FINE-TUNED IN-CONTEXT LEARNING TRANSFORMERS ARE EXCELLENT TABULAR DATA CLASSIFIERS

Anonymous authors
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ABSTRACT

The recently introduced TabPFN pretrains an In-Context Learning (ICL) transformer on synthetic data to perform tabular data classification. In this work, we extend TabPFN to the fine-tuning setting, resulting in a significant performance boost. We also discover that fine-tuning enables ICL-transformers to create complex decision boundaries, a property regular neural networks do not have. Based on this observation, we propose to pretrain ICL-transformers on a new forest dataset generator which creates datasets that are unrealistic, but have complex decision boundaries. TabForest, the ICL-transformer pretrained on this dataset generator, shows better fine-tuning performance when pretrained on more complex datasets. Additionally, TabForest outperforms TabPFN on some real-world datasets when fine-tuning, despiting having lower zero-shot performance due to the unrealistic nature of the pretraining datasets. By combining both dataset generators, we create TabForestPFN, an ICL-transformer that achieves excellent fine-tuning performance and good zero-shot performance.

1 INTRODUCTION

Tabular data classification is widespread across all industries, leading to an increased interest in the research field of deep learning for tabular data (Liakos et al., 2018; Zhang et al., 2020; Keith et al., 2021; Pang et al., 2022). This type of classification involves classifying a target variable based on a set of attributes, which are commonly stored in tabular format. Examples of tabular classification include predicting the existence of chronic kidney disease based on blood test results (Ogunleye & Wang, 2020), estimating the click-through rate of advertisements (Richardson et al., 2007), and predicting the stability of pillars in hard rock mines (Liang et al., 2020). Despite the significance of tabular data, major breakthroughs in AI, as demonstrated in vision and language domains, have yet to reach the tabular domain. In fact, neural networks are currently outperformed by tree-based machine learning algorithms such as XGBoost (Chen & Guestrin, 2016) and CatBoost (Prokhorenkova et al., 2018) in tabular classification tasks (Gorishniy et al., 2021; Grinsztajn et al., 2022; McElfresh et al., 2023).

In an attempt to bridge this performance gap, a recent method called *tabular prior-data fitted networks* (TabPFN) (Hollmann et al., 2023) introduces an *in-context learning* (ICL) (Dong et al., 2023) scheme, demonstrating promising results (Grinsztajn et al., 2022). This tabular ICL-transformer can predict test observations zero-shot: with only one forward pass using training observations included in the context. Hollmann et al. generate their pretraining data synthetically, focusing on creating realistic datasets that act as a “prior”. They make their datasets realistic by carefully crafting correlations between features, introducing variety in feature importance, and leveraging structural causal models to simulate causal relationships.

In this work, we extend TabPFN to the fine-tuning setting. We show that fine-tuning this ICL-transformer on downstream tasks boosts the performance, particularly on datasets with more than a thousand samples. We also find that increasing the context size provides a performance increase for both zero-shot and fine-tuning. Overall, we find that fine-tuning provides such a large performance boost that we recommend always using it over zero-shot when the number of observations exceeds a thousand, and using zero-shot only when inference speed is an issue.

During this process, we also discovered an interesting property of ICL-transformers. Fine-tuned ICL-transformers can create complex decision boundaries, see Figure 1 for an example. Intuitively,

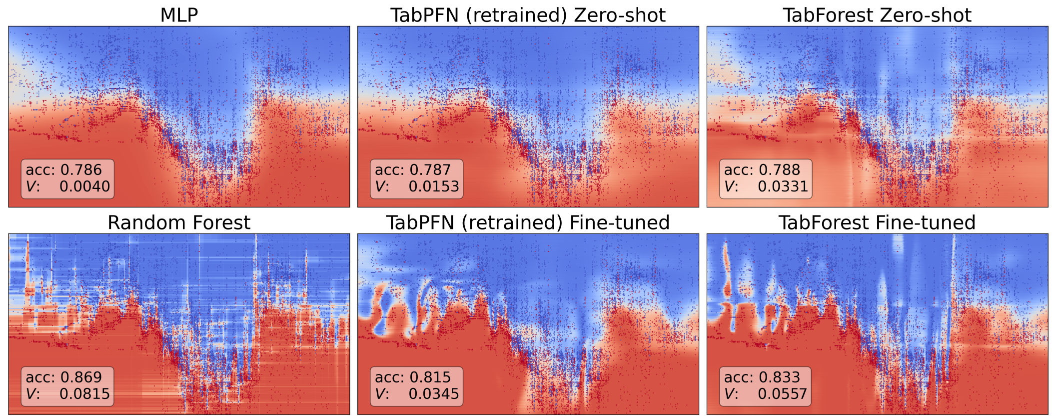


Figure 1: Comparison of decision boundaries for the Electricity dataset (OpenML ID 44156). Axis represent features, colors are predicted class probabilities, and dots are test observations. Fine-tuned variants show a higher complexity score V (see section 5.3) than zero-shot variants.

the complexity is determined by how far the decision boundary differs from a simple linear line. Neural networks trained from scratch on tabular data often have overly simple decision boundaries, a phenomenon known as simplicity bias (Shah et al., 2020), while tree-based methods do not suffer from this (Grinsztajn et al., 2022). We find that fine-tuned ICL-transformers, in contrast, are able to create these complex decision boundaries similar to tree-based methods.

Given this observation, we wonder whether pretraining on more complex data would improve the fine-tuning performance. To this end, we introduce the novel forest dataset generator, which creates highly complex synthetic datasets using a simple decision tree. By varying the parameters of the decision tree, we can control the complexity of the generated datasets. We observe that TabForest, the ICL-transformer pretrained on this forest dataset generator, achieves better fine-tuning performance as the complexity of the generated datasets increases.

Furthermore, TabForest shows fine-tuning performance that surpasses TabPFN on specific real-world datasets, even though the zero-shot performance of TabForest is significantly lacking compared to TabPFN. This suggests that for the fine-tuning performance of some real-world datasets, pretraining the ICL-transformer on highly complex datasets is more important than pretraining on realistic datasets, although for zero-shot, we would always prefer the TabPFN dataset generator.

As we would like to have a single ICL-transformer that performs well across all real-world tabular datasets, we mix the TabPFN and forest dataset generators to pretrain TabForestPFN. This model has excellent fine-tuning performance on two benchmarks (Grinsztajn et al., 2022; McElfresh et al., 2023), matching the performance of either TabForest or TabPFN. At the same time, mixing in the forest dataset generator does not seem to harm the zero-shot performance at all. This makes TabForestPFN the preferred ICL-transformer over TabForest and TabPFN.

In conclusion, fine-tuned ICL-transformers are highly effective tabular data classifiers, capable of creating complex decision boundaries. This new insight advances our understanding of tabular ICL-transformers and opens up new avenues for further research to enhance their performance. With further developments, we anticipate a significant shift in the field of tabular data, moving from tree-based methods towards ICL-transformers.

2 Related Works

There are three main branches of tools for tabular data classification: classical statistical methods like linear regression, K-nearest neighbors, Gaussian processes (Williams & Rasmussen, 1995), and support vector machines (Hearst et al., 1998); tree-based algorithms like XGBoost (Chen & Guestrin, 2016), CatBoost (Prokhorenkova et al., 2018), and LightGBM (Ke et al., 2017); and neural network-based methods such as the approach presented in this paper. There are several papers benchmarking the different methods (Gorishniy et al., 2021; Shwartz-Ziv & Armon, 2022; Grinsztajn et al., 2022; McElfresh et al., 2023; Zabërgja et al., 2024). Overall, tree-based methods stand at the top, with neural networks ranging from inferior to at best competitive.

Nonetheless, there have been numerous approaches that tackle tabular data classification with neural networks. First, we have the class of neural networks trained *from scratch*: training starts from random initialized weights and is only trained on the data at hand. Research has focused on architectures (Katzir et al., 2021; Somepalli et al., 2021; Arik & Pfister, 2021; Gorishniy et al., 2023; Huang et al., 2020; Chen et al., 2023a), embeddings (Ruiz et al., 2023; Gorishniy et al., 2022; Chen et al., 2023b), and regularization (Shavitt & Segal, 2018; Kadra et al., 2021).

In general, methods training from scratch can struggle because tabular datasets can be small. So, researchers have sought ways to use large volumes of tabular data or to change the training objective. Some employ self-supervised learning (Kossen et al., 2021; Yoon et al., 2020; Zhu et al., 2023; Bahri et al., 2022; Ucar et al., 2021; Sui et al., 2023), or closely related transfer learning techniques (Nam et al., 2023; Levin et al., 2023; Zhou et al., 2023). Others leverage pretrained LLMs or language data (Hegselmann et al., 2023; Zhang et al., 2023; Kim et al., 2024; Yan et al., 2024) to make predictions.

One of those related transfer learning methodologies is *tabular in-context learning*, a new field sparked by TabPFN (Hollmann et al., 2023). Currently, there is ongoing research on how to scale TabPFN to encompass more observations and features (Ma et al., 2023; Feuer et al., 2024; Thomas et al., 2024), as this architecture is limited by GPU memory. Our fine-tuning work can be seen as one approach to tackle this issue.

3 PRELIMINARIES

In tabular classification, we are interested in predicting targets $y \in \mathbb{N}$ given features $\boldsymbol{x} \in \mathbb{R}^d$, where d is the number of features. We predict y using an *in-context learning* (ICL) transformer pretrained on a synthetic dataset. The in-context learning allows the transformer to predict targets based on other observations included in the forward pass. In our work, *zero-shot* refers to one forward pass through the ICL-transformer without any fine-tuning, while *fine-tuning* refers to one forward pass through the ICL-transformer after fine-tuning. Our work builds on TabPFN (Hollmann et al., 2023), so below we explain their dataset generator and their transformer architecture.

3.1 TABPFN DATASET GENERATOR

The TabPFN authors create their own synthetic dataset using *Bayesian Neural Networks* (BNN) and *Structural Causal Models* (SCM). To construct a dataset, they first create a BNN or a SCM with random characteristics and with randomly initialized weights. Then they randomly draw an input $\boldsymbol{X}$ and pass it through the model to generate output $\boldsymbol{y}$. Their final dataset is given by $(\boldsymbol{X}, \boldsymbol{y})$. See their paper (Hollmann et al., 2023) for more details.

In their approach, they emphasize their ability to create realistic datasets, and even call their generator a "prior". They chose SCMs specifically because it can capture real-world causal mechanisms. One other aspect they focus on is simplicity, biasing the generator towards less complex input-output relationships. Additionally, they ensure the inputs $\boldsymbol{X}$ have natural correlations by correlating the features blockwise, and they vary their feature importance by tuning the magnitude of weights belonging to different features. These methods suggest the authors believe creating realistic datasets is important for achieving good performance.

3.2 ARCHITECTURE

In our work, we use the architecture from TabPFN, and make no changes to isolate the effect of the dataset generator. This ICL-transformer has as input the features $\boldsymbol{X}_{support} \in \mathbb{R}^{|S| \times d_f}$ and targets $\boldsymbol{y}_{support} \in \mathbb{N}^{|S|}$ from *support* set S and features $\boldsymbol{X}_{query} \in \mathbb{R}^{|Q| \times d_f}$ from *query* set Q. The output is a prediction for $\boldsymbol{y}_{query} \in \mathbb{R}^{|Q|}$. The query set Q represents the observations we want to predict, while the support set S includes the observations we base our prediction on. This architecture accepts a fixed number of features d_f, see also the preprocessing discussed in Appendix A.3.

In this transformer, a token with dimension d_{token} represents all features of a single observation. The creation of support tokens $H_{support} \in \mathbb{R}^{|S| \times d_{token}}$ and query tokens $H_{query} \in \mathbb{R}^{|Q| \times d_{token}}$ is

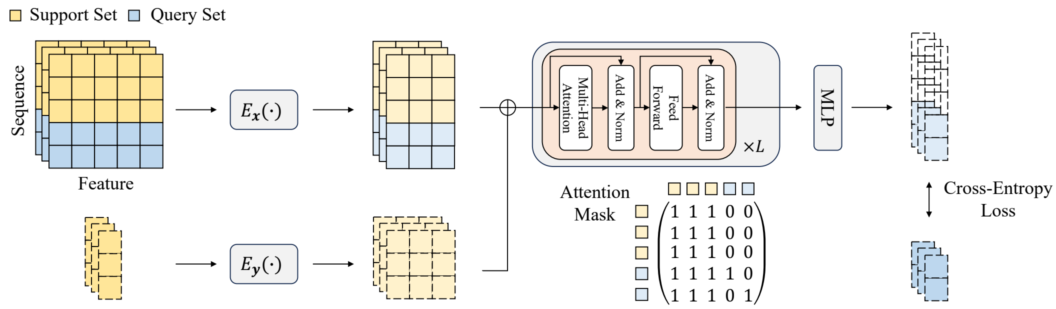


Figure 2: Base ICL-transformer architecture. On the left, dataset features and targets are separately encoded into tokens. On the right, the targets of the query dataset are used as label. In the middle is the ICL-transformer with the attention mask.

given by equations 1 and 2.

$$\boldsymbol{H}_{support} = \boldsymbol{X}_{support}\boldsymbol{W}_x + \boldsymbol{y}_{support}\boldsymbol{w}_y^T \tag{1}$$

$$\boldsymbol{H}_{query} = \boldsymbol{X}_{query}\boldsymbol{W}_x \tag{2}$$

Here, we embed the features linearly using weights $\boldsymbol{W}_x \in \mathbb{R}^{d_f \times d_{token}}$. Input classes $\boldsymbol{y}_{support}$ are also embedded using a linear layer with weights $\boldsymbol{w}_y \in \mathbb{R}^{d_{token}}$, in which $\boldsymbol{y}_{support}$ is treated as a float. Biases are used but omitted in the equations for conciseness. In Figure 2, E_x refers to the multiplication with $\boldsymbol{W}_x$ and E_y represents the product with $\boldsymbol{w}_y$.

After the embedding, we push the tokens through a standard transformer architecture with a special attention mask. Support tokens are only able to see other support tokens, and query tokens can only see all support tokens and themselves, with no attention to other query tokens. This attention mask ensures the prediction of an observation does not depend on which other test observations are included in the forward pass. The complete architecture is given in Figure 2.

4 METHODOLOGY

The full tabular data classification pipeline is given by: synthetic data generation (3.1 and 4.1), data preprocessing (A.3), architectural design (3.2) and fine-tuning (4.2). In this section, we introduce our new dataset generator and our proposed fine-tuning procedure.

4.1 FOREST DATASET GENERATION

Our goal is to create a simple dataset generator that produces datasets with complex patterns to train on, in contrast to the TabPFN (Hollmann et al., 2023) generator that aims to create realistic datasets. This forest dataset generator will better enable ICL-transformers to create complex decision boundaries. We base our dataset generator on decision trees, because of their ability to create highly complex decision boundaries with minimal computational cost. The idea is to *overfit* the decision tree to randomly generated features and targets. This fitted decision tree is then used as a data-generating process. See Algorithm 1 for the method and Figure 3 for examples of generated data.

Table 1: Hyperparameters for the Forest Dataset Generator

Hyperparameter	min	max
base size	1024	1024
dataset size	128	1024
tree depth	1	25
number of features	3	100
number of classes	2	10
ratio of categorical features	0.0	1.0

Our forest dataset generator allows datasets to vary in the number of classes, observations, numerical features, and categorical features. There are two parameters that contribute to the decision boundary complexity. The *base size* is the number of observations used to fit the decision tree; more observations means more places for the decision tree to split on. The *tree depth* determines how deep the decision tree will go before exiting the fitting algorithm, with higher depth leading to increased complexity.

Algorithm 1 Forest Dataset Generation

Require: *n_classes, n_features, base_size, dataset_size, tree_depth, categorical_perc*
  Draw $\boldsymbol{X} \sim \mathcal{N}(base\_size, n\_features)$
  Draw $\boldsymbol{y} \sim \mathcal{N}(base\_size)$
  Fit a decision tree on $(\boldsymbol{X}, \boldsymbol{y})$ of depth *tree_depth*.
  Draw $\boldsymbol{X}_2 \sim \mathcal{N}(dataset\_size, n\_features)$
  Convert *categorical_perc* features of $\boldsymbol{X}_2$ to categorical.
  Predict $\boldsymbol{y}_2$ using the decision tree on $\boldsymbol{X}_2$.
  Transform $\boldsymbol{y}_2$ using quantile transformation to uniform.
  Discretize $\boldsymbol{y}_2$ into *n_classes* classes.
Ensure: $(\boldsymbol{X}_2, \boldsymbol{y}_2)$

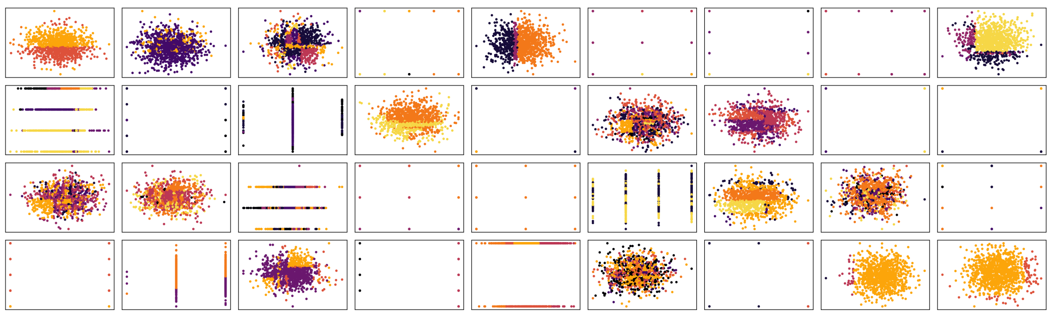


Figure 3: Generated forest data. Every box is a generated dataset with its own classes (color) and features (axes). The data clouds look unrealistic: decision boundaries are always orthogonal, and there is no feature correlation. Generated with base size of 1024, dataset size of 1024, maximum tree depth between 1 and 25, two features, and between 2 and 10 number of classes.

For every new synthetically generated dataset, we uniformly draw the hyperparameters from the bounds shown in Table 1. Because both hyperparameters influence the complexity, we decided to keep the base size fixed. In the final step of the algorithm, the targets $\boldsymbol{y}_2$ are discretized by uniformly drawing bucket boundaries between 0.0 and 1.0, and assigning a class to each bucket, creating varying degrees of class imbalance.

4.2 Fine-tuning Procedure

In our work, we introduce fine-tuning to the tabular ICL-transformer. When fine-tuning, we like to draw support and query sets from our training data such that the performance generalizes to the test set. This requires careful consideration of dataset splitting. The benchmark datasets already provide us with a training-validation-test split. We use this validation dataset for early stopping.

Every gradient descent step, we randomly draw a 80/20 support and query split from the training dataset. For validation, we draw the support set from the training set and draw the query set from the validation set. Every validation sample is seen exactly once, while the support samples are randomly drawn with replacement. We use early stopping based on the validation loss, which is calculated after every fine-tuning step.

The early stopping technique can decide to stop fine-tuning immediately if the validation loss increases in the first step of training, which allows us to fall back on the zero-shot performance in case fine-tuning harms the performance. This is especially important when using very small datasets, as they are prone to overfitting. At the same time, fine-tuning can leverage all samples in training dataset, while zero-shot cannot use more samples than that fit on the GPU.

5 Experiments

In our experiments we consider five pre-trained models, each with a zero-shot and a fine-tuned version:

- **TabPFN (original)** is the original implementation by the TabPFN (Hollmann et al., 2023) authors, fine-tuned by us. The weights are downloaded from their GitHub.
- **TabPFN (retrained)** is our implementation of TabPFN, trained by us on the TabPFN-dataset.
- **TabForest** is trained by us on our forest dataset.
- **TabForestPFN** is trained by us on both the TabPFN-dataset and our forest dataset.
- **TabScratch** is not pretrained. We include this as a baseline.

Comparing the behavior and performance allows us to understand the effect of the different synthetic datasets. Training and hyperparameter settings are given in appendix A.4, benchmarks used and results obtained are given below.

5.1 Introduction of the Benchmark Datasets

We show the results of our pre-trained architectures on two benchmarks, tested against publicly available results provided by the authors of the benchmarks. We include all their tested methods and datasets where possible. Appendix A.5 lists all used datasets.

The TabZilla (McElfresh et al., 2023) benchmark tests 20 algorithms on 176 classification datasets with sizes ranging from 32 observations to over a million. We selected 94 out of 176 datasets, see appendix A.5. The medium-sized benchmark which we refer to as WhyTrees (Grinsztajn et al., 2022) consists of 23 classification datasets with 2923 to a maximum of 10,000 observations. The benchmark is split into 7 datasets with only numerical features and 16 datasets with both numerical and categorical features.

Both benchmarks perform random hyperparameter search on their algorithms. TabZilla runs up to 30 times per algorithm and WhyTrees runs a few hundred times, up to 2500 runs. The ICL-transformers run only on default settings because we noticed little gains in performance when changing the fine-tuning hyperparameters.

5.2 Main Results of TabForestPFN

The results on the TabZilla benchmark are shown in Table 3, see Appendix A.7 for alternative presentations. For the WhyTrees benchmark, the comparison of fine-tuned TabForestPFN with the benchmark algorithms is shown in Figure 4, and the comparison with other ICL-transformer variants in Table 2, while results on individual datasets can be seen in Appendix A.8. We present the running time of TabForestPFN on all datasets in Appendix A.6.

Table 2: WhyTrees Results. Normalized accuracy for mixed and numerical features as shown in Figure 4.

	Mixed	Numerical
Zero-shot		
TabScratch	0.000	0.000
TabPFN (original)	**0.534**	0.624
TabPFN (retrained)	0.481	0.635
TabForest	0.388	0.536
TabForestPFN	0.473	**0.655**
Fine-tuned		
TabScratch	0.481	0.570
TabPFN (original)	0.742	0.775
TabPFN (retrained)	0.775	0.817
TabForest	**0.853**	**0.854**
TabForestPFN	0.842	0.849

In these figures and tables, we see that fine-tuning considerably improves the performance of ICL-transformers. Where the zero-shot variants perform very mediocre compared to XGBoost and the other baselines, the fine-tuned variants are extremely competitive. Given the poor performance of TabScratch, we can clearly see that both the pretraining and the fine-tuning are important.

When comparing the pretraining datasets, we see that the best method differs by benchmark. Fine-tuned TabForest is the best on WhyTrees, while fine-tuned TabPFN is favored on TabZilla. As TabForest strength comes from generating complex decision boundaries, we conjecture that TabZilla has many datasets for which this property is not helpful. The zero-shot variants on both benchmarks clearly favor TabPFN, which is unsurprising given the unrealistic nature of the forest dataset generator.

The TabForestPFN combines the best of both worlds. For WhyTrees, we can see that the fine-tuned TabForestPFN has almost the same performance as TabForest, and for TabZilla, it has almost the same performance as TabPFN. We can also see that mixing in the forest dataset does not deteriorate

Table 3: Main Results on TabZilla. N. Accuracy stands for Normalized accuracy. Rank compares the relative rank of a method compared to all other methods on that dataset.

Models	Rank				N. Accuracy	
	min	max	mean	median	mean	median
TabForestPFN - Fine-tuned	1	27	**8.4**	**7.0**	0.840	**0.902**
TabPFN (retrained) - Fine-tuned	1	26	**8.4**	7.5	**0.843**	0.891
CatBoost	1	**23**	9.6	9.0	0.842	0.874
TabPFN (original) - Fine-tuned	1	26	9.6	10.0	0.834	**0.902**
TabForestPFN - Zero-shot	1	25	9.7	9.2	0.819	0.883
XGBoost	1	23	9.8	9.8	0.836	0.899
TabForest - Fine-tuned	1	27	10.9	10.0	0.806	0.873
TabPFN (retrained) - Zero-shot	1	26	11.2	10.5	0.797	0.858
LightGBM	1	27	11.8	12.2	0.787	0.867
TabPFN (original) - Zero-shot	1	26	12.1	12.0	0.777	0.841
RandomForest	1	26	12.1	12.0	0.792	0.851
Resnet	1	27	12.8	12.0	0.727	0.837
NODE	1	27	12.9	13.5	0.751	0.833
SAINT	1	27	13.1	13.8	0.729	0.803
SVM	1	26	13.3	14.0	0.710	0.801
FT-Transformer	1	24	13.6	13.2	0.733	0.805
TabScratch - Fine-tuned	1	25	13.6	13.0	0.752	0.819
DANet	2	27	15.6	16.0	0.718	0.769
TabForest - Zero-shot	3	26	15.7	16.0	0.709	0.822
MLP-rtdl	1	27	16.9	19.0	0.619	0.736
STG	1	27	17.1	19.0	0.592	0.664
LinearRegression	1	27	18.5	21.0	0.564	0.593
MLP	2	27	18.8	21.0	0.570	0.586
TabNet	2	27	19.1	20.2	0.579	0.666
DecisionTree	1	27	19.7	21.5	0.502	0.551
KNN	2	27	20.5	23.0	0.473	0.478
VIME	3	27	22.9	25.0	0.343	0.241
TabScratch - Zero-shot	28	28	28.0	28.0	0.000	0.000

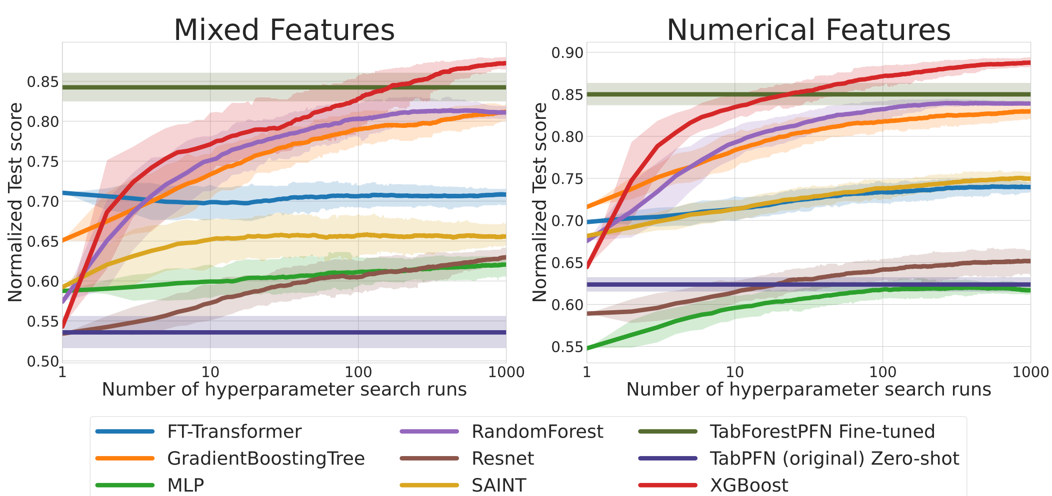


Figure 4: Main results on the WhyTrees Benchmark. TabForestPFN shows the mean over ten default runs for different fine-tuning seeds, all others use random search over the hyperparameters. See Table 2 for other ICL-transformers.

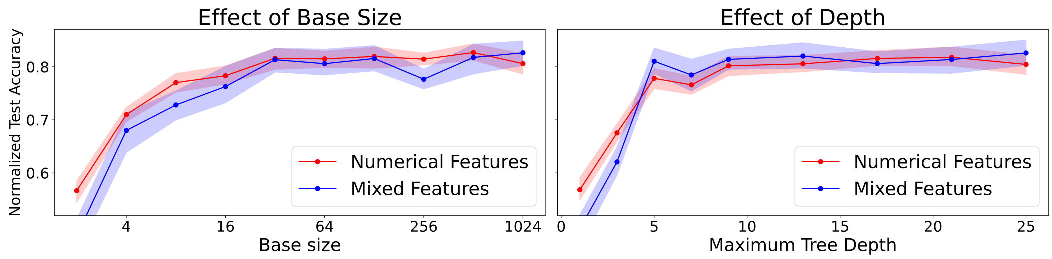


Figure 5: Ablation of the base size and maximum tree depth parameters of the Forest Dataset Generator. Figure shows normalized test accuracy of TabForest on the WhyTrees benchmark.

the zero-shot performance on either benchmark, which establishes the TabForestPFN as the clear best method among the ICL-transformer variants.

5.3 Complexity of ICL-Transformers' Decision Boundaries

In the previous section, we have seen that TabForest and TabPFN both achieve excellent performance as neural networks. Now we take a look at their decision boundaries. Repeating the analysis of the WhyTrees' authors (Grinsztajn et al., 2022), we use the Electricity dataset (OpenML ID: 44156) to predict a binary target on two features.

To capture the complexity of the decision boundary, we define the complexity score V. We split the feature space into a total of n grid cells where each cell has a predicted probability p_{ij} for grid cell indices (i, j). The complexity score V is defined as the sum of absolute values between neighbor cells:

$$V = \frac{1}{n} \sum_{ij} |p_{i+1,j} - p_{ij}| + |p_{i-1,j} - p_{i,j}| + |p_{i,j+1} - p_{ij}| + |p_{i,j-1} - p_{ij}|$$

The complexity score represents how fast the prediction changes when moving along the grid.

We plot the results in Figure 1. We see that when fine-tuning, both TabPFN and TabForest can create decision boundaries that are more complex than their zero-shot variants. The complexity of the decision boundaries was one of the characteristics that explained why tree-based methods outperformed neural networks (Grinsztajn et al., 2022). These results suggest ICL-transformers can also create complexity in their decision boundaries.

In our intuition, the ICL-transformer learns how to create these decision boundaries during pretraining. We can interpret this from a weight initialization perspective. The weights of the pretrained ICL-transformer provide a good initialization for the model to create complex decision boundaries, while an ICL-transformer trained from scratch lacks this ability. For this reason, TabForest can create decision boundaries of higher complexity than TabPFN.

5.4 Ablation of the Forest Dataset Generator

In Section 4.1, we discussed two ways to influence the complexity of the forest dataset generator: the tree depth and the base size, which is the number of observations to fit the tree algorithm. We expect the performance of TabForest to increase when the complexity of the forest dataset generator increases.

In Figure 5 we show the results of pretraining different settings of base size and maximum tree depth on the WhyTrees benchmark. The tree depth is set to 1-25 as the base size changes, and the base size is fixed to 1024 as the tree depth changes. When scaling up the base size from 2 to 32 and the tree depth from 1 to 9, we observe that the performance increases, and stabilizes for higher complexities. We provide figures of the data generated with these lower complexity hyperparameters in Appendix A.10 to give an impression. The correlation between performance and complexity supports our claim that learning complex decision boundaries is the driving force behind the performance of fine-tuned TabForest.

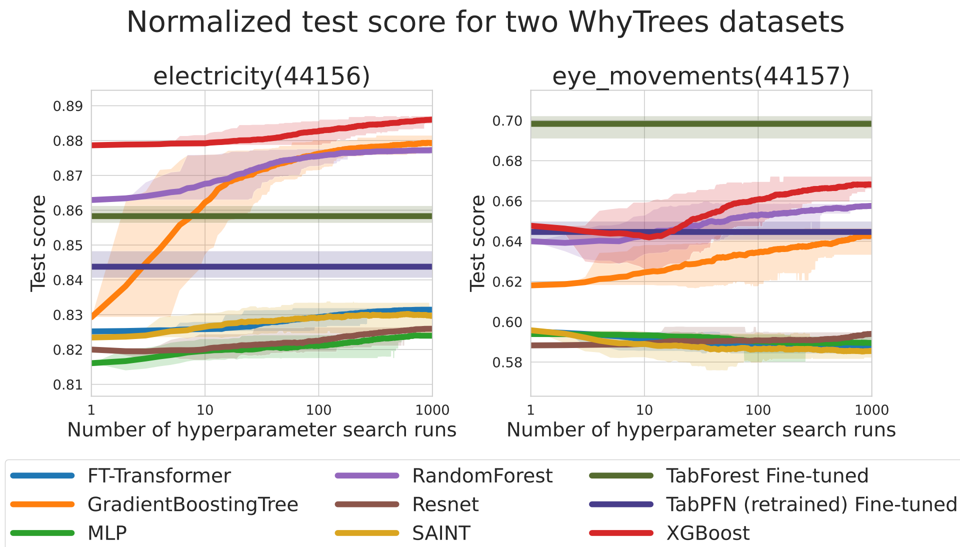


Figure 6: Comparison of fine-tuned TabForest and TabPFN on two datasets of the WhyTrees benchmark. These datasets show a big gap between neural networks and tree-based methods.

5.5 Case Study of the Gap between Neural Networks and Tree Algorithms.

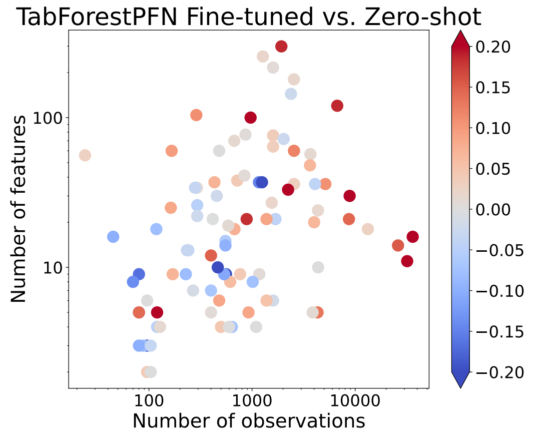
In Figure 6 we show the performance of fine-tuned TabPFN and TabForest on two specific datasets from WhyTrees. We selected these two datasets for the large gap between the neural networks (MLP, Resnet, SAINT, FT-Transformer) and the tree-based algorithms (XGBoost, GradientBoostingTree, RandomForest). The figure illustrates that ICL-transformers behave differently than other neural networks: their performance is closer to that of tree-based methods.

We propose the following explanation: these two datasets need highly complex decision boundaries. As tree-based methods are capable of creating these complex decision boundaries while neural networks struggle (Shah et al., 2020; Grinsztajn et al., 2022), fine-tuned ICL-transformers can also create them, as seen in Section 5.3. Furthermore, TabForest is naturally better at creating these decision boundaries than TabPFN, given that the forest dataset generator was specifically designed for this purpose. Figure 6 shows that TabForest significantly outperforms TabPFN on these two datasets. The explanation of the gap is further supported by Figure 1, as it illustrates the complexity of the decision boundaries for two variables from the Electricity dataset.

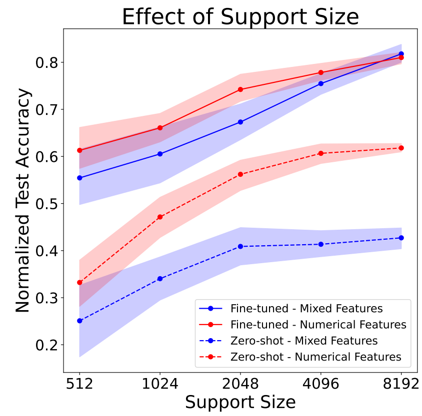
5.6 Improvement of Fine-tuning over Zero-shot

In the main results, we have seen that fine-tuning performs better than zero-shot. We look at this comparison in more detail. Figure 7a presents the performance of TabForestPFN on individual datasets from TabZilla. We can see clearly that fine-tuning strongly outperforms zero-shot when there are more than 10,000 observations. Overall, fine-tuning outperforms zero-shot on 57% of the datasets. This percentage decreases to 47% for datasets smaller than a 1000 observations and increases to 73% for datasets larger than a 1000 observations.

Figure 7b illustrates the effect of context length on the performance of TabForestPFN on the zero-shot and the fine-tuning task. We see that a higher support size is always better, which is why we set the support size in our paper to 8192, even though we only pretrained on a maximum size of 1024 observations. In conclusion, fine-tuning on the largest possible support size appears to be the most effective approach for ICL-transformers.



(a) Differences in normalized accuracy of individual datasets from TabZilla. The color red means fine-tuning is the best. The darkest red represents at least 0.20 normalized score points improvement, and dark blue at least 0.20 normalized accuracy points degradation.



(b) Effect of different support sizes on the WhyTrees benchmark. Both fine-tuning and zero-shot performance improves with context size.

Figure 7: Evaluation of TabForestPFN

6 Conclusion

The introduction of TabPFN (Hollmann et al., 2023) has opened up a new field of *in-context learning* (ICL)-transformers for tabular data classification. Our research has demonstrated that fine-tuned ICL-transformers achieve excellent performance and also learn to create complex decision boundaries. Furthermore, by adding the forest dataset to the pretraining mixture, we achieved performance levels competitive with tree-based methods.

Despite these advancements, there are still obstacles for ICL-transformers to overcome if we want them to replace tree-based methods in the realm of tabular data. One major challenge is the performance limitation of ICL-transformers due to GPU memory constraints. Our work uses fine-tuning as a solution to this problem, but it would be valuable to compare this approach to other concurrent research such as prompt tuning (Feuer et al., 2024), in-context distillation (Ma et al., 2023) and retrieval (Thomas et al., 2024). Moreover, our research focused solely on classification, although we expect that a simple switch from cross-entropy loss to mean-squared-error loss would suffice to tackle regression tasks. Another area that requires exploration is the setting with an exceptionally high number of features (Cherepanova et al., 2024), where the performance of ICL-transformers is unknown (McCarter, 2024). Lastly, tree-based methods can explain which features are important for their predictions, and research is needed to determine if ICL transformers can achieve a similar feat (Rundel et al., 2024). Overcoming these challenges will cement the ICL-transformer as the clear successor to tree-based methods.

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A APPENDIX

A.1 ETHICS AND SOCIAL IMPACT

Improving tabular data classification can provide major benefits to society. From medical to physics applications, better performance can save lives and money. There are, however, also more nefarious applications of tabular data classification, such as fraud risk detections based on ethnics or nationality; population analysis for micro-targeting political ad campaigns; and insurance premium discrimination based on underlying medical conditions.

Our models cannot detect the purpose for which the model is used. In contrast to large language models, our tabular data models take numerical data as input. Ethnicity, gender, or other sensitive information is represented by a class number. This means our models cannot recover the meaning behind the numbers.

A big benefit of this 'numerical anonymization' is privacy. In our paper, we use synthetic data, which is completely privacy risk free. But even when pretrained on real data, recovering the original data can be extremely hard due to the lack of labels and contextual information.

In light of the above, we decide to publish the model and open access to anyone. We do not know an effective way to create any form of safeguards against misuse, and we would welcome any advice from the research community that addresses this issue.

A.2 CODE AVAILABILITY

Code is attached to this submission.

The code includes everything: downloading datasets, preprocessing result benchmarks, training the ICL-transformers, pretrained weights on Google Drive, notebooks with analysis, and an easy example to get you started with applying the TabForestPFN to your dataset.

The code is built upon the works of Grinsztajn et al.; Hollmann et al. and McElfresh et al.. Although this resulted in a Frankenstein monster of a codebase, we have made great efforts to rewrite most of their code to integrate well. The code assumes a single server with access to 1 or more GPUs, with DistributedDataParallel used during pretraining and multiprocessing over different GPUs used during inference.

As currently there is no good tabular code base out there, we recommend anyone that is interested in doing research in tabular data to take a look at ours.

A.3 DATA PREPROCESSING

Before data is put into the neural network, the data is preprocessed. We use the exact same routine for both synthetic data and real-world data to ensure minimal differences in distribution and summary statistics of the input to the transformer. Algorithm 2 presents the procedure for preprocessing.

Algorithm 2 Data Preprocessing

Require: $\boldsymbol{X}_{raw}, \boldsymbol{y}_{raw}$
1: **Impute** NaN features with column mean.
2: **Remove** features with one unique value.
3: **Select** a subset of a hundred features.
4: **Transform** all features to normal using quantile transformation.
5: **Normalize** data to unit mean and variance.
6: **Scale** data based on number of features.
7: **Pad** the features to d_f features by adding zeros.
8: **if** Pretraining **then**
9:     **Shuffle** the order of the features and classes.
10: **end if**
Ensure: $\boldsymbol{X}_{preprocessed}, \boldsymbol{y}_{preprocessed}$

Because we fixed the input size of the neural network to $d_f = 100$ features, we first select a subset of a d_f features using scikit-learn's *SelectKBest* Pedregosa et al. (2011). If there are less than d_f features, we add zeros to ensure exactly d_f features. Following TabPFN, we scale by multiplying by $100/d_{f*}$, where d_{f*} is the number of features after selecting a subset. To be robust to skewness and outliers, we transform the data using scikit-learn's *QuantileTransformer* to follow a normal distribution. We make no distinction between numerical and categorical values in all our preprocessing.

In comparison to TabPFN, our data preprocessing follows roughly the same scheme. One change is the use of a quantile transformer, while they use standard input or a power transformer. We consider this a preference, both seem to work fine.

Furthermore, the TabPFN authors like to ensemble outputs of the TabPFN architecture, varying the transformation function between standard input and power transformer. In our paper, we use no ensembling at all.

A.4 Training Settings

All ICL-transformer architectures, including the original TabPFN, use the same model. The model consists of 12 layers, 4 attention heads, a hidden dimension of 512, and 10 classes as output dimension. Pretraining uses batch size 512, learning rate 1e-4, weight decay 0.00, AdamW optimizer with betas (0.9, 0.95), cosine scheduling, and maximum global gradient norm 1.0. Fine-tuning is performed under batch size 1, learning rate 1e-5, weight decay 0.00, no scheduling, with early stopping, and a maximum of 300 steps. To fit the model on an RTX 3090 with 24GB during fine-tuning, we set the maximum support size to 8192 samples and the maximum query size to 1024. Pre-training uses data generated with maximum support size 1024 and maximum query size 128. We choose these settings because the maximum support size affects performance, but the maximum query size only affects inference speed. On these settings, we train all ICL-transformers for 50,000 steps, which takes 4 GPU-days on one H100. Running all benchmarks takes one additional H100 GPU-day.

A.5 Benchmark Metadata

Of both the TabZilla and the WhyTrees benchmark, we show the OpenMLVanschoren et al. (2014) datasets we use as well as their characteristics. See Table 4 and Table 5. The TabZilla table presents the 94 datasets picked out of the 176 total datasets.

From the original 176 Tabzilla datasets, we excluded every dataset that does not have at least one completed run on default settings for every model, which brings the value to 99. Additionally, we exclude four datasets because they have more than 10 classes. The preprocessing code of one other dataset did not run without errors, and so is removed as well. The TabZilla authors did experiment with running TabPFN, but only on 62 datasets with a maximum support size of 3000 samples, so we redo their experiment.

Table 4: Metadata of the WhyTrees Benchmark. Splits refers to the number of cross validation splits.

OpenML		Observations				Features	Splits	Classes
ID	Name	All	Train	Valid	Test			
44089	credit	16714	10000	2014	4700	10	2	2
44120	electricity	38474	10000	8542	19932	7	1	2
44121	covertype	566602	10000	50000	50000	10	1	2
44122	pol	10082	7057	907	2118	26	3	2
44123	house_16H	13488	9441	1214	2833	16	3	2
44125	MagicTelescope	13376	9363	1203	2810	10	3	2
44126	bank-marketing	10578	7404	952	2222	7	3	2
44128	MiniBooNE	72998	10000	18899	44099	50	1	2
44129	Higgs	940160	10000	50000	50000	24	1	2
44130	eye_movements	7608	5325	684	1599	20	3	2
44156	electricity	38474	10000	8542	19932	8	1	2
44157	eye_movements	7608	5325	684	1599	23	3	2

44159	covertype	423680	10000	50000	50000	54	1	2
45019	Bioresponse	3434	2403	309	722	419	5	2
45020	default-of-cred...	13272	9290	1194	2788	20	3	2
45021	jannis	57580	10000	14274	33306	54	1	2
45022	Diabetes130US	71090	10000	18327	42763	7	1	2
45026	heloc	10000	7000	900	2100	22	3	2
45028	california	20634	10000	3190	7444	8	1	2
45035	albert	58252	10000	14475	33777	31	1	2
45036	default-of-cred...	13272	9290	1194	2788	21	3	2
45038	road-safety	111762	10000	30528	50000	32	1	2
45039	compas-two-year...	4966	3476	447	1043	11	3	2

Table 5: Metadata of the TabZilla Benchmark. Splits refers to the number of cross validation splits.

OpenML		Observations				Features	Splits	Classes
ID	Name	All	Train	Valid	Test			
3	kr-vs-kp	3196	2556	320	320	36	10	2
4	labor	57	45	6	6	16	10	2
9	autos	205	163	21	21	25	10	6
10	lymph	148	118	15	15	18	10	4
11	balance-scale	625	499	63	63	4	10	3
12	mfeat-factors	2000	1600	200	200	216	10	10
14	mfeat-fourier	2000	1600	200	200	76	10	10
15	breast-w	699	559	70	70	9	10	2
16	mfeat-karhunen	2000	1600	200	200	64	10	10
18	mfeat-morpholog...	2000	1600	200	200	6	10	10
23	cmc	1473	1177	148	148	9	10	3
25	colic	368	294	37	37	26	10	2
27	colic	368	294	37	37	22	10	2
29	credit-approval	690	552	69	69	15	10	2
30	page-blocks	5473	4377	548	548	10	10	5
35	dermatology	366	292	37	37	34	10	6
37	diabetes	768	614	77	77	8	10	2
39	sonar	208	166	21	21	60	10	2
40	glass	214	170	22	22	9	10	6
43	spambase	4601	3680	460	461	57	10	2
45	splice	3190	2552	319	319	60	10	3
47	tae	151	120	15	16	5	10	3
48	heart-c	303	241	31	31	13	10	2
49	tic-tac-toe	958	766	96	96	9	10	2
50	heart-h	294	234	30	30	13	10	2
53	vehicle	846	676	85	85	18	10	4
59	iris	150	120	15	15	4	10	3
2074	satimage	6430	5144	643	643	36	10	6
2079	eucalyptus	736	588	74	74	19	10	5
2867	anneal	898	718	90	90	38	10	5
3485	scene	2407	1925	241	241	299	10	2
3512	synthetic_contr...	600	480	60	60	60	10	6
3540	analcatdata_box...	120	96	12	12	3	10	2
3543	irish	500	400	50	50	5	10	2
3549	analcatdata_aut...	841	672	84	85	70	10	4
3560	analcatdata_dmf...	797	637	80	80	4	10	6
3561	profb	672	536	68	68	9	10	2
3602	visualizing_env...	111	88	11	12	3	10	2
3620	fri_c0_100_5	100	80	10	10	5	10	2
3647	rabe_266	120	96	12	12	2	10	2
3711	elevators	16599	13279	1660	1660	18	10	2
3731	visualizing_liv...	130	104	13	13	2	10	2
3739	analcatdata_chl...	100	80	10	10	3	10	2
3748	transplant	131	104	13	14	3	10	2
3779	fri_c3_100_5	100	80	10	10	5	10	2

3797	socmob	1156	924	116	116	5	10	2
3896	ada_agnostic	4562	3648	457	457	48	10	2
3902	pc4	1458	1166	146	146	37	10	2
3903	pc3	1563	1249	157	157	37	10	2
3904	jm1	10885	8707	1089	1089	21	10	2
3913	kc2	522	416	53	53	21	10	2
3917	kc1	2109	1687	211	211	21	10	2
3918	pc1	1109	887	111	111	21	10	2
3953	adult-census	32561	26048	3256	3257	14	10	2
9946	wdbc	569	455	57	57	30	10	2
9952	phoneme	5404	4322	541	541	5	10	2
9957	qsar-biodeg	1055	843	106	106	41	10	2
9960	wall-robot-navi...	5456	4364	546	546	24	10	4
9964	semeion	1593	1273	160	160	256	10	10
9971	ilpd	583	465	59	59	10	10	2
9978	ozone-level-8hr	2534	2026	254	254	72	10	2
9984	fertility	100	80	10	10	9	10	2
10089	acute-inflammat...	120	96	12	12	6	10	2
10093	banknote-authen...	1372	1096	138	138	4	10	2
10101	blood-transfusi...	748	598	75	75	4	10	2
14952	PhishingWebsite...	11055	8843	1106	1106	30	10	2
14954	cylinder-bands	540	432	54	54	37	10	2
14965	bank-marketing	45211	36168	4521	4522	16	10	2
14967	cjs	2796	2236	280	280	33	10	6
125920	dresses-sales	500	400	50	50	12	10	2
125921	LED-display-dom...	500	400	50	50	7	10	10
145793	yeast	1269	1015	127	127	8	10	4
145799	breast-cancer	286	228	29	29	9	10	2
145836	blood-transfusi...	748	598	75	75	4	10	2
145847	hill-valley	1212	968	122	122	100	10	2
145977	ecoli	336	268	34	34	7	10	8
145984	ionosphere	351	280	35	36	34	10	2
146024	lung-cancer	32	24	4	4	56	10	3
146063	hayes-roth	160	128	16	16	4	10	3
146065	monks-problems-...	601	480	60	61	6	10	2
146192	car-evaluation	1728	1382	173	173	21	10	4
146210	postoperative-p...	88	70	9	9	8	10	2
146607	SpeedDating	8378	6702	838	838	120	10	2
146800	MiceProtein	1080	864	108	108	77	10	8
146817	steel-plates-fa...	1941	1552	194	195	27	10	7
146818	Australian	690	552	69	69	14	10	2
146820	wilt	4839	3871	484	484	5	10	2
146821	car	1728	1382	173	173	6	10	4
167140	dna	3186	2548	319	319	180	10	3
167141	churn	5000	4000	500	500	20	10	2
167211	Satellite	5100	4080	510	510	36	10	2
168911	jasmine	2984	2386	299	299	144	10	2
190408	Click_predictio...	39948	31958	3995	3995	11	10	2
360948	libras	360	288	36	36	104	10	10

A.6 Run times

Table 6 and 7 present the run times of TabForestPFN on both the WhyTrees and the TabZilla benchmark. All fine-tuning runs take at most 220 seconds per cross validation split, with an average of 68 seconds. Runtimes differ by GPU, and creating a fair comparison with CPU-based methods is difficult due to the different hardware used. As main takeaway, we recommend to summarize the fine-tuning run time as ”a few minutes at most for a dataset of around 10,000 observations”.

Table 6: Run times of TabForestPFN of the WhyTrees Benchmark. The runtime is the end-to-end time in seconds for one cross validation split. End-to-end time includes loading, preprocessing, training and testing.

OpenML		Size		Run time (s)	
ID	Name	Obs.	Feat.	Zero-shot	Fine-tuned
44089	credit	10000	10	9	103
44120	electricity	10000	7	15	151
44121	covertype	10000	10	34	167
44122	pol	7057	26	6	57
44123	house_16H	9441	16	8	72
44125	MagicTelescope	9363	10	7	105
44126	bank-marketing	7404	7	7	68
44128	MiniBooNE	10000	50	28	126
44129	Higgs	10000	24	34	119
44130	eye_movements	5325	20	5	63
44156	electricity	10000	8	17	142
44157	eye_movements	5325	23	6	65
44159	covertype	10000	54	37	219
45019	Bioresponse	2403	419	8	34
45020	default-of-credit-card-clients	9290	20	7	81
45021	jannis	10000	54	23	130
45022	Diabetes130US	10000	7	25	95
45026	heloc	7000	22	6	56
45028	california	10000	8	11	112
45035	albert	10000	31	21	103
45036	default-of-credit-card-clients	9290	21	8	79
45038	road-safety	10000	32	30	153
45039	compas-two-years	3476	11	5	43

Table 7: Run times of TabForestPFN of the TabZilla Benchmark. The runtime is the end-to-end time in seconds for one cross validation split. End-to-end time includes loading, preprocessing, training and testing.

OpenML		Size		Run time (s)	
ID	Name	Obs.	Feat.	Zero-shot	Fine-tuned
3	kr-vs-kp	2556	36	4	29
4	labor	45	16	3	13
9	autos	163	25	3	11
10	lymph	118	18	3	9
11	balance-scale	499	4	3	32
12	mfeat-factors	1600	216	5	26
14	mfeat-fourier	1600	76	4	29
15	breast-w	559	9	3	19
16	mfeat-karhunen	1600	64	4	22
18	mfeat-morphological	1600	6	4	22
23	cmc	1177	9	4	20
25	colic	294	26	3	10
27	colic	294	22	3	11
29	credit-approval	552	15	4	22
30	page-blocks	4377	10	5	40
35	dermatology	292	34	3	13
37	diabetes	614	8	3	19
39	sonar	166	60	3	11
40	glass	170	9	3	10
43	spambase	3680	57	6	42
45	splice	2552	60	3	33
47	tae	120	5	3	11
48	heart-c	241	13	3	11

49	tic-tac-toe	766	9	3	20
50	heart-h	234	13	2	12
53	vehicle	676	18	3	23
59	iris	120	4	3	16
2074	satimage	5144	36	6	55
2079	eucalyptus	588	19	3	18
2867	anneal	718	38	3	26
3485	scene	1925	299	6	37
3512	synthetic_control	480	60	3	18
3540	analcatdata_boxing1	96	3	3	12
3543	irish	400	5	4	19
3549	analcatdata_authorship	672	70	4	25
3560	analcatdata_dmft	637	4	3	20
3561	profb	536	9	3	16
3602	visualizing_environmental	88	3	3	10
3620	fri_c0_100_5	80	5	3	13
3647	rabe_266	96	2	3	14
3711	elevators	13279	18	9	101
3731	visualizing_livestock	104	2	3	15
3739	analcatdata_chlamydia	80	3	3	16
3748	transplant	104	3	3	12
3779	fri_c3_100_5	80	5	3	13
3797	socmob	924	5	3	19
3896	ada_agnostic	3648	48	6	36
3902	pc4	1166	37	4	23
3903	pc3	1249	37	4	26
3904	jm1	8707	21	6	117
3913	kc2	416	21	3	26
3917	kc1	1687	21	4	48
3918	pc1	887	21	3	16
3953	adult-census	26048	14	14	175
9946	wdbc	455	30	4	17
9952	phoneme	4322	5	4	44
9957	qsar-biodeg	843	41	4	23
9960	wall-robot-navigation	4364	24	5	42
9964	semeion	1273	256	5	26
9971	ilpd	465	10	4	20
9978	ozone-level-8hr	2026	72	4	25
9984	fertility	80	9	3	13
10089	acute-inflammations	96	6	3	10
10093	banknote-authentication	1096	4	4	20
10101	blood-transfusion-service-center	598	4	3	20
14952	PhishingWebsites	8843	30	8	103
14954	cylinder-bands	432	37	4	16
14965	bank-marketing	36168	16	17	165
14967	cjs	2236	33	4	79
125920	dresses-sales	400	12	4	18
125921	LED-display-domain-7digit	400	7	4	16
145793	yeast	1015	8	4	19
145799	breast-cancer	228	9	3	11
145836	blood-transfusion-service-center	598	4	3	21
145847	hill-valley	968	100	4	47
145977	ecoli	268	7	3	12
145984	ionosphere	280	34	3	12
146024	lung-cancer	24	56	3	14
146063	hayes-roth	128	4	3	14
146065	monks-problems-2	480	6	2	22
146192	car-evaluation	1382	21	4	27
146210	postoperative-patient-data	70	8	3	13
146607	SpeedDating	6702	120	6	57
146800	MiceProtein	864	77	4	28
146817	steel-plates-fault	1552	27	4	22
146818	Australian	552	14	4	23
146820	wilt	3871	5	4	30
146821	car	1382	6	4	30

167140	dna	2548	180	4	26
167141	churn	4000	20	5	41
167211	Satellite	4080	36	5	40
168911	jasmine	2386	144	4	36
190408	Click_prediction_small	31958	11	14	129
360948	libras	288	104	3	11

A.7 TabZilla Further Results

In the TabZilla main results Table 3, we have shown the performance including all methods implemented by the TabZilla authors. Because the rank is calculated over all included methods, which ICL-transformer variants we include might change the results. Therefore, we check if the results are the same if we use calculate the rankings one ICL-transformer at the time.

Table 8 shows the results of only the fine-tuned TabForestPFN versus the rest of the benchmark. We do this for every ICL-transformer and aggregregate the results in Table 9. All results are qualitatively the same as in Table 3.

Table 8: Main Results on TabZilla. N. Accuracy stands for Normalized accuracy. Rank compares the relative rank of a method compared to all other methods on that dataset.

Models	Rank				N. Accuracy	
	min	max	mean	median	mean	median
TabForestPFN - Fine-tuned	1	19	**5.6**	**4.5**	0.846	**0.910**
CatBoost	1	**15**	6.2	5.0	**0.848**	0.876
XGBoost	1	16	6.3	5.0	0.841	0.901
LightGBM	1	19	7.7	6.0	0.792	0.871
RandomForest	1	18	7.9	8.0	0.797	0.852
NODE	1	19	8.4	8.0	0.754	0.839
Resnet	1	19	8.4	8.0	0.729	0.837
SAINT	1	19	8.5	8.0	0.733	0.817
SVM	1	18	8.6	8.0	0.713	0.801
FT-Transformer	1	16	8.9	8.5	0.737	0.805
DANet	2	19	10.0	10.0	0.721	0.768
MLP-rtdl	1	19	11.5	12.0	0.622	0.737
STG	1	19	11.5	12.0	0.594	0.672
LinearRegression	1	19	12.3	13.8	0.567	0.592
MLP	1	19	12.6	14.0	0.572	0.588
TabNet	2	19	12.8	13.2	0.583	0.672
DecisionTree	1	19	13.3	14.0	0.504	0.551
KNN	2	19	13.9	15.0	0.475	0.484
VIME	1	19	15.7	17.0	0.345	0.240

A.8 WhyTrees Further Results

The main results in Figure 4 report the normalized accuracy aggregated over all datasets. In Figure 8 and 9 we show the comparison between fine-tuned TabForestPFN and the original zero-shot version of TabPFN on all 23 datasets. In Figure 10 and 11 we show the same graphs but with fine-tuned TabPFN and fine-tuned TabForest.

A.9 One-by-One Comparisons

In Figure 12 we plot one-to-one comparisons of fine-tuned TabForestPFN versus CatBoost, TabForest and TabPFN. We see no clear correlations in the other comparisons between performance difference and model.

Table 9: Main Results on TabZilla. N. Accuracy stands for Normalized accuracy. Rank compares the relative rank of a method compared to all other methods on that dataset. This table displays individual results: Table 8 is run individually for all ICL-transformer variants, and the row of the ICL-transformer is copy-pasted here.

Models	Rank				N. Accuracy	
	min	max	mean	median	mean	median
Zero-shot						
TabScratch	19	19	19.0	19.0	0.000	0.000
TabPFN (original)	1	19	7.7	7.0	0.780	0.841
TabPFN (retrained)	1	18	7.0	**6.0**	0.803	0.860
TabForest	1	19	9.8	10.0	0.714	0.822
TabForestPFN	1	18	**6.3**	**6.0**	**0.824**	**0.900**
Fine-tuned						
TabScratch	1	18	8.3	7.0	0.757	0.819
TabPFN (original)	1	18	6.4	6.5	0.838	0.909
TabPFN (retrained)	1	18	**5.6**	5.0	**0.847**	0.891
TabForest	1	19	7.0	6.0	0.810	0.885
TabForestPFN	1	19	**5.6**	**4.5**	0.846	**0.910**

A.10 Synthetic Data with Lower Complexity

In the ablation we have seen that even with a forest dataset generator with lower complexity parameters, we still have similar performance. To give an idea of how complex the data is, here we showcase the generated data. Figure 13 displays generated data with base size 32, and Figure 14 displays generated data with maximum tree depth 9.

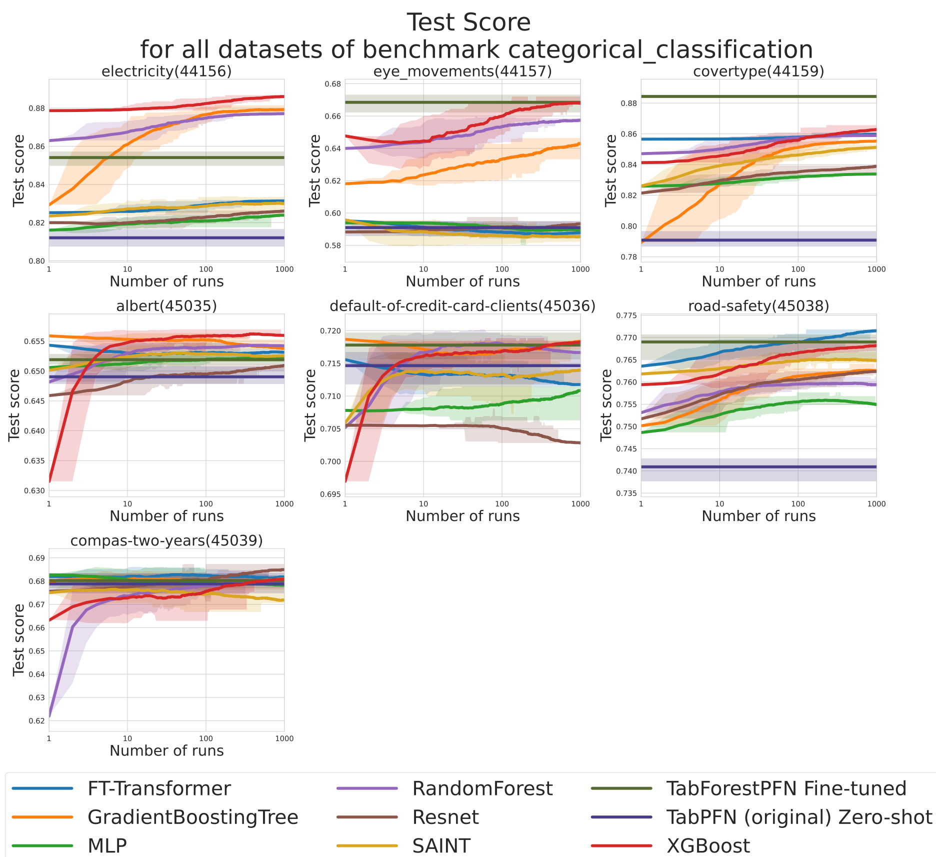

Figure 8: Comparison of fine-tuned TabForestPFN and the original zero-shot TabPFN on the WhyTrees benchmark with mixed features.

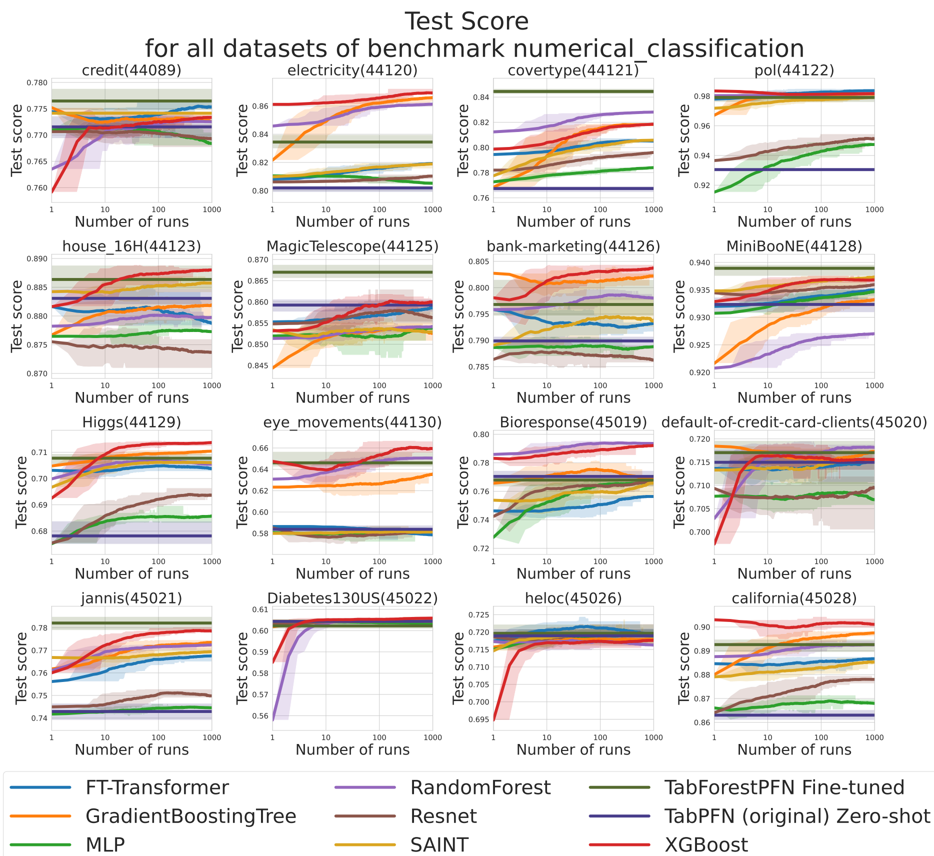

Figure 9: Comparison of fine-tuned TabForestPFN and the original zero-shot TabPFN on the WhyTrees benchmark with mixed features.

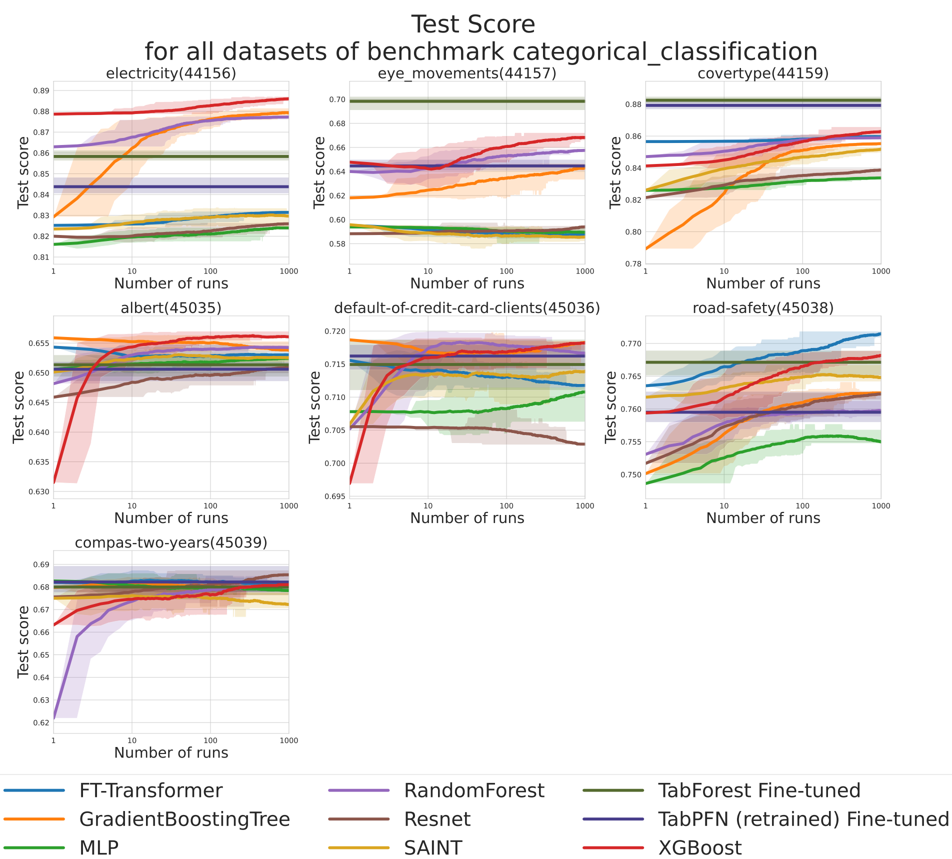

Figure 10: Comparison of fine-tuned TabForest and fine-tuned TabPFN on the WhyTrees benchmark with mixed features.

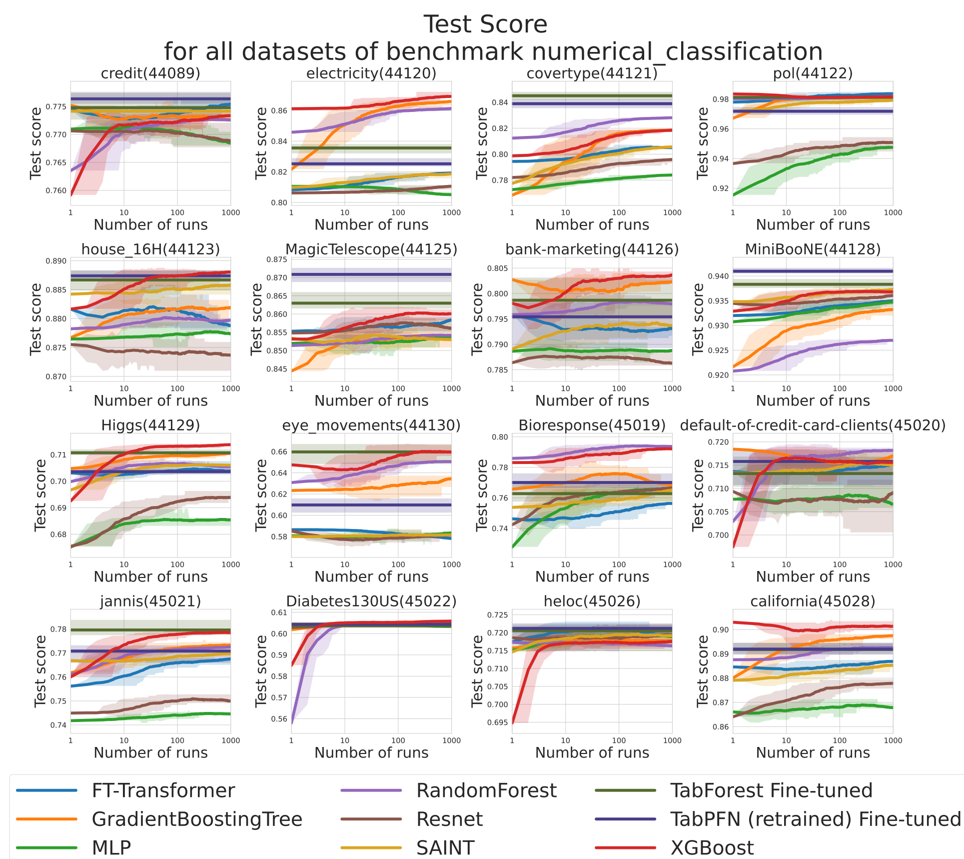

Figure 11: Comparison of fine-tuned TabForest and fine-tuned TabPFN on the WhyTrees benchmark with mixed features.

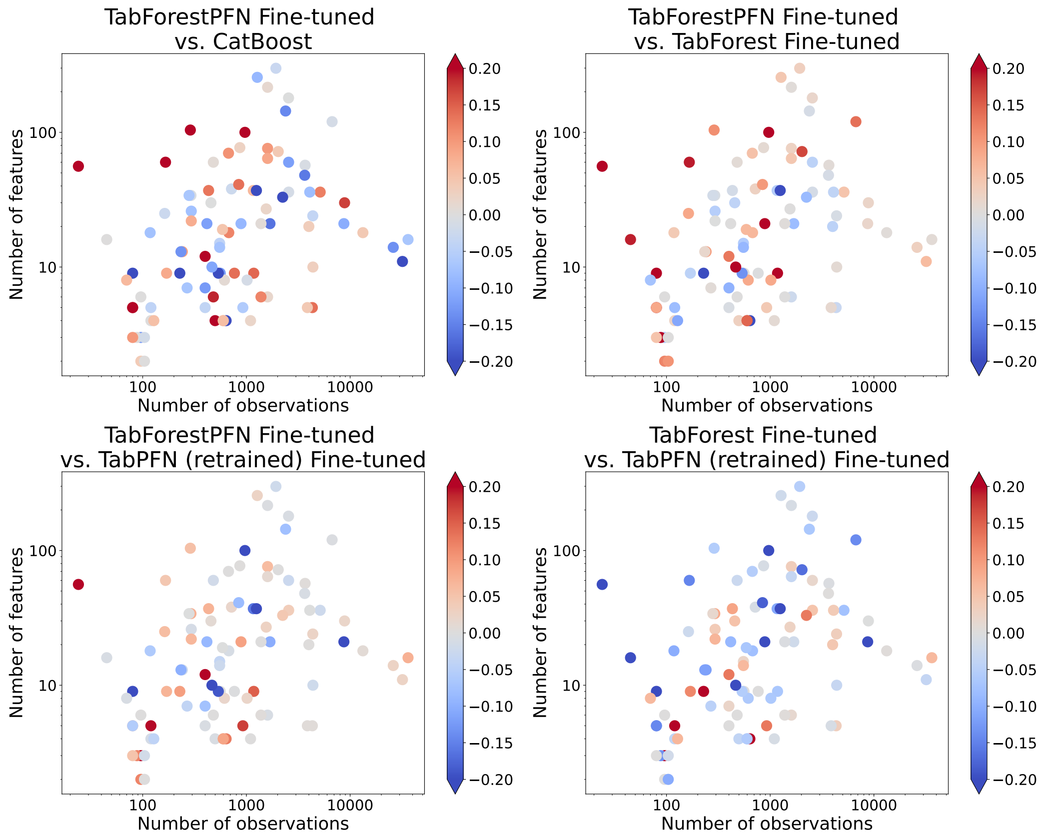

Figure 12: Differences in normalized accuracy of individual datasets from TabZilla. The color red means the left-mentioned method is the best, blue for the right-mentioned method. The darkest red represents at least 0.20 normalized score points improvement, and dark blue at least 0.20 normalized accuracy points degradation.

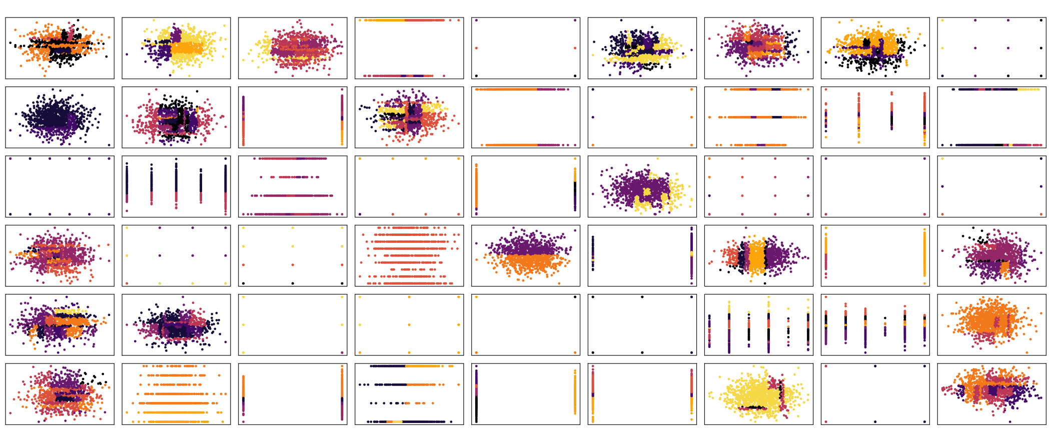

Figure 13: Generated forest data. Every box is a generated dataset with its own classes (color) and features (axes). Generated with base size 32, dataset size 1024, tree depth between 1 and 25, two features, and between 2 and 10 number of classes. See also Figures 3 and 14.

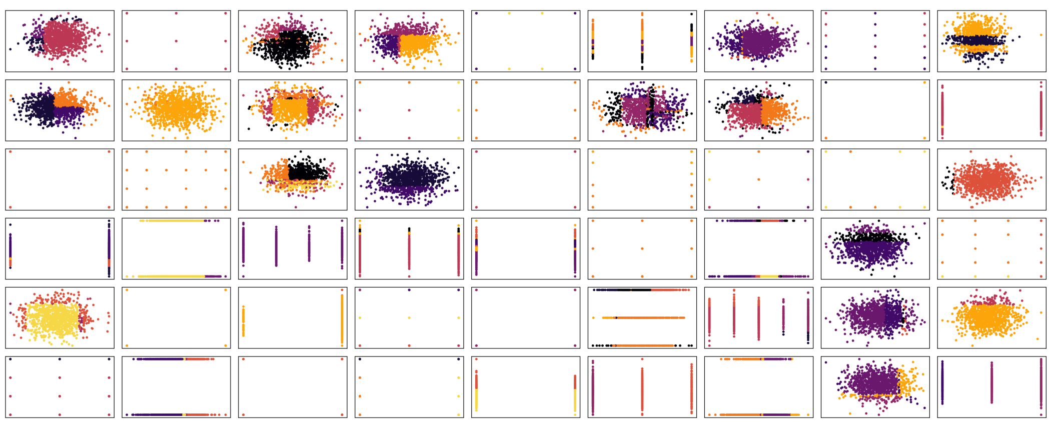

Figure 14: Generated forest data. Every box is a generated dataset with its own classes (color) and features (axes). Generated with base size 1024, dataset size 1024, tree depth between 1 and 9, two features, and between 2 and 10 number of classes. See also Figures 3 and 13.