A Pretraining details

We present all the training hyperparameters for the supernetwork (see Section 3.2 too) at different scales in Table 3. We train GPT-S, -M and -L scales for 4, 6 and 8 days, respectively, on 4 Nvidia A100 GPUs. GPT-XL is trained for 6 days across 40 A100 GPUs. As described in Section 3.2, we use the sandwich rule for the supernetwork training, which accumulates gradients from the smallest, largest and 2 random subnetworks of the supernetwork in each gradient update step.

Hyperparameter	Value
Trainer	
num_gpus	4
gradient_clip_val	1.0
max_steps	800000
precision	BFloat16 Mixed precision
seed	1234
Optimizer	
optimizer	AdamW
lr	0.000316
weight_decay	0.1
betas	[0.9, 0.95]
eps	1.0e-09
seed	1234
Optimizer Parameter Grouping	
bias_weight_decay	False
normalization_weight_decay	False
Scheduler	
num_warmup_steps	4000
num_training_steps	800000
decay_factor	0.1
schedule	cosine
Model	
block_size	1024
vocab_size	50254
padding_multiple	512
scale_embeddings	False
padded_vocab_size	50254
head_size	64
lm_head_bias	False
attn_dropout	0.1
resi_dropout	0.1
embed_dropout	0.1
shared_attention_norm	False
norm	LayerNorm
rope_condense_ratio	1
scale_attn_weights	True
scale_attn_by_inverse_layer_idx	True
shared_embedding	True
pos_embedding	False
rel_pos_enc	True
rotary_percentage	0.5
norm_eps	1e-5
rope_base	10000
parallel_residual	True
initializer_range	0.02
Data	
dataset	"openwebtext"
num_cpu_worker	32
batch_size	32(GPT-S), 8(GPT-M), 8(GPT-L), 1(GPT-XL-wide)
max_sample_len	1024
val_ratio	0.0005
val_split_seed	2357

Table 3: Supernet training hyperparameters.

B Hardware specifications and Properties

In Table 4, we present details of the 8 GPU devices and 5 CPU devices we used for profiling our 3 search spaces GPT-S, GPT-M and GPT-L. The devices we study capture a wide range of micro-architectures, number of cores and GPU/CPU memory. The considered GPUs capture a wide range of inference latencies and throughput [9].

Table 4: Hardware specifications.

Platform	Device Name	Micro Architecture	Number of Cores	Memory
GPU	NVIDIA RTX 2080	Turing	CUDA 2944	8GB GDDR6
	NVIDIA RTX 3080	Ampere	CUDA 8704	12GB GDDR6X
	NVIDIA RTX A6000	Ampere	CUDA 10752	48 GB GDDR6
	NVIDIA A100	Ampere	CUDA 6912	40GB HBM2e
	NVIDIA A40	Ampere	CUDA 10752	48GB GDDR6
	NVIDIA Tesla P100	Pascal	CUDA 3584	12GB HBM2
	NVIDIA Tesla V100	Volta	CUDA 5120	24GB GDDR6
	NVIDIA H100	Hopper	CUDA 16896	80GB HBM3
CPU	AMD 7452	Zen2	CPU Core 32	Cache 128 MB
	AMD 7513	Zen3	CPU Core 32	Cache 128MB
	AMD 7502	Zen2	CPU Core 32	Cache 128MB
	Intel Xeon Silver 4114	Intel P6	CPU Core 10	Cache 13.75MB
	Intel Xeon Gold 6242	Intel P6	CPU Core 16	Cache 22MB

C Surrogate models

In this section, we provide details of the latency and energy surrogate predictors used in HW-GPT-Bench. The surrogates are trained and evaluated on 8000 and 2000 fixed architectures, respectively.

C.1 PPL Surrogates

Data collection. We subsample 10% from the OpenWebText training set and use that as a validation set to compute the perplexity and accuracy metrics of architectures in the supernetwork, that inherit the trained supernetwork weights. The time to collect the perplexity pairs for 10k architectures was 8, 16, 24 and 32 days on 4 A100 GPUs for GPT-S, -M and -L and -XL-wide, respectively. Note that this computation is trivial to parallelize, as all architectures can be evaluated independently of each other, given the pretrained supernetwork weights. Afterwards, the (x, y) pairs, where x is the one-hot encoded architecture and y the corresponding perplexity value, are used to train an MLP (Multi Layer Perceptron) using the MSE loss to predict the perplexity on unseen (test) architectures.

Surrogate Architecture. The MLP contains 4 linear layers with hidden dimension of 128 and output dimension of 1 (the perplexity prediction). We use ReLU activations at every layer. The dimension of the one-hot encoding is 3 (3 choices for layers) + 3 (3 choices for embedding dimension) + max_layers$\times$3 (3 choices for number of heads for every layer) + max_layers$\times$3 (3 choices for MLP ratio for every layer). We train the MLP for 4000 epochs using the Adam optimizer with a learning rate of 10^{-3} and a batch size of 1024.

C.2 Hardware Surrogates

We now describe the different surrogates we study to model uncertainties in energy and latency prediction. Each of the surrogates is trained to predict mean and standard deviation of energy or latency predictions of a given architecture. For FLOPs, memory and number of parameters, we compute and predict a single observation per architecture. We use 8000 architectures for training our surrogates and 2000 to test the performance and calibration properties of our surrogates.

[9] GPU benchmark

Data collection. We measure energy and latency pairs across different devices multiple times to capture the noise in the energy and latency profiling. Additionally, we also profile hardware metrics like Floating Point Operations (FLOPs), Memory consumption (Float16 and BFloat16) and number of parameters for an architecture. Specifically, for every architecture, we compute 50 observations per architecture for energies on GPU and 10 observations for energies on CPU. Similarly, we compute 10 observations per architecture for latencies on both CPUs and GPUs. We use 8 CPU cores (per GPU) for all the latency and energy evaluations.

AutoGluon. AutoGluon simplifies the process of developing, training, and deploying machine learning models by automating key tasks such as feature engineering, model selection, and hyperparameter tuning. AutoGluon has two major components. First one is Bagging (bootstrap aggregation) on wide varieties of models like decision trees, random forests, nearest neighbors, linear models and neural networks. Second one is stacking, where predictions of models on the first level are fed as input to models at the next level. We use an AutoGluon model per metric (latency or energy) with `dynamic_stacking` = `False`, `num_stack_levels` = 1, `number_of_bag_folds` = 8 and `number_of_bag_sets` = 4. The input feature map to the model is simply a concatenation of chosen hyperparameters with choices for MLP ratio and number of heads set to -1 when a particular layer is not selected. We train two AutoGluon predictors, one to predict mean, and one to predict the standard deviation of the ground truth latency or energy measurements.

Ensemble (XGB). We use an ensemble of 27 Extreme Gradient Boosting (XGB) models with different hyperparameter combinations. Specifically, the models in the ensemble contain a cross product of `n_estimator` choices from `[200, 500, 800]`, `depth` choices from `[5,9,3]` and `learning_rate` choices from `[0.01,0.1,1.0]`. We then fit this ensemble, and predict the mean and standard deviation values for the metric at hand by aggregating the predictions of different models using bagging.

Ensemble (LightGBM). We use an ensemble of 36 Light Gradient Boosting Machine (LightGBM) models with different hyperparameter combinations. Specifically, the models in the ensemble contain a cross product of `n_estimator` choices from `[200, 500, 800]`, `depth` choices from `[5,9,3]` and `learning_rate` choices from `[0.01,0.1,0.001,1.0]`. We then fit this ensemble, and predict the mean and standard deviation values for the metric at hand by aggregating the predictions of different models using bagging.

Ensemble (MIX). In addition to ensembles based on XGB and LightGBM, we also fit an ensemble containing a mixture of different machine learning models. Specifically, this ensemble contains 4 XGB and LightGBM regressors (default: `[n_estimators = 500,max_depth = 5 ,learning_rate = 0.01]`,`[n_estimators = 800,max_depth = 3,learning_rate = 0.1]`, `[n_estimators = 200,max_depth = 9,learning_rate = 1]`), as well as LinearRegression, Ridge and RandomForestRegressor from `sklearn` with their default hyperparameters.

C.3 Memory Surrogate.

We model the memory consumption using a simple MLP (similar to perplexity). The MLP has 4 layers with a hidden dimension of 128 and uses ReLU activations. The input to the MLP is the normalized feature map corresponding to the concatenation of the architecture parameters. The MLP is trained using Adam, with learning rate of 10^{-4} and a batch size of 1024, for 4000 epochs.

D Accuracy and Calibration of Surrogate models

In this section we provide a more detailed description on the metrics we used to evaluate our surrogate models in Section 3.3, as well as additional results that complement results shown in Table 2 and Figure 4.

D.1 Accuracy and Calibration Metrics

Given a finite dataset $D = \{(x_i, y_i)_{i=1}^N\}$ and a regression model that predicts the mean value $\hat{y}$, we use standard accuracy metrics:

Root Mean Squared Error (RMSE): $RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2}$

Mean Absolute Error (MAE): $MAE = \frac{1}{N}\sum_{i=1}^{N}|\hat{y}_i - y_i|$

Median Absolute Error (MDAE): Median of the absolute differences between predicted and actual values, in ascending order.

$$MDAE = med(\{|\hat{y}_i - y_i|\}_{i=1}^{N})$$

Mean Absolute Percentage Relative Deviation (MARPD): A similar metric to MAE but scaled by the sum of the absolute values of predicted and actual values. This scaling can be beneficial when dealing with a wider range of values, especially when the predicted or actual values are very close to zero.

$$MARPD = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{2\cdot(\hat{y}_i - y_i)}{|\hat{y}_i| + |y_i|}\right| \cdot 100$$

Coefficient of Determination (R^2): Tells us about the proportion of variance in the dependent variable (y) explained by the independent variable (x) through the model. Denoting by $\bar{y} = \sum_{i=1}^{N} y_i$ the mean of the ground truth data, R^2 is defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(\hat{y}_i - y_i)^2}{\sum_{i=1}^{N}(\bar{y} - y_i)^2}$$

Correlation Coefficient: The Pearson correlation coefficient (r) measures the strength and direction of the linear relationship between predicted values ($\hat{y}_i$) and actual values (y_i) of the data. It ranges from -1 to 1.

$$r = \frac{\sum_{i=1}^{N}(\hat{y}_i - \bar{y})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N}(\hat{y}_i - \bar{y})^2 \sum_{i=1}^{N}(y_i - \bar{y})^2}}$$

Root Mean Squared Calibration Error (RMS Cal.): A metric used to evaluate the calibration of probabilistic predictions in regression models, particularly in the context of uncertainty quantification. It measures the discrepancy between predicted and observed quantiles. For a model to be well-calibrated, the proportion of observations below a given predicted quantile should match the quantile value. For example, the 90th percentile prediction should contain the true outcome 90% of the time. RMS Cal. is computed as the root mean square of the difference between the predicted quantile levels and the observed frequencies over all quantiles:

$$\text{RMS Cal.} = \sqrt{\frac{1}{K}\sum_{k=1}^{K}\left(P(Y \leq Q_k) - q_k\right)^2},$$

where Q_k is the k-th predicted quantile, q_k is the corresponding quantile level, and $P(Y \leq Q_k) = \frac{1}{N}\sum_{i=1}^{N}\mathbb{I}[y_i \leq Q_k(x_i)]$ is the empirical frequency of the target variables $Y = \{y_i\}_{i=1}^{N}$ being less than or equal to Q_k. $\mathbb{I}$ stands for the indicator function. A lower RMS Cal. indicates better calibration, reflecting that the predicted uncertainties are accurate and reliable.

Mean Absolute Calibration Error (MA Cal.): MA Cal. is computed as the average absolute difference between the predicted quantile levels and the observed frequencies over all quantiles:

$$\text{MA Cal.} = \frac{1}{K}\sum_{k=1}^{K}\left|P(Y \leq Q_k) - q_k\right|.$$

D.2 Additional Results on the Accuracy and Calibration of Surrogates

In Tables 5-10 and Figures 9-34 we show additional results that complement results shown in Table 2 and Figure 4.

Table 5: Various performance metrics of surrogates evaluated to predict latencies and energies on GPT-S for different GPUs. The arrow on the side of the metric name indicates if lower or higher is better.

GPU	Surrogate	Accuracy												Calibration					
		MAE ↓		RMSE ↓		MDAE ↓		MARPD ↓		R^2 ↑		Corr. ↑		RMS Cal. ↓		MA Cal. ↓		Miscal. Area ↓	
		latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies
A100	**AutoGluon**	**0.39**	**0.03**	**0.50**	**0.28**	**0.33**	**0.02**	**0.23**	**5.68**	**1.00**	**0.17**	**1.00**	**0.42**	**0.46**	0.09	**0.40**	0.08	**0.41**	0.08
	Ensemble (XGB)	1.81	0.05	2.37	0.29	1.48	0.02	1.03	8.32	1.00	0.10	1.00	0.34	0.54	**0.08**	0.47	0.07	0.47	0.07
	Ensemble (LGB)	8.74	0.05	10.14	0.29	8.37	0.03	5.06	9.70	0.97	0.14	1.00	0.37	0.57	0.08	0.49	**0.06**	0.49	**0.06**
	Ensemble (Mix)	1.93	0.04	2.51	0.29	1.57	0.02	1.09	7.42	1.00	0.14	1.00	0.38	0.55	0.08	0.47	0.07	0.47	0.07
A40	**AutoGluon**	**0.52**	**0.09**	**0.76**	**0.15**	**0.32**	**0.03**	**0.18**	**6.16**	**1.00**	**0.93**	**1.00**	**0.96**	**0.35**	0.21	**0.31**	0.18	**0.31**	0.18
	Ensemble (XGB)	3.16	0.09	4.19	0.16	2.43	0.03	1.26	6.56	1.00	0.92	1.00	0.96	0.54	0.16	0.46	0.14	0.47	0.15
	Ensemble (LGB)	14.90	0.12	17.40	0.18	14.80	0.08	6.21	11.26	0.97	0.90	1.00	0.96	0.57	**0.09**	0.49	**0.07**	0.49	**0.08**
	Ensemble (Mix)	3.16	0.09	4.32	0.15	2.30	0.03	1.20	6.49	1.00	0.93	1.00	0.96	0.54	0.17	0.46	0.15	0.47	0.15
H100	**AutoGluon**	**0.18**	**0.02**	**0.25**	**0.03**	**0.14**	**0.01**	**0.23**	**3.34**	**1.00**	**0.90**	**1.00**	**0.95**	**0.19**	**0.05**	**0.17**	**0.04**	**0.17**	**0.04**
	Ensemble (XGB)	0.76	0.02	0.99	0.03	0.61	0.01	0.98	3.57	1.00	0.90	1.00	0.95	0.48	0.05	0.41	0.05	0.42	0.05
	Ensemble (LGB)	3.45	0.02	4.02	0.04	3.34	0.02	4.44	4.64	0.97	0.87	1.00	0.95	0.55	0.18	0.48	0.16	0.48	0.16
	Ensemble (Mix)	0.77	0.02	1.00	0.03	0.64	0.01	0.99	3.50	1.00	0.90	1.00	0.95	0.47	0.05	0.41	0.05	0.42	0.05
RTX2080	**AutoGluon**	**20.01**	**0.09**	**28.40**	**0.14**	**11.91**	**0.07**	**4.54**	**6.45**	**0.98**	**0.99**	**0.99**	**0.99**	**0.35**	0.26	**0.29**	0.23	**0.29**	0.23
	Ensemble (XGB)	20.59	0.10	29.58	0.15	12.17	0.07	4.60	6.95	0.97	0.98	0.99	0.99	0.42	0.24	0.35	0.21	0.36	0.21
	Ensemble (LGB)	32.25	0.20	42.97	0.25	22.52	0.18	7.14	14.77	0.94	0.96	0.99	0.99	0.53	**0.05**	0.46	**0.04**	0.46	**0.04**
	Ensemble (Mix)	20.79	0.10	29.25	0.15	13.27	0.08	4.71	7.52	0.97	0.98	0.99	0.99	0.42	0.21	0.36	0.19	0.37	0.20
RTX3080	**AutoGluon**	**6.21**	**0.06**	**8.83**	**0.12**	**3.69**	**0.03**	**1.97**	**4.10**	**1.00**	**0.96**	**1.00**	**0.98**	**0.43**	0.03	**0.36**	0.03	**0.37**	0.03
	Ensemble (XGB)	7.18	0.06	10.25	0.12	4.26	0.04	2.21	4.67	1.00	0.95	1.00	0.98	0.47	**0.02**	0.41	**0.02**	0.41	**0.02**
	Ensemble (LGB)	22.76	0.10	27.36	0.16	21.79	0.08	7.45	8.40	0.97	0.92	1.00	0.98	0.56	0.25	0.48	0.22	0.49	0.23
	Ensemble (Mix)	7.49	0.07	10.43	0.13	5.05	0.04	2.37	4.74	1.00	0.95	1.00	0.98	0.48	0.02	0.42	0.02	0.42	0.02
A6000	**AutoGluon**	**1.74**	**0.05**	**2.68**	**0.06**	**1.03**	**0.04**	**0.85**	**5.95**	**1.00**	**0.93**	**1.00**	**0.96**	**0.47**	0.04	**0.40**	0.03	**0.41**	0.03
	Ensemble (XGB)	3.34	0.05	4.45	0.06	2.42	0.04	1.54	6.17	1.00	0.92	1.00	0.96	0.53	**0.02**	0.45	**0.02**	0.46	**0.02**
	Ensemble (LGB)	13.46	0.05	15.83	0.07	13.16	0.04	6.48	6.85	0.97	0.90	1.00	0.96	0.57	0.04	0.49	0.04	0.49	0.04
	Ensemble (Mix)	3.39	0.05	4.54	0.06	2.50	0.04	1.54	6.22	1.00	0.92	1.00	0.96	0.54	0.03	0.46	0.03	0.47	0.03
V100	**AutoGluon**	**7.49**	**0.02**	**10.51**	**0.14**	**3.94**	**0.01**	**2.21**	**2.64**	**0.99**	**0.70**	**1.00**	**0.84**	**0.44**	**0.36**	**0.38**	**0.32**	**0.39**	**0.33**
	Ensemble (XGB)	8.03	0.02	11.42	0.15	4.60	0.01	2.41	3.68	0.99	0.64	1.00	0.80	0.47	0.37	0.41	0.33	0.41	0.33
	Ensemble (LGB)	18.87	0.04	23.54	0.15	16.73	0.03	6.32	7.22	0.96	0.66	1.00	0.83	0.55	0.52	0.47	0.45	0.48	0.45
	Ensemble (Mix)	8.10	0.02	11.40	0.14	4.82	0.01	2.43	3.40	0.99	0.69	1.00	0.83	0.48	0.37	0.42	0.32	0.42	0.33
P100	**AutoGluon**	**3.62**	**0.30**	**5.31**	**0.40**	**2.36**	**0.23**	**0.21**	**6.13**	**1.00**	**1.00**	**1.00**	**1.00**	**0.24**	0.26	**0.22**	0.23	**0.22**	0.23
	Ensemble (XGB)	22.53	0.34	31.55	0.45	16.57	0.27	1.35	7.06	1.00	1.00	1.00	1.00	0.52	0.21	0.45	0.19	0.45	0.19
	Ensemble (LGB)	140.75	0.99	160.96	1.18	144.00	1.04	9.42	22.64	0.97	0.97	1.00	1.00	0.57	0.21	0.49	**0.16**	0.49	**0.16**
	Ensemble (Mix)	26.29	0.39	36.45	0.49	19.65	0.33	1.55	7.87	1.00	0.99	1.00	1.00	0.52	**0.18**	0.45	0.16	0.46	0.16

Table 6: Various performance metrics of surrogates evaluated to predict latencies and energies on GPT-S for different CPUs. The arrow on the side of the metric name indicates if lower or higher is better.

CPU	Surrogate	Accuracy												Calibration					
		MAE ↓		RMSE ↓		MDAE ↓		MARPD ↓		R^2 ↑		Corr. ↑		RMS Cal. ↓		MA Cal. ↓		Miscal. Area ↓	
		latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies
Xeon Silver	**AutoGluon**	**1534.66**	**8.94**	**1982.43**	**11.88**	**1242.68**	**6.52**	**3.89**	**11.69**	**0.99**	**0.91**	**1.00**	**0.95**	**0.14**	**0.50**	**0.13**	**0.43**	**0.13**	**0.43**
	Ensemble (XGB)	1606.20	9.14	2107.51	12.21	1297.02	6.92	4.11	12.08	0.99	0.90	0.99	0.95	0.21	0.53	0.19	0.45	0.20	0.46
	Ensemble (LGB)	3243.75	10.09	4020.23	13.66	2833.39	8.42	9.15	14.42	0.96	0.88	0.99	0.95	0.39	0.54	0.34	0.46	0.35	0.47
	Ensemble (Mix)	1633.05	9.05	2146.05	12.09	1285.48	6.95	4.14	11.81	0.99	0.90	0.99	0.95	0.22	0.52	0.20	0.45	0.20	0.46
Xeon Gold	**AutoGluon**	**1161.51**	**2.62**	**1634.77**	**3.37**	**833.97**	**2.08**	**6.49**	**9.40**	**0.96**	**0.92**	**0.98**	**0.96**	0.12	**0.02**	0.10	**0.02**	0.10	**0.02**
	Ensemble (XGB)	1224.12	2.69	1695.22	3.47	896.84	2.19	6.88	9.66	0.95	0.92	0.98	0.96	**0.06**	0.04	**0.05**	0.04	**0.05**	0.04
	Ensemble (LGB)	1690.01	3.20	2144.80	3.98	1456.95	2.78	9.58	11.52	0.93	0.89	0.98	0.96	0.09	0.12	0.09	0.11	0.09	0.11
	Ensemble (Mix)	1200.12	2.65	1677.90	3.42	874.13	2.16	6.68	9.47	0.95	0.92	0.98	0.96	0.07	0.04	0.06	0.04	0.06	0.04
AMD 7502	**AutoGluon**	**1570.47**	**15.84**	**2297.45**	**22.15**	**1021.43**	**11.24**	**3.84**	**4.89**	**0.99**	**0.98**	**0.99**	**0.99**	**0.17**	**0.35**	**0.15**	**0.31**	**0.15**	**0.31**
	Ensemble (XGB)	1697.98	16.83	2420.66	23.22	1107.53	12.16	4.12	5.16	0.99	0.98	0.99	0.99	0.20	0.39	0.17	0.34	0.17	0.35
	Ensemble (LGB)	3764.57	31.28	4531.32	38.53	3489.26	26.99	9.94	10.26	0.96	0.95	0.99	0.99	0.45	0.51	0.39	0.44	0.40	0.44
	Ensemble (Mix)	1693.33	16.82	2425.90	23.07	1110.10	12.23	4.13	5.21	0.99	0.98	0.99	0.99	0.20	0.41	0.17	0.36	0.17	0.36
AMD 7513	**AutoGluon**	**3321.83**	**150.24**	**5518.96**	**221.10**	**2174.08**	**103.02**	**2.76**	**10.55**	**0.99**	**0.93**	**1.00**	**0.96**	**0.38**	**0.53**	**0.34**	**0.46**	**0.34**	**0.46**
	Ensemble (XGB)	3761.37	157.08	6054.88	230.02	2633.74	108.79	3.23	11.14	0.99	0.92	1.00	0.96	0.41	0.54	0.36	0.46	0.36	0.47
	Ensemble (LGB)	11204.40	187.74	13456.74	268.02	10465.21	150.15	10.68	14.91	0.96	0.89	1.00	0.96	0.55	0.54	0.47	0.47	0.48	0.47
	Ensemble (Mix)	3852.39	154.29	6098.78	226.36	2635.35	104.72	3.22	10.85	0.99	0.92	1.00	0.96	0.41	0.54	0.36	0.47	0.36	0.47
AMD 7452	**AutoGluon**	**4879.20**	**14.75**	**6100.78**	**18.95**	3820.30	11.39	**9.02**	**9.21**	**0.95**	**0.95**	**0.98**	**0.97**	**0.41**	**0.47**	**0.36**	**0.41**	**0.37**	**0.41**
	Ensemble (XGB)	4930.64	15.06	6253.26	19.54	3817.53	11.60	9.16	9.46	0.95	0.95	0.98	0.97	0.44	0.47	0.39	0.41	0.39	0.42
	Ensemble (LGB)	5907.72	18.06	7569.56	23.38	4669.03	14.40	11.97	12.29	0.93	0.92	0.98	0.97	0.45	0.48	0.40	0.41	0.40	0.42
	Ensemble (Mix)	4903.38	14.94	6172.90	19.31	**3738.50**	**11.25**	9.12	9.36	0.95	0.95	0.98	0.97	0.46	0.48	0.40	0.42	0.40	0.42

Table 7: Various performance metrics of surrogates evaluated to predict latencies and energies on GPT-M for different GPUs. The arrow on the side of the metric name indicates if lower or higher is better.

GPU	Surrogate	Accuracy												Calibration					
		MAE ↓		RMSE ↓		MDAE ↓		MARPD ↓		R^2 ↑		Corr. ↑		RMS Cal. ↓		MA Cal. ↓		Miscal. Area ↓	
		latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies
A100	**AutoGluon**	**2.31**	**0.10**	**3.59**	**0.36**	**1.17**	**0.06**	**0.74**	**6.50**	**1.00**	**0.84**	**1.00**	**0.92**	**0.45**	0.40	**0.39**	0.35	**0.39**	0.36
	Ensemble (XGB)	3.35	0.13	4.66	0.39	2.30	0.07	1.17	7.94	1.00	0.81	1.00	0.90	0.50	0.36	0.43	0.32	0.44	0.32
	Ensemble (LGB)	13.88	0.16	16.12	0.39	13.82	0.13	5.37	12.00	0.97	0.81	1.00	0.91	0.57	**0.24**	0.49	**0.21**	0.49	**0.22**
	Ensemble (Mix)	3.21	0.12	4.50	0.37	2.21	0.07	1.11	7.32	1.00	0.82	1.00	0.91	0.48	0.37	0.42	0.33	0.43	0.33
A40	**AutoGluon**	**1.12**	**0.26**	**1.68**	**0.35**	**0.67**	**0.18**	**0.28**	**6.38**	**1.00**	**0.98**	**1.00**	**0.99**	**0.45**	0.20	**0.39**	0.18	**0.40**	0.18
	Ensemble (XGB)	4.16	0.27	5.58	0.36	3.19	0.20	1.17	6.82	1.00	0.98	1.00	0.99	0.54	0.18	0.47	0.16	0.47	0.16
	Ensemble (LGB)	23.39	0.48	26.62	0.56	24.93	0.45	7.11	13.17	0.97	0.95	1.00	0.99	0.57	**0.08**	0.49	**0.08**	0.49	**0.08**
	Ensemble (Mix)	4.01	0.27	5.47	0.36	2.94	0.19	1.09	6.63	1.00	0.98	1.00	0.99	0.54	0.19	0.46	0.17	0.47	0.1
H100	**AutoGluon**	**0.27**	**0.05**	**0.37**	**0.07**	**0.21**	**0.04**	**0.24**	**4.57**	**1.00**	**0.95**	**1.00**	**0.98**	**0.22**	**0.24**	**0.19**	**0.21**	**0.20**	**0.21**
	Ensemble (XGB)	0.91	0.05	1.19	0.07	0.74	0.04	0.81	4.72	1.00	0.95	1.00	0.98	0.45	0.24	0.39	0.22	0.40	0.22
	Ensemble (LGB)	4.49	0.07	5.14	0.09	4.54	0.06	4.04	6.25	0.97	0.92	1.00	0.98	0.56	0.31	0.48	0.27	0.48	0.27
	Ensemble (Mix)	0.87	0.05	1.15	0.07	0.68	0.04	0.76	4.68	1.00	0.95	1.00	0.98	0.45	0.24	0.39	0.21	0.40	0.22
RTX2080	**AutoGluon**	**9.13**	**0.17**	**12.76**	**0.23**	**6.70**	**0.12**	**1.36**	**3.04**	**1.00**	**1.00**	**1.00**	**1.00**	**0.11**	0.35	**0.07**	0.31	**0.07**	0.31
	Ensemble (XGB)	11.91	0.19	16.15	0.27	8.86	0.14	1.83	3.35	0.99	1.00	1.00	1.00	0.16	0.32	0.12	0.28	0.12	0.29
	Ensemble (LGB)	34.99	0.60	41.31	0.70	34.08	0.57	5.73	9.74	0.97	0.97	1.00	1.00	0.37	**0.09**	0.33	**0.07**	0.33	**0.07**
	Ensemble (Mix)	11.58	0.20	15.82	0.27	8.78	0.15	1.76	3.43	0.99	1.00	1.00	1.00	0.16	0.32	0.12	0.28	0.13	0.28
RTX3080	**AutoGluon**	**2.90**	**0.82**	**4.62**	**1.06**	**1.70**	**0.59**	**0.54**	16.97	**1.00**	**0.93**	**1.00**	**0.97**	**0.14**	**0.20**	**0.11**	**0.18**	**0.11**	**0.19**
	Ensemble (XGB)	5.82	0.83	8.10	1.08	4.52	0.63	1.28	17.18	1.00	0.93	1.00	0.96	0.26	0.24	0.21	0.21	0.21	0.21
	Ensemble (LGB)	34.62	1.00	38.99	1.28	36.60	0.87	7.87	22.33	0.97	0.90	1.00	0.96	0.55	0.32	0.47	0.27	0.48	0.27
	Ensemble (Mix)	5.95	0.83	8.17	1.07	4.63	0.63	1.30	**16.84**	1.00	0.93	1.00	0.96	0.27	0.24	0.22	0.21	0.22	0.21
A6000	**AutoGluon**	**0.70**	**0.11**	**1.06**	**0.18**	**0.46**	**0.07**	**0.21**	**3.97**	**1.00**	**0.99**	**1.00**	**0.99**	**0.32**	0.20	**0.28**	0.18	**0.28**	0.18
	Ensemble (XGB)	3.66	0.12	4.93	0.19	2.82	0.07	1.16	4.25	1.00	0.99	1.00	0.99	0.52	0.18	0.45	0.16	0.46	0.16
	Ensemble (LGB)	20.92	0.27	23.81	0.34	22.15	0.23	7.19	10.84	0.97	0.96	1.00	0.99	0.57	0.21	0.49	0.19	0.49	0.19
	Ensemble (Mix)	3.52	0.14	4.86	0.20	2.57	0.10	1.08	5.25	1.00	0.99	1.00	0.99	0.52	**0.10**	0.45	**0.09**	0.46	**0.09**
V100	**AutoGluon**	**9.43**	**0.16**	**11.64**	**0.35**	**7.92**	**0.05**	**2.60**	**4.46**	**0.99**	**0.99**	**1.00**	**0.99**	**0.37**	**0.08**	**0.33**	**0.07**	**0.33**	**0.07**
	Ensemble (XGB)	10.24	0.24	12.67	0.45	8.31	0.10	2.71	7.80	0.99	0.98	1.00	0.99	0.42	0.20	0.37	0.15	0.37	0.15
	Ensemble (LGB)	26.38	0.54	30.14	0.67	25.11	0.42	6.63	25.46	0.97	0.96	1.00	0.99	0.54	0.40	0.46	0.34	0.47	0.35
	Ensemble (Mix)	10.46	0.32	12.69	0.46	9.43	0.23	2.81	15.49	0.99	0.98	1.00	0.99	0.42	0.31	0.37	0.25	0.37	0.25
P100	**AutoGluon**	**6.87**	**0.66**	**10.69**	**0.96**	**4.52**	**0.42**	**0.28**	**2.38**	**1.00**	**1.00**	**1.00**	**1.00**	**0.32**	0.06	**0.28**	0.04	**0.28**	0.04
	Ensemble (XGB)	33.86	0.73	48.02	1.06	24.22	0.46	1.39	2.63	1.00	1.00	1.00	1.00	0.52	**0.03**	0.45	**0.03**	0.46	**0.03**
	Ensemble (LGB)	213.74	2.55	241.02	3.03	224.82	2.33	10.04	11.36	0.97	0.97	1.00	1.00	0.57	0.43	0.49	0.38	0.49	0.38
	Ensemble (Mix)	38.65	0.89	52.59	1.21	28.81	0.69	1.60	3.61	1.00	0.99	1.00	1.00	0.53	0.08	0.46	0.06	0.47	0.07

Table 8: Various performance metrics of surrogates evaluated to predict latencies and energies on GPT-M for different CPUs. The arrow on the side of the metric name indicates if lower or higher is better.

CPU	Surrogate	Accuracy												Calibration					
		MAE ↓		RMSE ↓		MDAE ↓		MARPD ↓		R^2 ↑		Corr. ↑		RMS Cal. ↓		MA Cal. ↓		Miscal. Area ↓	
		latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies
Xeon Silver	**AutoGluon**	**1713.09**	**13.02**	**2355.46**	**16.40**	**1261.81**	10.12	**3.50**	**11.85**	**0.99**	**0.94**	**1.00**	**0.97**	**0.08**	0.54	**0.07**	0.46	**0.07**	0.47
	Ensemble (XGB)	1867.00	13.19	2544.82	16.74	1379.22	10.25	3.78	12.04	0.99	0.93	1.00	0.97	0.14	**0.54**	0.12	**0.46**	0.12	**0.47**
	Ensemble (LGB)	5077.16	15.70	5981.26	20.00	4830.55	13.47	10.78	15.19	0.97	0.91	1.00	0.97	0.44	0.54	0.38	0.46	0.39	0.47
	Ensemble (Mix)	1913.78	13.05	2597.53	16.48	1464.40	**9.92**	3.87	11.93	0.99	0.94	1.00	0.97	0.14	0.54	0.12	0.46	0.12	0.47
Xeon Gold	**AutoGluon**	**997.52**	**1.78**	**1342.44**	**2.36**	**749.29**	**1.37**	**4.66**	**5.51**	**0.99**	**0.98**	**0.99**	**0.99**	0.21	**0.02**	0.19	**0.02**	0.19	**0.02**
	Ensemble (XGB)	1059.66	1.88	1399.18	2.46	835.65	1.49	5.00	5.82	0.99	0.98	0.99	0.99	0.19	0.02	0.17	0.02	0.17	0.02
	Ensemble (LGB)	2038.55	3.23	2439.66	3.88	1886.11	2.99	9.75	9.79	0.96	0.96	0.99	0.99	**0.08**	0.22	**0.07**	0.20	**0.07**	0.20
	Ensemble (Mix)	1042.62	1.88	1395.96	2.47	795.68	1.47	4.81	5.74	0.99	0.98	0.99	0.99	0.20	0.02	0.18	0.02	0.18	0.02
AMD 7502	**AutoGluon**	**2793.38**	**22.27**	**3832.68**	**29.64**	**2039.52**	**16.81**	**4.75**	**4.81**	**0.99**	**0.99**	**0.99**	**0.99**	**0.36**	**0.45**	**0.32**	**0.40**	**0.32**	**0.40**
	Ensemble (XGB)	2889.71	22.93	3927.64	30.61	2083.31	17.06	4.95	4.98	0.99	0.99	0.99	0.99	0.41	0.47	0.36	0.41	0.36	0.41
	Ensemble (LGB)	5664.76	44.12	6951.41	54.57	5092.86	39.69	11.17	11.02	0.96	0.96	0.99	0.99	0.51	0.51	0.44	0.44	0.44	0.45
	Ensemble (Mix)	2888.22	22.81	3930.69	30.58	2101.56	16.93	4.95	4.94	0.99	0.99	0.99	0.99	0.41	0.46	0.36	0.40	0.36	0.40
AMD 7513	**AutoGluon**	**3297.57**	**315.32**	**6512.33**	**708.51**	**1709.93**	**174.70**	**1.92**	**14.36**	**1.00**	**0.74**	**1.00**	**0.86**	**0.46**	0.55	**0.40**	0.48	**0.40**	0.48
	Ensemble (XGB)	4020.05	344.26	7071.85	724.33	2639.66	200.98	2.55	15.96	1.00	0.72	1.00	0.85	0.49	0.55	0.43	0.48	0.43	0.48
	Ensemble (LGB)	15744.34	367.84	18417.64	744.75	15733.28	256.65	11.25	19.37	0.97	0.71	1.00	0.85	0.57	0.56	0.49	0.48	0.49	0.49
	Ensemble (Mix)	4390.21	329.13	7277.61	717.62	3043.23	183.58	2.72	14.82	0.99	0.73	1.00	0.85	0.50	**0.55**	0.44	**0.48**	0.44	**0.48**
AMD 7452	**AutoGluon**	**6422.40**	**19.16**	**8400.06**	**25.91**	**4603.69**	**13.53**	**8.76**	**8.80**	**0.96**	**0.96**	**0.98**	**0.98**	**0.40**	**0.43**	**0.34**	**0.37**	**0.35**	**0.38**
	Ensemble (XGB)	6583.99	19.77	8650.39	26.64	4800.54	14.12	9.01	9.17	0.96	0.96	0.98	0.98	0.46	0.47	0.40	0.41	0.41	0.42
	Ensemble (LGB)	8414.41	25.28	11082.78	33.29	6746.91	20.86	13.18	13.17	0.93	0.93	0.98	0.98	0.49	0.51	0.43	0.44	0.43	0.44
	Ensemble (Mix)	6535.60	19.66	8556.66	26.48	5013.65	14.41	8.93	9.06	0.96	0.96	0.98	0.98	0.46	0.47	0.40	0.41	0.40	0.41

Table 9: Various performance metrics of surrogates evaluated to predict latencies and energies on GPT-L for different GPUs. The arrow on the side of the metric name indicates if lower or higher is better.

GPU	Surrogate	Accuracy												Calibration					
		MAE ↓		RMSE ↓		MDAE ↓		MARPD ↓		R^2 ↑		Corr. ↑		RMS Cal. ↓		MA Cal. ↓		Miscal. Area ↓	
		latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies
A100	**AutoGluon**	**1.43**	**0.34**	**1.97**	**0.56**	**1.14**	**0.16**	**0.70**	**6.63**	**1.00**	**0.98**	**1.00**	**0.99**	0.31	0.39	0.24	0.34	0.24	0.34
	Ensemble (XGB)	2.07	0.36	2.85	0.58	1.55	0.18	1.00	7.55	1.00	0.97	1.00	0.99	0.30	0.35	0.22	0.31	0.23	0.32
	Ensemble (LGB)	9.28	0.67	10.63	0.84	9.24	0.54	4.75	18.27	0.97	0.95	1.00	0.99	0.46	**0.13**	0.41	**0.10**	0.41	**0.10**
	Ensemble (Mix)	2.16	0.38	2.94	0.58	1.68	0.21	1.04	8.26	1.00	0.97	1.00	0.99	**0.29**	0.34	**0.22**	0.30	**0.22**	0.31
A40	**AutoGluon**	**0.61**	**0.18**	**0.90**	**0.23**	**0.41**	**0.15**	**0.27**	**2.43**	**1.00**	**1.00**	**1.00**	**1.00**	**0.44**	0.38	**0.39**	0.34	**0.39**	0.35
	Ensemble (XGB)	2.44	0.23	3.37	0.28	1.81	0.19	1.11	2.88	1.00	1.00	1.00	1.00	0.54	0.36	0.47	0.32	0.47	0.32
	Ensemble (LGB)	15.23	0.83	17.17	0.95	16.50	0.87	7.69	10.53	0.97	0.97	1.00	1.00	0.57	**0.06**	0.49	**0.05**	0.49	**0.05**
	Ensemble (Mix)	2.41	0.22	3.34	0.28	1.74	0.19	1.07	2.79	1.00	1.00	1.00	1.00	0.54	0.36	0.47	0.32	0.47	0.33
H100	**AutoGluon**	**0.15**	**0.13**	**0.21**	**0.17**	**0.11**	0.09	**0.15**	**5.37**	**1.00**	**0.96**	**1.00**	**0.98**	**0.22**	0.16	**0.20**	0.14	**0.20**	0.14
	Ensemble (XGB)	0.62	0.13	0.83	0.18	0.47	0.09	0.63	5.50	1.00	0.96	1.00	0.98	0.48	0.16	0.42	0.14	0.42	0.14
	Ensemble (LGB)	3.61	0.18	4.11	0.23	3.79	0.15	3.84	8.09	0.97	0.93	1.00	0.98	0.56	0.27	0.48	0.25	0.49	0.25
	Ensemble (Mix)	0.57	0.13	0.78	0.17	0.41	**0.08**	0.57	5.41	1.00	0.96	1.00	0.98	0.47	**0.16**	0.41	**0.14**	0.41	**0.14**
RTX2080	**AutoGluon**	**2.40**	**1.80**	**3.43**	**2.58**	**1.53**	1.12	**0.59**	**10.68**	**1.00**	**0.90**	**1.00**	**0.95**	0.16	**0.24**	0.14	**0.22**	0.14	**0.22**
	Ensemble (XGB)	5.21	1.83	6.98	2.63	4.06	1.15	1.30	10.91	1.00	0.90	1.00	0.95	**0.16**	0.29	**0.13**	0.25	**0.13**	0.25
	Ensemble (LGB)	28.00	2.09	31.84	2.92	30.68	1.42	7.61	13.14	0.97	0.88	1.00	0.95	0.35	0.35	0.32	0.30	0.32	0.31
	Ensemble (Mix)	4.79	1.83	6.60	2.62	3.46	**1.09**	1.14	10.92	1.00	0.90	1.00	0.95	0.16	0.30	0.13	0.26	0.13	0.27
RTX3080	**AutoGluon**	**1.49**	**0.68**	**2.13**	**0.77**	**0.99**	0.66	**0.50**	**6.50**	**1.00**	**0.99**	**1.00**	**1.00**	**0.13**	0.07	**0.12**	0.06	**0.12**	0.06
	Ensemble (XGB)	3.95	0.70	5.40	0.81	2.89	0.65	1.36	6.59	1.00	0.99	1.00	1.00	0.21	0.07	0.15	0.06	0.16	0.06
	Ensemble (LGB)	22.68	1.46	25.65	1.71	24.92	1.42	8.86	12.08	0.97	0.96	1.00	1.00	0.52	0.12	0.45	0.11	0.46	0.11
	Ensemble (Mix)	3.86	0.69	5.32	0.81	2.78	**0.65**	1.32	6.56	1.00	0.99	1.00	1.00	0.23	**0.07**	0.17	**0.06**	0.17	**0.06**
A6000	**AutoGluon**	**1.56**	**0.45**	**2.24**	**0.61**	**1.08**	**0.33**	**0.74**	**7.13**	**1.00**	**0.98**	**1.00**	**0.99**	**0.48**	0.20	**0.42**	0.17	**0.42**	0.18
	Ensemble (XGB)	2.22	0.47	3.06	0.63	1.57	0.34	1.11	7.21	1.00	0.98	1.00	0.99	0.51	0.19	0.44	0.17	0.45	0.17
	Ensemble (LGB)	13.40	0.84	15.18	1.04	14.58	0.67	7.47	12.16	0.97	0.95	1.00	0.99	0.57	**0.03**	0.49	**0.02**	0.49	**0.02**
	Ensemble (Mix)	2.08	0.46	2.95	0.63	1.45	0.34	0.99	7.36	1.00	0.98	1.00	0.99	0.50	0.17	0.43	0.15	0.44	0.15
V100	**AutoGluon**	11.61	**0.30**	**13.29**	**2.99**	11.30	**0.15**	4.23	**3.74**	**0.98**	**0.86**	**0.99**	**0.93**	**0.52**	0.21	**0.45**	0.19	**0.45**	0.19
	Ensemble (XGB)	**11.50**	0.44	13.66	3.02	**10.46**	0.25	**4.16**	6.43	0.98	0.86	0.99	0.93	0.54	**0.05**	0.47	**0.05**	0.47	**0.05**
	Ensemble (LGB)	17.77	1.32	22.53	3.31	13.23	1.34	6.55	25.45	0.96	0.83	0.99	0.93	0.54	0.34	0.46	0.30	0.47	0.30
	Ensemble (Mix)	11.84	0.43	13.63	3.03	10.69	0.24	4.35	6.30	0.98	0.86	0.99	0.93	0.55	0.07	0.47	0.06	0.48	0.06
P100	**AutoGluon**	**5.59**	**0.78**	**7.81**	**1.27**	**4.28**	**0.40**	**0.52**	**1.31**	**1.00**	**1.00**	**1.00**	**1.00**	**0.29**	0.13	**0.26**	0.11	**0.26**	0.12
	Ensemble (XGB)	21.84	1.17	29.68	1.77	16.52	0.73	1.61	2.18	1.00	1.00	1.00	1.00	0.49	**0.06**	0.43	**0.06**	0.43	**0.06**
	Ensemble (LGB)	131.33	5.74	146.45	6.60	139.03	5.69	10.74	13.53	0.97	0.97	1.00	1.00	0.57	0.50	0.49	0.44	0.49	0.44
	Ensemble (Mix)	23.97	1.64	31.74	2.20	18.94	1.30	1.76	3.66	1.00	1.00	1.00	1.00	0.49	0.20	0.42	0.18	0.43	0.18

Table 10: Various performance metrics of surrogates evaluated to predict latencies and energies on GPT-L for different CPUs. The arrow on the side of the metric name indicates if lower or higher is better.

CPU	Surrogate	Accuracy												Calibration					
		MAE ↓		RMSE ↓		MDAE ↓		MARPD ↓		R^2 ↑		Corr. ↑		RMS Cal. ↓		MA Cal. ↓		Miscal. Area ↓	
		latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies	latencies	energies
Xeon Silver	**AutoGluon**	**636.15**	5.61	**864.06**	**7.70**	**494.13**	3.93	**2.54**	**9.84**	**1.00**	**0.96**	**1.00**	**0.98**	0.17	0.44	0.15	0.38	0.15	0.39
	Ensemble (XGB)	753.47	5.72	1025.05	7.81	578.99	4.01	2.96	10.02	1.00	0.96	1.00	0.98	0.08	**0.42**	0.07	**0.36**	0.07	**0.37**
	Ensemble (LGB)	2824.18	8.02	3236.41	9.97	2733.85	6.99	11.64	14.87	0.97	0.93	1.00	0.98	0.41	0.48	0.37	0.41	0.37	0.42
	Ensemble (Mix)	794.59	**5.60**	1061.38	7.73	619.52	**3.82**	3.12	10.00	1.00	0.96	1.00	0.98	**0.06**	0.42	**0.05**	0.36	**0.06**	0.37
Xeon Gold	**AutoGluon**	**1808.83**	**2.94**	**4993.72**	**9.06**	**961.39**	**1.64**	**12.44**	**12.52**	**0.65**	**0.60**	**0.81**	**0.77**	**0.04**	**0.22**	**0.03**	**0.20**	**0.03**	**0.20**
	Ensemble (XGB)	2071.91	3.33	5172.30	9.21	1192.99	2.01	14.28	14.39	0.62	0.58	0.79	0.76	0.23	0.36	0.21	0.32	0.21	0.32
	Ensemble (LGB)	2276.83	3.72	5208.21	9.42	1546.31	2.52	16.82	17.10	0.62	0.56	0.80	0.76	0.32	0.42	0.28	0.37	0.28	0.37
	Ensemble (Mix)	1956.75	3.15	5056.95	9.17	1058.07	1.74	13.15	13.29	0.64	0.59	0.80	0.77	0.21	0.35	0.18	0.31	0.18	0.31
AMD 7502	**AutoGluon**	**979.59**	**10.85**	**1401.41**	**15.13**	**637.77**	**7.47**	**3.47**	**4.78**	**0.99**	**0.99**	**1.00**	**0.99**	**0.32**	0.46	**0.29**	0.40	**0.29**	0.41
	Ensemble (XGB)	1061.60	11.30	1488.69	15.60	747.04	8.16	3.90	5.16	0.99	0.99	1.00	0.99	0.36	0.47	0.32	0.41	0.32	0.41
	Ensemble (LGB)	2963.13	24.72	3487.50	29.94	2788.52	22.54	12.75	13.26	0.96	0.96	1.00	0.99	0.53	0.54	0.46	0.47	0.46	0.47
	Ensemble (Mix)	1077.05	11.22	1504.92	15.53	777.37	8.19	3.88	4.97	0.99	0.99	1.00	0.99	0.34	**0.44**	0.30	**0.38**	0.31	**0.39**
AMD 7513	**AutoGluon**	**1341.23**	**138.82**	**2336.42**	**193.98**	**747.38**	**92.12**	**1.55**	**13.84**	**1.00**	**0.91**	**1.00**	**0.96**	**0.48**	**0.55**	**0.42**	**0.48**	**0.42**	**0.48**
	Ensemble (XGB)	1821.68	141.56	2867.87	198.08	1203.03	97.95	2.32	14.26	1.00	0.91	1.00	0.95	0.53	0.56	0.45	0.48	0.46	0.48
	Ensemble (LGB)	8438.54	158.86	9602.56	224.77	8622.26	129.98	12.73	18.19	0.97	0.88	1.00	0.95	0.57	0.56	0.49	0.48	0.49	0.49
	Ensemble (Mix)	1990.32	141.12	2967.07	197.03	1402.25	103.07	2.56	14.02	1.00	0.91	1.00	0.95	0.53	0.56	0.46	0.48	0.46	0.49
AMD 7452	**AutoGluon**	**766.81**	**4.16**	**1101.54**	**6.15**	**535.75**	**2.72**	**2.52**	**4.20**	**1.00**	**0.99**	**1.00**	**1.00**	**0.05**	**0.26**	**0.04**	**0.23**	**0.05**	**0.23**
	Ensemble (XGB)	895.53	4.40	1262.25	6.44	636.53	3.02	2.98	4.55	1.00	0.99	1.00	1.00	0.14	0.29	0.12	0.26	0.13	0.26
	Ensemble (LGB)	3265.62	10.37	3747.71	12.55	3294.40	9.69	12.28	12.92	0.97	0.96	1.00	0.99	0.50	0.50	0.43	0.43	0.44	0.44
	Ensemble (Mix)	920.19	4.45	1277.03	6.47	681.07	2.98	3.07	4.57	1.00	0.99	1.00	0.99	0.14	0.29	0.13	0.26	0.13	0.26

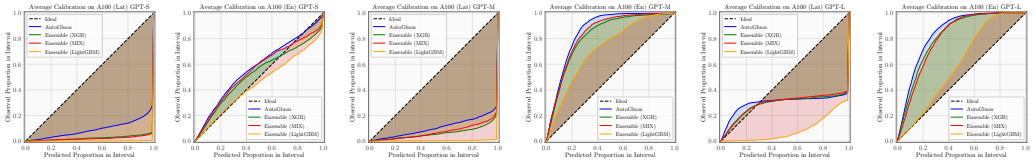


Figure 9: Calibration Areas A100

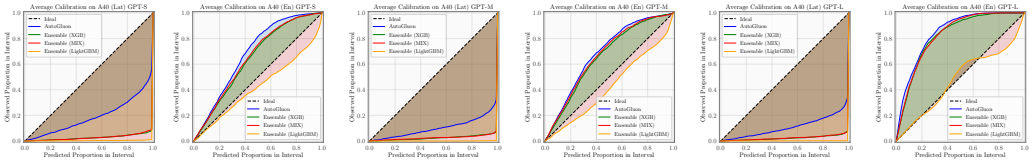


Figure 10: Calibration Areas A40

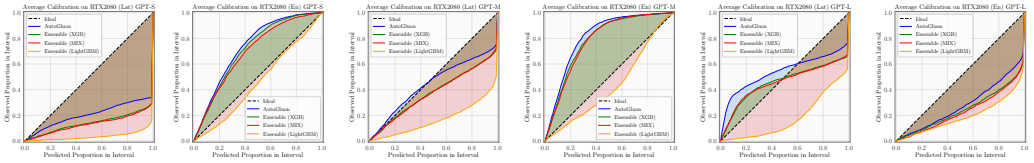


Figure 11: Calibration Areas RTX2080

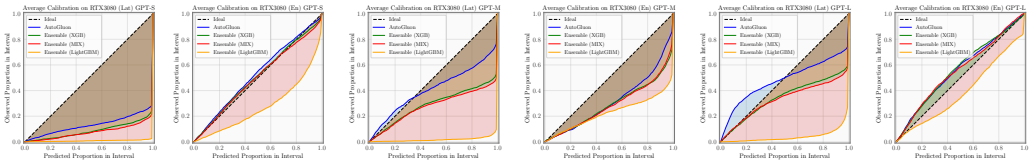


Figure 12: Calibration Areas RTX3080

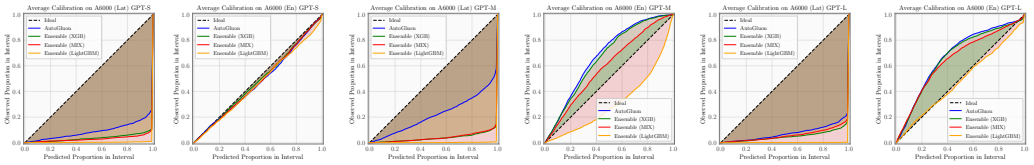


Figure 13: Calibration Areas A6000

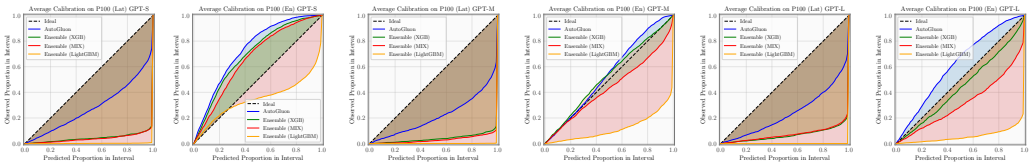


Figure 14: Calibration Areas P100

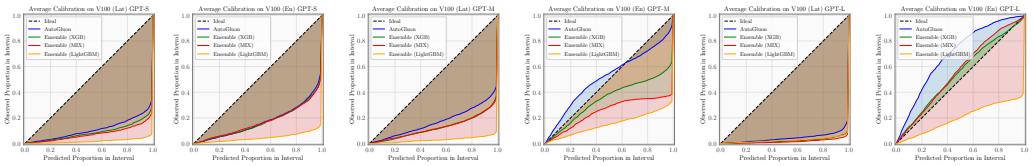


Figure 15: Calibration Areas V100

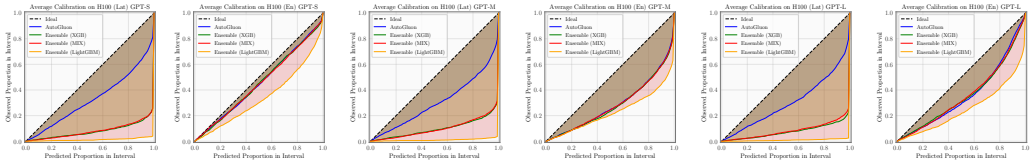


Figure 16: Calibration Areas H100

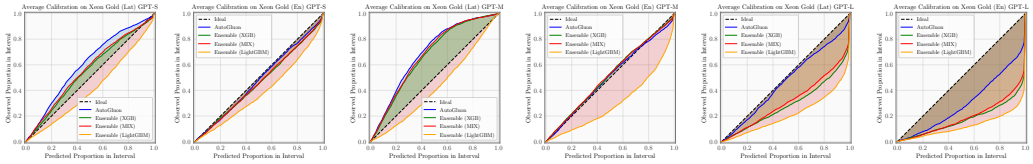


Figure 17: Calibration Areas Xeon Gold

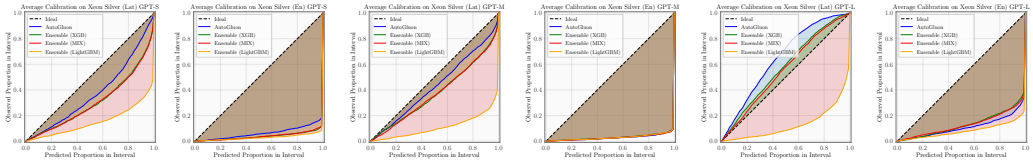


Figure 18: Calibration Areas Xeon Silver

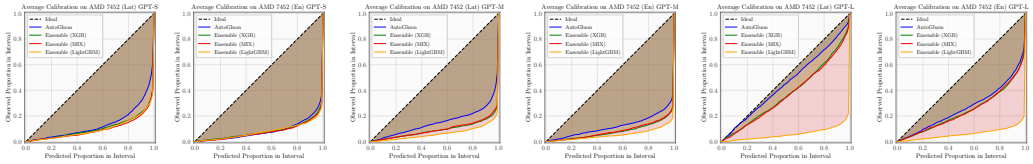


Figure 19: Calibration Areas CPU AMD 7452

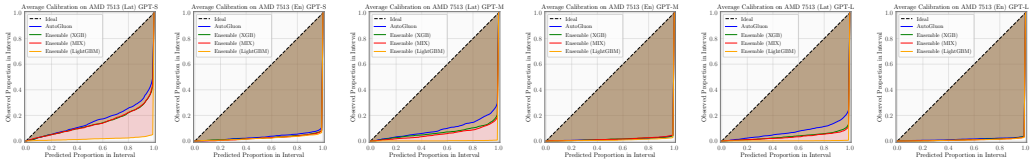


Figure 20: Calibration Areas CPU AMD 7513

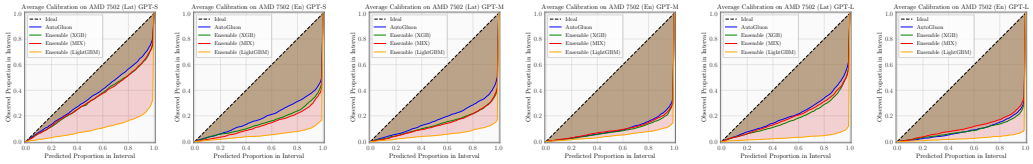


Figure 21: Calibration Areas CPU AMD 7502

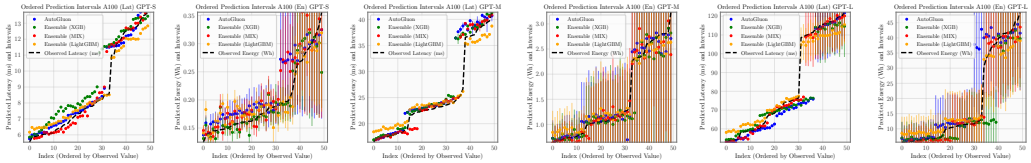


Figure 22: Prediction Intervals A100

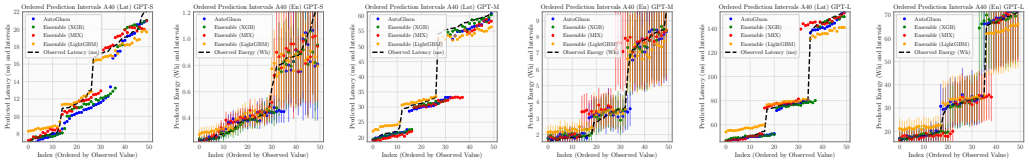


Figure 23: Prediction Intervals A40

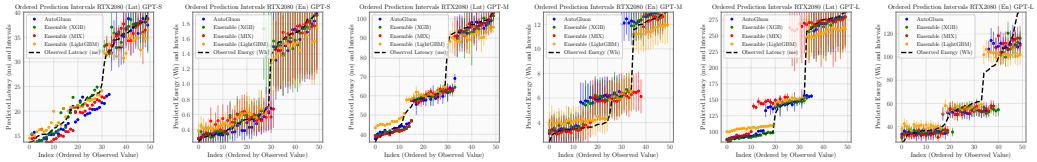


Figure 24: Prediction Intervals RTX2080

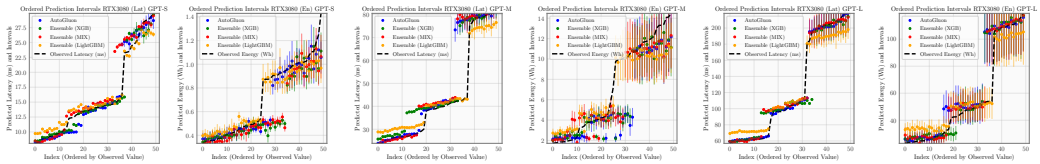


Figure 25: Prediction Intervals RTX3080

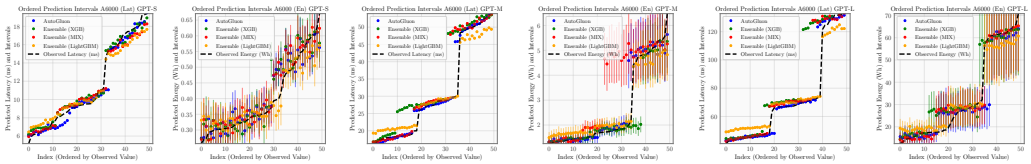


Figure 26: Prediction Intervals A6000

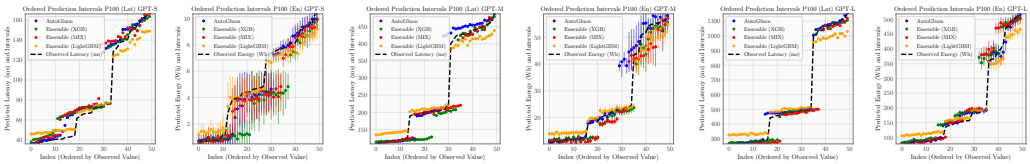


Figure 27: Prediction Intervals P100

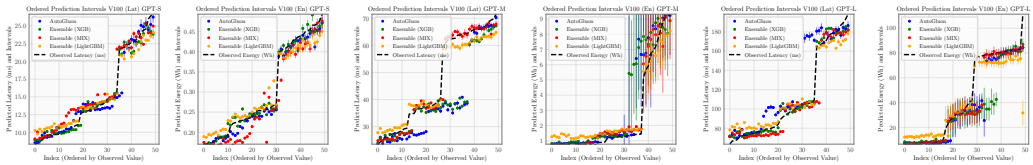


Figure 28: Prediction Intervals V100

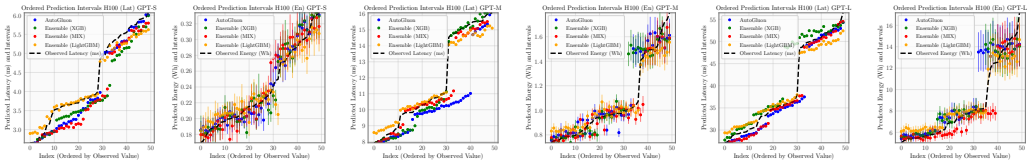


Figure 29: Prediction Intervals H100

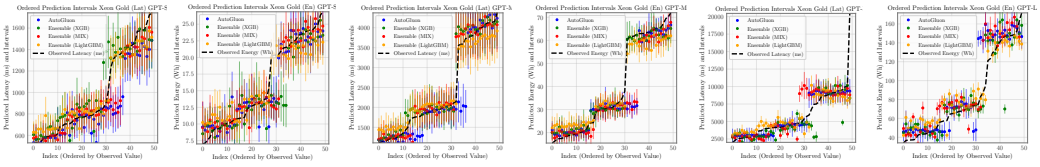


Figure 30: Prediction Intervals Xeon Gold

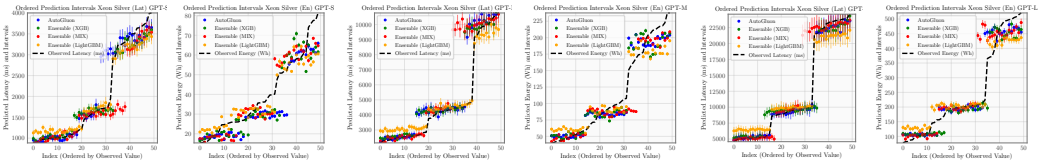


Figure 31: Prediction Intervals Xeon Silver

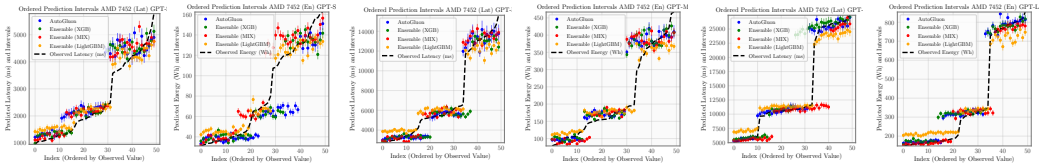


Figure 32: Prediction Intervals CPU AMD 7452

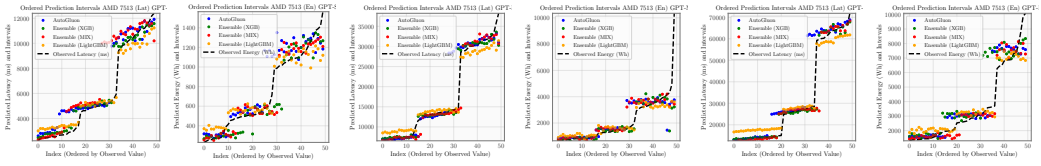


Figure 33: Prediction Intervals CPU AMD 7513

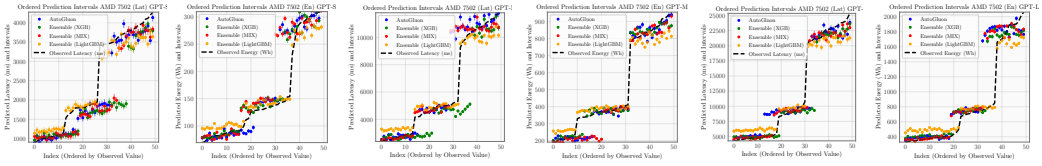


Figure 34: Prediction Intervals CPU AMD 7502

E Comparison with NAS-Bench-301

Given the immense size of the search spaces (approximately 10^{36}), training architectures from scratch is impractical. Our work is inspired by surrogate benchmarks such as those proposed by [88]. However, HW-GPT-Bench presents several key differences compared to NB301. First, unlike NB301, which trains architectures from scratch—impractical for larger models and dataset sizes—we utilize an efficient weight-sharing-based supernet. The performance of the inherited subnetwork directly serves as a reliable performance estimation proxy, and these architectures can be fine-tuned if necessary. We also employ a sandwich scheme to train the supernet by sampling the largest, smallest, and a set of random architectures. Second, while NB301 uses the DARTS pre-training pipeline, we introduce three novel search spaces and design a training pipeline specifically for supernet training. Additionally, we focus on the application domain of language modeling, in contrast to NB301's primary focus on image classification. Lastly, unlike NB301, our work supports a range of hardware devices and provides well-calibrated latency predictions. To our knowledge, we are the first to study the calibration of surrogate models for latency predictions.

F Importance Analysis

In this section, we provide details on the methods we used throughout the paper to analyze and interpret the data collected from the HW-GPT-Bench search space.

F.1 OLS Covariate Analysis.

Ordinary Least Squares (OLS) is a statistical method used for estimating the parameters of a linear regression model. The primary goal of OLS is to minimize the sum of the squared residuals, which are the differences between the observed values and the values predicted by the model. In the context of OLS, covariate analysis involves examining the relationships between independent variables (covariates) and the dependent variable. This analysis helps to understand how each covariate contributes to the prediction of the dependent variable and the overall model performance. To fit the linear regression model and conduct the analysis we used `statsmodel.regression.linear_model.OLS` [10].

F.1.1 Key Concepts in OLS

Linear Regression Model: The model assumes a linear relationship between the dependent variable Y (perplexity) and one or more independent variables (covariates). The general form of the model is:

$$Y = \beta_0 + \beta_1 e + \beta_2 l + \sum_{i=1}^{l} \beta_{i+2} h^i + \sum_{i=1}^{l} \beta_{i+2+l} m^i + \beta_{2l+3} b + \epsilon,$$

where β_0 is the intercept, β_i (for $i = 1, \ldots, 2l + 3$) are the coefficients of the covariates, and ϵ represents the error term. l is the number of layers, e is the embedding dimension, m^i and h^i are the MLP ratio and number of heads on layer i, respectively, and b is the bias.

Objective of OLS: The goal is to estimate the coefficients β such that we minimize the sum of the squared residuals (SSR):

$$SSR = \sum_{i=1}^{N} (Y_i - \hat{Y}_i)^2,$$

where Y_i is the observed ground truth perplexity and $\hat{Y}_i$ is the predicted perplexity by the Linear Regression model.

F.1.2 Covariate Analysis

Covariate analysis in the context of OLS involves investigating the effect of each independent variable (embedding dimension, number of layers, etc.) on the dependent variable, i.e. perplexity. This includes:

[10] https://www.statsmodels.org/dev/examples/notebooks/generated/ols.html

- **Estimating Coefficients**: Determining the values of $\beta_1, \beta_2, \ldots, \beta_{2l+3}$ which represent the change in perplexity for a one-unit change in the respective architectural dimension, holding other variables constant.
- **Statistical Significance**: Assessing the significance of each coefficient using t-tests. The null hypothesis H_0 states that the coefficient is zero (no effect). The p-value indicates whether the null hypothesis can be rejected.
- **Standard Errors**: Providing a measure of the variability of the coefficient estimates. Smaller standard errors suggest more precise estimates.
- **Goodness-of-Fit**: Evaluating how well the model explains the variability of perplexity using metrics such as R-squared and adjusted R-squared. R-squared indicates the proportion of the variance in perplexity that is predictable from the independent variables.

The results of the OLS analysis for perplexity on the collected samples are presented below. These results include:

1. **Coefficients (β)**: Estimates for each covariate.
2. **Standard Errors**: Indicate the precision of the coefficient estimates.
3. **t-Values**: Used to test the hypothesis that a coefficient is significantly different from zero.
4. **P-Values**: Indicate the significance level of each coefficient.
5. $\mathbf{R}^2$: The proportion of the variance in the dependent variable explained by the model.
6. **Adjusted R-squared**: Adjusted for the number of predictors in the model, providing a more accurate measure of goodness-of-fit for models with multiple covariates.

OLS Regression Results GPT-L

Dep. Variable:	perplexity	R-squared:	0.901			
Model:	OLS	Adj. R-squared:	0.901			
Method:	Least Squares	F-statistic:	1.817e+04			
No. Observations:	10000	AIC:	3.395e+04			
Df Residuals:	9994	BIC:	3.399e+04			
Df Model:	5					
Covariance Type:	nonrobust					

	coef	std err	t	P>|t|	[0.025	0.975]
const	23.6263	0.013	1788.886	0.000	23.600	23.652
num_layers	-0.0426	0.013	-3.227	0.001	-0.069	-0.017
embed_dim	-3.9787	0.013	-301.209	0.000	-4.005	-3.953
mean_mlp_ratio	-0.1164	0.013	-8.812	0.000	-0.142	-0.091
mean_heads	-0.0612	0.013	-4.634	0.000	-0.087	-0.035
bias	-0.0630	0.013	-4.769	0.000	-0.089	-0.037

Omnibus:	75511.319	Durbin-Watson:	2.026
Prob(Omnibus):	0.000	Jarque-Bera (JB):	1537.046
Skew:	-0.635	Prob(JB):	0.00
Kurtosis:	1.559	Cond. No.	1.03

OLS Regression Results GPT-M

Dep. Variable:	perplexity	R-squared:	0.914
Model:	OLS	Adj. R-squared:	0.914
Method:	Least Squares	F-statistic:	2.117e+04
No. Observations:	10000	AIC:	3.791e+04
Df Residuals:	9994	BIC:	3.796e+04

```
Df Model:                           5
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         28.1305      0.016   1747.009      0.000      28.099      28.162
num_layers    -0.0983      0.016     -6.104      0.000      -0.130      -0.067
embed_dim     -5.2315      0.016   -324.795      0.000      -5.263      -5.200
mean_mlp_ratio -0.1445     0.016     -8.975      0.000      -0.176      -0.113
mean_heads    -0.0744      0.016     -4.623      0.000      -0.106      -0.043
bias          -0.0650      0.016     -4.035      0.000      -0.097      -0.033
==============================================================================
Omnibus:                    66013.096   Durbin-Watson:                   2.021
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1509.031
Skew:                          -0.600   Prob(JB):                         0.00
Kurtosis:                       1.524   Cond. No.                         1.03
==============================================================================

==============================================================================
                        OLS Regression Results GPT-S
==============================================================================
Dep. Variable:              perplexity   R-squared:                       0.949
Model:                             OLS   Adj. R-squared:                  0.949
Method:                  Least Squares   F-statistic:                 3.754e+04
No. Observations:                10000   AIC:                         3.667e+04
Df Residuals:                     9994   BIC:                         3.671e+04
Df Model:                            5
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         32.3973      0.015   2141.130      0.000      32.368      32.427
num_layers    -0.4912      0.015    -32.459      0.000      -0.521      -0.462
embed_dim     -6.5321      0.015   -431.656      0.000      -6.562      -6.502
mean_mlp_ratio -0.2199     0.015    -14.530      0.000      -0.250      -0.190
mean_heads    -0.2739      0.015    -18.096      0.000      -0.304      -0.244
bias          -0.0251      0.015     -1.661      0.097      -0.055       0.005
==============================================================================
Omnibus:                    88675.889   Durbin-Watson:                   2.044
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1321.623
Skew:                          -0.544   Prob(JB):                     1.03e-287
Kurtosis:                       1.589   Cond. No.                         1.03
==============================================================================
```

F.2 Power-laws for GPT-wide spaces

We define the power-law fits for GPT-wide spaces below. Similar to the observation in 4, we see that the embedding size has the most effect on perplexity, followed by number of layers, mlp expansion ratio and number of heads. The bias plays a minimal role in determining perplexity of an architecture.

$$\text{GPT-S-wide:} \quad y = 1116.453 \cdot l^{-0.212} \cdot e^{-0.3770} \cdot m^{-0.0514} \cdot h^{-0.0647} \cdot b^{-0.000190},$$

$$\text{GPT-M-wide:} \quad y = 618.0753 \cdot l^{-0.1795} \cdot e^{-0.3401} \cdot m^{-0.0711} \cdot h^{-0.0556} \cdot b^{-0.0050},$$

$$\text{GPT-L-wide:} \quad y = 498.9920 \cdot l^{-0.1659} \cdot e^{-0.3204} \cdot m^{-0.0692} \cdot h^{-0.053} \cdot b^{-0.0081}.$$

F.3 Recursive Feature Elimination

Recursive Feature Elimination (RFE) is a feature selection method used in machine learning to identify the most relevant features in a dataset. It works by recursively fitting a model and removing the least important feature(s) based on model coefficients or importance scores until the maximum

number of features is reached. Features in our case are the architectural choices, i.e. embedding dimension size, number of layers, etc. The process involves the following steps:

1. **Model Fitting**: The model is initially trained on the entire set of features.
2. **Feature Ranking**: Features are ranked based on their importance scores derived from the fitted model.
3. **Feature Elimination**: The least important feature(s) are removed from the dataset.
4. **Repetition**: Steps 1-3 are repeated recursively on the pruned feature set until the desired number of features is reached or only a single feature remains.

We implement RFE using `sklearn` [11], which provides an efficient and easy-to-use RFE function. We employ a `RandomForest` regressor as the base model due to its ability to handle high-dimensional data and capture non-linear relationships. Specifically, we use a `RandomForest` regressor with 50 estimators, which balances model complexity and computational efficiency. In Figures 35, 36 and 37, we present the ranking of all search space dimensions for GPT-S, GPT-M and GPT-L spaces.

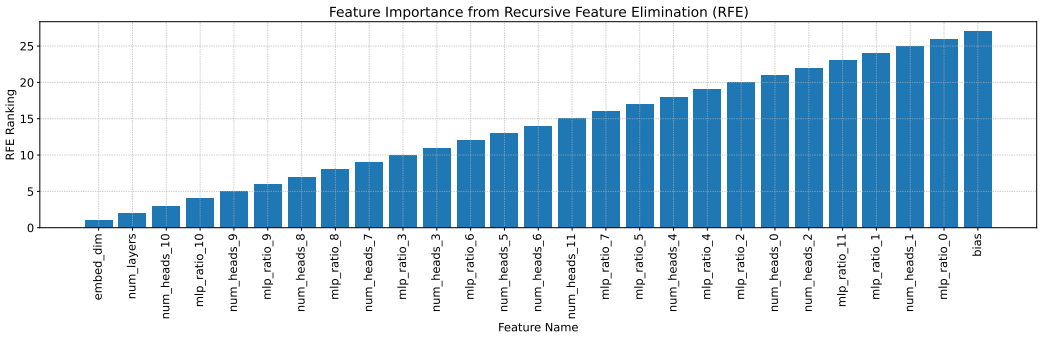


Figure 35: Detailed feature ranking from RFE for GPT-S.

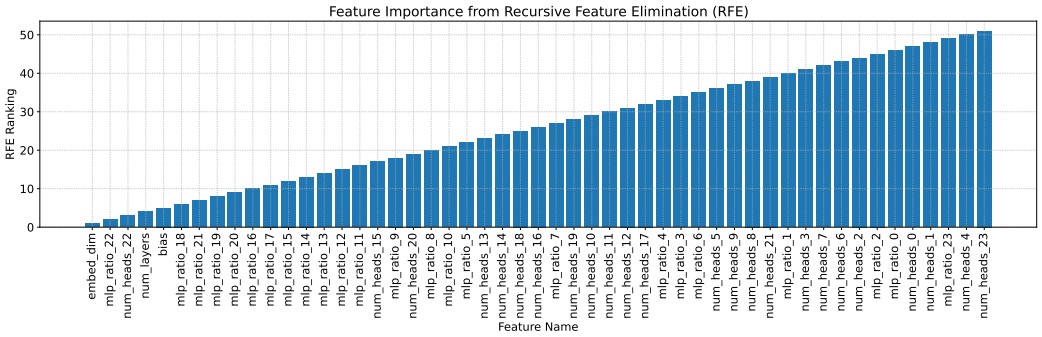


Figure 36: Detailed feature ranking from RFE for GPT-M.

G Details on Empirical Attainment Function (EAF)

Running multi-objective optimization algorithms multiple times can yield different Pareto fronts. Computing uncertainty estimates of Pareto fronts over multiple runs of an algorithm is important to ensure that we appropriately compare different algorithms in a statistically meaningful way. Simply superimposing the Pareto fronts across multiple runs is insufficient in depicting how the Pareto fronts tend to vary. The Empirical Attainment Function (EAF) [25, 47] is a statistical measure used in

[11] https://scikit-learn.org/stable/auto_examples/feature_selection/plot_rfe_digits.html

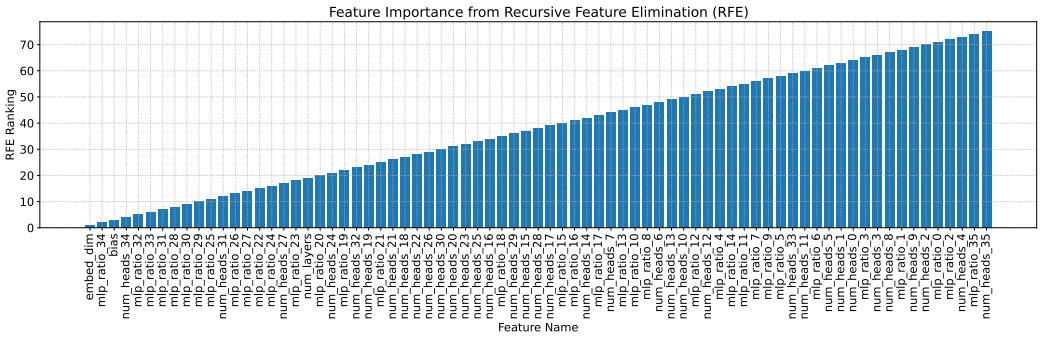


Figure 37: Detailed feature ranking from RFE for GPT-L.

multi-objective optimization to describe the distribution of outcomes achieved by an optimization algorithm over multiple runs. It provides a way to empirically estimate the probability that a given point in the objective space is attained (i.e., dominated or matched) by the solutions generated by the algorithm.

For two solution vectors of the multi-objective function, $\mathbf{y}$ and $\mathbf{z}$, $\mathbf{y}$ weakly dominates $\mathbf{z}$ ($\mathbf{y} \preceq \mathbf{z}$) if the following conditions hold:

1. **Not worse on any objective:** $\mathbf{y}$ is at least as good as $\mathbf{z}$ on all objectives. This means for each objective function, the value in $\mathbf{y}$ is either equal to or better than the corresponding value in $\mathbf{z}$.
2. **Strictly better on at least one objective (or indifferent on all):** $\mathbf{y}$ must be strictly better than $\mathbf{z}$ on at least one objective function. Alternatively, it can be equal on all objectives.

Given a set of Pareto fronts $\{F^1, \ldots, F^n\}$ obtained from n independent runs with different random seeds, the EAF is defined by the following empirical attainment function:

$$\varepsilon(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}[F^i \preceq \mathbf{z}],$$

where $\varepsilon(\mathbf{z})$ represents the EAF value for a specific objective vector $\mathbf{z}$ in the objective space. $\mathbb{I}[F^i \preceq \mathbf{z}]$ is an indicator function that is 1 if the objective vector $\mathbf{z}$ is weakly dominated by the F^i, i.e. the Pareto front from the i-th run, and 0 otherwise. $F^i \preceq \mathbf{z}$ means that there exists at least an objective vector $\mathbf{y}$ in F^i at least as good as $\mathbf{z}$. This doesn't necessarily mean every single run achieved a better outcome than $\mathbf{z}$, but at least one did. In simpler terms, the EAF value at a given objective vector $\mathbf{z}$ represents the portion of independent runs where a Pareto front achieved at least that good of an objective vector (weakly dominated $\mathbf{z}$).

The EAF can be used to visualize uncertainty in the Pareto front by plotting different EAS levels. For example, $S^{1/2}$ represents the set of objective vectors that are weakly dominated by at least half of the independent runs (50% EAF level). To compute the Empirical Attainment Surfaces (EAS) in this paper we used the implementation from Watanabe [80] [12].

H Inheriting v/s Finetuning Subnetworks

We validate the effectiveness of out perplexity surrogate by inheriting randomly sampled 100 subnetworks and comparing the correlation between the perplexity on simply inheriting the subnetworks v/s finetuning the subnetworks further upon inheritance for 5000 update steps. We observe that the inherited subnetwork performance strongly correlates with fine-tuned subnetworks as indicated by Table 11.

I Distribution of Architecture Latencies

We fit a kernel-density-estimator to the collected subnetwork latencies. As observed in Figure 38 and 39, the distribution of CPU latency is more noisier than GPU latency.

[12] https://github.com/nabenabe0928/empirical-attainment-func

Supernet	Kendall-Tau
GPT-S	0.9626
GPT-M	0.9580
GPT-L	0.9286

Table 11: Kendall-Tau values between perplexities after inheriting and perplexities after finetuning (for 5000 steps) for different Supernets for a set of 100 random architectures

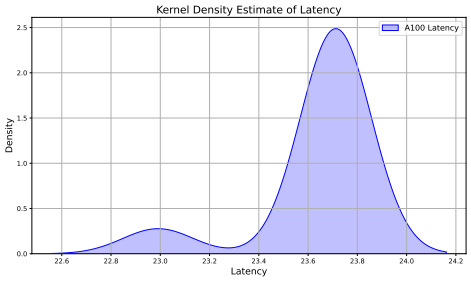


Figure 38: GPU-A100

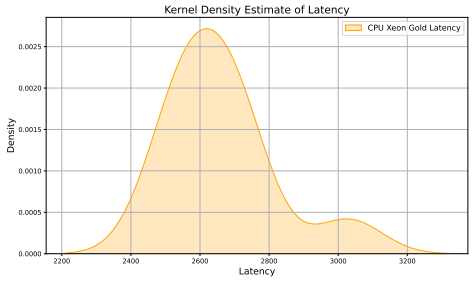


Figure 39: CPU-Xeon Gold

Figure 40: Distribution of Latencies on different devices

J Scatter Plots for GPT-wide

We introduced 4 new search spaces (with more widely spaced choices), mainly GPT-S-wide, GPT-M-wide, GPT-L-wide and GPT-XL-wide and present the scatter plots on the collected ground truth subnetworks for these spaces in Figure 41.

K Multi-objective NAS algorithms

In this section, we provide more details on the multi-objective NAS methods we run on HW-GPT-Bench in Section 5. We use their implementation in SyneTune [62][13].

- **Random Search (RS)**. RS has been shown to be a strong baseline for single [40] and multi-objective [10, 31, 69] architecture search. For this baseline we sample architectures uniformly at random from the search space and then compute the Pareto-Front from these architecture samples. In larger search space, random search, while being embarrasingly parallel and often performant, is not guaranteed to yield the optimal architectures.
- **Multi-Objective Regularized Evolution Algorithm (MOREA).** Regularized Evolution (RE) or Aging Evolution [59] has been quite successfully applied for neural architecture search. Regularized Evolution works by evolving a population of candidates using mutation and periodically discarding the oldest members of the population, inducing a *regularization* effect. In SyneTune RE is extended to Multi-Objective Regularized Evolution (MOREA) by scoring the population via a multi-objective priority based on non-dominated sorting. Parents are then be sampled from the population based on this priority score.
- **Non-dominated Sorting Genetic Algorithm II (NSGA-II)**. NSGA-II [16], is a multi-objective evolutionary algorithm to obtain a Pareto-Set of architectures. It employs non-dominated sorting to rank architecures based on their dominance relationships and **crowding distance** to maintain a diverse population. Through selection, crossover, and mutation, NSGA-II iteratively evolves populations toward the Pareto front, offering a range of trade-off solutions.
- **Local Seach (LS).** SyneTune adapts LS to explore the vicinity of Pareto-optimal points in multi-objective optimization problems, aiming to iteratively refine Pareto-optimal solutions solutions within defined neighborhoods. The method is described in more detail in Klein et al. [36].
- **Bayesian Optimization with Random Scalarizations (RSBO).** RSBO [55] uses an acquisition function that takes as input multiple random scalarizations of the objectives being optimized, to obtain the Pareto-optimal set which minimizes the Bayesian regret.

[13] https://syne-tune.readthedocs.io/en/latest/getting_started.html#supported-multi-objective-optimization-methods

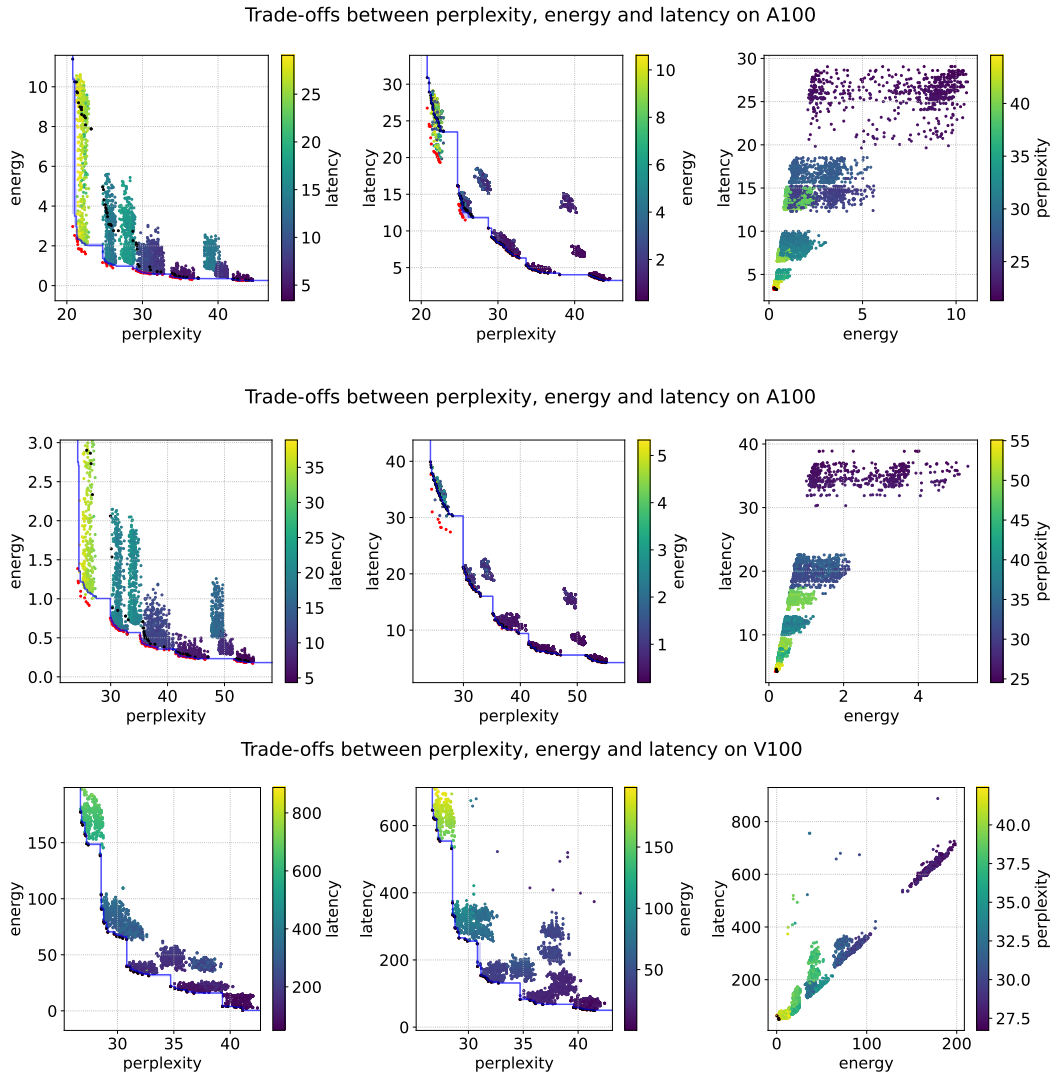


Figure 41: Trade-off scatter plots for GPT-M-wide, GPT-L-wide and GPT-XL-wide

- **Bayesian Optimization with Linear Scalarizations (LSBO).** Similar to RSBO, this method optimizes a single objective corresponding to a fixed linear combination of two objectives instead of randomizing the scalarizations at each BO iteration.
- **Expected Hypervolume Improvement (EHVI).** EHVI [15] is a Bayesian optimization method with an acquisition function designed to efficiently explore the Pareto front in multi-objective optimization problems. It quantifies the expected improvement in hypervolume, which measures the volume of the objective space dominated by Pareto-optimal solutions, that a candidate solution can offer. EHVI guides the search towards regions of the objective space likely to contain better trade-offs, aiding in the discovery of diverse Pareto-optimal solutions.
- **Multi-objective Asynchronous Successive Halving (MOASHA).** MOASHA [65] is a multi-fidelity approach that leverages an asynchronous successive halving scheduler [41] along with non-dominating sorting for budget allocation. It employs the NSGA-II selection mechanism and the ϵ-net [63] exploration strategy, which ranks candidates within the same Pareto set by iteratively choosing the one with the greatest Euclidean distance from the previously selected candidates.

L Additional experiments with MOO methods

In addition to the results presented in the paper we also run MOO methods on our benchmark for latencies and perplexity across different devices and search spaces in Figures 42-54. We present the EAFs resulting from running the baselines for multiple seeds and the hypervolume of the baselines

over the number of surrogate evaluations. Furthermore, we also present the results of running different MOO methods on the energy-perplexity objectives for different devices on GPT-L in Figures 55-59. Interestingly for these two objectives local search is often very performant at higher budgets, outperforming other baselines like NSGA-2 and EHVI.

L.1 Experiments with 2 Objectives

We observe from Figures 42-59 that NSGA-II and EHVI are amongst the top performing methods (even at lower budgets). LS typically has a low hypervolume in the beginning, however, often outperforms other methods with enough budget.

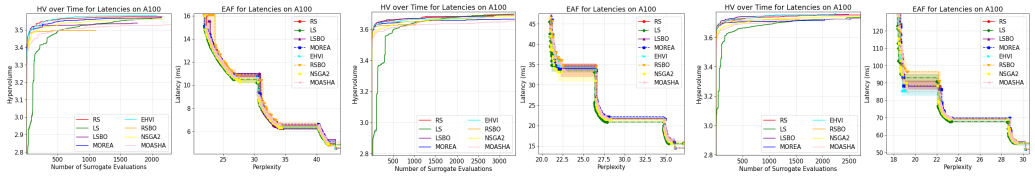


Figure 42: Pareto fronts and HV over time on A100 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

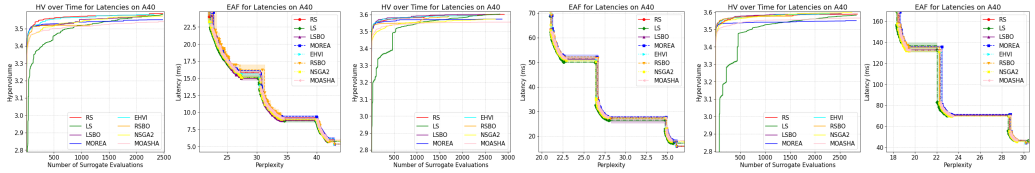


Figure 43: Pareto fronts and HV over time on A40 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

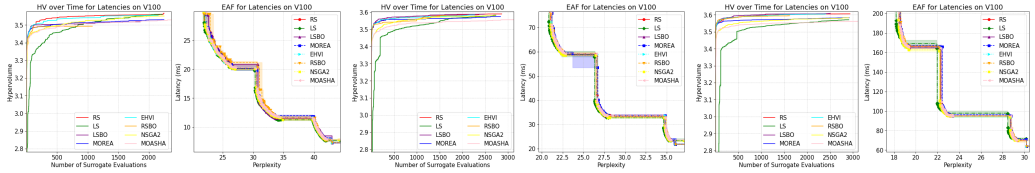


Figure 44: Pareto fronts and HV over time on V100 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

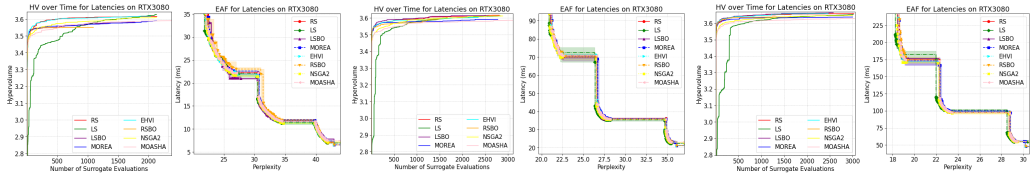


Figure 45: Pareto fronts and HV over time on RTX3080 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

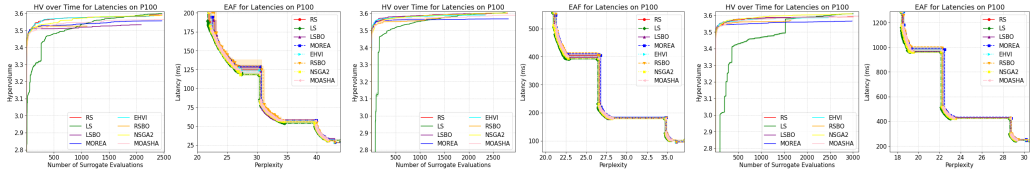


Figure 46: Pareto fronts and HV over time on P100 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

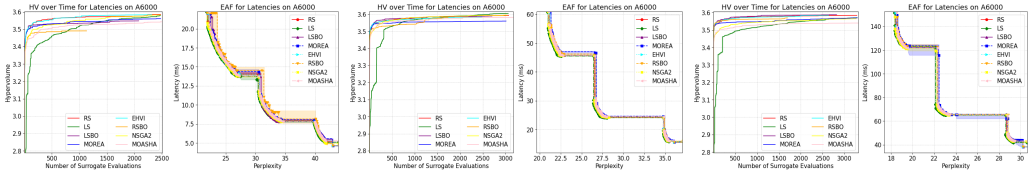


Figure 47: Pareto fronts and HV over time on A6000 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

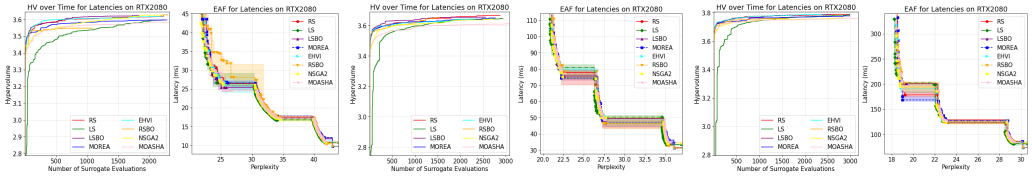


Figure 48: Pareto fronts and HV over time on RTX2080 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

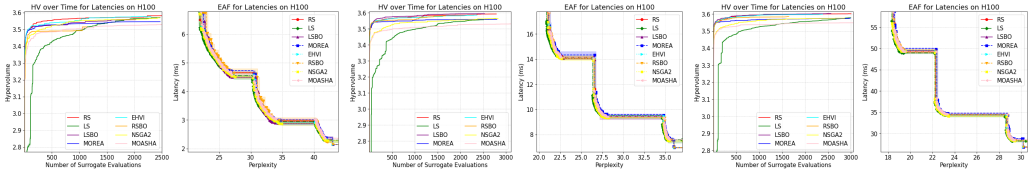


Figure 49: Pareto fronts and HV over time on H100 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

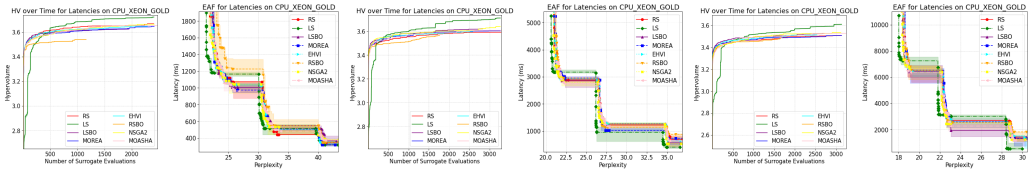


Figure 50: Pareto fronts and HV over time on CPU Xeon Gold for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

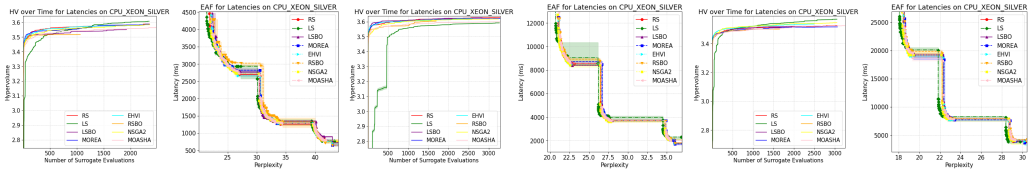


Figure 51: Pareto fronts and HV over time on CPU Xeon Silver for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

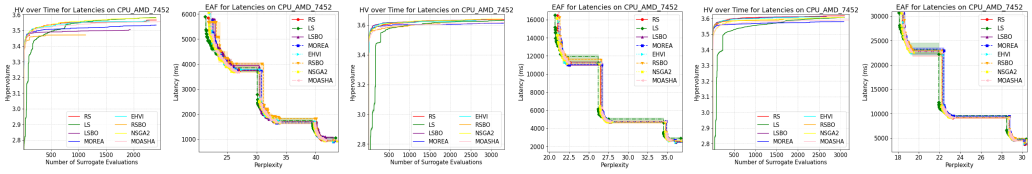


Figure 52: Pareto fronts and HV over time on CPU AMD 7452 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

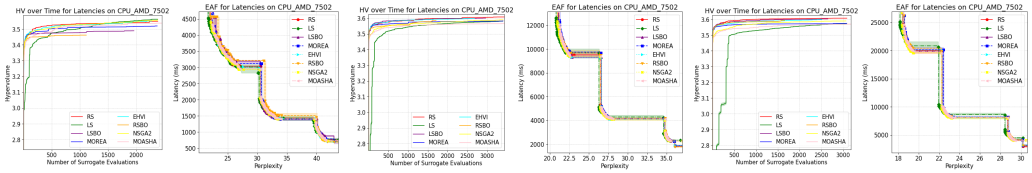


Figure 53: Pareto fronts and HV over time on CPU AMD 7402 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

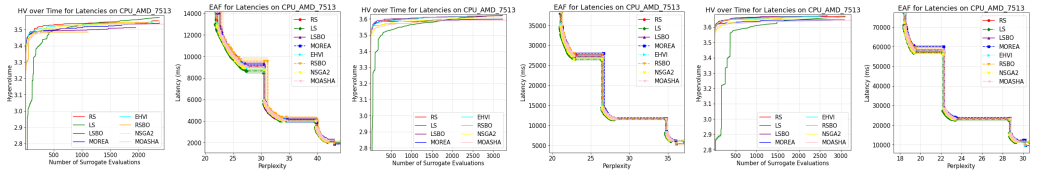


Figure 54: Pareto fronts and HV over time on CPU AMD 7513 for GPT-S (first two), GPT-M (second two) and GPT-L (last two).

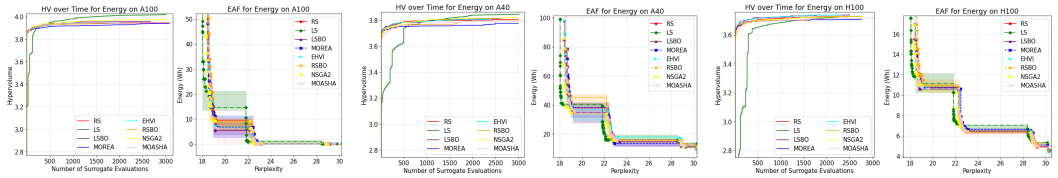


Figure 55: Pareto Fronts and HV on A100 (first 2), A40 (second 2) and H100 (last 2) for GPT-L

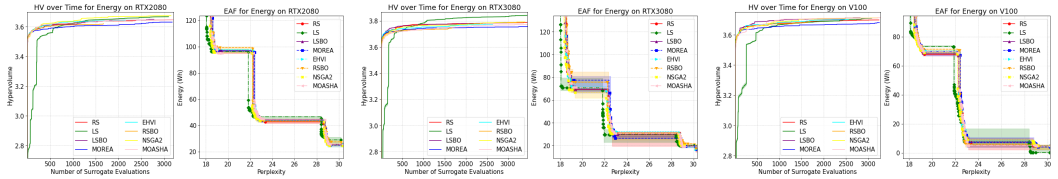


Figure 56: Pareto Fronts and HV on RX2080 (first 2), RTX3080 (second 2) and V100 (last 2) for GPT-L

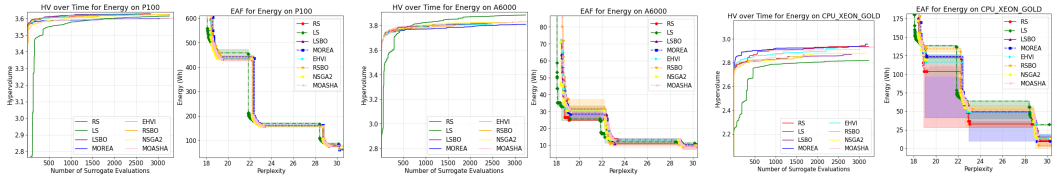


Figure 57: Pareto Fronts and HV on P100 (first 2), A6000 (second 2) and Xeon Gold CPU (last 2) for GPT-L

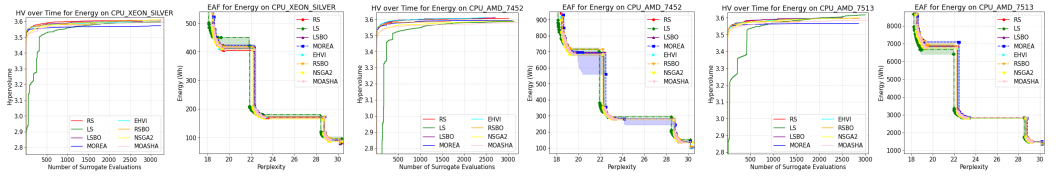


Figure 58: Pareto Fronts and HV on Xeon Silver (first 2), AMD 7452 (second 2) and AMD 7513 (last 2) for GPT-L

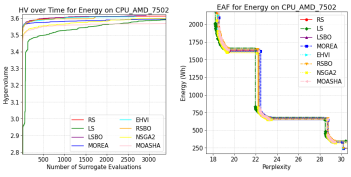


Figure 59: Pareto Fronts and HV on AMD 7502 for GPT-L.

L.2 Experiments with 3 Objectives

In addition, we also use our benchmark to optimize energies and latencies, in conjunction with perplexity, on different devices for the GPT-L space, as presented in Figure 60 and Figure 61. We run these experiments for a smaller time budget of 3 hours using SyneTune. We observe that at smaller time budgets random search and MOO methods based on Bayesian optimization are the top methods.

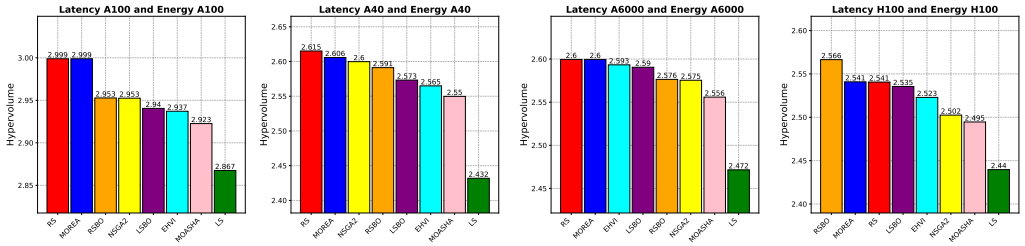


Figure 60: Hypervolumes of baselines optimizing for perplexity, latency and energy usage on A100, A40, A6000 and H100.

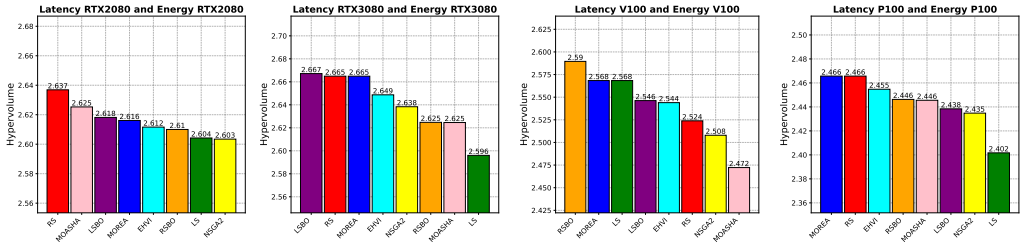


Figure 61: Hypervolumes of baselines optimizing for perplexity, latency and energy usage on RTX2080, RTX3080, V100 and P100.

M Correlations between different metrics

Figures 62,63, 64 show the Kendall-τ rank correlation coefficient across all the metrics supported in HW-GPT-Bench. Given two sets of n observations $\{y_i\}_{i=1}^n$ and $\{z_i\}_{i=1}^n$, the τ coefficient is computed as:

$$\tau = \frac{C - D}{\frac{1}{2}n(n-1)},$$

where C and D are the number of concordant and discordant pairs, respectively. For every pair (i, j) where $1 \leq i < j \leq n$:

1. A pair is **concordant** if the order of both elements in the pair is the same in both datasets: $(y_i < y_j$ and $z_i < z_j)$ or $(y_i > y_j$ and $z_i > z_j)$.
2. A pair is **discordant** if the order of the elements in the pair is different in the two datasets: $(y_i < y_j$ and $z_i > z_j)$ or $(y_i > y_j$ and $z_i < z_j)$.

To compute these values, we use the same 10k ($n = 10000$) ground truth observations that we use to train the surrogate models. For metrics that contain multiple observations, such as latency and energy usage, we use the median value. For easier visualization, we stratify the aforementioned correlation plots by metrics relevant to GPUs (Figures 68,69, 70) and CPUs (Figures 65,66, 67).

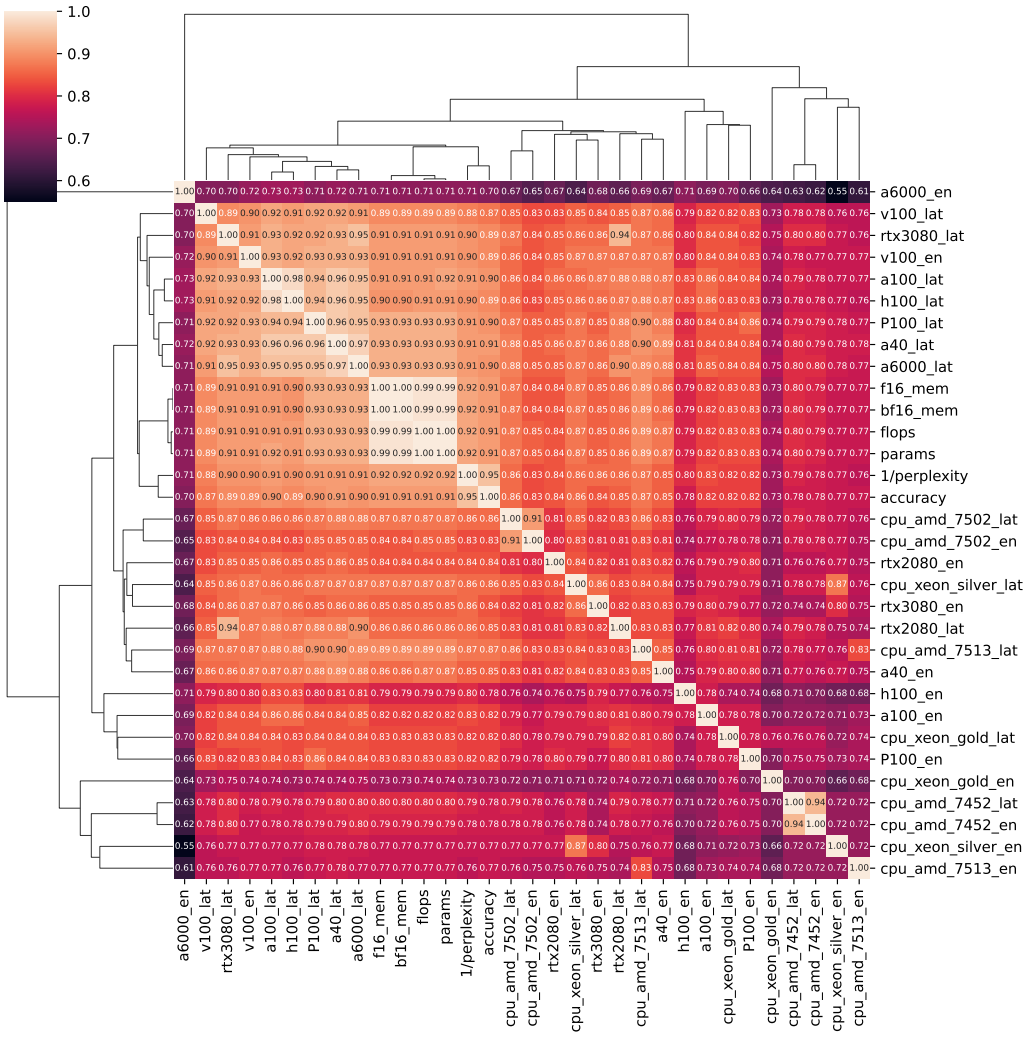


Figure 62: Cross-Metric kendall-tau correlation plots for GPT-S

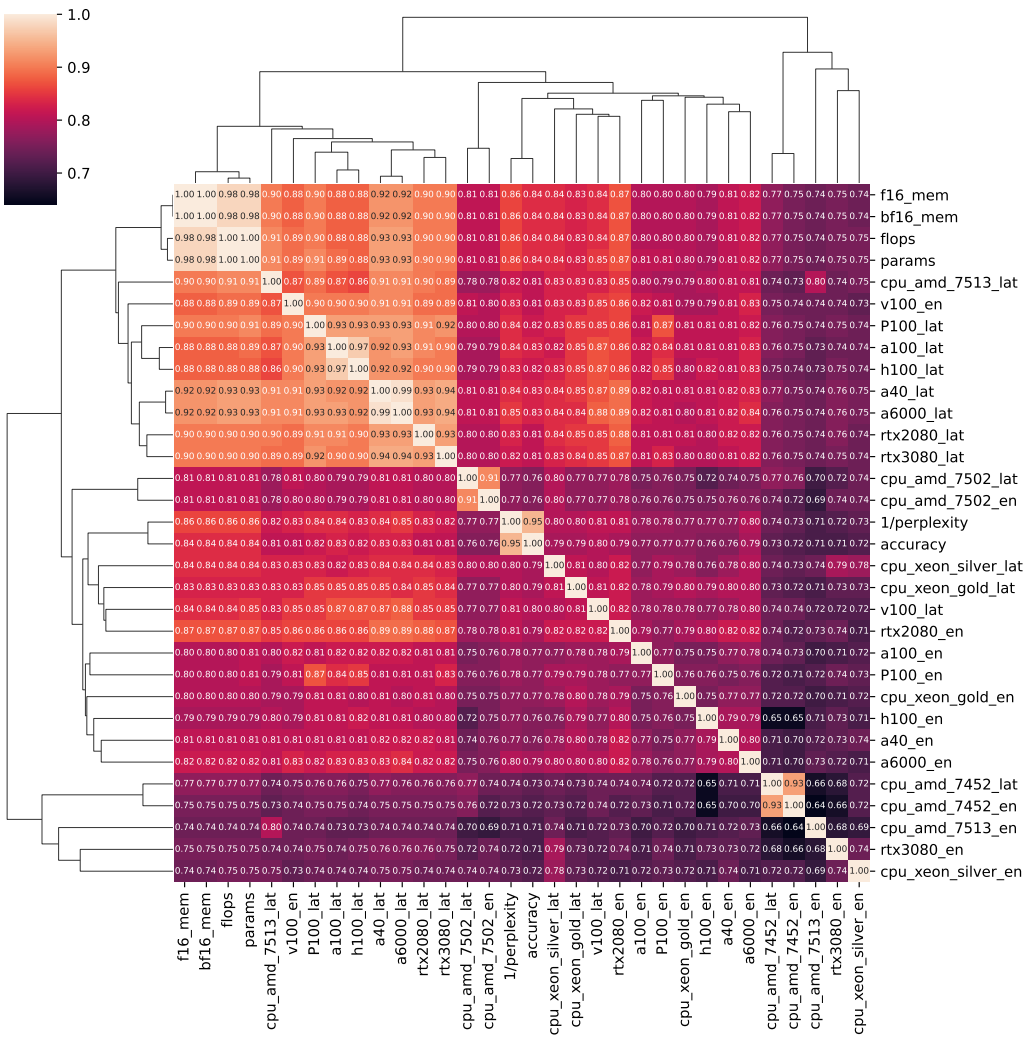


Figure 63: Cross-metric Kendall-τ correlation plots for GPT-M.

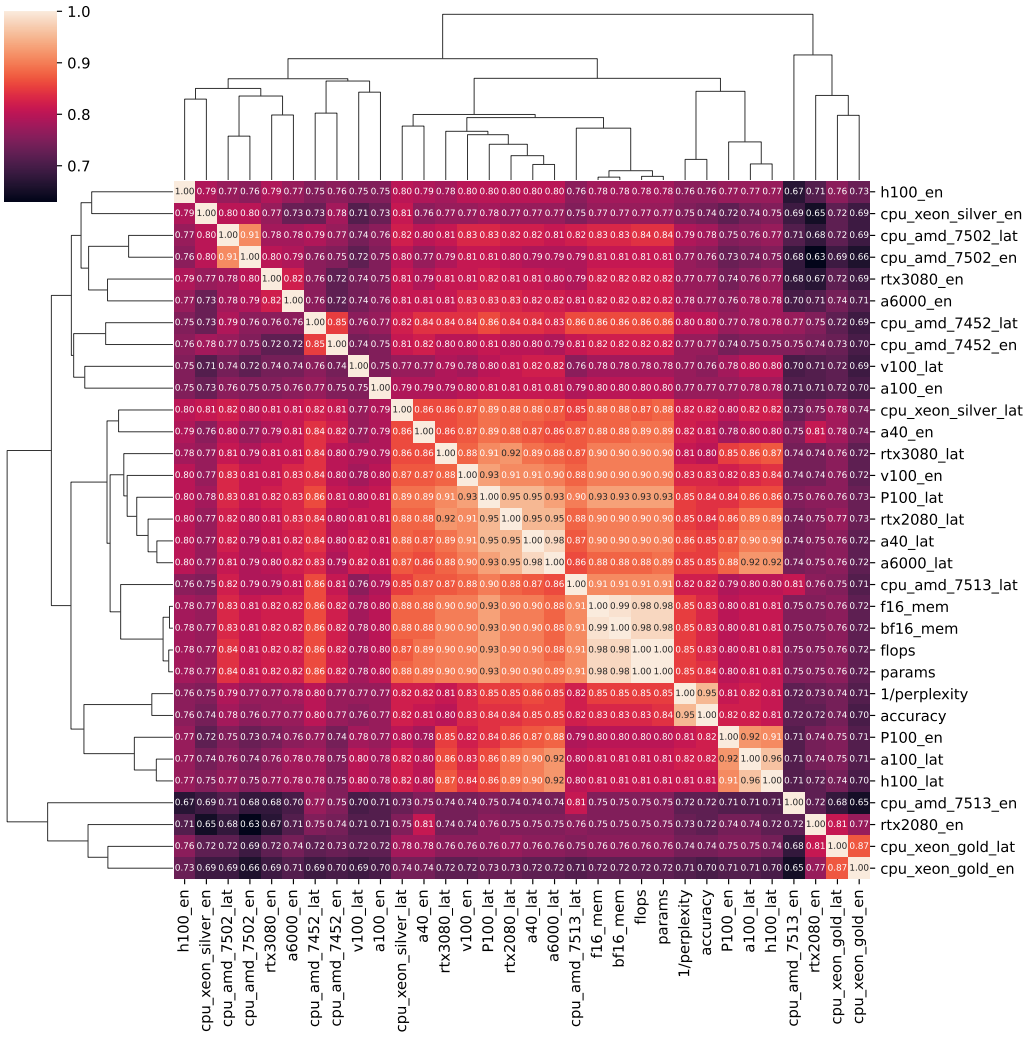


Figure 64: Cross-metric Kendall-τ correlation plots for GPT-L.

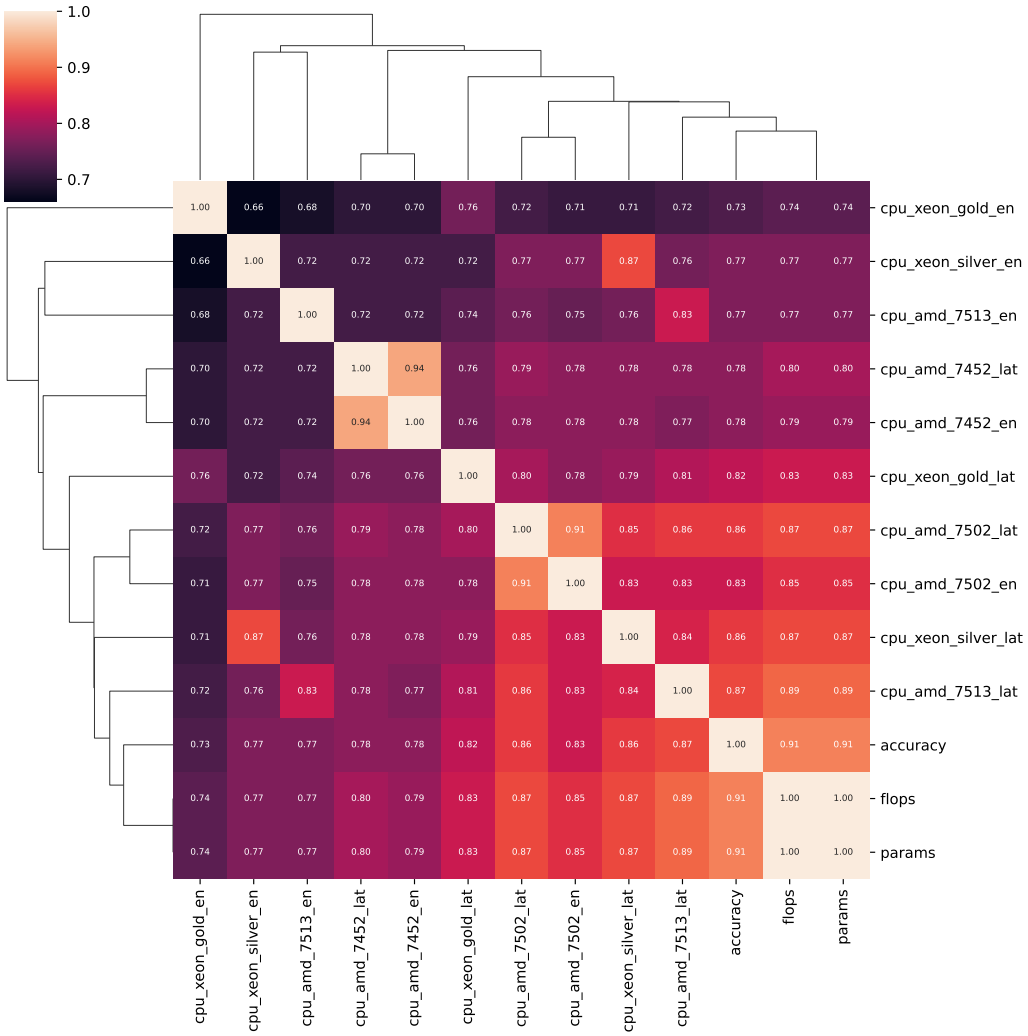


Figure 65: Cross-metric Kendall-τ correlation plots for GPT-S (only CPU devices).

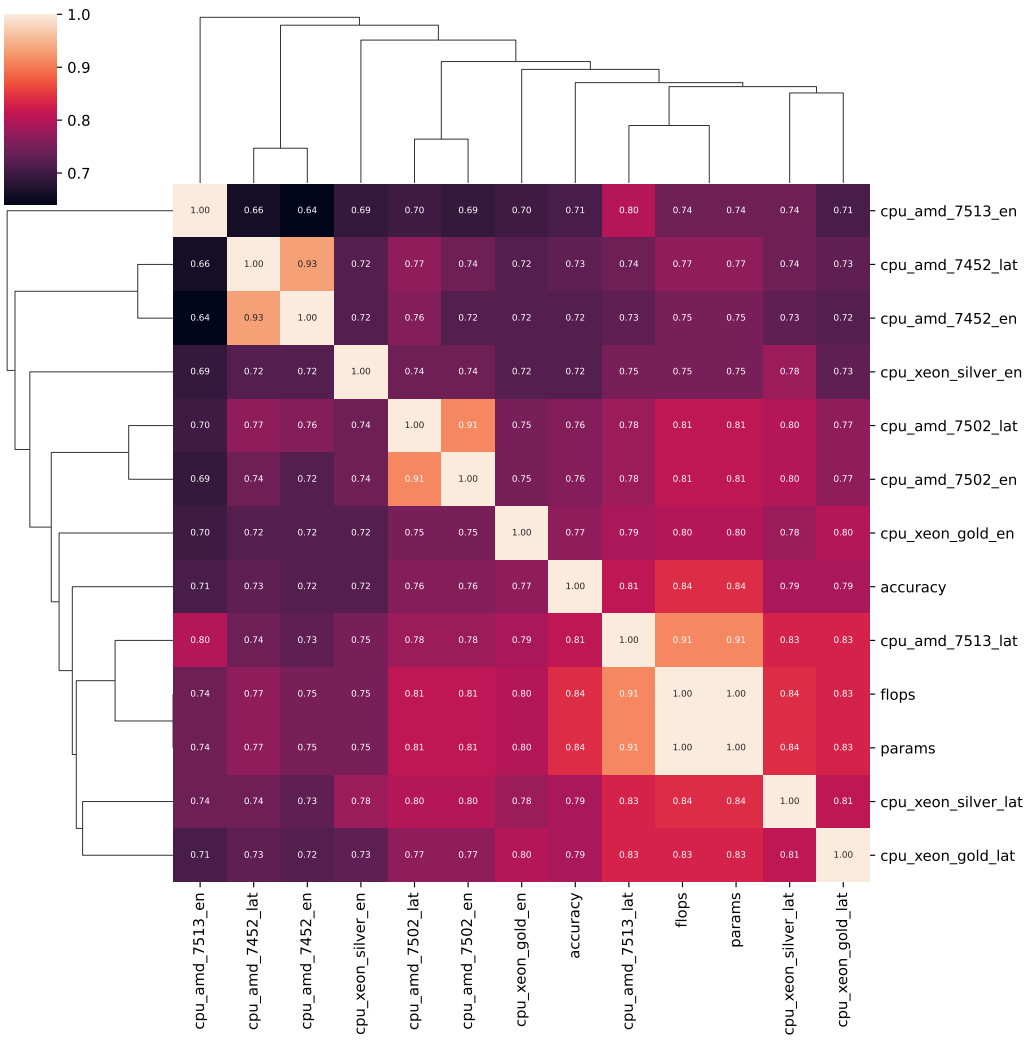


Figure 66: Cross-metric Kendall-τ correlation plots for GPT-M (only CPU devices).

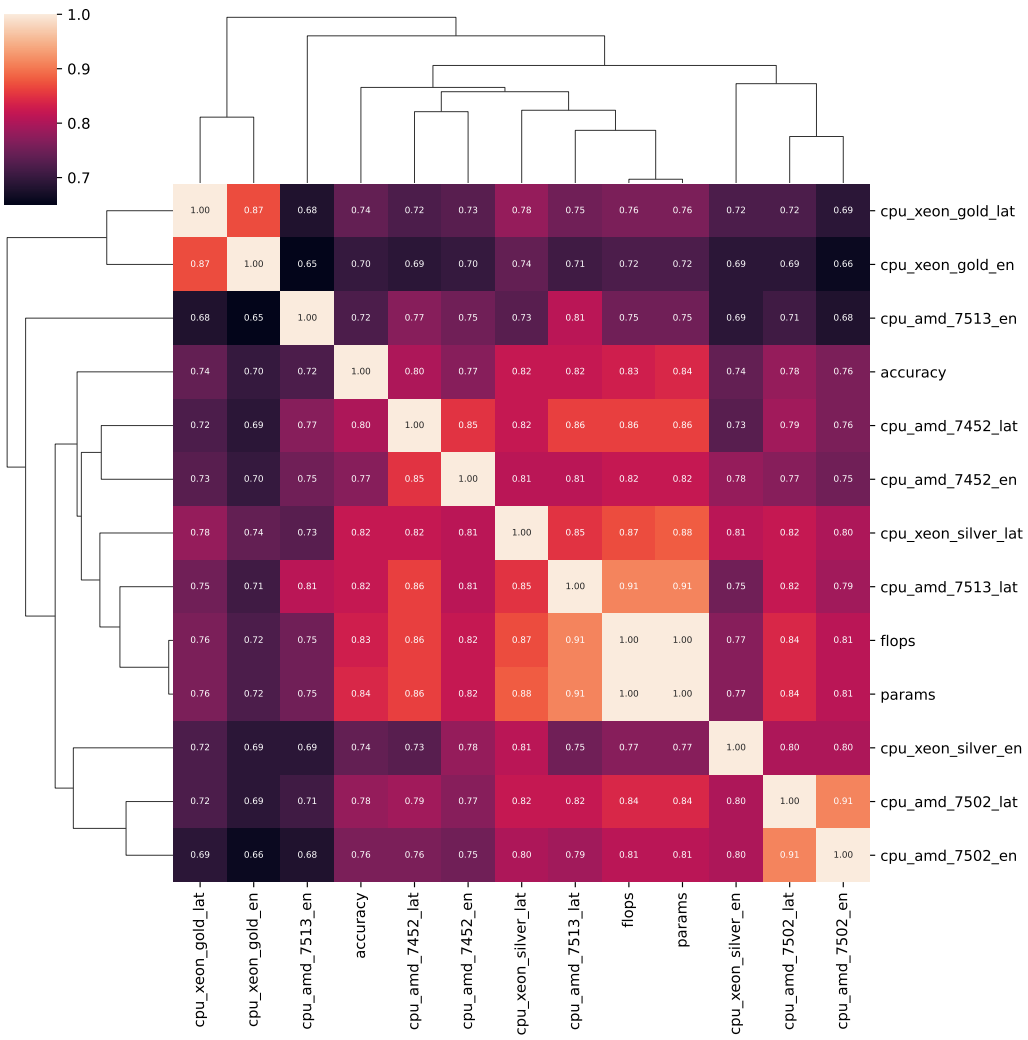


Figure 67: Cross-metric Kendall-τ correlation plots for GPT-L (only CPU device).

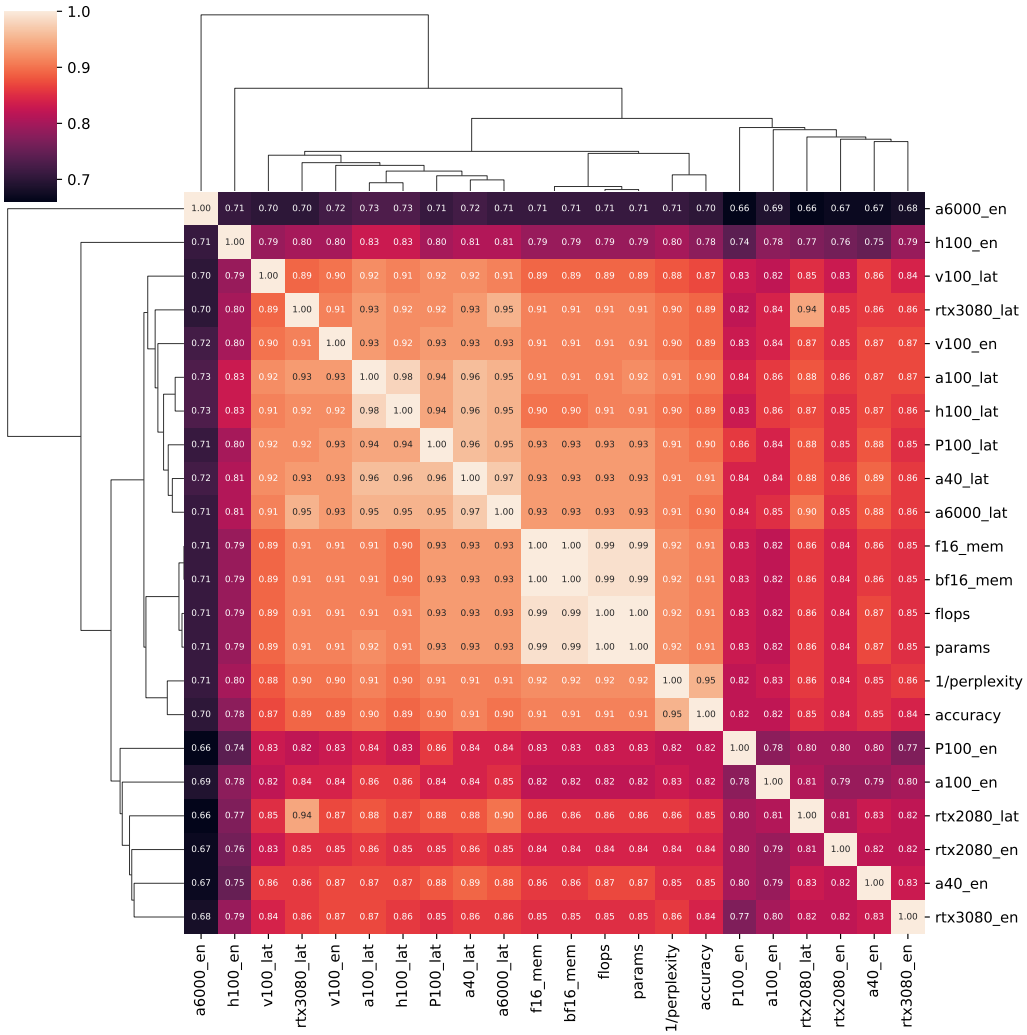


Figure 68: Cross-metric Kendall-τ correlation plots for GPT-S (only GPU devices).

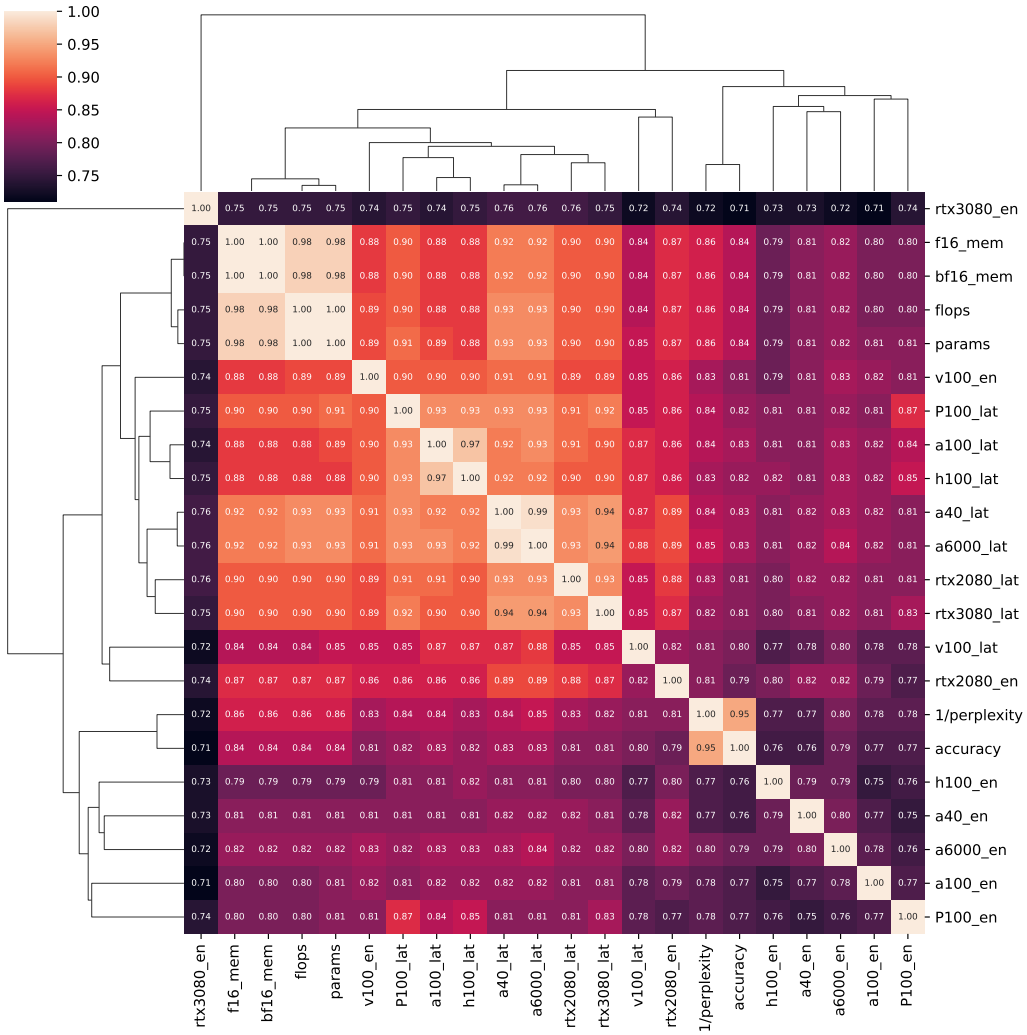


Figure 69: Cross-metric Kendall-τ correlation plots for GPT-M (only GPU devices).

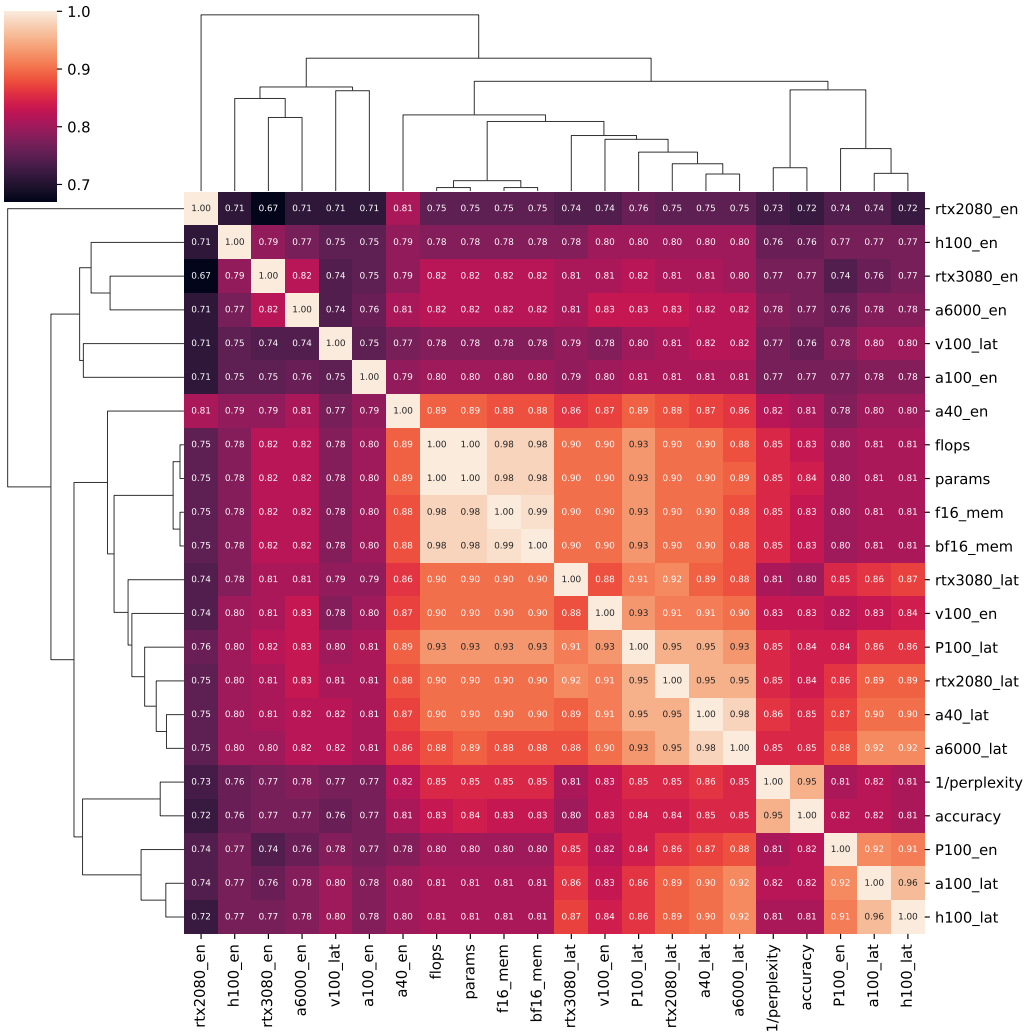
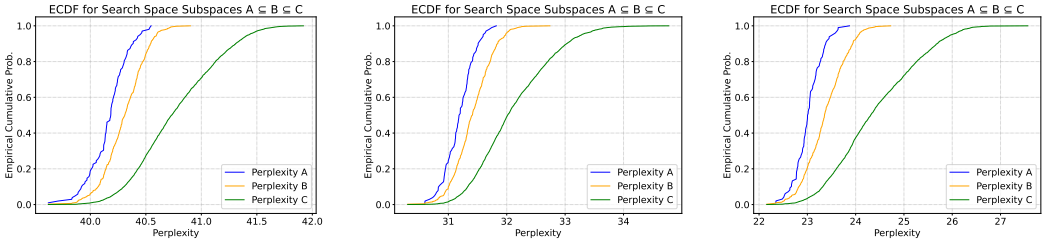


Figure 70: Cross-metric Kendall-τ correlation plots for GPT-L (only GPU devices).

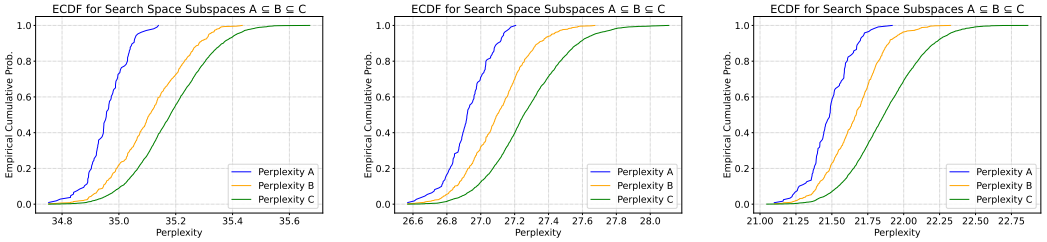
N Additional ECDF plots

In this section, we present the ECDF plots of perplexity on different search space scales, computed using the 10k ground truth observations from the supernetwork. The largest set, C, contains all architectures for a fixed embedding dimension size. B, a subset of C, contains all architectures that, in addition to the fixed embedding dimension e, have the number of layers set to the largest possible value $l = l_3$, namely 12, 24, and 36 for GPT-S, -M and -L, respectively. A, a subset of B, contains all architectures that, in addition to the number of layers set to largest possible values, have the average MLP ratio and number of heads greater than a fixed threshold. We show results for all 3 Transformer scales: GPT-S, -M and -L, in Figures 71, 72 and 73, respectively.



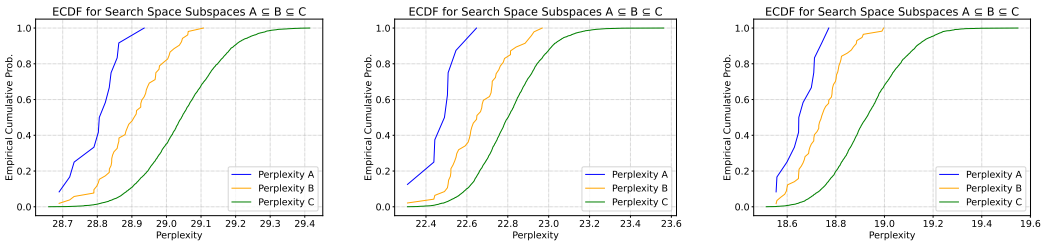
(a) Embedding dimension 192 (b) Embedding dimension 384 (c) Embedding dimension 768

Figure 71: ECDF plots for GPT-S.



(a) Embedding dimension 256 (b) Embedding dimension 512 (c) Embedding dimension 1024

Figure 72: ECDF plots for GPT-M.



(a) Embedding dimension 320 (b) Embedding dimension 640 (c) Embedding dimension 1280

Figure 73: ECDF plots for GPT-L.

O HW-GPT-Bench API Examples

```
from hwgpt.api import HWGPT
api = HWGPT(search_space="m") # initialize API for GPT-M
random_arch = api.sample_arch() # sample random arch
api.set_arch(random_arch) # set  arch
flops = api.query(metric="flops") # query flops for the architecture
params = api.query(metric="params") # query params for the architecture
float16_memory = api.query(metric="f16mem") # query float16 memory for the architecture
bfloat16_memory = api.query(metric="bf16mem") # query bfloat16 memory for the architecture
```

Snippet 2: Hardware agnostic metric using the HW-GPT-Bench API.

```
from hwgpt.api import HWGPT
api = HWGPT(search_space="m") # initialize API for GPT-M
random_arch = api.sample_arch_gt() # sample random arch from amongst the 10k ground truth archs
api.set_arch(random_arch) # set  arch
results = api.query(gt=True) # get all ground truth results for the architecture
energy = api.query(metric="energy",gt=True)  # get ground truth energy observations for all
     architectures
rtx2080 = api.query(device="rtx2080",gt=True) # get all hw metrics for rtx2080 device
```

Snippet 3: Ground truth observations using the HW-GPT-Bench API.

```
from hwgpt.api import HWGPT
api = HWGPT(search_space="m") # initialize API for GPT-M
nsga2_results_2d = api.run_baseline(method="nsga2", device="h100", metrics=["energy","perplexity"],
     ppl_predictor="mlp") # nsga-2d
nsga2_results_3d = api.run_baseline_3d(method="nsga2", device="h100", metrics=["energy","perplexity","
     latency"],ppl_predictor="mlp") #nsga-3d
```

Snippet 4: Running MOO with 3 objectives using the HW-GPT-Bench API.

P HW-GPT-Bench Release and Maintainance

HW-GPT-Bench will be distributed under the Apache 2.0 License, tailored explicitly for academic research. The Apache 2.0 License is chosen for its permissive characteristics within the open-source community, permitting users to freely utilize, modify, and distribute the software under the condition of proper attribution and adherence to Apache 2.0 stipulations. This licensing strategy is pivotal in fostering broad adoption of HW-GPT-Bench.

In addition to its release, we are committed to fostering community engagement with the benchmark. We will actively monitor and respond to inquiries, issues, and suggestions related to HW-GPT-Bench, thereby cultivating a collaborative environment conducive to ongoing improvement and innovation.

Looking forward, our development roadmap includes plans to expand HW-GPT-Bench to encompass a wider range of devices and language model spaces. This expansion aims to bolster the benchmark's utility and relevance, accommodating emerging research demands and technological advancements in the field

Q Limitations and Future Work

While our work is the first one to efficiently benchmark different decoder-only architectures on a variety of gpu and cpu devices, there are several possible enhancements possible, which we leave to future work. Firstly, currently the benchmark is limited to decoder only models and we believe it would be interesting to extend to encoder-decoder models and state-space models. Secondly, currently the benchmark trains supernetworks from scratch and scaling to very large models (eg: Llama 3.1 405b), would require expensive retraining. Initializing from pretrained models and exploring parameter-efficient finetuning methods for supernet finetuning, is important to avoid retraining and make most efficient use of available compute. Furthermore, since the benchmark is developed primarily in an academic setting, we couldn't profile the architectures on edge devices and specifically edge devices which are optimized for LLM inference. However, provide a plug and play framework by releasing all our profiling scripts and hope for community contributions to enhance the benchmark for newer hardware devices.

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