImageNet. Each bar represents the target models whose similarity to source models falls within the corresponding range. The normalized estimation gap is defined as shown in equation 20. On average, AIPW outperforms RANDOM-SAMPLING, even with half the data. However, RANDOM-SAMPLING shows better performance when model similarity is low.

D.2 Ablation on Core-set Size

We conduct an ablation study on the size of the core-set n. We experiment with $n \in \{10, 20, 50, 100, 200\}$, and the summarized results are shown in Table 1 (detailed results can be found in Figures 6, 7, 8, 9, 10, 11, 12, 13, 14, and 15. As expected, the estimation gap generally decreases as n increases for most methods. Our previous conclusions remain valid across both settings. With larger core-set sizes, most methods continue to perform better than RANDOM-SAMPLING in the interpolation split but fail to do so in the extrapolation model split. Interestingly, we also find that RANDOM-SAMPLING outperforms all other methods when given twice as much data, even in the interpolation model split.

AIPW remains effective in both settings. However, its advantage over RANDOM-SAMPLING diminishes as n increases. While AIPW reduces the estimation gap by -30.4% in interpolation and -12.6% in extrapolation for n=50, these advantages shrink to -12.4% in interpolation and a mere -2.3% in extrapolation for n=200. This is because the estimator variance reduction factor of AIPW is up to $\frac{1}{1+\frac{n}{N}}\rho(\hat{s}^(f,z),s(f,z))^2$. On the other hand, the advantage of AIPW remains significant when the dataset is large and thus $\frac{n}{N}$ is small. Figure 5 compares AIPW with n=50 to RANDOM-SAMPLING with n=100 data points using ImageNet. AIPW achieves a lower average normalized estimation gap compared to RANDOM-SAMPLING, despite using only half the data. However, the normalized estimation gap under RANDOM-SAMPLING remains largely neutral regarding model similarity. Consequently, while AIPW reduces the average, it produces a higher gap for models with low similarity compared to RANDOM-SAMPLING with twice the data.

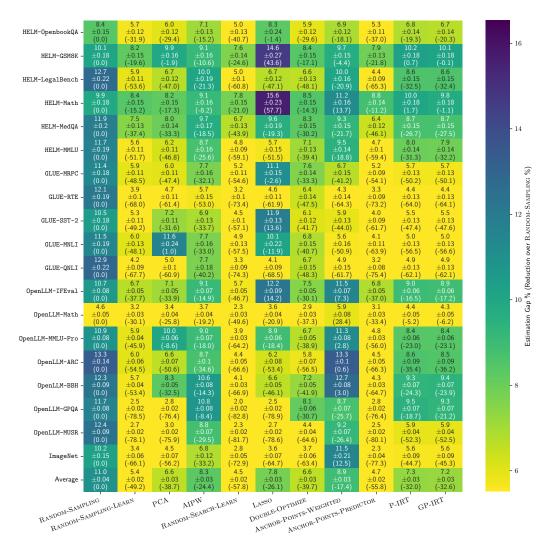


Figure 6: The estimation gaps (\downarrow) for target models (calculated as equation 1) under interpolation model split, where source models are identically distributed with target models. Each target model can only be evaluated on n=10 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

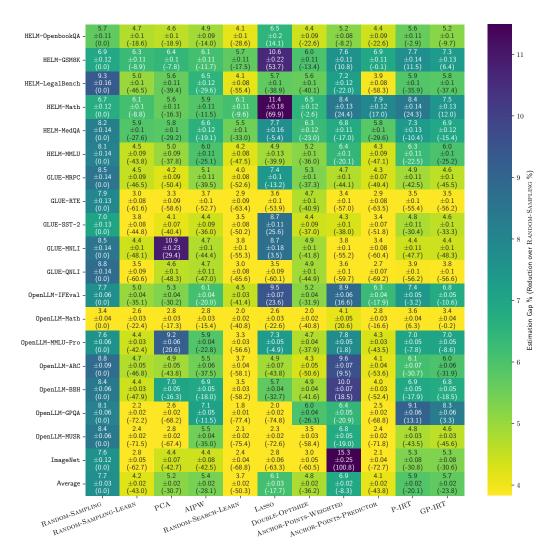


Figure 7: The estimation gaps (\downarrow) for target models (calculated as equation 1) under interpolation model split, where source models are identically distributed with target models. Each target model can only be evaluated on n=20 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

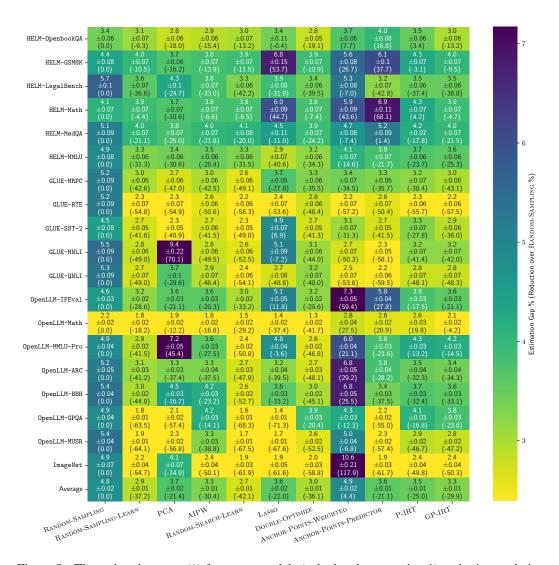


Figure 8: The estimation gaps (\downarrow) for target models (calculated as equation 1) under interpolation model split, where source models are identically distributed with target models. Each target model can only be evaluated on n=50 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

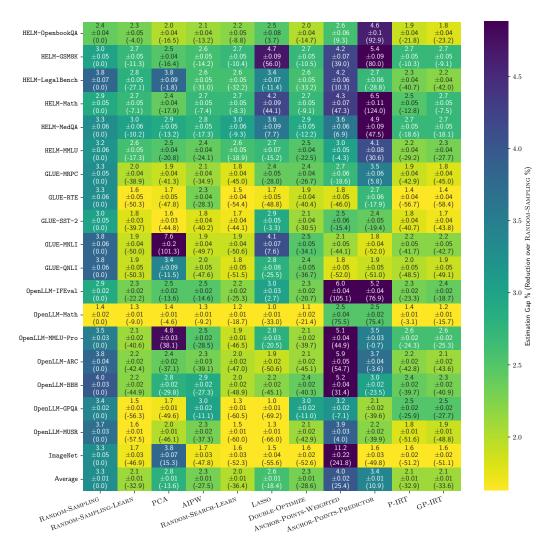


Figure 9: The estimation gaps (\downarrow) for target models (calculated as equation 1) under interpolation model split, where source models are identically distributed with target models. Each target model can only be evaluated on n=100 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

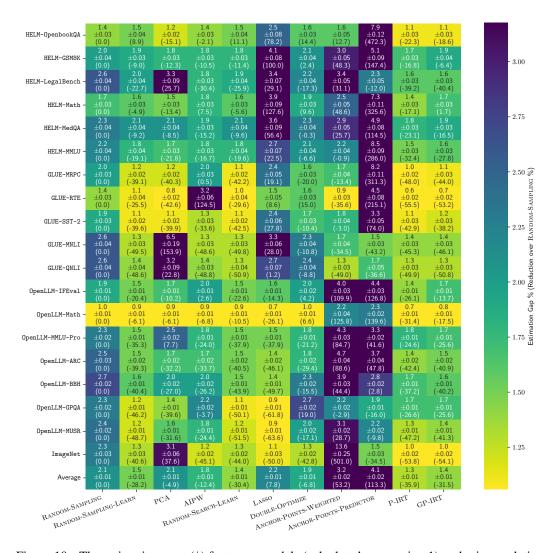


Figure 10: The estimation gaps (\downarrow) for target models (calculated as equation 1) under interpolation model split, where source models are identically distributed with target models. Each target model can only be evaluated on n=200 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

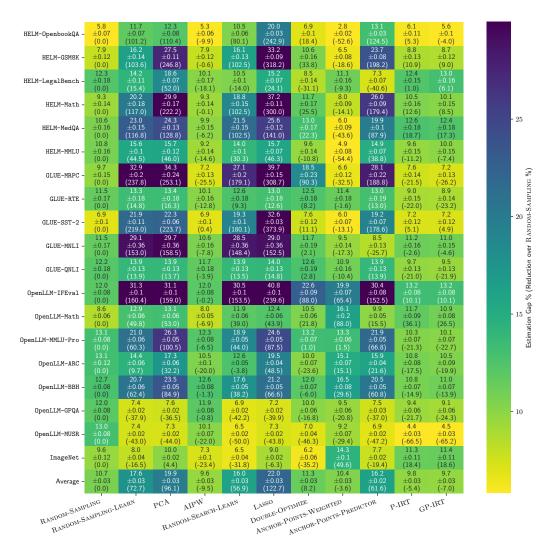


Figure 11: The estimation gaps (\downarrow) for target models (calculated as equation 1) under extrapolation model split, where source models are the lowest-performing 50%, and target models are the top 30% based on average performance over the full benchmark. Each target model can only be evaluated on n=10 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

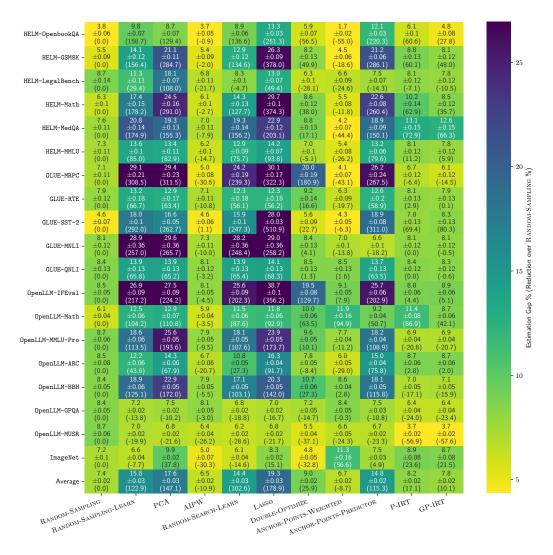


Figure 12: The estimation gaps (\downarrow) for target models (calculated as equation 1) under extrapolation model split, where source models are the lowest-performing 50%, and target models are the top 30% based on average performance over the full benchmark. Each target model can only be evaluated on n=20 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

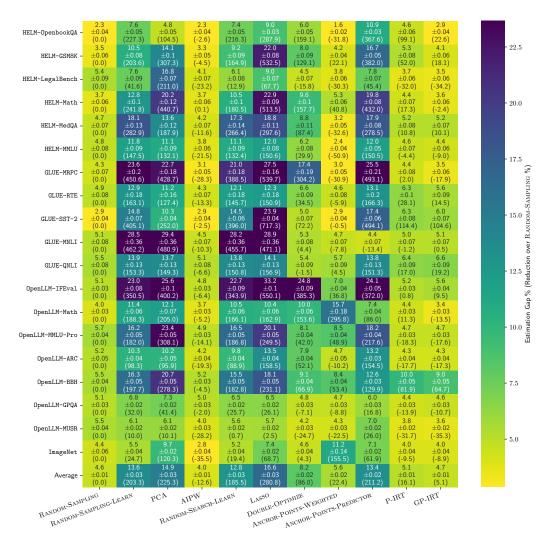


Figure 13: The estimation gaps (\downarrow) for target models (calculated as equation 1) under extrapolation model split, where source models are the lowest-performing 50%, and target models are the top 30% based on average performance over the full benchmark. Each target model can only be evaluated on n=50 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

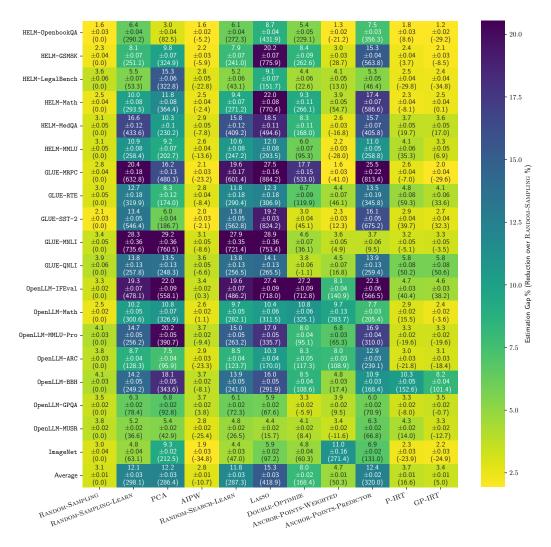


Figure 14: The estimation gaps (\downarrow) for target models (calculated as equation 1) under extrapolation model split, where source models are the lowest-performing 50%, and target models are the top 30% based on average performance over the full benchmark. Each target model can only be evaluated on n=100 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

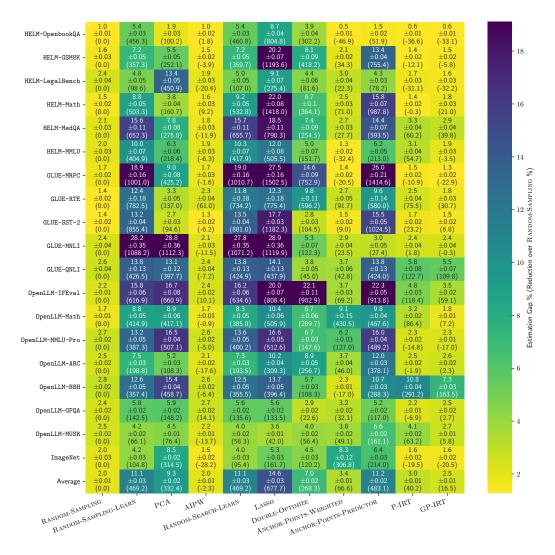


Figure 15: The estimation gaps (\downarrow) for target models (calculated as equation 1) under extrapolation model split, where source models are the lowest-performing 50%, and target models are the top 30% based on average performance over the full benchmark. Each target model can only be evaluated on n=200 data points. We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

Table 2: Training and inference time of each method on ImageNet with N=50000 data points and $|\mathcal{F}|=110$ models. Training is based on 83 source models, and inference is on 27 target models.

	Training Time (s)	Inference Time (s)
RANDOM-SAMPLING	0.00	0.00
RANDOM-SAMPLING-LEARN	0.02	0.00
PCA	0.59	19.20
AIPW	0.00	0.27
RANDOM-SEARCH-LEARN	81.02	0.00
Lasso	105.58	0.01
DOUBLE-OPTIMIZE	4.88	0.00
ANCHOR-POINTS-WEIGHTED	84.26	0.00
ANCHOR-POINTS-PREDICTOR	197.71	0.26
P-IRT	585.72	0.90
GP-IRT	1750.20	0.89

Table 3: Average estimation gap between the predicted rankings based on the coreset and the actual rankings based on the full benchmark, measured by Kendall's τ (\uparrow). The results are averaged over all benchmarks.

	Interpolation					Extrapolation					
	n = 10	n = 20	n = 50	n = 100	n = 200	n = 10	n = 20	n = 50	n = 100	n = 200	
RANDOM-SAMPLING	0.52	0.61	0.70	0.78	0.84	0.36	0.43	0.53	0.63	0.73	
RANDOM-SAMPLING-LEARN	0.57	0.66	0.75	0.81	0.86	0.07	0.12	0.18	0.27	0.36	
PCA	0.55	0.63	0.72	0.78	0.83	0.04	0.10	0.21	0.40	0.57	
AIPW	0.52	0.62	0.72	0.79	0.84	0.33	0.40	0.51	0.61	0.70	
RANDOM-SEARCH-LEARN	0.66	0.70	0.76	0.82	0.86	0.13	0.13	0.20	0.29	0.38	
LASSO	0.68	0.71	0.77	0.81	0.82	0.05	0.06	0.12	0.19	0.22	
DOUBLE-OPTIMIZE	0.58	0.66	0.76	0.81	0.84	0.31	0.36	0.44	0.50	0.58	
ANCHOR-POINTS-WEIGHTED	0.65	0.70	0.76	0.81	0.85	0.37	0.43	0.50	0.60	0.69	
ANCHOR-POINTS-PREDICTOR	0.67	0.72	0.77	0.80	0.80	0.21	0.25	0.32	0.38	0.44	
P-IRT	0.52	0.58	0.71	0.80	0.87	0.28	0.31	0.42	0.56	0.69	
GP-IRT	0.53	0.59	0.72	0.80	0.86	0.28	0.33	0.45	0.59	0.71	

D.3 Running time

While some of the benchmark prediction methods could potentially benefit from the use of GPUs, we opted to run all methods without them, as they are sufficiently fast on standard hardware. Table 2 presents the training and inference times for each method on ImageNet. Among the models, GPIRT is the slowest during training because it involves fitting a large Item Response Theory (IRT) model. During inference, PCA is the slowest, as it requires multiple imputations of the entire matrix. Although AIPW needs training a separate regressor for each target model during inference, the regressor is small, making the inference process remain efficient.

D.4 Ranking Preservation

We further compare the predicted rankings of target models with the actual rankings based on the full benchmark using Kendall's τ . Specifically, we calculate Kendall's τ for each random trial and average the results over 100 trials. Our conclusions mostly remain unchanged, with almost all benchmark prediction methods outperforming Random Sampling under interpolation, while none can surpass RANDOM-SAMPLING under extrapolation.

841 D.5 Case Studies

We further investigate two additional experimental settings that deviate from the primary setting in the main paper.

Fewer source models under interpolation. Different from the previous interpolation setting that utilized 75% of models as source models, we now use only 10 models as source models for each benchmark and use the rest as target models. All other settings remain unchanged. This setting allows us to assess the effectiveness of benchmark prediction when "training data" from source models is more limited. Results are shown in Figure 16. Consistent with the findings in the paper, most methods still outperform RANDOM-SAMPLING, while RANDOM-SEARCH-LEARN and RANDOM-SAMPLING-LEARN remain to be the best-performing methods.

Near extrapolation. We modify the previous extrapolation setting, which used the lowest-performing 50% of models as source models and the top 30% as target models. In this new setting, we designate the top 25% of models as target models and utilize all remaining models as source models. All other settings remain unchanged. This setup enables us to examine whether benchmark prediction methods demonstrate improved performance when the distribution gap between source and target models is reduced. Results are shown in Figure 17. Consistent with the findings in the paper, most methods fail to consistently outperform RANDOM-SAMPLING, except for AIPW.

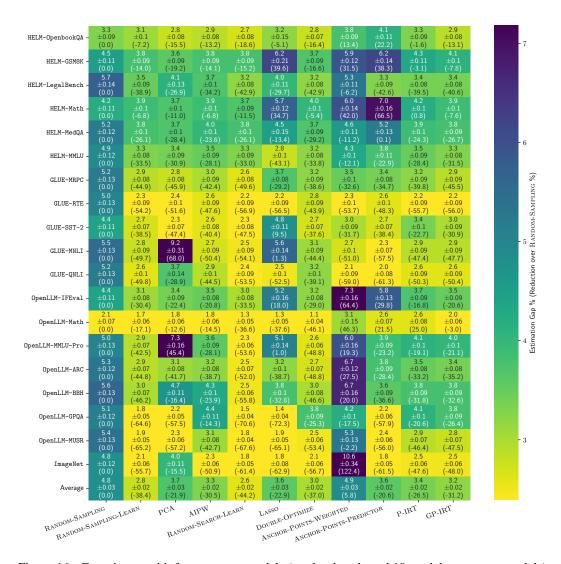


Figure 16: Experiment with fewer source models (randomly selected 10 models as source models) under the interpolation model split. We report the estimation gaps (\downarrow) for target models (calculated as equation 1). We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over Random-Sampling in parentheses. A negative reduction implies that the method achieves a lower estimation gap than Random-Sampling. % is omitted. Best viewed in color.

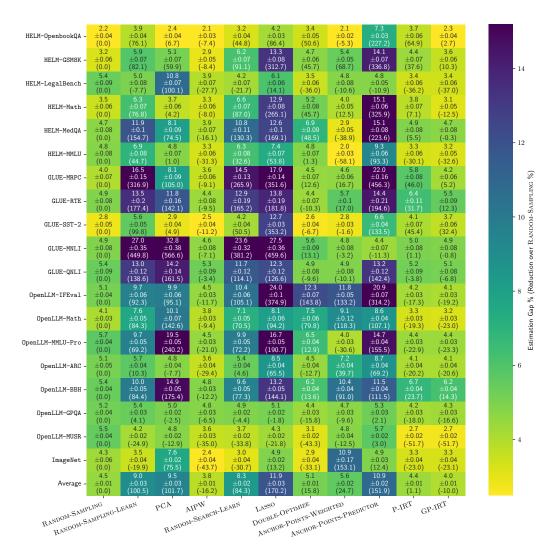


Figure 17: Experiment with the near extrapolation model split by using the top 25% of available models as target models and the remaining bottom 75% models as source models. We report the estimation gaps (\downarrow) for target models (calculated as equation 1). We also report \pm the standard error of the mean and the estimation gap reduction (\downarrow) over RANDOM-SAMPLING in parentheses. A negative reduction implies that the method achieves a lower estimation gap than RANDOM-SAMPLING. % is omitted. Best viewed in color.

E Detailed Conclusion

In this paper, we study the problem of benchmark prediction from fewer data and examine 11 859 benchmark prediction methods. Our findings call into question the necessity of meticulous core-set 860 selection and reveal that these methods are most proficient at interpolating scores among similar 861 models. However, except RANDOM-SAMPLING and AIPW, all methods face significant difficulties 862 when predicting target models that differ substantially from those they have encountered before. 863 We caution against the indiscriminate use of benchmark prediction techniques, as their dependence on 864 model similarity causes most of them to fail precisely when most needed: at the evaluation frontier, 865 where the aim is to assess new models with unknown capabilities. Even in the context of interpolation, 866 no method outperforms RANDOM-SAMPLING, when that simple baseline is given access to twice as 867 much data. Thus, while we recommend to use AIPW as a consistent estimator with lower variance, 868 this suggests that simply raising the sampling budget for RANDOM-SAMPLING can be competitive, 869 especially in settings where predictions of other models for fitting AIPW are costly to obtain. 870

871 F Broarder Impacts and Limitations

This paper addresses the benchmark prediction problem in scenarios with limited data. One potential limitation of our study is the relatively small number of models examined. For both the HELM-Lite and GLUE benchmarks, we have collected full benchmark results for fewer than 100 models. Despite conducting 100 random trials for each experiment, including additional and more diverse models could further strengthen the comprehensiveness and robustness of our analysis.

We do not anticipate any direct societal impacts from this work, such as potential malicious or unintended uses, nor do we foresee any significant concerns involving fairness, privacy, or security considerations. Additionally, we have not identified potential harms resulting from the application of this technology.