OmniPred: Towards Language Models as Universal Regressors

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Abstract

Over the broad landscape of experimental design, regression has been a powerful tool to accurately predict the outcome metrics of a system or model given a set of parameters, but has been traditionally restricted to methods which are only applicable to a specific task. In this paper, we propose OmniPred, a framework for training language models as universal end-to-end regressors over (x, y) evaluation data from diverse real world experiments. Using data sourced from a large proprietary blackbox optimization database, our extensive experiments demonstrate that through only textual representations of mathematical parameters and values, language models are capable of very precise numerical regression, and if given the opportunity to train over multiple tasks, can significantly outperform traditional regression models.

1 Introduction

Regression is a fundamental task in experimental design, over many domains such as hyperparameter tuning, computer software, industrial engineering, and chemical discovery. The goal of regression is to predict a metric y of a general system given a set of input features x. Such regressors can later be used for various applications, such as offline optimization (Kumar et al., 2022; Trabucco et al., 2022), online optimization (Cai et al., 2020), low-cost benchmarking (Zela et al., 2022; Eggensperger et al., 2015) and simulation (Mendis et al., 2019; Hashemi et al., 2018; Kaufman et al., 2021).

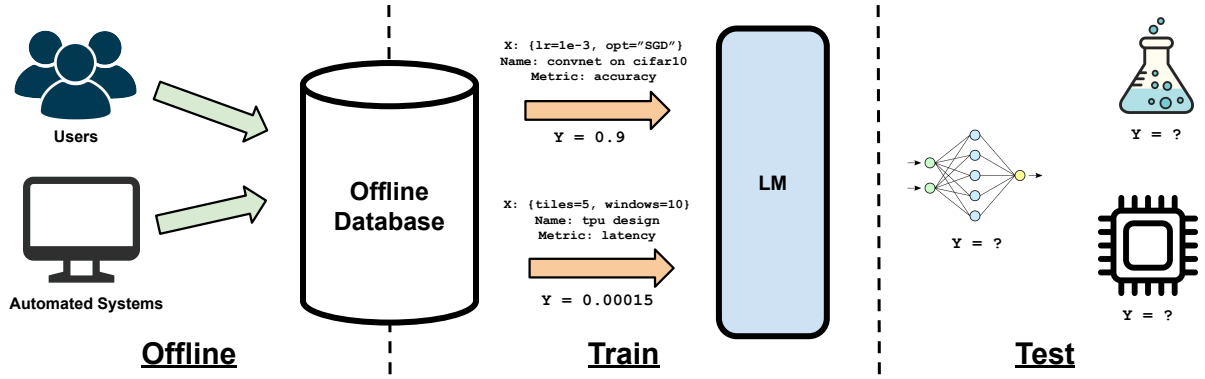


Figure 1: Overview of our method. Using heterogenous offline blackbox function evaluations collected from a variety of sources, we train a LM-based regressor.

In recent years, large language models (LLMs) have emerged as powerful tools for processing textual representations at scale over massive heterogeneous datasets to represent complex relationships between input features and output labels. Given that LLMs have been shown to be effective for a variety of tasks beyond natural language processing, such as coding (Li et al., 2022), symbolic mathematics (Lewkowycz et al., 2022), and scientific reasoning (Singhal et al., 2022), it is reasonable to wonder: *Can language models be used for numeric regression?*

Answering this question is highly important not only for the traditional field of experimental design, but also for the ever-changing field of LLM research, especially due to recent interest in the ability to forecast outcomes of complex systems (Gruver et al., 2023) and reward modeling in reinforcement learning fine-tuning (Ziegler et al., 2019). The textual processing abilities of LLMs are particularly attractive, as they can potentially bypass the need to tediously featurize inputs (i.e. the x's) into raw numerical tensors. Prior to our work, there has been no such research specifically addressing the feasibility and utility of training a "universal" metric predictor over a large heterogenous offline dataset.

Our core contributions in summary, are as follows:

- To the best of our knowledge, we propose OmniPred, the first scalable yet simple metric prediction framework based on free-form textual representations, applicable to general input spaces.
- Through only these text and token-based representations, OmniPred is capable of very accurate metric predictions over experimental design data.
- By simultaneously multi-task learning across vastly different input spaces and objectives, in many cases OmniPred can outperform traditional regression models such as MLPs and boosted trees.
- These transfer learning benefits persist even on unseen tasks after locally finetuning OmniPred on small amounts of new evaluation data.

2 Related Work and Motivation

Traditional regression methods have widely used statistical techniques such as Gaussian Processes (GPs), tree-based methods, and multilayer perceptrons (MLPs), to predict a scalar objective given a fixed-length feature vector, commonly seen in tabular data settings. Multitask (Bonilla et al., 2007) and contextual (Krause & Ong, 2011) variants have been further proposed for transfer learning purposes, but still require fixed-length tensor representations of x, and can thus only use previous x from the same input space. Additional recent works utilizing deep learning-based regressors include Transformers (Hollmann et al., 2023; Huang et al., 2020), recurrent neural networks (Hashemi et al., 2018), graph neural networks (Lukasik et al., 2020; Gao et al., 2023), and deep-hierarchical GPs (Fan et al., 2024), which allow length-independence. Even so, a frequent issue is still the reliance on *tensor representations* of (x, y).

Tensor representations are commonly *problem-dependent*, where each tensor element may need to be in a reasonable numerical range (e.g. in $[-1, 1]$) as inputs to a model. Thus to represent x, every categorical feature must be one-hot embedded against user-provided choices, and scalar features may need to be rescaled against user-provided bounds. Dynamic yet minor input space changes such as new bounds or additional categories, are incompatible with this static representation. To represent y, a raw objective in $\mathbb{R}$ may also need to be rescaled, which can be problematic at test-time when encountering outlier y-values. Dealing with this issue leads to implementing complicated nonlinear warpings (Daimon, 2011; Yeo & Johnson, 2000), many of which are also data-dependent (e.g. require storing min/max values from training data).

Regressor	Dynamic Input Spaces?	Can Multitask?	Tensorize?	Rescale?
MLP	No	Only fixed spaces	Yes	Yes
Tree-based	No	Only fixed spaces	Yes	Optional
Gaussian Process (GP)	No	Only fixed spaces	Yes	Yes
GNN / Transformer / RNN	No	Only fixed domains	Yes	Yes
OmniPred (Ours)	**Yes**	**Yes**	**No**	**No**

Table 1: Comparisons between the flexibilties of different typical regressors.

These issues are summarized in Table 1. In principle, an ideal regressor should process x and output y, both **in absolute terms**, independent of changing external statistics or search constraints. For example, if the objective is $f(x) = \exp(x)$, then the regressor's prediction for $f(2)$ should be invariant regardless if the constraint is $x \in [1, 5]$ or $x \in [0, 100]$. One way to accomplish this is to represent x with an independent universal tokenizer without problem-specific numeric transformations (Zhou et al., 2023). This immediately

unlocks a large amount of transferrability when dealing with variable-length inputs and additional contextual metadata.

This token-based paradigm has shown great success in the case of reinforcement learning from human feedback (Ziegler et al., 2019), where regression over textual responses (the "x"), also known as *reward modelling*, has been crucial to the success of recent interactive LLMs such as ChatGPT (OpenAI, 2022) and Gemini (Team, 2024). Here, LLMs are able to imitate human ratings in the form of pairwise rankings (the "y") or probabilistic scores within a fixed range, e.g. $y \in [0, 1]$ (Bradley & Terry, 1952).

While the overwhelming current focus has been on subjective *human-based* feedback needed for determining aspects such as creativity, safety, and personality, much less attention has been given towards language models for evaluating complex and natural systems common to experimental design, which consist of much more objective and numeric-based data where $y \in \mathbb{R}$. Given multiple works which have shown the brittleness and unreliability of numerical processing in language models (Hendrycks et al., 2021; Nogueira et al., 2021), it is not immediately obvious that language models are capable of high-precision numerical prediction over token-based representations. This is a crucial technical challenge which our paper resolves in the quest for a general-purpose predictor.

3 Methodology

3.1 Preliminaries and Problem Definition

Based on standard blackbox optimization terminology (Golovin et al., 2017; Liaw et al., 2018), for a given task $\mathcal{T} = (\mathcal{X}, f, \mathcal{D}, m)$, we assume there is an inherent objective function $f : \mathcal{X} \to \mathbb{R}$ for which we obtain *trials* (x, y) from evaluating suggestions x, selected from a (possibly implicit) input space $\mathcal{X}$. We define a *study* as an offline collection of trials $\mathcal{D} = \{(x_1, y_1), ..., (x_T, y_T)\}$. To distinguish between different tasks, there may be observable task-level metadata m, which can additionally characterize the task and potentially even describes the behavior of the corresponding objective $f(x)$.

The goal of standard metric prediction is to obtain a distribution function $s : \mathcal{X} \to \mathcal{P}(\mathbb{R})$ such that $s(x)$ accurately approximates $f(x)$ over a distribution of inputs from $\mathcal{X}$, provided that a training set $\mathcal{D}^{train}$ is given. In our particular case, we also provide our language model with multi-task training data $\cup\{\mathcal{D}_1^{train}, \mathcal{D}_2^{train}, ...\}$ from other tasks $\{\mathcal{T}_1, \mathcal{T}_2, ...\}$. While these extraneous tasks do not contain exact evaluations over the f at hand and may even have different input spaces, training on such additional extraneous data may still lead to transferrability, especially for similar tasks.

A common and unified way to measure the accuracy of predictors (deterministic or stochastic) is to compute the gap between a final pointwise prediction against the true objective value, using a regressor-dependent aggregator $\alpha : \mathcal{P}(\mathbb{R}) \to \mathbb{R}$ such as median or mean. However, since different studies can have vastly different objective scales (e.g. CIFAR10 accuracies are within $[0, 1]$ while synthetic objectives are within $[10^2, 10^9]$), we must therefore normalize the difference based on per-study statistics, i.e. for a specific task, we define the study error as a normalized mean absolute error (MAE):

$$\frac{1}{y_{\max} - y_{\min}} \frac{1}{|\mathcal{D}^{test}|} \sum_{(x,y) \in \mathcal{D}^{test}} |\alpha(s(x)) - y| \tag{1}$$

To prevent outlier predictions from significantly swaying average errors, we further clip error maximums to 1.0, equivalent to when the regressor simply outputs boundary values from $\{y_{\min}, y_{\max}\}$.

3.2 Language Model

In this paper, we focus on the standard multi-task regression setting, in which for a given trial (x, y) and task-level metadata m, the prompt is (x, m) and response is y, compatible with both encoder-decoder and decoder-only settings. For simplicity, we train a relatively small 200M parameter T5 encoder-decoder (Raffel et al., 2020) *from scratch* to avoid any confounding effects from typical generative language pre-training. We wish to learn a single set of weights θ, which can be used to form a predictor $s_\theta(\cdot)$ given any arbitrary task

$\mathcal{T}$. In contrast to settings such as (1) traditional regression requiring training a separate model θ_t for each task $\mathcal{D}_t$ or (2) requiring completely evaluated trajectories over specialized trial tokenizations for in-context learning (Chen et al., 2022; Hollmann et al., 2023), our setting maximizes the usage of training data, much of which may contain unfinished trajectories or non-standard x-formats.

Representation: To facilitate training a single model over multiple heterogeneous studies, a crucial guiding principle as mentioned before, is to express x and y in *absolute* fashion, independent of the input space and numeric scaling of the specific study. Thus, we express x in a *key-value* format, directly mapping parameter names to values, but do **not** represent[1] the input space $\mathcal{X}$, allowing generalizability to conditional parameters and dynamic constraints. We represent y with fixed-length custom tokens to guarantee proper decoding via token logit masking, using specific tokens to express sign, exponent, and significant digits. An example is illustrated in Table 2. Ablations over different tokenizations are conducted in Appendix A.1.

	Language Model Textual Representation
x	`batch_size:128,kernel:'rbf',learning_rate:0.5,model:'svm',optimizer:'sgd'`
m	`title:'classification',user:'some-person',description:'spam detection',objective:'accuracy'`
y	`<+><1><2><3><E-2>`

Table 2: Textual representations used for OmniPred. `<*>` represents a single custom token. Input space and x is the same as in Figure 2. Example y tokenization represents a value of 1.23.

Training: To maintain simplicity and normalization-independence, we minimize standard cross-entropy loss over the y-value tokens, consistent with typical language model training. The model will thus implicitly learn numeric distances from training data.

Sampling and Decoding: Through regular temperature decoding, we can repeatedly sample $\hat{y} \sim s_\theta(x)$, to approximate the underlying distribution defined over $\mathbb{R}$. To remain robust to strong outliers, we aggregate samples using the empirical median, with ablations over different aggregation methods in Section 6.1. Since the model may need to predict over unseen regions of the input space, we can also assess the model's uncertainty by observing the concentration of sampled $\hat{y}$ and additionally specific log probabilities across every decoded token.

Local Finetuning: To adapt to an unseen task $\mathcal{T}_u$, the model can further be quickly finetuned over the tasks's corresponding training data $\mathcal{D}_u^{train}$. This is a common requirement during regressor-guided search, where online function evaluations should be taken into account, e.g. in Wistuba & Grabocka (2021). Finetuning may also help to refocus over seen data, when the model is not fully optimized against a specific study, e.g. if the pretraining dataset was too large.

Appendix B contains additional implementation details such as the specific architecture and vocabulary used.

4 Data

4.1 OSS Vizier Format

The abstractions in Section 3.1 above are concretely implemented in Open Source (OSS) Vizier (Song et al., 2022), a research interface for blackbox and hyperparameter optimization. Every space $\mathcal{X}$ is defined by a list of *parameters*, each of type `DOUBLE`, `INTEGER`, `DISCRETE`, or `CATEGORICAL` with an associated value set. Every parameter may also potentially be a *child parameter*, only active when the corresponding parent parameter is a specific value (e.g. "beta" is active only if a parent categorical parameter selects "Adam", but not "SGD"). An example is shown in Figure 2.

Task-level metadata m consists of a title, owner username, description, objective name, and optional free-form text. Since the OSS Vizier API is meant to provide an optimization service for users, there can be many sources of transferrability due to user-specific settings. These include:

[1]In applications such as code search, it is even infeasible to express the space of all possible programs.

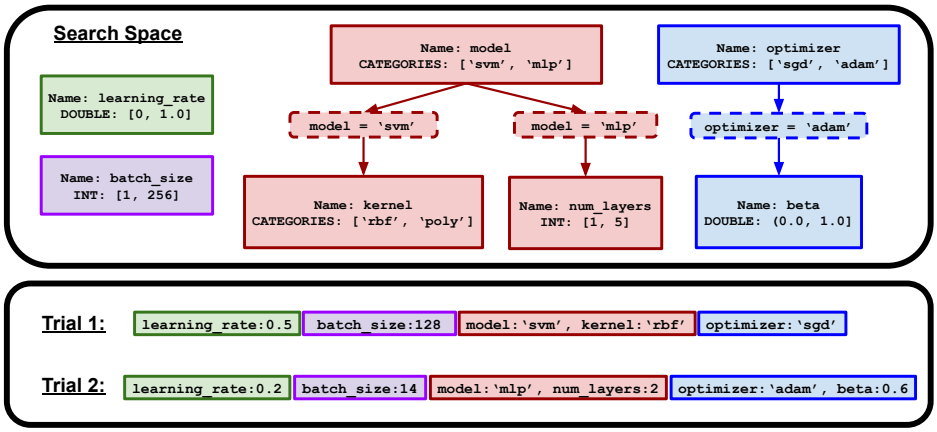


Figure 2: Common example of a (possibly nested) space and suggestions x in OSS Vizier.

- A single user or team regularly tuning similar experiments.
- Multiple different users tuning similar experiments (e.g. training ResNets on CIFAR10).
- Similar parameters used across different experiments (e.g. "learning rate").
- Metadata m describing the nature of the objective function.

4.2 Datasets

BBOB (Shifted): For precise controlled experiments where we can generate synthetic datasets and perform online evaluations, we create a multi-task version of the BBOB benchmark (ElHara et al., 2019) containing 24 different synthetic functions, by applying random domain shifts c to transform a vanilla synthetic $f(x)$ into $f(x - c)$, and ranging the dimension over $[2, 6]$. Thus each task $\mathcal{T}$ is parameterized by controllable $m =$ (function class, dimension, shift), and the corresponding objective can be seen as $f(x, m)$, allowing evaluation over unseen m. For a specific task $\mathcal{T}_i$, we minimize the *in-study training data* size $\mathcal{D}_i^{train}$ but freely vary *inter-study* training data $\{\mathcal{D}_j^{train}\}_{j \neq i}$ from different tasks $\{\mathcal{T}_j\}_{\neq i}$. Thus traditional regressors (e.g. MLPs) which can only train from a single $\mathcal{D}_i^{train}$ will struggle to regress the corresponding f_i under this limited data condition. In contrast, the LM may perform better as it will have seen trials from other tasks whose functions share similarities with f_i.

Real World Data: To investigate metric prediction over real world data which contain a rich variety of tasks, we will use a proprietary database. Because we are not constrained to only training over fully completed trajectories over flat input spaces, our training data availability can be larger than the 750K studies for training the OptFormer (Chen et al., 2022), as seen from Table 3.

Property	Statistic
# Studies	$\mathcal{O}$(70M+)
# Trials	$\mathcal{O}$(120B+)
# Distinct Users	$\mathcal{O}$(14K)

Table 3: Relevant statistics on the real world database. We provide order estimates as there may be numerous ways to define e.g. "legitimate" studies or trials. See Appendix D for further details and data breakdown.

Since the offline dataset is collected from users' blackbox optimization trajectories, we for the most part do not have online access to an actual objective $f(x)$, rather only data samples $\mathcal{D}$, and thus we must evaluate our predictor's accuracy via a test set $\mathcal{D}^{test} \subset \mathcal{D}$. We thus need to take into account how much $\mathcal{D}_{train}$ sufficiently covers the space $\mathcal{X}$, which affects the difficulty of achieving high accuracy on the task. Influencing factors include:

- Trial count: Users can decide when to stop tuning, and thus the size of a study can be on the order of 10^0 to 10^5.

- Diversity of trials: By default, a study's trials $\{(x_1, y_1), ..., (x_T, y_T)\}$ form the trajectory of an optimization loop, and thus later trials may converge towards a single local optimum.
- Space size: Approximate cardinality of a space $\mathcal{X}$ is exponential with respect to parameter count, and thus large input spaces will naturally be less explored.

While we apply practical processing steps such as (1) setting a maximum initial trial limit per study and (2) randomly shuffling the trials and then (3) deciding on a fixed train/validation/test splitting ratio (default 0.8/0.1/0.1), we cannot fully control whether each $\mathcal{D}$ saturates its space $\mathcal{X}$, or essentially how "easy" the task is. Instead, we use a baseline regressor trained only on $\mathcal{D}^{train}$ and evaluated on corresponding $\mathcal{D}^{test}$ as a proxy metric of the difficulty of the task.

5 Experiments

We answer the following key questions:

1. Is it possible to simultaneously regress on multiple tasks of different input spaces and objective scales?
2. Are there benefits to multi-task training and are textual signals useful for transfer learning?
3. Can finetuning improve accuracy over unseen studies outside of the pretraining set?

5.1 Simultaneous Regression

In Figure 3, we visually present how a BBOB-trained model captures the overall shape of analytical functions of vastly different objective scales with high precision. Furthermore, the model is capable of expressing uncertainty estimates via i.i.d. prediction samples.

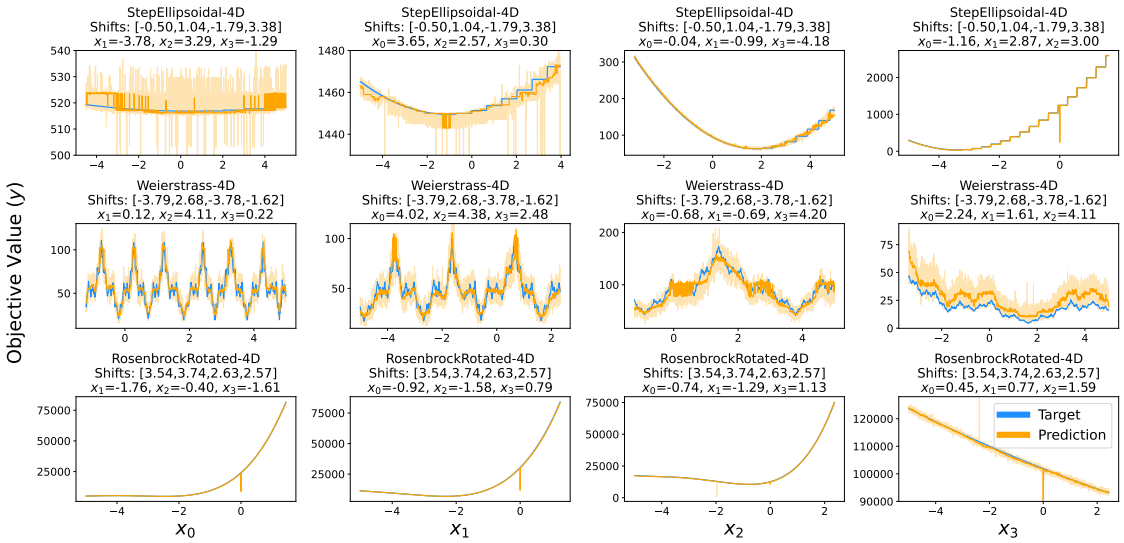
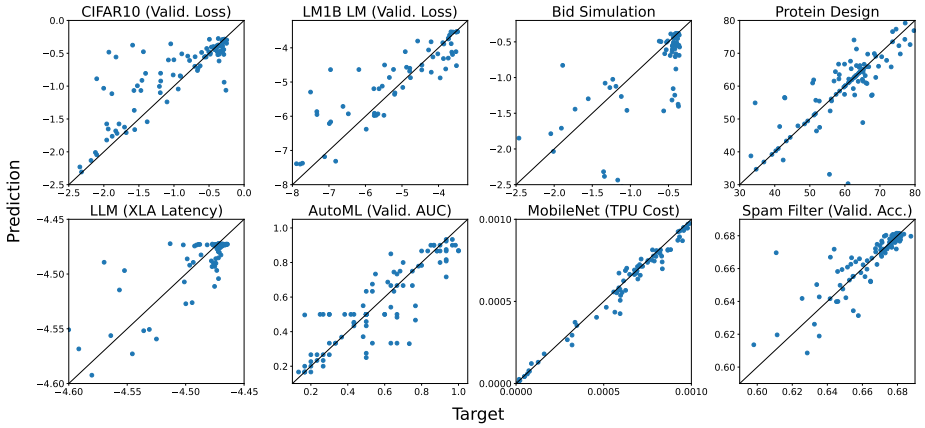


Figure 3: Model prediction samples over selected 4D BBOB functions with unseen shifts. Empirical mode (bolded) and min/max are shown from 10 samples. Over all BBOB functions, we vary the coordinate value x_i while keeping others $x_{j \neq i}$ fixed.

In Figure 4 for a model trained over real world data, we present an analogous visualization over hand-selected studies with drastically different input spaces, representative of objectives tuned commonly in real world settings. These include standard machine learning (e.g. image classification and language modeling), production systems (e.g. bid simulation, LLM inference latency), and scientific research (e.g. protein and hardware design).



Name	Space
CIFAR10	4 Double
LM1B LM	4 Double
Bid Simulation	4 Double
Protein Design	60 Categories
LLM Latency	31 Hybrid
AutoML	3-H, 42-T
MobileNet	10 Discrete
Spam Filter	13-H, 15-T

Figure 4: **Left:** Diagonal fit (/) is better. Model's y-prediction vs. ground truth over varying studies. Corporate-specific objective names are redacted. **Right:** Corresponding input spaces. "#-H, $-T" is shorthand for a conditional hybrid input space with # root parameters and $ total possible parameters.

5.2 Multi-task Transferrability

In this subsection, we demonstrate the model's ability to transfer learn, i.e. improve accuracy over a specific task using knowledge gained from other similar but non-equivalent tasks, in contrast to "single-task" regressors (described in Appendix C) which only observe training data from the task being evaluated. Note that single-task baselines such as MLPs are incapable of multi-task training when tasks have different dimensionalities.

In Figure 5, we clearly see that the model's accuracy improves with more tasks seen in training and eventually outperforms all traditional baselines. For AutoML studies the error is averaged from a fixed subset of encountered studies. For BBOB, we can further demonstrate the model's inter-study generalization capabilities over metadata m (as opposed to x) by evaluating on unseen tasks with new shifts not encountered during training.

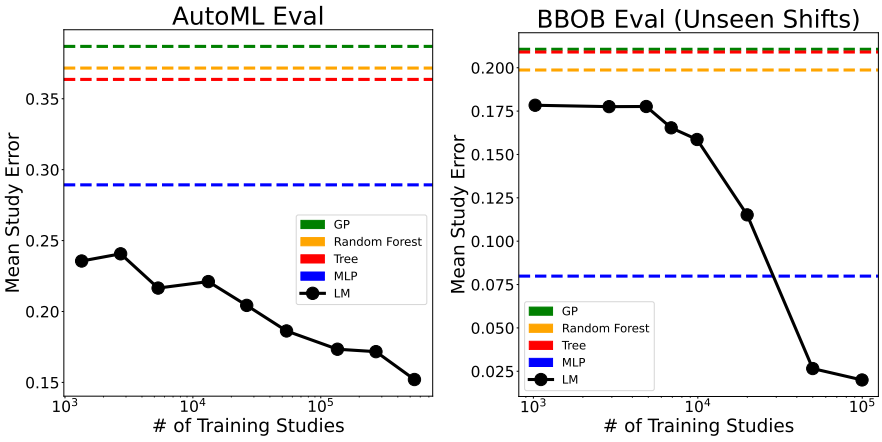


Figure 5: Lower (↓) is better. Mean study prediction error of the model when varying the amount of different studies used in training (log scale). Colored horizontal lines display single-task baseline errors.

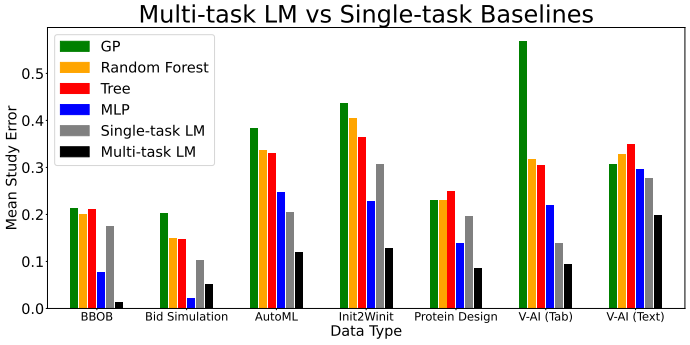
To verify whether the model is performing transfer learning by reading textual cues, in Table 4 we compare results against the case when data is "anonymized" using a study-dependent hash function. For BBOB, we hash metadata m which originally displayed (function class, dimension, shift). For AutoML, we hash parameter names and string values. Each study can still be uniquely identified and trained over, but the

model can no longer observe useful correlations from common textual clues. Interestingly, the model fails to train over the full anonymized BBOB dataset, a case when the data is too large and heterogeneous.

In Figure 6, we further see that for the model, multi-task training consistently improves over single-task training, and in regimes with relatively lower input space saturation (i.e. low trial to parameter count ratio) from training data, multi-task models outperform traditional baselines over several different domains. Interestingly, a single-task model trained from scratch remains a competitive choice and for certain domains such as AutoML, can even outperform all other single-task baselines. We hypothesize this is due to language-based representations being more appropriate for the conditional structures of these domains (e.g. AutoML).

Datasets (# Training Studies)	Mean Study Error (↓) Original	Anonymized
BBOB (50K)	**0.03**	0.46
BBOB (Full 1M)	**0.01**	FAIL
AutoML (26.3K)	**0.19**	0.44
AutoML (Full 540K)	**0.15**	0.43

Table 4: Lower (↓) is better. Comparisons between models trained on original vs anonymized data, across BBOB-Shifted and AutoML test trials. "FAIL" means the model failed to even train.



Name	# Studies	Avg. TpS	Avg. SS
BBOB	1M	30	4.0
Bid Simulation	22K	698	4.6
AutoML	540K	250	(3.3, 29.9)
Init2winit	2K	176	3.6
Protein Design	54K	584	125.6
Vertex AI (Tabular)	1.4M	88	(4.6, 42.4)
Vertex AI (Text)	544K	118	56.0

Figure 6: **Left:** Lower (↓) is better. Aggregate error across different domains. **Right:** Statistics on domains. Shorthand notation: "TpS" = Trials per Study, "SS" = Space Size, with brackets (#, $) denoting conditional space with # root parameters and $ total possible parameters. Note that all baselines are single-task regressors.

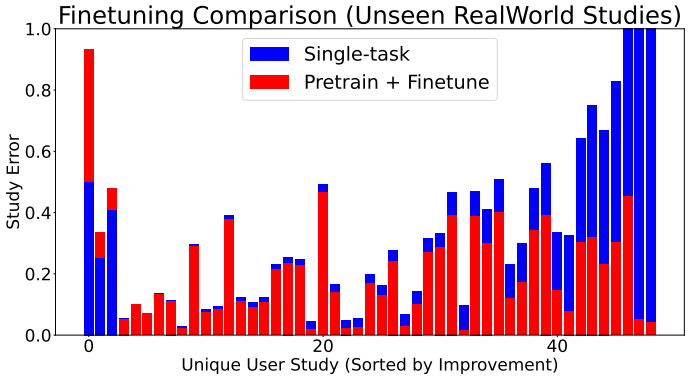
5.3 Finetuning Analysis

We first examine the conditions in which finetuning may be beneficial. In Table 5, we finetune various pretrained models over AutoML studies. While there is negligible benefit in finetuning the AutoML model on its data again, we see that a model pretrained over the entire real world dataset is able to finetune to the same level of accuracy as a pretrained AutoML model, while a BBOB-pretrained model leads to significantly worse results than even a single-task model. This suggests that knowledge obtained from pretraining can have a large (positive or negative) influence on transferrability over specific domains such as AutoML.

Pretraining Dataset	Mean Study Error (↓) on AutoML Before Finetuning	After Finetuning
None (Single-Task)	0.98	0.20
BBOB	0.98	0.45
AutoML	**0.15**	**0.15**
All RealWorldData	0.31	**0.15**

Table 5: Lower (↓) is better. Mean study errors of pretrained models and their corresponding finetuned versions.

We further examine this effect by evaluating over unseen tasks, i.e. those which were newly created after the original training set was scraped, and can contain studies from new users and objectives. In Figure 7, we compare initialization from scratch (leading to single-task training) against a pretrained model on older real world data. We see that knowledge obtained from pretraining can significantly transfer over and help



Method	Mean Study Error (↓)
Single-task (LM)	0.28
Pretrain (LM)	0.68
Pretrain + Finetune (LM)	**0.21**
MLP Baseline	0.25
Tree Baseline	0.32
Random Forest	0.32
Gaussian Process	0.42

Figure 7: **Left:** Lower (↓) is better. Example LM study errors over unseen studies filtered over random distinct users. **Right:** Aggregate comparisons across different methods over 1000 unseen studies.

predictions over new tasks, although as seen on the left with three studies, there are few cases of negative transfer.

6 Ablations

We further ablate certain important settings and scenarios which affect the model's prediction accuracy below. Appendix A contains additional ablations, specifically (1) around our choice of y-tokenization and (2) experimental outcomes when using ranking-based regression metrics.

6.1 Effect of Sampling

The LM can output extreme outliers in its y-prediction, usually due to an inaccurate prediction on the exponent token or significant digits. While such issues do not occur once the model has nearly perfectly regressed on a task (e.g. BBOB), they occur frequently on realistic tasks with nontrivial error (e.g. AutoML) and thus require techniques for correction. One obvious method to reduce error is to increase sample count, as demonstrated in Figure 8.

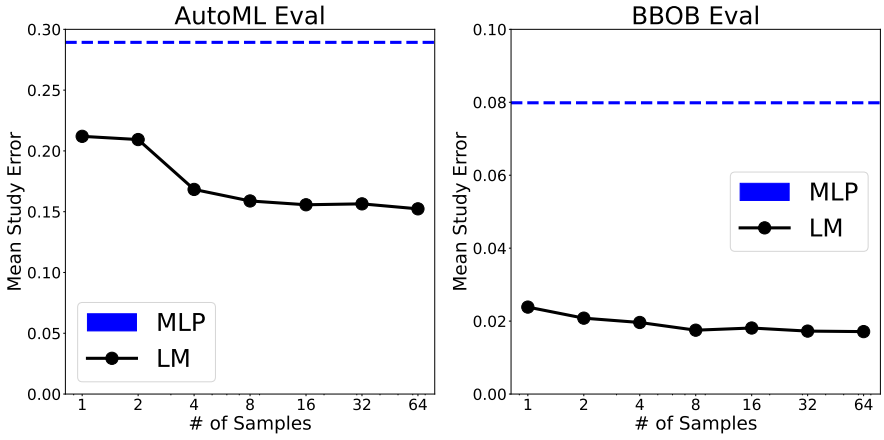


Figure 8: Lower (↓) is better. Mean study error when varying the samples used during inference (log scale).

An additional method is to change the method of aggregation across samples. In Table 6, we see that using the median considerably outperforms both max-likelihood and mean. We hypothesize this is due to the median's robustness to hallucinated outlier samples which can occur with relatively high probability and can also skew the mean.

Empirical Aggregation Method	Mean Study Error (↓) AutoML (Full 540K)	BBOB (Full 1M)
Median (default)	**0.15**	0.01
Max-likelihood	0.22	0.01
Mean	0.23	0.01

Table 6: Lower (↓) is better. Comparisons between different sample aggregation methods when using 64 samples.

6.2 Uncertainty Calibration

Although the main metric used throughout our work is based on pointwise prediction, an important ability for regressors is to express uncertainty when they are unable to provide an accurate prediction. This is particularly useful in applications such as Bayesian Optimization, where uncertainty can be used as an exploration proxy. In this section, we examine whether the model can quantify uncertainty even if we did not calibrate or tune any of the models for such purposes.

We begin by demonstrating the LM's ability to nonparametrically express distributions with multiple modes in Figure 9 when we train the model against randomly sign-flipped BBOB objectives. In contrast, traditional methods such as ensembled MLPs (Havasi et al., 2021) and Gaussian Process mixtures (Bonilla et al., 2007) must specify the mixture count a priori.

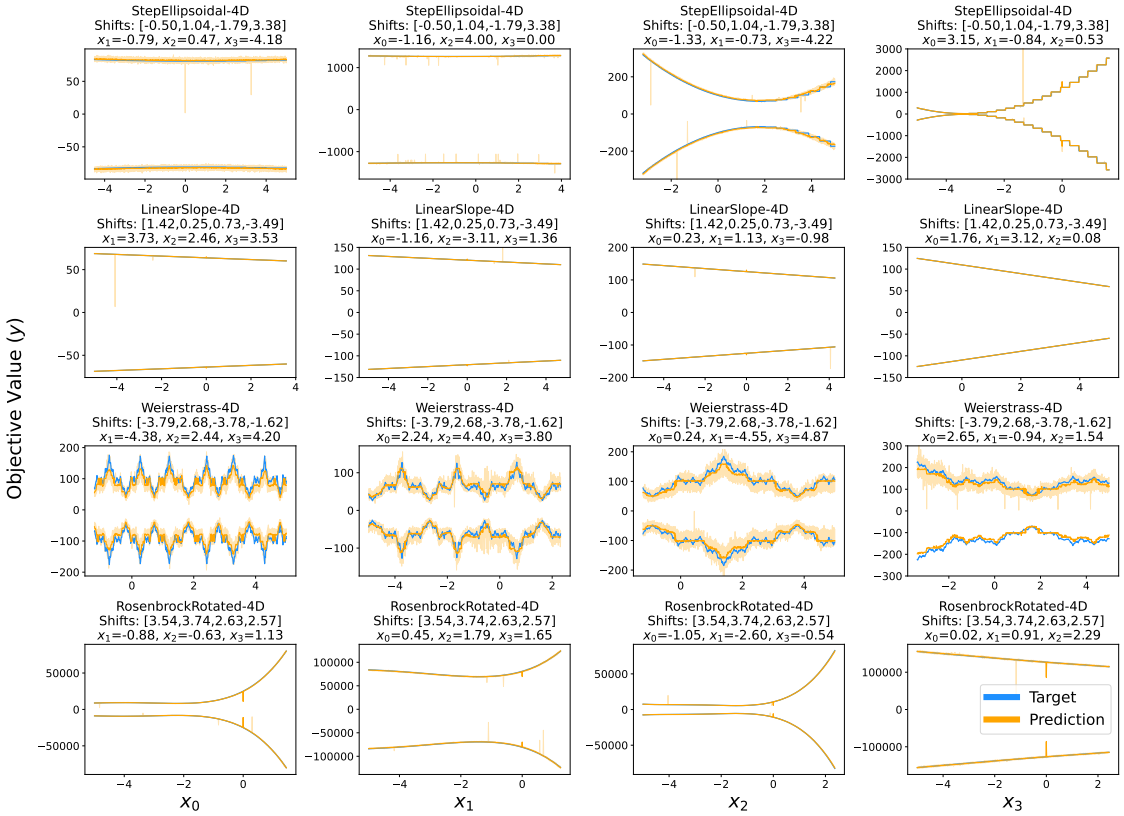


Figure 9: Setting similar to Figure 3, but with bimodality.

Furthermore, we measured the correlation between uncertainty and error on each study. In Table 7, we report the average correlation across studies. Interestingly, although Table 6 demonstrated that mean aggregation over LM samples is worse for prediction than median aggregation, the errors are well correlated with the standard deviation of the samples.

Regressor	Uncertainty Metric	Pearson, Kendall-Tau, Spearman Correlation (↑) AutoML	BBOB
Gaussian Process	Predicted SD	0.254, 0.230, 0.307	0.018, 0.068, 0.048
LM w/ mean aggregation	Sample SD	0.560, 0.487, 0.625	0.360, 0.366, 0.454
LM w/ median aggregation	Harrell-Davis SE	0.525, 0.412, 0.539	0.360, 0.293, 0.380

Table 7: Higher (↑) is better. Rank correlation between quantified uncertainty (SD = standard deviation, SE = standard error) and actual error over studies with at least 10 test trials (all BBOB studies and 641 AutoML studies)

6.3 Study Size vs. Multi-task Gain

Intuitively, as a task's space becomes more saturated with trials, single-task training becomes more sufficient for accurate prediction. In Figure 10, we plot the gains from multi-task LM training over the single-task MLP baseline to validate this hypothesis. Gains are maximized at roughly ≈ 50 training trials and diminish as the number of training trials increases. Note that maximal gains do not occur with ≈ 0 trials, as presumably *some* training trials are still needed to identify the structure of a task.

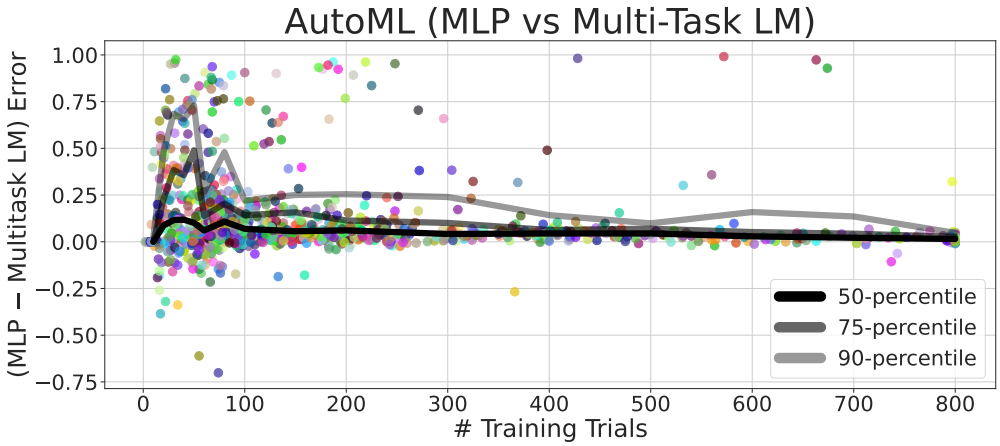


Figure 10: Higher (↑) is better. Study error differences between MLP and multi-task LM over individual AutoML tasks. Percentiles are computed after binning the x-axis appropriately.

7 Discussion: Limitations and Extensions

In this work, our emphasis was to demonstrate the promise of applying language modelling to general-purpose regression, and thus our design choices remained relatively simple to avoid confounding factors. We list some limitations of our specific design, which opens many more potential areas of exploration.

Hallucinations: By giving the model the freedom to sample y-values over approximately all of $\mathbb{R}$, wildly inaccurate outlier predictions are now possible. This can be exacerbated by a wrong prediction over a significant float token (e.g. leading digit or exponent). Although for convenience, we used an unweighted cross-entropy loss in which all float tokens are of equal importance, prediction accuracy can be improved by weighting more significant tokens, making the training loss more aware of numerical distances over $\mathbb{R}$.

Prompt-Side Numeric Tokenization: In this work, we directly represented numeric parameter values from x into the default human readable format (e.g. 1234.5 is serialized simply to `'1234.5'`) to be consistent with LLM literature. This may be suboptimal, as the corresponding tokens may not exactly be digit-by-digit (e.g. SentencePiece tokenization leads to tokens {`'12'`, `'3'`, `'4.5'`}). One may instead potentially reuse the custom tokenization for y-values (e.g. `<+><1><2><3><4><E0>`) or in text-space, represent using other serializations which emphasize digits atomically, e.g. `'[1 10e2 2 10e1 3 10e0 4 10e-1 ]'`) as in (Nogueira et al., 2021).

Pretrained English Encoder: Since x includes parameter names and metadata which contain English words, warm-starting from a model pretrained on English text may improve accuracy. However, most checkpoints comparable to our model's size (<1B params) such as T5-small and T5-medium are not pretrained over experimental data and are unlikely to understand the numerical meaning of e.g. `'learning_rate'`. Furthermore, when using a pretrained English model, there are numerous confounding technical choices to consider (e.g. whether to freeze the encoder, tune the learning rate, embed additional custom float tokens, and use more English-based representations of x and m), but this topic is worth pursuing in the future. In this work, we have already found that training a relatively small model from scratch can still achieve regression, thus suggesting our technique's broad applicability even without English understanding.

Computational Costs: Compared to traditional baselines, a language model requires accelerator usage and has a relatively higher computational cost for both training and finetuning, in addition to higher inference times. In this work, we purposely designed the model to minimize costs by using $\approx$ 220M params which only requires at most 8 GPUs for training and 1 GPU for inference (see Appendix B).

Other Input Spaces: The OSS Vizier API primarily focuses on hyperparameter tuning spaces. Traditionally, more complex spaces such as combinatorics and graphs require sophisticated modeling techniques to form regressors, largely in part to difficulties in representing the x's as tensors. In addition, many applications with non-expressible spaces such program synthesis are impossible to traditionally regress over. We believe that text and token-based representations are highly promising and are widely applicable to domains previously unexplored in the field of experimental design.

Other Metadata: While we performed ablations which anonymized m and parameter names, more investigation could be made on what types of metadata are particularly useful for prediction. Such metadata could contain *proxy metrics* introduced by previous domain-specific works, such as Jacobian Covariance for neural architecture search (Mellor et al., 2021) and neural-network norms (Jiang et al., 2020) for the study of generalization. The relevant *code* implementing machine learning or programming tasks may be especially important.

8 Impact Statement

This research addresses the ability to regress metrics against textual data. Since any textual metadata may be collected, user-specific information may be used, which raises privacy concerns. This would be particularly true on sensitive topics (e.g. predicting metrics related to personal protected characteristics).

Our research does not involve such sensitive topics for regression, as it is performed over blackbox optimization data. We followed ethical guidelines as all users in our proprietary dataset have consented to have their tuning data saved and used for offline analysis. The proprietary real world dataset does not contain any sensitive personal information other than usernames. Furthermore, we do not released any of the trained checkpoints, as it may be possible to reverse-engineer parts of the training data, which can lead privacy violations and data leakage.

9 Conclusion

Our OmniPred framework is a first step towards a universal regressor, capable of performing high-precision predictions over objectives of any scale from vastly different input spaces and applications. Its simple and scalable design allows transfer learning from large amounts of offline diverse evaluations, while its single-task variant can still perform competitively against a wide variety of gold-standard baselines. Furthermore, it is capable of adapting to unseen data through finetuning, while still transferring knowledge from previous data. This research lays the groundwork for exciting new potential expansions in the field of experimental design.

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Appendix

A Additional Ablations

We further ablate certain settings and scenarios which affect the model's prediction accuracy below.

A.1 y-Tokenization

There are multiple possible ways to represent a float (e.g. 123.4) using custom tokens. Using examples from (Charton, 2022; Nogueira et al., 2021; d'Ascoli et al., 2022), the following are all possible representations:

- (Default) Separate Sign and Digit-by-Digit: `<+><1><2><3><4><E-2>`
- Merged Mantissa: `<+1234><E-2>`
- Exponent Before Mantissa: `<+><E-2><1><2><3><4>`

In Table 8, we see that these tokenization differences do not matter with large training data (e.g. multi-task), but matter very much in low data regimes (e.g. single-task). The poor accuracy using "Merged Mantissa" is especially apparent as it requires large amounts of data to learn differences between 18K possible mantissa tokens.

	AutoML		BBOB	
Tokenization Method	Single-Task	Multi-Task	Single-Task	Multi-Task
Default	0.21	0.15	0.17	0.01
Merged Mantissa	0.73	0.15	0.41	0.01
Exponent Before Mantissa	0.24	0.15	0.17	0.01

Table 8: Mean Study Error (↓) comparisons between different tokenization methods.

A.2 Ranking and Correlation Metrics

Although our paper focuses on pointwise predictions which are maximally informative, we can trivially bootstrap our predictions into ranking-based metrics, which may be of downstream use for evolutionary algorithms which are agnostic to y-scaling. We see that in general, the multi-task LM generally maintains competitive ranking metrics.

	Kendall-Tau, Spearman Correlation (↑)						
Regressor	BBOB	Bid Simulation	AutoML	Init2Winit	Protein Design	V-AI (Tab)	V-AI (Text)
Gaussian Process	0.69, 0.80	0.80, 0.91	0.04, 0.06	0.15, **0.81**	0.35, 0.43	-0.03, -0.05	0.30, 0.39
Random Forest	0.59, 0.75	0.71, 0.84	0.45, 0.57	0.55, 0.67	0.40, 0.52	0.56, 0.71	0.29, 0.38
Tree	0.60, 0.74	**0.82, 0.93**	0.37, 0.48	0.59, 0.71	0.44, 0.57	0.55, 0.70	0.28, 0.36
MLP	0.63, 0.76	0.73, 0.85	0.37, 0.49	0.53, 0.63	0.47, 0.60	0.50, 0.64	0.25, 0.34
Single-task LM	0.01, 0.01	0.19, 0.28	0.21, 0.28	0.05, 0.08	0.15, 0.20	0.18, 0.24	0.11, 0.16
Multi-task LM	**0.92, 0.96**	0.70, 0.84	**0.61, 0.73**	**0.65, 0.74**	**0.72, 0.81**	**0.57, 0.72**	**0.49, 0.58**

Table 9: Higher (↑) is better. Ranking metrics across different regressors and tasks.

B Model Details

B.1 Pretraining

We pretrained our model using T5X (Raffel et al., 2020), which can be found in the open-source codebase `https://github.com/google-research/t5x`. Important hyperparameters, most of which are defaulted, include:

- Architecture size: 12 encoder layers, 12 decoder layers, 12 heads, 64 head dimension, 768 embedding dimension, 2048 MLP dimension.
- Optimizer: Adafactor with base learning rate 0.01 and square root decay. Batch size 256.
- Vocabulary and Tokenizer: SentencePiece tokenizer (Kudo & Richardson, 2018) with a vocabulary of 32000 subword tokens, in addition to the custom tokens for representing y-objectives.
- Early stopping: We train for a maximum of 1 million steps, but early stop based on validation loss if overfitting is detected.

The model ($\approx$ 200M parameters) was pretrained using a 4x4 TPU V3.

B.2 Local Training

During local training, data is only sourced from a single study's limited trials (at most 1000). The training set size can be lower than the batch size (256), and thus we must define one epoch as seeing the training data once, i.e. only one gradient step if training size $\leq$ batch size, but multiple gradient steps otherwise.

We use the same settings from pretraining for consistency, but allow a maximum of 30 epochs. For early stopping, validation loss is now measured over the entire validation set rather than sampled batches. Further specific changes:

- **Single-task training:** Since the model is initialized randomly, we use a larger constant learning rate of 10^3, consistent with early learning rates encountered during pretraining.
- **Finetuning:** We reload the weights in addition to the optimizer state (containing e.g. momentum parameters) from a checkpoint. We use a smaller fixed learning rate of 10^{-5}, which is 10x lower than the $\mathcal{O}(10^{-4})$ learning rate normally encountered during late stages of training.

Due to the small training set and relatively low finetuning steps, we used a single 1x1 TPU V3.

B.3 Inference

At inference time, we perform temperature sampling with a temperature of 1.0. We restrict the logits to only decode the custom floating point tokens for representing y-values. To maximize batch size for a 1x1 TPU V3, we generate 64 samples and select the empirical median of these floating point samples as our final prediction when computing error.

C Baseline Details

C.1 Vizier Input Space

The space is defined as a list of `ParameterConfig`s, each of which is one of the four primitives:

- `DOUBLE`: Specifies the search range $[l, u]$.
- `DISCRETE`: Specifies a finite subset of $\mathbb{R}$.
- `INTEGER`: Specifies an integer range $[l, u]$.
- `CATEGORICAL`: Specifies a set of strings.

Numeric (`DOUBLE, DISCRETE` and `INTEGER`) parameters may specify optional log or reverse-log scaling. The log scaling is most commonly used for tuning learning rates.

C.2 Data Processing for Flat Space

A *flat space* is where every trial in the study specifies every parameter configured in the space. In this case, we convert the parameters into the unit hypercube $[0, 1]^d$. For numeric parameters, we scale all values to $[0, 1]$ range, using the linear scaling by default unless (reverse)-log scaling was configured. For `CATEGORICAL` parameters, we use a one-hot encoding.

C.3 Data Processing for Conditional Space

A *conditional space* is where depending on one parameter's value, another parameter may be unused by the blackbox function. Conditional spaces commonly appear in AutoML settings where different model classes require a different set of parameters to be tuned. Another common use case is when we wish to optimize a numeric hyperparameter in the log scale but include 0 in the search (e.g. dropout rate, regularization coefficient), i.e. $\{\texttt{UNUSED}\} \cup [l, u]$ where $l > 0$.

For a categorical parameter, we simply add an extra out-of-vocabulary dimension for the one hot encoding.

For a numeric parameter, we first convert parameter values to $\texttt{NaN} \cup [0, 1]$, using the same scaling as in the flat space but mapping all `UNUSED` to `NaN`. We then add a custom layer (one per parameter) which is defined as:

$$x \mapsto \begin{cases} v_p & \text{if } x \text{ is } \texttt{NaN}, \\ x & \text{otherwise} \end{cases}$$

where v_p is a parameter that is trained together with the rest of the model.

C.4 Regressor Baselines

Below, we list out the specific implementation details of our regressor baselines. One nuanced issue is of hyperparameter tuning the regressors themselves, which could affect results. In order to be reasonably fair to all regressors (including our own OmniPred which has its own hyperparameters), for each regressor, we used a reasonable fixed set of hyperparameters for consistent throughout all experiments.

We emphasize in our paper on the concept of flexible string-based regression using language models and large-scale multi-task training data, rather than claiming replacement over widely accepted baselines in single-task, apples-to-apples comparisons.

Gaussian Process: The GP regressor model is from the GP-Bandit implementation found Open Source Vizier at `https://github.com/google/vizier` and consists of the following:

- $\alpha \sim$ TruncatedLogNormal controls the amplitude of Matern5/2 kernel.

- $\lambda_i \sim$ TruncatedLogNormal (i.i.d. for each dimension i) controls the length scale for the i-th dimension.
- $\sigma \sim$ TruncatedLogNormal controls the Gaussian noise.
- $z \sim \text{Normal}(0, \sigma)$ is the observation noise.
- $f \sim \text{GP}(\lambda, \alpha)$ is the function.
- $y \sim f(x) + z$ is the noisy function.

The algorithm then uses L-BFGS to obtain the MAP estimate of α, λ and σ.

One caveat here is that this model requires a non-linear preprocessing on the observations and thus predicts y in the preprocessed space. This preprocessing is found to be critical to achieving stable regression across Vizier studies, which have a wide variety of value ranges. Since the preprocessing is non-linear, we cannot obtain the predictive distribution over the raw observation in a closed form. Instead, we take 1000 samples from the GP, apply the inverse of the preprocessor, and then take the mean.

Tree and Random Forest: We use the standard API (`XGBRegressor`, `XGBRFRegressor`) found in XGBoost (`https://github.com/dmlc/xgboost`) with default hyperparameters. Although tree-based methods do not generally require rescaling, we still applied consistent x-preprocessing (in particular to deal with optional log or reverse-log scaling).

Multilayer Perceptron: The base architecture consists of a 2-layer ReLU dense network of hidden size 256 with a final scalar output. y-values are normalized using `tf.keras.layers.Normalization` which subtracts mean and divides by standard deviation computed empirically from the training data. Training was performed with an Adam optimizer using learning rate 10^{-2}, full batch training over 100 epochs, and mean squared error.

D Real World Data

D.1 Study Preprocessing

Since the real world data is sourced from an optimization service in which users control evaluations, much of the raw study data can be quite chaotic. We apply certain preprocessing techniques to make the data more conducive to training and evaluation.

Removing bad trials: Users may ignore or fail to evaluate a proposed x. Furthermore, during some trials, the y-objective may be denoted with a special "infeasible" value (e.g. if a high batch size led to GPU out-of-memory, or training encountered NaNs). We remove such trials from consideration in our work, although one can extend our y-tokenization to support infeasibility in later works.

Trial count hard limit: Some raw studies can contain trials in upwards of 10^5 trials, which could dominate the data distribution. We therefore apply a hard limit and only consider the first 10^3 trials per study.

Filtering specific users: There are specific human and automated "power users" which produce orders of magnitude more studies than the average user. Some automated users in particular are simply automatic unit tests involving the use of OSS Vizier. We disregard studies from these users to prevent them from dominating the data distribution.

D.2 Real World Data Descriptions

(Overall) Entire Database: No filters were applied. All studies from the database were exported on March 31, 2023. Finetuning experiments involving unseen studies consist of studies created after this date.

Bid Simulation: Contains hyperparameters for proprietary bid simulation. The simulator estimates how advertisements might have performed in terms of key metrics such as cost, impressions, clicks, and conversion volume.

AutoML: Collection of proprietary AutoML data for tuning user objectives.

Init2Winit: Data from running deterministic, scalable, and well-documented deep learning experiments, with a particular emphasis on optimization and tuning experiments (e.g. ResNets on CIFAR10, Transformers on LM1B). Public codebase can be found in `https://github.com/google/init2winit`.

Protein Design: Each space consists of 50+ parameters, each of which denotes a categorical protein building block.

Vertex AI (Tabular and Text): A Vertex AI platform for automated ML model selection and training for tabular or text data. For tabular data, Vertex AI searches over a tree of model and optimizer types, their hyperparameters, data transformation, and other components in the ML pipeline. For text, Vertex AI trains an ML model to classify text data, extract information, or understand the sentiment of the authors. See `https://cloud.google.com/vertex-ai?#train-models-with-minimal-ml-expertise`.

D.3 Serialization Examples

For transparency, we provide examples of text representations seen by the model. **Disclaimer:** Due to privacy policies, we redacted (in red) some parameter names and values.

Dataset	Example x	Example m
AutoML	batch_size: 128 model_type: REDACTED activation_fn: "tanh" batch_norm: "True" dropout: 0.143 embedding_combiner: "mean" gradient_clip_norm: 1.63e+03 num_hidden_layers: 1 hidden_units[0]: 359 optimizer_type: "AdamOptimizer" beta1: 0.9 beta2: 0.999 learning_rate: 0.926 nlp_vocabulary_strategy: "adjusted_mutual_info" vocabulary_strategy: "adjusted_mutual_info"	title: "n-w597ng99i7lj0-q40zcboi1ea7l" user: REDACTED description: "" objective: "val_categorical_cross_entropy" amc_model_version: REDACTED task_type: "multi_class_classification"
Init2Winit	dropout_rate: 0.6 decay_factor: 0.0379 label_smoothing: 0.378 lr_hparams.base_lr: 0.00285 lr_hparams.decay_steps_factor: 0.854 lr_hparams.power: 1.94 opt_hparams.one_minus_momentum: 0.0557	title: "d_sp1-lm1b_trfmr-b1024-2021aug20" user: REDACTED description: "" objective: "valid/ce_loss"
Protein Design	p00000000:"9" p00000001:"16" p00000002:"1" p00000003:"11" p00000004:"16" p00000006:"9" p00000006:"0" p00000007:"14" ... p00000047:"13"	title: "871cac30956711eab5bef371aa1bb25a" user: REDACTED description:"" objective:""
Vertex AI Text	universal_model_type: "single_dense_feature" token_model_type: "cnn" token_bow_combiner: "sqrtn" token_model_type: "bow" rand:0 batch_size: 4 convnet: "2:3:4*100pa" dropout_keep_prob: 1 hidden_layer_dims: 50 max_length: 1.54e+03 max_num_classes_for_per_class_metric: 0 max_token_vocab_size: 1e+05 merge_word_embeddings_vocab_size: 1e+05 token_freq_cutoff: 1 tokenizer_spec: "delimiter" word_embedding: REDACTED word_embedding_dim: 100	title: "20220228-621c9aea-0000-2c94" user: REDACTED description: REDACTED objective:"micro-auc-pr-label0_label" atc_study_dataset_tag:"" atc_study_notes:""