Overhyped? Can ML Models Reliably Predict Stock Returns?[∗]

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Abstract

Hyperparameters determine the architecture of machine learning (ML) models and can greatly affect their forecasting performance, yet there is little consensus on how to choose the range and grid of hyperparameters to search over. We provide an extensive examination of which hyperparameters are most important for popular ML models' out-of-sample forecasting performance using a large U.S. dataset on individual stock returns and firm characteristics. We find that some choices of hyperparameters virtually guarantee good out-of-sample return forecasts while others lock in poor forecasts. This poses a challenge because many empirical studies fail to provide details on how they set their hyperparameters. We also find that time-series validation methods do not offer a definitive solution to the dependence of out-of-sample return forecasting performance on the underlying range of hyperparameters.

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1 Introduction

Machine learning (ML) methods are now widely used in empirical asset pricing, with many studies finding that these methods can produce more accurate forecasts of stock and bond returns and improve portfolio performance compared to traditional time-series approaches.^{[1](#page-1-0)} While early empirical results have been promising, evaluating forecasts generated by ML methods poses new challenges related to the additional levers and flexibility these methods introduce. In particular, the forecasting performance of ML methods such as random forests, boosted regression trees and neural nets depends on a potentially large set of hyperparameters that determine their ability to capture complex interaction effects and non-linearities. In contrast, conventional (linear) return prediction models focus on which predictors to include. This boils down to determining how to set a penalty term for inclusion of individual variables or groups of predictors from a candidate list and how much to shrink their coefficients. Both choices involve relatively simple and well-understood decisions.

The myriad of hyperparameters that users of ML methods must decide on can be illustrated by Feed-Forward Neural Networks (NNs). First, a researcher needs to decide on the number of hidden layers to use as well as their shape. Next, the researcher needs to select an activation function for the hidden units within the hidden layers, typically either linear or rectified linear unit. Because NNs update the input weights recursively (in epochs) the researcher needs to select a loss function (e.g., MSE, Huber) for each hidden unit. Moreover, because the loss function is not concave, the researcher needs to select an optimization algorithm, e.g., gradient descent or Adaptive Moment Estimation, and an associated learning rate. Lastly, decisions have to be made on batch normalization, dropout rate, whether to use early stopping, and regularization in the kernel of hidden units.^{[2](#page-1-1)}

Given these many choices, in practice how do researchers go about setting the range of values considered for the hyperparameters of ML models? Table [1](#page-6-0) summarizes the choices reported in recent studies that use ML methods. Random Forests (RF), Gradient Boosted

¹Prominent studies that use ML methods to predict stock returns include [Gu et al.](#page-41-0) [\(2020\)](#page-41-0), [Gu et al.](#page-41-1) [\(2021\)](#page-41-1), [Jiang et al.](#page-41-2) [\(2023\)](#page-41-2), and [Han et al.](#page-41-3) [\(2023\)](#page-41-3). [Kelly et al.](#page-41-4) [\(2023\)](#page-41-4) provide a comprehensive recent review of the literature.

²This list of hyperparameters and architectural choices is not comprehensive but represents some of the main desiderata researchers must consider when training neural networks.

Trees (GBT), and Neural Networks (NN) are the most popular algorithms. The table illustrates that there is no broad consensus on the hyperparameter used by these algorithms. Indeed, because these parameters typically have no economic interpretation, there is gen-erally no universal way to determine which ranges to search over.^{[3](#page-2-0)} Some hyperparameters are simply set ex ante, appealing to prior studies or "convention", while others are chosen through validation methods. Both strategies require an understanding of how the hyperparameters influence forecasting performance and how they possibly interact.

Computational constraints typically make it infeasible to consider all possible combinations of hyperparameters. In practice, researchers can therefore only conduct their search within a subset of the high-dimensional space of hyperparameters and are forced to make judgment calls on the range and grid of hyperparameters to focus on.

Despite their central role for ML models, how the range and grid of hyperparameters affects the performance of return predictability models has largely gone unexamined with some studies effectively providing examples of particular combinations of hyperparameters that seem to produce good forecasting results. In this paper we fill this void by undertaking a comprehensive study of how sensitive the performance of return forecasts generated by different ML models is with respect to their choice of hyperparameters, the implications of this sensitivity with regards to inference about (out-of-sample) forecasting performance, and possible solutions in the form of validation schemes.[4](#page-2-1)

Our empirical analysis uses the updated characteristics dataset of [Gu et al.](#page-41-0) [\(2020\)](#page-41-0) which we merge with stock return data obtained from the Center for Research in Security Prices (CRSP). As the data contains many missing characteristics, we use the local backward B-XS model of [Bryzgalova et al.](#page-40-0) [\(2024\)](#page-40-0) to impute missing characteristics based on historical data and contemporaneous cross-sectional asset information without introducing any look-ahead biases through information leakage. Our monthly data runs from January 1977 through December 2021, spanning almost 7,000 unique firms and 140 features.

To examine the sensitivity of the out-of-sample forecasting performance to different hy-

³For example, the learning rate of the Adam optimization algorithm is difficult to choose based on economic intuition or insights.

⁴This is also related to the literature on nonstandard errors (see, e.g., [Menkveld et al.,](#page-42-0) [2024\)](#page-42-0), which examines how research design choices, such as the selection and transformation of explanatory and target variables, influence results. We leave this aspect for future research.

perparameters and identify the most critical ones, our analysis proceeds by fixing one dimension of the hyperparameter space (i.e., one hyperparameter) while letting the remaining dimensions vary freely. For penalized linear models such as the Lasso and Elastic Net, predictive accuracy depends mostly on the shrinkage parameter that determines the cutoff for a predictor to be included in the model. For Random Forests, the depth of the trees and number of features are the most important hyperparameters while for Extreme Gradient Boosted Trees (XGBoost) the depth of the trees and the learning rate are key determinants of out-of-sample forecasting performance.[5](#page-3-0) Lastly, the out-of-sample predictive performance of NNs depends critically on the learning rate, followed by kernel *l*¹ shrinkage. Though they still matter, the choice of the number of hidden layers, loss function, and activation function appear to be relatively less consequential.

Building on these insights, we next show that the range of values for the key hyperparameters can matter greatly to out-of-sample predictive performance. For example, a very low shrinkage parameter for the Lasso or Elastic Net results in too many predictors being included with return forecasts that are dominated by noise and perform poorly out-of-sample. For XGBoost, a low depth of the trees combined with a low learning rate tends to produce overly conservative models, resulting in underfitting, while high depth paired with a high learning rate leads to overfitting and instability in the learning process. Similarly, a high learning rate for extreme gradient boosted trees or NNs results in a set of models whose out-of-sample predictive accuracy is far lower on average with a far higher chance of serious underperformance than models using a lower learning rate.

Several important insights emerge from this analysis. Across all ML methods, our results show that it is possible to fix a subset ("corner") of the space of hyperparameters such that good out-of-sample forecasting performance is achieved regardless of how the remaining hyperparameters are chosen. However, the opposite also holds: the space of hyperparameters can be restricted so that poor forecasting performance is, if not guaranteed, highly likely regardless of whether other hyperparameters are chosen optimally. This situation typically occurs as a result of using flexible models and a high learning rate.

We also show that the spread in out-of-sample predictive performance can be much wider

⁵Conversely, choices such as the number of trees matters less.

for some ML approaches such as neural nets compared to that of traditional linear models. This increases the risk that the out-of-sample forecasting performance of these methods is overstated ("hyped") since it is often possible to select a combination of values for the hyperparameters such that forecasts appear to be accurate even out-of-sample.^{[6](#page-4-0)}

Importantly, however, the much wider distribution in out-of-sample forecasting performance of ML models compared to traditional linear forecasting models is not symmetric but heavily left-skewed. In other words, across a wide set of configurations of hyperparameters there is, in practice, an upper bound on the maximum out-of-sample accuracy achievable by ML return forecasts. Conversely, the forecasting performance of the worst ML models, with hyperparameters set to make forecasts overly sensitive to noise, can become arbitrarily poor.

These conclusions on the average forecasting performance of ML models carry over to differences in cross-sectional measures of return predictability. Specifically, We find that the cross-sectional spread in forecasting accuracy across individual stocks is much wider for flexible ML models than for penalized linear models. Moreover, ML forecasting methods tend to perform relatively poorly for large cap stocks and stocks with high trading volume, raising concerns about whether such forecasts can be implemented in a profitable investment strategy net of transactions costs.

Having established these findings, we finally examine whether validation methods provide a convincing solution for choosing the hyperparameters. In many empirical applications, researchers split the data into training, validation, and test samples with the validation set used to select the hyperparameters. This procedure involves another set of choices such as validation method, the length of the validation sample, the range and grid of hyperparameters under consideration, the method being used to search over the space of hyperparameters, and whether or not to implement early stopping.

We find that these choices can have an important impact on out-of-sample forecasting performance. For instance, we demonstrate that the out-of-sample performance of XGBoost and neural networks is highly dependent on the initially selected hyperparameter grid even

⁶This phenomenon is distinct from over-fitting which is concerned with flexible ML models' ability to provide an arbitrarily good (in-sample) fit on the training data. We show instead that the out-of-sample predictive performance results have a far wider dispersion for ML methods than for conventional linear forecasting regressions.

when employing an efficient grid search algorithm that dynamically adjusts the hyperparameter search space, increasing the likelihood of finding a (near-)optimal hyperparameter configuration. In practice, validation is therefore no panacea to the issue of how to choose hyperparameters.

While economic reasoning does not suggest a specific range of values over which to search for the best hyperparameters of a given ML approach, an understanding of how the architecture of different ML methods, as determined by their hyperparameters, affects forecasting performance can be used to determine strategies for choosing reasonable ranges for regulating the bias-variance trade-off that is essential to out-of-sample forecasting performance.

The remainder of the paper proceeds as follows. Section [2](#page-7-0) describes the ML methods we consider, emphasizing the hyperparameters each method uses. Section [3](#page-17-0) introduces the main features of our data along with the estimation and forecasting procedure. Section [4](#page-22-0) provides a detailed analysis of the ML models' out-of-sample forecasting performance for different regions of the space of hyperparameters. Section [5](#page-29-0) examines the forecasting performance under different validation schemes used to select the hyperparameters. Finally, Section [6](#page-38-0) concludes.

Table 1: Hyperparameter grids used by previous studies

Note: RF refers to random forest, GBT to gradient boosted trees, NN to neural networks, and CV to cross-validation. "NA" indicates use of the algorithm but no mention of the hyperparameter grid. "-" indicates GBT to gradi

2 Methodology

This section sets out the forecast modeling problem that is the focus of our analysis and introduces the different classes of ML models considered in the paper.

2.1 The Modeling Problem

Let $r_{i,t}$ denote the return of stock i at time t , measured in excess of the risk-free rate, where $i = 1, \ldots, N_t$ and $t = 1, \ldots, T$. We add a *t* subscript to *N* to note the unbalanced structure of the panel. However, to simplify notation, we refer to the number of stocks in each period as *N* in the remainder.

We can decompose excess returns into its conditional expectation given the information set available at time $t - 1$, \mathcal{I}_{t-1} , and an orthogonal residual, $\varepsilon_{i,t}$:

$$
r_{i,t} = \mathbb{E}[r_{i,t} | \mathcal{I}_{t-1}] + \varepsilon_{i,t}.
$$
 (1)

Our objective is to model the expectation of $r_{i,t}$ conditional on a set of K predictor variables $X_{i,t-1}$ ∈ \mathcal{I}_{t-1} :

$$
\mathbb{E}[r_{i,t} \mid \mathcal{I}_{t-1}] = g(X_{i,t-1}; \theta),\tag{2}
$$

where $g(\cdot)$ is a flexible function of $X_{i,t-1}$ parameterized through θ . As in [Gu et al.](#page-41-0) [\(2020\)](#page-41-0), the functional form of $g(\cdot)$ is assumed to be the same across stocks and over time.

2.2 Hyperparameters

Machine learning methods involve two sets of parameters. *Hyperparameters* (θ_H) control the complexity of the models and are determined a priori by the researcher before estimating the full model. Given a set of hyperparameters, the *model parameters* (θ_M) are estimated with the objective of minimizing a given loss function. This second step is conceptually (though not necessarily computationally) simple. Identifying suitable hyperparameters is often complex and varies with the particular optimization problem at hand. In equity premium prediction, there is little theoretical guidance on how to choose a good set of hyperparameters. It is therefore common either to use a pre-defined set of hyperparameters or to search over a grid of a priori determined hyperparameters. The configuration of this grid—its granularity and range—is often overlooked due to the reliance on validation techniques, but is the key focus of our analysis.

Why not choose hyperparameters by optimizing the objective function with regards to these parameters just as with the regular model parameters? In many cases, this turns out to be computationally infeasible. For example, with only five hyperparameters, each evaluated on a grid of ten different values, nearly 10 million different models would need to be examined. Researchers therefore tend to either use predetermined values appealing to "common practice", or use validation methods, an approach we return to in Section [5.](#page-29-0)

To evaluate the sensitivity of forecasting performance to the choice of hyperparameters, we examine model performance on a large grid of hyperparameters. Specifically, to capture the marginal effect of a particular hyperparameter, θ_{H1} , we fix this at some value, $\theta_{H1} = \theta_{H1,fix}$ and examine forecasting performance across the full grid of values taken by all other hyperparameters θ_{H1}^C . In other words, our computational experiments optimize over the model parameters in the training set but keep one dimension of the hyperparameter space fixed. Specifically, for a given set of hyperparameters, we split the dataset into two samples, the training sample and test sample. We use the training sample to estimate the model parameters based on a training loss function, \mathcal{L}_{loss} . The objective function, $\mathcal{L}(\theta)$, takes the following general form

$$
\mathcal{L}(\theta) = \mathcal{L}_{loss}(\theta) + \mathcal{P}(\theta),\tag{3}
$$

where $\mathcal{P}(\theta)$ is a penalty term. Following common practice (e.g., [Gu et al.,](#page-41-0) [2020\)](#page-41-0), we determine the parameters of our models using the mean squared error (MSE) objective, l_2 , over the training set corresponding to the loss function

$$
\mathcal{L}_{l_2}(r_{i,t}, \theta) = \left(r_{i,t} - g(X_{i,t-1}; \theta)\right)^2.
$$
\n(4)

The MSE loss function in [\(4\)](#page-8-0) penalizes large errors quite, making it sensitive to outliers. As a more robust training criterion we also consider the Huber loss function for the ensemble models and neural networks:

$$
\mathcal{L}_{\delta}(r_{i,t},\theta;\delta) = \begin{cases} \left(r_{i,t} - g(X_{i,t-1};\theta)\right)^2, & \text{if } |r_{i,t} - g(X_{i,t-1};\theta)| \leq \delta\\ 2\delta\left(|r_{i,t} - g(X_{i,t-1};\theta)| - \delta^2\right), & \text{if } |r_{i,t} - g(X_{i,t-1};\theta)| > \delta. \end{cases}
$$
(5)

We set δ to the 99.9th percentile of the data following [Gu et al.](#page-41-0) [\(2020\)](#page-41-0). This loss function tends to produce more stable forecasts.

2.3 Linear Models

For linear machine learning algorithms we focus on penalized regression models, namely, the Lasso and Elastic Net. For these models, we have

$$
g(X_{i,t-1};\beta) = \beta' X_{i,t-1},\tag{6}
$$

such that the conditional expectation is approximated by a linear function of the predictor variables and parameter vector *β*. Penalized regression models minimize Equation [\(3\)](#page-8-1), with the conventional least squares objective function and a penalty term. The Lasso approach includes an l_1 penalization and the Elastic Net includes both l_1 and l_2 penalization terms:

$$
\mathcal{P}(\beta; \alpha, \lambda) = \begin{cases} \alpha \sum_{k=0}^{K} |\beta_k|, & \text{Lasso}, \\ \alpha \lambda \sum_{k=0}^{K} |\beta_k| + \frac{\alpha(1-\lambda)}{2} \sum_{k=0}^{K} \beta_k^2, & \text{Elastic Net.} \end{cases}
$$
(7)

Here, α is the shrinkage hyperparameter on the coefficients and λ is the mixing hyperparameter determining how the l_1 and l_2 penalizations get weighted. For the Lasso approach $\lambda = 1$, so the loss function only depends on the penalty parameter α .

We do not tune the penalty parameters α and λ . Instead we use a grid of penalty parameters and generate one-month ahead forecasts recursively for each combination of hyperparameters. We refit the model every year, such that the parameters β are updated every twelve months. For Lasso we consider an evenly spaced grid of 20 values of the *α* hyperparameter between 0.0001 and 0.015. The lowest value (0.0001) corresponds to a very small penalty term while the upper value effectively excludes any predictor variables from being included, so higher values yield the same results. For Elastic Net we use the same grid for α while for λ we consider a grid between 0.2 and 0.8, with 0.05 increments, resulting in

13 settings. For λ there is a natural range between zero and one, so the main issue is how fine a mesh to use.^{[7](#page-10-0)}

2.4 Tree-based Models

Tree-based methods have been widely used in the ML literature. We focus on Random Forests and Gradient Boosted Trees, specifically Extreme Gradient Boosting, as regularization methods. Both offer non-parametric flexibility and are distinctive from traditional econometric methods.

Trees aim to identify groups of observations exhibiting similar behavior. A tree grows by sequential branching; data with similar behavior and characteristics are selected, forming the foundation for subsequent growth and branching of the tree. These branches, created in subsequent steps, group the remaining data from previous stages and organize them into bins or suitable intervals, approximating the functional form $g(\cdot)$ in Equation [\(2\)](#page-7-1).^{[8](#page-10-1)}

At each node *l* of the tree, the algorithm evaluates potential splits by considering a subset of the predictors (features).^{[9](#page-10-2)} Let $F_l \subseteq \{1, 2, ..., K\}$ denote the set of features considered at node *l*, and $F = |F_l|$ the number of features. The splitting criterion is based on minimizing the impurity of the three, following an l_2 penalty quantified by the loss function $\mathcal{L}_{cart}(\theta_l, C_l)$:

$$
\mathcal{L}_{cart}(\theta_l, C_l) = \frac{1}{|C_l|} \sum_{X_{i,t-1} \in C_l} \left(r_{i,t} - \theta_l \right)^2,\tag{8}
$$

where $|C_l|$ is the number of samples at node *l* and the mean target value at node *l* is

$$
\theta_l = \frac{1}{|C_l|} \sum_{X_{i,t-1} \in C_l} r_{i,t}.\tag{9}
$$

For each feature $j \in F_l$ and potential split value *s*, the dataset C_l is divided into two

⁷When producing forecasts with the Lasso and the Elastic Net methods, we also allow a constant to be included in the feature space. However, at each point of re-estimation and for each penalty parameter, we allow the model the flexibility to determine whether or not to include the constant.

⁸Bagging and boosting algorithms both utilize classification and regression trees (CART) [\(Breiman et al.,](#page-40-8) [1984\)](#page-40-8) as the foundation for constructing individual trees. The defining characteristic of CART is its binary splitting process, where each node divides into exactly two child nodes.

⁹The growth of the tree starts with the root node l_0 which contains all samples in the training set, S_{l_0} .

Figure 1: Example of a Classification and Regression Tree

Example of a classification and regression tree with depth $D = 3$ and $L = 4$ leaves. Here, $X_{i,t-1,j}$ denotes the value of feature *j* for asset *i* at time $t - 1$. Each node determines the optimal splitting feature j^* and value s^* via Equation [\(10\)](#page-11-0). Leaf values θ_l represent the outcomes at each terminal node.

subsets $C_{l,1}(j, s)$ and $C_{l,2}(j, s)$. The optimal split (j^*, s^*) is then determined as

$$
(j^*, s^*) = \underset{j,s}{\arg\min} \left[\mathcal{L}_{cart}(\theta_{l,1}, C_{l,1}(j,s)) + \mathcal{L}_{cart}(\theta_{l,2}, C_{l,2}(j,s)) \right]. \tag{10}
$$

This process is applied recursively until a stopping criterion is reached: when the tree expansion reaches the predefined maximum depth *D*, the number of samples at node *l* drops below S_l , or the resulting leaf nodes would have fewer samples than S_L ^{[10](#page-11-1)}

The final prediction is based on the average target values present in the samples of each leaf node in Equation [\(9\)](#page-10-3). The prediction for a given feature set $X_{i,t-1}$ is computed using the combined contributions from all *L* leaf nodes of tree *b*:

$$
\hat{r}_{i,t}^{(b)} = \sum_{l=1}^{L} \theta_l \, 1_{\{X_{i,t-1} \in C_l\}},\tag{11}
$$

where $1_{\{X_{i,t-1}\in C_l\}}$ is an indicator function which equals 1 when $X_{i,t-1}$ falls within the sample space of leaf node *l*, and is 0 otherwise.

A tree of depth *D* has the ability to capture (*D*−1)-way interactions but this flexibility of tree models comes at the cost of being highly prone to overfitting. Regularization techniques are used to overcome this problem. We consider Random Forests and Boosting. Both use

¹⁰As we re-estimate the model parameters, the splits and consequently θ_l depends on time *t*. For ease of notation, we omit the subscript t from θ_l .

ensemble methods to combine forecasts from a set of individual tree predictors.

2.4.1 Random Forest

The Random Forest (RF) method introduced by [Breiman](#page-40-9) [\(2001\)](#page-40-9) employs a bagging procedure over a collection of decision trees to minimize the variance in predictions. This process draws multiple bootstrap samples from the dataset and, for each sample $b = 1, ..., B$, constructs a regression tree based on the CART procedure.

The predictive power of the RF method comes from its ability to average forecasts from the individual trees, reducing the risk of overfitting and improving the overall predictive accuracy. The aggregated final prediction of the Random Forest is

$$
g(X_{i,t-1};\theta) = \frac{1}{B} \sum_{b=1}^{B} \hat{r}_{i,t}^{(b)},
$$
\n(12)

where $\hat{r}_{i,t}^{(b)}$ is the prediction from an individual tree in the forest.

Our choice of hyper parameter grid configuration focuses on evaluating the most influ-ential hyperparameters that impact model performance [\(Probst et al.,](#page-42-4) [2019\)](#page-42-4):^{[11](#page-12-0)}

Number of trees in the forest, *B*. This hyperparameter influences the model's ability to generalize; more trees usually lead to better performance but also increase the computational complexity. We consider $B \in \{30, 100, 500\}.$

Maximum depth of a tree, *D*. A deeper tree can model more complex relationships by allowing more splits but also increases the risk of overfitting. *D* is a critical parameter for controlling the balance between bias and variance. We set $D \in \{1, 2, 4, 6, 8\}.$

Features in each split, *F*. The parameter *F* represents the number of features to consider at each split in the individual tree, dictating the size of the subset of features selected randomly from the total of *K* explanatory variables for evaluation at each decision node. We consider the grid $F \in \{1, 3, 10, 50, 70\}.$

¹¹We also considered varying the hyperparameters for the minimum internal node size and the minimum node size. However, these do not have a significant impact on out-of-sample performance.

2.4.2 Extreme Gradient Boosting

Extreme Gradient Boosting (XGBoost), an advanced implementation of Gradient Boosted Trees [\(Friedman,](#page-41-6) [2001\)](#page-41-6), is a highly efficient and scalable algorithm for tree boosting. Unlike the traditional GBT that incrementally builds trees to minimize predictor bias through weak learners, XGBoost, developed by [Chen and Guestrin](#page-40-10) [\(2016\)](#page-40-10), applies gradient descent optimization within the context of boosting, enabling the recursive construction of trees. An advantage of XGBoost over methods like Random Forest is its approach to ensemble learning which involves optimizing Equation (8) . This loss includes l_1 and l_2 regularization terms, crucial for controlling model complexity and preventing overfitting.^{[12](#page-13-0)}

The core of XGBoost lies in the sequential addition of trees with each tree designed to correct the residuals of all previous trees. These trees are commonly referred to as weak learners. In each boosting round *b*, a tree f_b is trained using the features $X_{i,t-1}$ with the objective to predict the residuals from the predictions made in round *b* − 1. Here, $f_b(X_{i,t-1})$ denotes the output of the *b*-th tree. The learning rate, *η*, is crucial in this process—controlling the contribution of each new tree and ensuring a controlled learning process. The cumulative prediction, $\hat{r}_{i,t}^{(b)}$, is updated sequentially by adding the contribution of the *b*-th tree to the previous prediction;

$$
\hat{r}_{i,t}^{(b)} = \hat{r}_{i,t}^{(b-1)} + \eta f_b(X_{i,t-1}).\tag{13}
$$

The boosting process continues until the maximum number of rounds *B* is reached or other stopping criteria are met. Again, we consider a range of settings for the hyperparameters:

Number of trees in the forest, *B*. This hyperparameter influences the model's ability to generalize; more trees usually lead to better performance but also increases computational complexity. We consider $B \in \{1, 100, 500\}.$

Maximum depth of each tree in the forest, *D*. Deeper trees can model more complex relations by allowing more splits, but also increase the risk of overfitting. *D* is a critical

¹²Extreme Gradient Boosting constructs binary trees where each internal node is split into two child nodes. This methodology parallels the fundamental structure of CART, but XGBoost diverges from CART's greedy algorithm. Instead of making the best immediate split based on an MSE criterion, XGBoost uses a gradient boosting mechanism—allowing for an objective function of the general loss function form in Equation [\(3\)](#page-8-1) with penalty term. This mechanism involves calculating the gradients and Hessian of the loss function, enabling the algorithm to efficiently determine the optimal splits by evaluating how effective each split is in reducing the overall loss.

parameter for controlling the balance between bias and variance. We set $D \in \{1, 2, 4, 6\}$.

Learning rate, *η*. The learning rate controls the step size of the prediction updating process. This parameter helps to ensure gradual improvement and prevent overfitting. We consider the grid $\eta \in \{0.0001, 0.001, 0.01, 0.1, 0.2, 0.3, 0.4\}$, which includes the default value of 0.3 and covers the range often found to be optimal in empirical applications, typically between 0.01 and 0.2 (see, e.g., [Chen and Guestrin](#page-40-10) [\(2016\)](#page-40-10) and the corresponding [XGBoost](https://xgboost.readthedocs.io/en/stable/parameter.html) [documentation\)](https://xgboost.readthedocs.io/en/stable/parameter.html).

We use histogram-based boosting as the booster method, which is a fast implementation that approximates the greedy algorithm. The l_1 and l_2 regularization on the weights are set to $\alpha = 0$ and $\lambda = 1$, respectively.^{[13](#page-14-0)}

Further, *early stopping* is a well-known technique employed in machine learning to prevent overfitting and enhance model generalization. The model is trained on a training set, and the performance is evaluated on a validation set. The training process is halted when the model's performance on the validation dataset ceases to improve or starts to degrade, ensuring that the model does not become overly specialized to the training data. We set the patience parameter to 5, indicating the number of consecutive iterations during which no improvement is observed in the model's performance—see Algorithm [1.](#page-46-0) When early stopping is used, we do not retrain the model on both the training and validation sets and instead use the model to directly make predictions on the test set. This approach helps ensure that the model's evaluation on the test set remains consistent with its ability to generalize to unseen data.

2.5 Neural Networks

Neural networks are anchored in their ability to approximate a broad range of continuous functions [\(Kolmogorov,](#page-41-7) [1957;](#page-41-7) [Cybenko,](#page-41-8) [1989;](#page-41-8) [Hornik et al.,](#page-41-9) [1989\)](#page-41-9). Specifically, a Feed-Forward Neural Network (FNN) with a single hidden layer and a finite number of neurons can approximate any continuous function on compact subsets of real numbers, given appropriate parameters and activation functions. In FNNs, data travels exclusively forward starting from

¹³Note that in the context of XGBoost, the parameters α and λ have definitions that differ slightly from their usage in the Elastic Net. Here, they directly correspond to the l_1 and l_2 penalization, respectively. Additionally, we investigate a range of values for α and λ , as well as the proportions of observations and features randomly sampled for each tree. However, these values do not affect the model's performance.

Figure 2: Example of a Feed Forward Neural Network

Example of a Feed Forward Neural Network with $H = 1$ hidden layer. There are K blue input nodes corresponding to each feature, *Xi,t*−1*,k*. The hidden layer contains 3 neurons, marked in orange, and the output layer is the pink node. The function $f(\cdot)$ in the hidden neurons denotes the activation function.

the input layer, passing through (multiple) hidden layers, and aggregating in the output layer. Each neuron in the hidden layers represents a distinct feature of the data. The initial input layer receives the predictor input, which then gets processed and transformed non-linearly through *H* hidden layers. The output layer aggregates the transformed data, yielding a prediction. Thus, $g(\cdot)$ in Equation [\(2\)](#page-7-1) is approximated by the hidden layers. Figure [2](#page-15-0) shows a visual representation of a FFN with one hidden layer containing three neurons.

We construct the FNNs in the following way. Let $\tilde{x}_{k}^{(\ell)}$ denote the output coming from neuron *k* in layer ℓ , and let $\tilde{x}^{(\ell)} = (\tilde{x}_1^{(\ell)})$ $\widetilde{x}_{1}^{(\ell)},...,\widetilde{x}_{K^{\ell}}^{(\ell)}$ $\binom{\ell}{K^{\ell}}'$, with K^{ℓ} being the number of neurons in layer ℓ . The input layer takes data $\tilde{x}^{(0)} = X'_{i,t-1}$ and forwards it to the fully connected first hidden layer. We recursively construct the output of each neuron k in layer $\ell > 0$ as

$$
\widetilde{x}_{k}^{(\ell)} = f\left(\widetilde{x}^{(\ell-1)\prime}\omega_{k}^{(\ell)} + \omega_{0}^{(\ell)}\right),\tag{14}
$$

where $\omega_k^{(\ell)}$ $\alpha_k^{(\ell)}$ are the weights of neuron *k* in layer ℓ . The bias term $\omega_0^{(\ell)}$ $\int_0^{(\ell)}$ in layer ℓ allows the activation function to shift, enabling the model to effectively fit the data regardless of input values. Further, $f(\cdot)$ is the activation function. Finally, the prediction $\hat{r}_{i,t}$ is computed as

$$
g(X_{i,t-1};\theta) = \tilde{x}^{(H)}\omega^{(H+1)} + \omega_0^{(H)},
$$
\n(15)

where $\tilde{x}^{(H)}$ denotes the output from the last hidden layer, $\omega^{(H+1)}$ the weights linking these to the final layer and $\omega_0^{(H)}$ $_0^{(H)}$ the final layer bias term, summarizing the contributions of each neuron in the last hidden layer for the prediction.

To determine the optimal weights of the neural nets $\omega_k^{(\ell)}$ $k^{(l)}$, we consider two loss functions, namely mean squared error of Equation [\(4\)](#page-8-0) and Huber loss of Equation [\(5\)](#page-9-0). Determining the optimal weights of a neural network is often computationally inefficient using standard stochastic gradient descent. We use the Adaptive Moment Estimation (Adam) optimizer from [Kingma and Ba](#page-41-10) [\(2014\)](#page-41-10), which enhances efficiency by adjusting the learning rate for each parameter during training. Let ω_d represent the weights and biases across all layers at step *d*. The weight update mechanism at step *d* operates as follows;

$$
\omega_d = \omega_{d-1} - \frac{\eta \cdot \hat{m}_d}{\sqrt{\hat{v}_d} + \epsilon},\tag{16}
$$

where η is the Adam learning rate, \hat{m}_d and \hat{v}_d are bias-corrected estimates of the gradient's first and second moments of the loss function, and $\epsilon = 10^{-8}$ prevents division by zero. The Adam optimizer is shown in Algorithm [2.](#page-46-1)

We follow [Gu et al.](#page-41-0) [\(2020\)](#page-41-0) and consider five types of FNNs, labeled FNN1 through FNN5, corresponding to $H = 1$ to $H = 5$ hidden layers, respectively. The number of neurons decreases by half for each subsequent layer and follow a geometric pyramid that starts from 32. FNN1 thus has a single layer with 32 neurons and FNN5 features five layers with 32, 16, 8, 4, and 2 neurons, respectively. As in Figure [2,](#page-15-0) all layers are fully connected such that every neuron receives its input from the preceding neurons.

Activation function $f(\cdot)$. We focus on the linear activation function and the rectified linear unit (ReLU) activation function; $ReLU = max(0, x)$. The ReLU function allows for faster derivative evaluation and favors sparsity. However, ReLU can result in zero outputs, stopping learning in some neurons. To mitigate this, we also use Leaky $ReLU = max(0.01x, x)$, which maintains a nonzero gradient for inactive units, ensuring continuous learning.^{[14](#page-17-1)}

Adam learning rate η. The learning rate of the optimizer in Equation [\(16\)](#page-16-0), is critical for performance, as demonstrated by [Bergstra and Bengio](#page-40-11) [\(2012\)](#page-40-11) on seven datasets. We consider the set $\eta \in \{0.0001, 0.001, 0.01, 0.1\}$, which includes the default value of 0.01 as suggested by [Kingma and Ba](#page-41-10) [\(2014\)](#page-41-10) and contains and extends those used in prior financial literature (Table [1\)](#page-6-0).

Shrinkage penalty α . As neural nets are heavily parameterized, some form of regularization needs to be introduced. We therefore introduce an l_1 penalty term on the weights in the loss function, similar to the Lasso approach. In practice, $\alpha = 0.01$ is often used. We consider $\alpha \in \{0.0001, 0.001, 0.01, 0.1\}.$

As in XGBoosting, we also perform *early stopping* in the feed-forward neural networks. [Amari et al.](#page-40-12) [\(1995\)](#page-40-12) show that early stopping in neural networks always decreases the generalization error, leading to better performance on unseen data. We use a validation set for the stopping criteria. If the objective function does not improve after 5 iterations, we stop the training. For training, we use 100 epochs.^{[15](#page-17-2)}

2.6 Summary of Hyperparameter Ranges

For each model type, Table [2](#page-18-0) summarizes which hyperparameters we vary along with the range of values taken. The total number of hyperparameters under consideration is obtained, for each model type, as the product of each set of hyperparameter listed in the table and ranges from 20 for the Lasso approach to 260 for Elastic Net models.

3 Data

Our data consists of monthly values of firm-level stock returns and characteristics obtained from CRSP and Dacheng Xiu's [website,](https://dachxiu.chicagobooth.edu) respectively. We measure returns in excess of the

¹⁴The Sigmoid and Tanh function are also common choices as activation functions. However, these functions are susceptible to saturation with low signal-to-noise input, leading to a vanishing gradient [\(Glorot](#page-41-11) [and Bengio,](#page-41-11) [2010\)](#page-41-11). This limits the model's ability to learn from weak signals.

¹⁵[Prechelt](#page-42-5) [\(2002\)](#page-42-5) shows that increasing the patience results in small improvements at the cost of increased computation time. Further, increasing the number of epochs has minimal effect on the performance.

Model Type	Model	Hyperparameter		Grid size	Grid range
Linear	Lasso	Shrinkage strength	α	20	$\{0.0001, 0.009, \ldots, 0.015\}$
Linear	Elastic Net	Shrinkage strength (l_1, l_2) penalty mix	α λ	260	$\{0.0001, 0.009, , 0.015\}$ $\{0.2, 0.25, , 0.8\}$
Tree-based	Random Forest (RF)	Number of trees Maximum depth of tree Number features in split	\boldsymbol{B} \overline{D} $\,F$	75	$\{30, 100, 500\}$ $\{1, 2, 4, 6, 8\}$ $\{1, 3, 10, 50, 70\}$
Tree-based	Extreme Gradient Boosting (XGB)	Number of trees Maximum depth of tree Learning rate	В D η	84	$\{1, 100, 500\}$ $\{1, 2, 4, 6\}$ $\{0.0001, 0.001, 0.01, 0.1, 0.2, 0.3, 0.4\}$
Neural Nets	Feed Forward NN 1-5	Activation functions Loss function Adam learning rate l_1 shrinkage penalty	$f(\cdot)$ $\mathcal{L}(\cdot)$ η α	96	${Leaky, linear, ReLU}$ ${MSE, Huber}$ $\{0.0001, 0.001, 0.01, 0.1\}$ $\{0.0001, 0.001, 0.01, 0.1\}$

Table 2: Ranges of hyperparameters for the ML models

risk-free rate proxied by the 1-month Treasury Bill rate obtained from Kenneth French's [website.](https://mba.tuck.dartmouth.edu/pages/faculty/ken.french/data_library.html) As in [Gu et al.](#page-41-0) [\(2020\)](#page-41-0), we assume that monthly, quarterly, and annual data are accessible to investors with one-month, four-month, and six-month lags. Details on the frequency and description of the characteristics are reported in Table [A.1.](#page-43-0)

The dataset contains many missing entries. For every month we only consider firms from which the monthly return is available since our goal is to predict excess returns. Although the original data goes further back in time, to balance the cross-sectional and time-series dimension, we choose a dataset that ranges from January 1977 to December 2021, contains 92 firm- or stock-level characteristics and 48 industry-specific dummies, resulting in 140 features.[16](#page-18-1) Before 1985, there are between 300 and 800 firms in our dataset each month. After 1985, the number of firms averages 1500 per month. In total there are 6,840 unique firm numbers.

3.1 Missing Characteristics and Data Transformations

Missing data points are typically not random draws and so need to be carefully handled. Data missing earlier in our sample arises primarily due to coverage issues while missing data later in the sample occur mostly because of the Global Financial Crisis (GFC) and the COVID pandemic. To address the issue of missing characteristics in our dataset, we follow

¹⁶The original panel of characteristics goes back to January 1957. However, data prior to 1977 has many missing entries.

[Bryzgalova et al.](#page-40-0) [\(2024\)](#page-40-0) and consider data from January 1977 onward since the frequency of missing characteristics is significantly lower after 1976. Furthermore, we consider 92 characteristics instead of 94, since two of these (real estate holdings and secured debt) are only available from 1985 onward, and even then, only sparsely available across time.

Next, we employ the local backward (B-XS) model of [Bryzgalova et al.](#page-40-0) [\(2024\)](#page-40-0) which fills data by using contemporaneous cross-sectional information and recent historical characteristics.[17](#page-19-0) The B-XS model is the best-performing model that does not use forward-looking information for imputing characteristics in terms of out-of-sample mean squared error. For cross-sectional fitting we use the settings of [Bryzgalova et al.](#page-40-0) [\(2024\)](#page-40-0). That is, we capture the cross-sectional dependence using six latent factors, we only consider stocks that have at least ten characteristics observed at each point in time, and we use the covariance structure between the characteristics of January 1985 to avoid look-ahead bias. After converting the characteristics to rank percentiles, we impute the missing data and then transform the imputed rank quantiles back to their original values using the empirical distribution.[18](#page-19-1)

The characteristics are measured on different scales and so are not directly comparable. To handle this issue, we cross-sectionally rank the explanatory variables for each period and scale them to the $[-1, 1]$ range, as proposed in [Gu et al.](#page-41-0) (2020) . This method is more robust to outliers than conventional standardization method because it imposes boundaries at −1 and 1. However, it also has some drawbacks. Cross-sectionally ranking the variables between −1 and 1 erases information about the level of the variables. We further construct dummies based on the first two digits of the Standard Industrial Classification (SIC) codes.^{[19](#page-19-2)} To obtain as granular a grouping as possible, but with a sufficient number of firms, we group some of the first two digits of the SIC numbers which results in 48 dummies. 20 20 20

¹⁷We are grateful to Markus Pelger and Sven Lerner for sharing their code with us.

¹⁸Note that we handle missing data very differently from [Gu et al.](#page-41-0) [\(2020\)](#page-41-0) who fill firm-level missing characteristics with zeros.

¹⁹Appendix Table [A.2](#page-45-0) shows the grouping we use.

 20 We exclude macroeconomic predictors because the scaling process eliminates the information these variables contain. Because our most flexible ML models can capture complex non-linear relations and interaction terms we do not take the Kronecker product between characteristics and macro variables.

Figure 3: Training, Validation, and Test Samples

Panel (a) shows the training (estimation) window for the procedure that uses fixed hyperparameters. The model undergoes training using the training dataset, shown in light blue, and performs out-of-sample predictions on the test dataset, shown in purple. Panel (b) shows the estimation process incorporating a 2-year validation period. If validation or early stopping mechanisms are applied, the model is trained with the training set (light blue) and validated on the validation set (dark blue). If early stopping is not employed, the model parameters are re-estimated using both the training and validation sets before making out-ofsample predictions on the test set (purple).

3.2 Training and Test Set

To examine the sensitivity of our return predictability results with respect to the values of the hyperparameters, we split our data into training and test sets. The training set is used to estimate the model parameters and our initial training uses the first 20 years from January 1977 to December 1996. The test sample evaluates the performance of the model on unseen data and is the 25-year out-of-sample period from January 1997 to December 2021 (300 months). Using an expanding estimation window, we update the model parameters every 12 months as visualized in the upper panel in Figure [3.](#page-20-0) The validation procedure (shown in the lower panel of Figure [3\)](#page-20-0) is discussed in Section [5.](#page-29-0)

3.3 Evaluation of Forecasts

We evaluate predictive performance by means of the widely used out-of-sample *R*² measure of [Campbell and Thompson](#page-40-13) [\(2008\)](#page-40-13) generalized to account for multiple stocks:

$$
R_{OoS}^2 = 1 - \frac{(T - T_0)^{-1} \sum_{i=1}^{N_t} N_t^{-1} \sum_{t=T_0+1}^T (r_{i,t} - \hat{r}_{i,t}^{(m)})^2}{(T - T_0)^{-1} \sum_{i=1}^{N_t} N_t^{-1} \sum_{t=T_0+1}^T (r_{i,t} - \hat{r}_{i,t}^{(bm)})^2},
$$
(17)

where T_0 is the start of the test sample which ends at time T , N_t is the number of firms in existence at time *t*, $\hat{r}_{i,t}^{(m)}$ denotes the predicted excess returns from model *m*, $\hat{r}_{i,t}^{(bm)}$ is the benchmark forecast, and $r_{i,t}$ is the realized excess return of stock *i* at time *t*. R_{OoS}^2 is a relative measure tracking the predictive accuracy of model *m* relative to the benchmark forecasts with positive values indicating outperformance. As in [Gu et al.](#page-41-0) [\(2020\)](#page-41-0), we use zero prediction as the benchmark model, i.e., $\hat{r}_{i,t}^{(bm)} = 0$ for all *i* and t .^{[21](#page-21-0)}

We use the Diebold-Mariano (DM) test [\(Diebold and Mariano,](#page-41-12) [1995\)](#page-41-12) to test for significance in the differences between the out-of-sample predictive accuracy of our models and the zero prediction. Specifically, we use a cross-sectional adaptation of the DM test to test forecast accuracy. The prediction error differential for time *t* is defined as

$$
d_t = \frac{1}{N_t} \sum_{i=1}^{N_t} \left(\left(\hat{e}_{i,t}^{(bm)} \right)^2 - \left(\hat{e}_{i,t}^{(m)} \right)^2 \right).
$$
 (18)

where $\hat{e}_{i,t}^{(bm)} = r_{i,t}$ and $\hat{e}_{i,t}^{(m)} = r_{i,t} - \hat{r}_{i,t}^{(m)}$. The DM statistic for model m is then $DM_m = \overline{d}_m / \hat{\sigma}_{\overline{d}_m}$, where d_m is the time series average of d_t and $\hat{\sigma}_{\overline{d}_m}$ is the Newey-West standard error.

To track the time-series evolution in the predictive accuracy of model *m* versus the benchmark, we also plot the cumulative sum of squared error differences $CSSED_{\tau} = \sum_{t=t_0}^{\tau} d_t$ over the test set.

²¹Alternatively, one could use the prevailing mean, $\overline{r}_{i,t} = \frac{1}{t-1} \sum_{\tau=0}^{t-1} r_{i,\tau}$, which is the average excess return of firm *i* until *t* − 1, as a benchmark. However, the prevailing mean is noisy and generates a 4.5% higher MSE compared to the zero prediction for individual stocks.

4 Results

In this section, we report the forecasting performance of the models introduced in Section [3.](#page-17-0) We summarize the sensitivity of our R_{Os}^2 measure of predictive accuracy with respect to hyperparameter values through boxplots constructed by fixing one hyperparameter at a given value while allowing the remaining hyperparameters to vary across the grid values listed in Table 2. Each boxplot, complete with whiskers, displays the range of R_{OoS}^2 values achievable as we vary the other hyperparameters within a predetermined grid. Our boxplots follow standard practice: the central box encompasses the interquartile range (*IQR*) between the 25th percentile, $q_{0.25}$, and the 75th percentile, $q_{0.75}$, so $IQR = q_{0.75} - q_{0.25}$. The line inside the box corresponds to the median, $q_{0.50}$. Whiskers visualize the range of R_{OoS}^2 values outside the middle 50%, using the $1.5 \times IQR$ rule. Hence, the lower whisker extends from the first quartile $(q_{0.25})$ to the lowest data point not below $q_{0.25} - 1.5 \times IQR$ while the upper whisker goes from the third quartile $(q_{0.75})$ to the highest data point not above $q_{0.75} + 1.5 \times IQR$. Values outside the boundaries of the whiskers are plotted as individual points and are considered outliers.[22](#page-22-1)

4.1 Linear Models

Figure [4](#page-23-0) panel (a) shows the sensitivity of the out-of-sample performance of Lasso across values of the single hyperparameter, α , which controls the amount of shrinkage with larger values of α corresponding to a higher level of regularization. The R_{OoS}^2 ranges from -0.2 for penalty terms approaching zero to 0.38 for small α values. The R_{OoS}^2 curve is flat at zero for $\alpha > 0.01$ because the Lasso approach does not select any predictor variables. Supporting this interpretation, Panel (b) of Figure [4](#page-23-0) plots the percentage of non-zero coefficients over the estimation window. When $\alpha > 0.01$, the estimated coefficients for all models are reduced to zero across every window.

²²For example, for a random forest model we fix hyperparameter *B* at 30, and let the hyperparameters *D* and *F* vary over the grid, which could result in the following range of R_{OoS}^2 values: $\{-0.05, 0.18, 0.22, 0.23, 0.28, 0.3, 0.35, 0.39, 0.41\}$. The corresponding central box ranges from 0.22 to 0.35, as the corresponding percentiles are $q_{0.25} = 0.22$ and $q_{0.75} = 0.35$, and $IQR = 0.13$. The median is 0.28. The lower whisker is determined by the smallest value still above $q_{0.25} - 1.5 \times IQR = 0.025$, which is 0.18. The upper whisker is 0.41, which is the highest value still below $q_{0.75} + 1.5 \times IQR = 0.545$. The value -0.05 is shown by a dot.

Figure 4: Sensitivity of R^2_{OoS} to Lasso hyperparameter (α)

Panel (a) shows the sensitivity of R_{OoS}^2 , expressed as a percentage, with respect to different choices of α . Panel (b) shows the percentage of variables $X_{i,t}$ included by Lasso for different values of α .

Figure [5](#page-24-0) shows the sensitivity of R_{OoS}^2 for the Elastic Net across the range of values for the two hyperparameters, α and λ . Panel (a) shows the sensitivity of $R_{O_0S}^2$ when keeping the amount of shrinkage (α) fixed at a given value while varying the (l_1, l_2) penalty mix *λ*. For $\alpha = 0.0001$, the range of R_{OoS}^2 values is between −0.5 and −0.25 consistent with underperformance against the zero benchmark. Performance improves when α is fixed around 0.001 and gets a further boost once we increase α to 0.003 or 0.004 which raises the average R_{OoS}^2 value and narrows its range so that even the worst model across the grid of λ values performs better than the median performer for $\alpha = 0.001$. Increasing α beyond these values pulls the R_{OoS}^2 towards zero and expands the range of R_{OoS}^2 values, thus increasing the risk of selecting a model with poor forecasting performance.

Panel (b) of Figure [5](#page-24-0) shows the range of R_{OoS}^2 values for a given value of the (l_1, l_2) penalty mix parameter λ while varying α . The performance of both the median and best models is less sensitive to the choice of λ than to the choice of α . Outliers marked by dots occur for the lowest value $\alpha = 0.0001$ which results in too many predictors being selected and noisy forecasts. Higher values of λ tend to increase the minimum R_{OoS}^2 value.

Figure 5: Sensitivity of R^2_{OoS} to hyperparameters for Elastic Net

The figure displays the sensitivity of the out-of-sample R_{OoS}^2 in percentage for the panel of individual stocks on the test sample from January 1997 to December 2021 for the Elastic Net. Panel (a) varies the level of shrinkage (α) while Panel (b) varies the penalty mix parameter (λ) .

4.2 Tree-based Models

Figure [6](#page-25-0) panel (a) presents the range of R_{OoS}^2 values for the random forest models whose hyperparameters are *B*, the number of trees averaged over by the random forest; *D*, the maximum depth of each tree; and *F*, the number of features considered for each split. Outof-sample performance for the median, top-quartile and best model is robust with regards to the choice of the number of trees (*B*). Conversely, the worst and bottom-quartile models perform notably poorer when $B = 30$ than when $B = 500$. The maximum depth of the trees (*D*) is more important. For $D = 1$, the range of $R_{O_0S}^2$ values is narrow and centered around 0.30. Increasing *D* shifts the median value of R_{OoS}^2 down and increases the range of values so that, when $D = 6$, the median model generates a negative $R^2_{O_0S}$. A similar pattern is observed from increasing the number of features in the split, F . When $F = 1$, the range of R_{OoS}^2 values is narrow and centered around 0.30. Increasing F beyond this value reduces the average R_{OoS}^2 and expands its range.^{[23](#page-24-1)} Limiting the number of features to just one per tree increases diversity among the trees in the ensemble, in contrast to using many features which can lead to trees splitting on similar information. This increased diversity strengthens model generalization, resulting in a consistently narrow range of performance metrics as the Random Forest averages the outputs of these diverse trees.

²³The minimal internal and leaf node size barely affect the out-of-sample performance.

Figure 6: Sensitivity of R^2_{OoS} to hyperparameters for tree-based models

This figure shows the sensitivity of the out-of-sample R_{OoS}^2 in percentage for the panel of individual stocks from January 1997 to December 2021 for Random Forest and Extreme Gradient Boosted Trees. For Random Forests, Panel (a) displays the sensitivity to the number of trees *B*, tree depth *D*, and the number of features *F*. For Extreme Gradient Boosted Trees Panel (b) shows the sensitivity to the number of trees *B*, tree depth *D*, and the learning rate *η*. The Boosted trees are trained with early stopping with a patience of 5, where the early stopping criteria are based on the lowest MSE within a 2-year validation set.

Figure [6](#page-25-0) panel (b) shows the R_{OoS}^2 for the Extreme Gradient Boosted Regression Trees.^{[24](#page-25-1)} The number of trees (B) has little effect on predictive performance. In contrast, the maximum depth of the trees and the learning rate are both important. Shallow trees (low *D*) perform best and settings $D = 4, 6$ result not only in a decline in the median model's performance but also widens the range of R^2_{OoS} values with the bottom-quartile model having a negative R_{OoS}^2 value. The learning rate also has a large impact on R_{OoS}^2 values with $\eta = 0.3, 0.4$ leading to poor performance for the bottom-quartile models which now generate a R_{OoS}^2 value close to -1 and -2 , respectively.

The interplay between the learning rate and tree depth in XGBoost is key to understanding its out-of-sample forecasting performance. A combination of low depth and a high

 24 Note that the specified number of trees does not reflect the actual number of constructed trees or boosting rounds since we use early stopping.

learning rate generally strikes a good balance between model complexity and learning efficiency. Low depth together with a low learning rate tends to produce overly conservative models and is indicative of underfitting. High depth with a low learning rate results in conservative performance, while a high depth alongside a high learning rate typically leads to poor model performance due to overfitting and instability in the learning process.

4.3 Neural Networks

We finally turn to the NN models. Panel (a) in Figure [7](#page-27-0) shows out-of-sample forecasting performance across NN models that fix the number of hidden layers *H* between 1 and 5 and vary all other hyperparameters, resulting in a total of 96 settings per NN specification. The box plots feature a broken *y*-axis to accommodate the wide variation in performance. The lower segment of the axis is deliberately capped at −30. For each hidden layer count (*H*), the figure features three box plots: the first utilizes a 6-month set for early stopping, the second a 2-year set, and the third a 10-year set for this purpose. For all architectures, both the median and the worst-performing models exhibit better out-of-sample performance on the 2-year set compared to the 6-month and 10-year period. The improved out-of-sample performance achieved with a 2-year early stopping period suggests that there is a tradeoff between incorporating more recent data into the training process and maintaining a sufficiently large early stopping set. Moreover, the use of a larger (smaller) early stopping sample has the potential to result in underfitting (overfitting) during training, consequently leading to a decline in out-of-sample performance.

Figure [7](#page-27-0) panel (b) focuses on the performance of a specific network architecture, NN2, over a 2-year validation period. To conserve space, we only report the NN2 architecture for the 2-year validation set as the results are very similar. The ReLU activation function performs best in terms of median performance and downside risk. Further, the out-of-sample performance is not much affected by the training loss function. For both validation periods, choosing the slowest learning rate $\eta = 0.0001$ or the second slowest rate $\eta = 0.001$ yields the best results overall. For both the 6-month and 10-year validation period, performance can be preserved by choosing a very slow learning rate. The performance differential between

Figure 7: Sensitivity of R^2_{OoS} to architecture and hyperparameters for the Feed-**Forward Neural Networks**

This figure shows the out-of-sample R_{Os}^2 sensitivity, expressed in percentage, for the range of individual stocks from January 1997 to December 2021. Panel (a) shows the sensitivity across architectures and different set sizes used to define the early stopping criteria. The *y*-axis is capped at −30%. Panel (b) shows the sensitivity across the hyperparameters of Neural Networks with $H = 2$ hidden layers, utilizing a 2-year period to implement early stopping. The *y*-axis is capped at −12%. All models apply early stopping with a patience of 5 based on achieving the lowest MSE during this period.

(a) NN1 to NN5 with varying early stopping period

the validation periods can be linked to the l_1 shrinkage penalty α . For both the 6-month and 10-year validation period, the smaller value of $\alpha = 0.0001$ results in underperformance, likely due to overfitting. All in all, the best approach here is to have a smaller validation set of for example 2-years, a relatively deep neural net architecture and apply a slow learning rate, with some regularization.[25](#page-27-1)

²⁵In deeper neural networks with 4 or more layers, predictions become constant due to large biases $\omega_0^{(\ell)}$ dominating the effects of inputs multiplied by weights in Equation [\(14\)](#page-15-1), pushing activation functions into saturation. This saturation results in outputs that are insensitive to input variations, thereby hindering the network's ability to learn effectively from data.

4.4 Summary of Results

We summarize the key insights from our analysis as follows. First, our results show that it is possible to fix a subset of the hyperparameters such that good out-of-sample forecasting performance is achieved regardless of how the remaining hyperparameters are chosen. For the RF method this occurs when the maximum depth *D* equals 1 or 2 or when only a single feature is included $(F = 1)$. For XGBoost, this is achieved when the maximum depth $D = 1, 2$ or when the learning rate is very low. For NNs, similarly a very slow learning rate is likely to lead to accurate forecasts regardless of how the other hyperparameters are set.

Second, the opposite also holds: the hyperparameters can be set so that poor forecasting performance is, if not guaranteed, highly likely even when the regular parameters are chosen optimally. For penalized linear models such as the Lasso or Elastic Net, this happens when the shrinkage parameter (α) is very low. For the RF models this occurs when the maximum depth or the number of features are high (e.g, $D = 8$ or $F = 70$) and for XGBoost when $D = 6$ or the learning rate, η , is high. Similarly, a high learning rate tends to "noise up" forecasts generated by NNs, leading to poor out-of-sample forecasting performance regardless of how other hyperparameters are chosen.

Third, due to their extra flexibility, varying the grid of hyperparameters of the nonlinear ML models tends to expand the range of R^2_{OoS} values far more than that generated by varying the shrinkage and penalty hyperparameters of the linear models. This widening in the range of out-of-sample performance means that extra caution has to be exercised when evaluating the predictive accuracy of ML methods to avoid spurious outcomes even after accounting for the tendency of out-of-sample forecasting methods towards being conservative.

Fourth, The widening of the range of out-of-sample forecasting performance of ML models relative to conventional linear models is highly asymmetric and left-skewed. In particular, we see a clear upper limit on the maximum degree of outperformance achievable by these models while, conversely, ML models with hyperparameters chosen so they are sensitive to noise are prone to generate extremely poor out-of-sample forecasts. This pronounced "downside" risk calls for caution by investors and portfolio managers using these models to generate forecasts of asset returns.

5 Validation

So far we demonstrated the sensitivity of the predictive accuracy of return forecasts to the choice of hyper parameters by fixing the latter across a range of values as shown in Table [2.](#page-18-0) In this section, we present model performance using time series validation and the economic value of return forecasts.

Because there is little theoretical guidance on selecting hyperparameters, it is common practice in finance (e.g., [Gu et al.,](#page-41-0) [2020;](#page-41-0) [Bianchi et al.,](#page-40-2) [2021;](#page-40-2) [Bali et al.,](#page-40-6) [2023\)](#page-40-6) to undertake time-series validation on a pseudo out-of-sample period. Validated models use data to determine the hyperparameters based on performance in the validation sample, rather than setting them a priori. The validation sample is formed by partitioning the original training sample into a training and validation sample, and is used to tune hyperparameters. The objective of the validation procedure is to determine the optimal set of hyperparameters by identifying the configuration that yields the best fit in the validation set.

In this section, we set out to examine whether validation methods can be used to select hyperparameters in a way that avoids poor out-of-sample forecasting performance.

5.1 Validation Analysis and Results

Validation methods do not offer a fully automated solution to the hyperparameter selection problem. Researchers must choose whether to use time-series validation or cross-validation, the length of the validation window, how to split a given sample into training, validation and test samples (sample split), and establish the initial hyperparameter grid for conducting the validation procedure. Lastly, researchers need to decide whether early stopping is suitable or not.[26](#page-29-1) All of these choices affect out-of-sample forecasting performance.

Following common practice in finance, we use time-series validation in our analysis as illustrated in the bottom panel of Figure [3.](#page-20-0) To tune hyperparameters, we consider validation sets with lengths of 6 months, 2 years, and 10 years, covering the common choices in literature

²⁶If early stopping is implemented, the model is trained solely on the training set with the optimal hyperparameters without re-estimating the model parameters on the combined training and validation sets. Conversely, if early stopping is not used, the model is re-estimated using both the training and validation sets after determining the optimal hyperparameters.

Table 3: Performance statistics for the validated models

We report the monthly R_{Os}^2 in percentage, and the corresponding Diebold-Mariano (DM) statistic for the validated models with different validation periods, where the MSE is used as the evaluation metric. For XGBoost and neural networks, e.s. refers to early stopping which is based on the same period as the validation procedure.The DM statistic is asymptotically normally distributed.

	Lasso		Elastic Net					Random Forest		$XGBoost$ (e.s.)	$NN2$ (e.s.)			$NN5$ (e.s.)
	DM	R_{Os}^2	DΜ	R_{Os}^2	DM	R_{Os}^2	DM	R_{Os}^2	DM	R_{Os}^2	DΜ	R_{Os}^2		
6 months	0.401	0.069	0.323	0.059	-0.475	-0.242	-1.398	-0.795	-3.294	-2.753	-3.755	-3.204		
2 years	0.624	0.153	$1.056\,$	0.254	0.160	0.013	0.648	0.221	-1.310	-0.451	-1.836	-0.669		
10 years	0.828	0.170	0.395	0.081	0.526	0.143	0.636	0.197	0.785	0.195	1.170	0.282		

[\(Gu et al.,](#page-41-0) [2020;](#page-41-0) [Bali et al.,](#page-40-6) [2023\)](#page-40-6). The shorter validation set ensures that the model captures the latest information while the 10-year set captures a broader range of economic conditions which could improve the model's ability to generalize across different scenarios. We use the hyperparameter grids shown in Table [2](#page-18-0) for the the validation exercise.

Table [3](#page-30-0) reports $R_{O_0S}^2$ values for different validation windows. The length of the validation window is crucial to the models' performance. Specifically, tree-based models and neural networks exhibit subpar performance with a validation set of 6 months. For longer validation windows such as 10 years, performance is generally similar to or worse than for a 2-year period although NNs show more robust performance on the 10-year validation set.

Table [3](#page-30-0) also reports the associated DM-statistics. None of the validated models significantly outperform the zero benchmark throughout the out-of-sample test sample. Conversely, the NN2 and NN5 models based on the shortest validation window significantly underperform this benchmark.

5.2 Breakdown in Forecasting Performance

Table [3](#page-30-0) reports the sample-average forecasting performance for different models but does not provide any indication of how this evolves over time or whether forecasting performance breaks down in certain periods. To examine this issue, Figure [8](#page-31-0) displays the cumulative sum of squared error differentials (CSSED) for our validated models against the zero prediction benchmark, with NBER recession periods marked by vertical grey shaded areas. Each panel focuses on a different model: Panel (a) for Random Forest and Extreme Gradient Boosting, and Panel (b) for Neural Networks with 2 and 5 hidden layers.

Figure 8: Cumulative sum of squared error differentials

This figure displays Cumulative Sum of Squared Error Differentials (CSSED) with positive and increasing values indicating that the validated model is more accurate than the zero prediction benchmark. The data covers the test sample from January 1997 to December 2021. Grey shaded areas correspond to NBER recession periods. Panel (a) shows the CSSED of Random Forest and Extreme Gradient Boosting, while Panel (b) shows the performance for two Neural Networks, where the *y*-axis is capped at −0*.*11. Performance deteriorates until −0*.*35.

The forecasting performance of the tree-based models in Panel (a) deteriorates markedly during the three recessions in our sample, most notably during the GFC. This holds across all validation windows with the forecasts based on the six-month window experiencing the worst deterioration in performance during these periods. Panel (b) displays the performance of the shallow (NN2) and deep (NN5) neural network architectures, respectively. The worst performance is again observed for a 6-month validation window while a 10-year validation window produces better performance. The deeper architecture, NN5, shows slightly more variability in performance compared to NN2.[27](#page-31-1)

²⁷The CSSED for Lasso and Elastic Net are reported in Appendix Table [C.3.](#page-51-0) Shorter validation windows

Overall, the performance observed across different ML models and validation windows exhibit similar patterns and no single model specification consistently surpasses the others throughout the entire test period.

5.3 Cross-sectional Variation in Predictive Accuracy

The top panel of Figure [9](#page-33-0) reports percentiles of the cross-sectional distribution of $R_{i,OoS}^2$. For most models, the R_{OoS}^2 is negative for between 25% and 50% of the stocks. The non-linear ML models generate a significantly greater cross-sectional spread in forecasting performance across stocks.

The bottom panel of Figure [9](#page-33-0) illustrates how $R_{i,OoS}^2$ varies across firm size, captured by sorting stocks into $d = 10$ market-cap deciles. The smallest firms achieve the highest $R_{i,00}^2$ values across all models. These are generally also the firms that would have been most costly to trade, calling into question whether the return forecasts could have been exploited to generate economic gains. All models underperform for the largest firms, with $R_{i,OoS}^2$ values turning negative from the seventh decile and onward. The performance of the Neural Networks is, once again, particularly poor for the largest stocks.

While size is a proxy for how liquid a stock is, trading volume may provide an even better measure of how easy it would have been to convert forecasting signals from the ML models into trading positions. We therefore next examine results for portfolios of stocks sorted on trading volume. Table [4](#page-34-0) shows strong evidence that stocks with the lowest trading volume also exhibit the strongest out-of-sample return predictability. Conversely, most methods tend to generate negative or very small positive R_{OoS}^2 values for stocks in the top three volumesorted deciles. This raises concerns about whether the return predictability identified by the ML methods could have been exploited for economic gains.

To evaluate this issue more formally, we report *t*-statistics as well as *p*-values for the Monotonic Relation (MR) test of [Patton and Timmermann](#page-42-6) [\(2010\)](#page-42-6) designed to test if there is a monotonically increasing relation between trading volume and return predictability.

help mitigate downturns during crises by turning to a zero prediction. The 2-year validation set typically yields the best results, while the 6-month window is the least accurate.

Figure 9: Out-of-sample performance across firms

Panel (a) displays firm-level $R_{i,OoS}^2$ values sorted into percentiles *p* while Panel (b) displays firm-level R_{OoS}^2 values for stocks grouped into ten deciles based on their firm size (cut off at −1*.*6%. For *d* = 10, the performance deteriorates to −2% and −2*.*2% for NN2 and NN5, respectively). The validated models use a 2-year validation set. All measures are reported for firms with at least 60 observations in the test set, encompassing a total of 2774 firms. The test set ranges from January 1997 to December 2021.

(a) Percentiles (p) of stock-level $R_{i,OoS}^2$

Table [4](#page-34-0) shows that the opposite holds and that stocks with the highest trading volume tend to be significantly less predictable than stocks with lower trading volume. Combined with our results on the size-predictability relation, these findings suggest that converting the return forecasts from the ML models into profitable trading strategies, after accounting for the higher trading costs of small caps with low trading volume, would have been difficult or offered an unattractive risk-return trade-off.

Table 4: Out-of-sample R^2_{OoS} performance for portfolios sorted on trading volume

We report the R_{OoS}^2 (monthly, percentage) forecasting performance for equal-weighted decile portfolios sorted on trading volume. We test the statistical significance of the H–L spread using HAC standard errors with **, and * denoting significance at the 1%, 5% levels, respectively. Additionally, we report the [Patton and](#page-42-6) [Timmermann](#page-42-6) [\(2010\)](#page-42-6) monotonicity tests in the rows marked "MR Test", for which the null hypothesis is $H_0: \mu_i \leq \mu_{i-1}$, where μ_i is the R_{OoS}^2 value for the *i*th portfolio, versus the alternative $H_1: \mu_i > \mu_{i-1}$. Hence, a rejection (low *p*-value) is consistent with monotonically increasing R_{OoS}^2 values.

	Lasso				Enet			RF			XGBR				
	6m	2y	10y	6m	2y	10y	6m	2y	10v	6m	2y	10y			
Low	0.47	0.63	0.53	0.62	0.79	0.40	0.34	0.75	0.48	-0.11	0.48	0.70			
$\overline{2}$	0.09	0.32	0.37	0.21	0.46	0.25	-0.20	0.18	0.24	-3.52	0.33	0.42			
3	0.18	0.35	0.30	0.29	0.48	0.20	0.05	0.33	0.39	-1.65	0.39	0.33			
4	0.17	0.31	0.24	0.20	0.43	0.15	-0.24	0.12	0.28	-0.23	0.43	0.24			
5	-0.14	0.07	0.12	-0.10	0.15	0.04	-0.28	-0.21	0.08	-0.49	0.18	0.15			
$\,6\,$	0.17	0.26	0.20	0.13	0.37	0.10	-0.22	-0.13	0.13	-0.35	0.23	0.13			
$\overline{7}$	0.06	0.05	0.04	-0.01	0.11	-0.03	-0.19	-0.17	0.04	-0.25	0.11	0.07			
8	-0.04	-0.06	0.01	-0.20	-0.01	-0.08	-0.55	-0.26	-0.01	-0.29	0.18	0.07			
9	-0.15	-0.27	-0.09	-0.34	-0.17	-0.17	-0.73	-0.29	-0.25	-0.67	0.00	-0.03			
High	0.00	-0.19	-0.01	-0.17	-0.12	-0.09	-0.38	-0.17	-0.08	-0.69	-0.08	-0.10			
$H-L$	$-0.47*$	$-0.82**-0.54$			$-0.79** -0.91** -0.49$		-0.73	-0.92	-0.56	-0.58	-0.56	$-0.80*$			
MR Test $(p$ -value)	0.95	0.783	0.296	0.78	0.754	0.287	0.815	0.722	0.569	0.307	0.481	0.41			
	NN1			NN2			NN ₃			NN4			NN ₅		
	6m	2v	10v	6m	2v	10v	6m	2v	10v	6m	2y	10v	6m	2y	10v
Low	0.29	0.35	-1.66	0.29	0.44	-1.86	0.01	0.38	-1.84	-0.10	0.39	-2.34	-0.29	0.37	
2	-0.32	0.29	-2.54	-0.33	0.42	-2.64	-0.51	0.37	-2.56	-0.55	0.32	-2.96	-0.70	0.30	
3	-0.22	0.29	-2.48	-0.18	0.40	-2.62	-0.42	0.36	-2.58	-0.46	0.37	-3.01	-0.62	0.36	
$\overline{4}$	-0.14	0.25	-2.34	-0.17	0.31	-2.48	-0.33	0.29	-2.43	-0.40	0.33	-2.79	-0.48	0.36	
5	-0.54	0.16	-3.02	-0.57	0.21	-3.06	-0.64	0.17	-2.98	-0.58	0.28	-3.37	-0.69	0.30	
6	-0.28	0.13	-2.94	-0.32	0.17	-3.15	-0.52	0.17	-3.13	-0.55	0.30	-3.54	-0.64	0.34	
$\overline{7}$	-0.25	0.04	-2.30	-0.35	0.06	-2.42	-0.41	0.08	-2.40	-0.43	0.17	-2.64	-0.45	0.22	
8	-0.60	0.07	-3.36	-0.81	0.07	-3.51	-0.81	0.09	-3.45	-0.72	0.25	-3.79	-0.75	0.31	
9	-0.86	-0.08	-3.73	-1.08	-0.08	-3.98	-1.13	-0.08	-3.84	-1.01	0.10	-4.24	-1.08	0.15	
High	-0.52	0.00	-2.73	-0.82	-0.04	-2.82	-0.78	-0.02	-2.77	-0.66	0.11	-3.06	-0.66	0.17	
$H-L$		$-0.81**-0.35*$	-1.06		$-1.11***$ $-0.48**$ -0.96		$-0.79**-0.39$					$-0.94***$ $-0.55***$ $-0.28**$ $-0.71**$ $-0.37**$ -0.20			
MR Test $(p$ -value	0.71	0.78	0.25	0.88	0.69	0.33	0.84	0.49	0.30	0.80	0.70	0.38	0.82	0.67	0.60

5.4 Economic Value of Return Forecasts

We next examine the economic value of our return forecasts. We sort individual stocks into deciles based on their predicted returns for the following month and form equal-weighted portfolios. We then construct long-short portfolios taking a long positions in stocks in the top decile of expected returns and short positions in stocks in the bottom decile.[28](#page-34-1)

Table [5](#page-36-0) reports annualized average returns (Panel A) and Sharpe ratios (Panel B) of the prediction sorted portfolios. The high minus low (H–L) average return spread is significant

²⁸[Gu et al.](#page-41-0) [\(2020\)](#page-41-0) and [Avramov et al.](#page-40-4) [\(2023\)](#page-40-4) follow this procedure to evaluate the economic significance of return forecasts. In contrast, [Coulombe et al.](#page-40-5) [\(2022\)](#page-40-5) develop a method based on Shapley values to estimate the contributions to portfolio performance of individual variables or groups of predictors.

across all models and validation sets except for the NN2 and NN5 models with 10-year validation sets, demonstrating that economic performance improves for stocks with the highest predicted return. However, we do not find any significant spreads for the Sharpe ratios.

We further evaluate whether the average returns of the decile portfolios sorted on return forecasts are monotonically increasing using the MR test of [Patton and Timmermann](#page-42-6) [\(2010\)](#page-42-6). Formally, we test the null of $H_0: \mu_i \leq \mu_{i-1}$ against the alternative $H_1: \mu_i > \mu_{i-1}$ so that rejections (small *p*-values) show that economic performance is higher for stocks with the highest predicted return while a failure to reject the null suggests the opposite. We reject the null for at most two validation windows across the Lasso, Enet, and RF methods (Panel A). In contrast, we fail to find significant evidence of a monotonically increasing relation for the portfolios based on the forecasts from the XGBR, NN2 and NN5 models.[29](#page-35-0) Panel B of the table shows that the evidence is even weaker for the Sharpe ratios for which we only find a single case (Enet with a 2-year validation window) with a significantly increasing Sharpe ratio.

In conclusion, these results do not provide conclusive evidence that the return forecasts generated by applying validation to choose the hyperparameters of a range of ML methods could have been used to significantly improve economic performance.

 29 We also build 18 value-weighted portfolios using size, book to market, operating profitability, and investment as sorting variables. These sorts did not establish any particular patterns in return predictability across firm characteristics beyond the size effect.

Table 5: Economic performance of prediction-sorted stock portfolios

We report annualized average returns in Panel A and Sharpe ratios in Panel B for portfolios sorted on return predictions from six machine learning models: Lasso, Elastic Net (Enet), Random Forest (RF), Extreme Gradient Boosted Trees (XGBoost), and feed-forward neural networks with ² and ⁵ hidden layers (NN2, NN5). The machine learning models are validated using windows of ⁶ months (6m), ² years (2y), and ¹⁰ years (10y). We test the statistical significance of the H–L spread using HAC standard errors with **, and * denoting significance at the 1%, 5% levels, respectively.Additionally, we report the Patton and [Timmermann](#page-42-7) [\(2010\)](#page-42-7) monotonicity tests in the rows marked "MR Test (p-value)", for which the null hypothesis is $H_0: \mu_i \leq \mu_{i-1}$, where μ_i is the mean of the return measure for the i^{th} portfolio, versus the alternative $H_1: \mu_i > \mu_{i-1}$. Hence, a rejection (low *^p*-value) is consistent with monotonically increasing mean returns or Sharpe ratios. All portfolios are equal-weighted.

5.5 Efficient Grid Search

Many studies support the use of efficient algorithms such as hyperband for hyperparameter optimization. However, the performance of these algorithms is significantly influenced by the initial grid of hyperparameters. We next examine whether an efficient search algorithm applied to a wide grid is sufficient.

Specifically, to evaluate the implications of the choice of grid for the initial hyperparameters on out-of-sample predictive accuracy, we use Optuna [\(Akiba et al.,](#page-40-14) [2019\)](#page-40-14) to efficiently search across the hyperparameter grids. Optuna is an open-source hyperparameter optimization framework designed for machine learning applications. Given the computational intensity of exploring all possible hyperparameters, Optuna efficiently searches the hyperparameter grid leading to a near-optimal solution. As for all other methods, a search space needs to be specified for the hyperparameters to initiate the optimization process.

Optuna uses the Tree-structured Parzen Estimator (TPE) to facilitate this exploration by estimating the likelihood that a given set of hyperparameters will improve performance. TPE separates the set of hyperparameters into two groups: the best-performing set and the remaining set. Leveraging this partition, TPE prioritizes areas of the search space expected to produce superior outcomes. A key efficiency feature of Optuna is its pruning mechanism which conservatively allocates computational resources by discontinuing trials that perform significantly worse than the current best trial at earlier checkpoints. Moreover, Optuna can dynamically adjust the hyperparameter search space in response to insights gained from completed trials. This adaptability focuses the search on the most promising region of hyperparameters, enhancing the likelihood of finding the (near-)optimal hyperparameter configurations with minimal computational costs.[30](#page-37-0)

Table [6](#page-38-1) shows the out-of-sample performance of various grids for Extreme Gradient Boosting and Neural Networks with 2 and 5 hidden layers. As expected, the baseline results are similar to our results in Table [3](#page-30-0) as Optuna conducts an efficient grid search. The out-ofsample performance depends on the initial grid that is chosen for the validation, regardless of the validation period. Thus, choosing a wide hyperparameter grid does not guarantee

³⁰The combination of XGBoost and Optuna is often used in Kaggle forecasting competitions (see, e.g., [Filho,](#page-41-13) [2023\)](#page-41-13), and recently also by [Coulombe et al.](#page-40-1) [\(2023\)](#page-40-1).

Table 6: Performance statistics for the validated models using Optuna

We report the monthly R_{OoS}^2 in percentage, and the corresponding Diebold-Mariano (DM) statistic for the validated models with different validation periods, where the MSE is used as the evaluation metric, and for different initial grids. Here, e.s. refers to early stopping, which is based on the same period as the validation procedure. Results are based on 100 trials.

			Extreme Gradient Boosting (e.s.)			Neural Networks $H = 2$ (e.s.)								
	6 months		2 years			10 years		6 months		2 years		10 years		
Grid	DМ	R_{Os}^2	DM	R_{Os}^2	DΜ	R_{Os}^2	DМ	R_{Os}^2	DМ	R_{Os}^2	DM	R_{OoS}^2		
Wide	-1.911	-0.834	1.134	0.304	0.677	0.159	-3.871	-3.001	-2.028	-0.818	1.080	0.245		
Baseline	-0.403	-0.161	0.641	0.227	0.774	0.217	-3.430	-3.566	-1.722	-0.607	0.947	0.226		
Restricted	1.454	0.410	1.653	0.454	0.708	0.188	0.165	0.015	0.575	0.174	1.239	0.287		
			Neural Networks $H = 5$ (e.s.)											
		6 months	2 years			10 years								
Grid	DM	R_{Os}^2	DΜ	R_{OoS}^2	DМ	R_{Os}^2								
Wide	3.619	-3.198	-1.747	-0.609	1.133	0.266								
Baseline	-3.358	-1.991	-1.901	-0.672	1.047	0.240								
Restricted	-0.119	-0.045	0.252	0.077	1.226	0.291								

Note: "Baseline" refers to the initial search grids stated in Table [2.](#page-18-0) For XGBoost, "Wide" refers to the initial grid of $B = 1000$, $D \in [1, 12]$, $\eta \in [0.0001, 0.7], \ \alpha \in [0, 0.5], \ \lambda \in [0, 1],$ both sub sample and column sample between [0, 1], and $\mathcal{L}(\cdot) \in \{MSE, Huber\}$, and "Restricted" to $B = 1000, D \in [1, 2], \eta \in [0.0001, 0.1],$ all with early stopping and a patience of 5. For NN2 and NN5, wide refers to $\eta \in [0.00001, 0.1],$ $\alpha \in [0.0001, 0.1], \ell_2 \in [0.0001, 0.1], \ f(\cdot) \in \{\texttt{Leaky}, \texttt{Relu}, \texttt{Sigmoid}, \texttt{linear}, \texttt{Tanh}, \texttt{Softmax}\}, \ \mathcal{L}(\cdot) \in \{\texttt{MSE}, \texttt{Huber}\}, \ \texttt{dropout} \in \{0, 0.1, 0.2, 0.5\}, \ \texttt{Input} \in \{0.0001, 0.1, 0.2, 0.5\}$ batch size \in {2000, 10000, none}, and "Restricted" to $\eta \in [0.0001, 0.001]$, $\alpha \in [0.0001, 0.01]$, $f(\cdot) \in$ {Leaky, ReLu}, $\mathcal{L}(\cdot) \in \{MSE, Huber\}$.

good forecasting performance and, in fact, the chosen initial grid fed to Optuna for every validation period critically affects forecasting performance.

6 Conclusion

Machine learning models such as random forests, gradient boosted trees, and neural networks, have shown considerable promise in empirical asset pricing studies. This capacity, however, comes with the challenge of managing a broad array of hyperparameters—from the number of hidden layers in neural networks to the depth of trees in random forests—each impacting model performance. These hyperparameters determine the ML models' basic architecture and how they regulate the bias-variance trade-off that is key to forecasting performance especially for variables as noisy as stock returns.

The risk of overfitting and spurious forecasting performance is not particular to ML methods and has been a constant theme in evaluating the forecasting performance even of linear models. However, ML methods display a degree of flexibility that significantly heightens this danger. Our empirical analysis analysis shows that the distribution of outof-sample forecasting performance is much wider and highly left-skewed for ML methods compared to linear models. Risk related to model misspecification and parameter estimation error is, thus, notably elevated for flexible ML models that attempt to account for nonlinear dynamics and complex interaction terms. This flexibility can come at the cost of enhanced sensitivity to noisy data and outliers.

Our extensive analysis of the importance of hyperparameters for ML models' forecasting performance shows that there is a ("guaranteed success") range of values for a subset of one or two hyperparameters which results in impressive out-of-sample forecasting performance regardless of how the other hyperparameters are chosen. Conversely, there is also a ("lost cause") range of values for a subset of hyperparameters for which poor out-of-sample forecasting performance occurs regardless of how the other hyperparameters are chosen.

Importantly, time-series validation schemes which use data-driven methods to choose the optimal combination of hyperparameters do not provide a definitive solution to the dependence of forecasting performance on the chosen hyperparameters. Validation methods themselves depend on features such as the choice of validation window and the grid of hyper parameter values included in the search and these choices tend to have important effects on forecasting performance.

Our results highlight that the current lack of guidelines for setting the range of values examined for the hyperparameters heightens the risk of false inference in asset pricing studies based on out-of-sample forecasting performance. At a minimum, an implication of our findings is that empirical studies should carefully document the range of hyperparameters being considered along with details of any validation schemes being used.

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Appendix for

"Overhyped? Can ML Models Reliably Predict Stock Returns?"

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This supplementary material for "Overhyped? Can ML Models Reliably Predict Stock Returns?" complements the paper with details on the data and additional empirical results.

A Data

Table [A.1](#page-43-0) reports details on the firm characteristics used in our paper. Table [A.2](#page-45-0) presents the categorization of our dataset based on the Standard Industry Classification system used to generate industry dummies. For each grey block in the table, a separate dummy is constructed, generating a total of 48 distinct dummy variables.

No.	Acronym	Firm characteristic description	Update frequency
1	absacc	Absolute accruals	Annual
$\overline{2}$	acc	Working capital accruals	Annual
3	aeavol	Abnormal earnings announcement volume	Quarterly
$\overline{4}$	age	No. of years since first Compustat coverage	Annual
5	agr	Asset growth	Annual
6	baspread	Bid-ask spread	Monthly
7	beta	Market beta	Monthly
8	betasq	Market beta squared	Monthly
9	bm	Book-to-market	Annual
10	bm_ia	Industry-adjusted book to market	Annual
11	cash	Cash holdings	Quarterly
12	cashdebt	Cash flow to debt	Annual
13	cashpr	Cash productivity	Annual
14	cfp	Cash flow to price ratio	Annual
15	cf p _{-ia}	Industry-adjusted cash flow to price ratio	Annual
16	chatoia	Industry-adjusted change in asset turnover	Annual
17	chcsho	Change in shares outstanding	Annual
18	chempia	Industry-adjusted change in employees	Annual
19	chiny	Change in inventory	Annual
20	chmom	Change in 6-month momentum	Monthly
21	chpmia	Industry-adjusted change in profit margin	Annual
22	chtx	Change in tax expense	Quarterly
23	cinvest	Corporate investment	Quarterly
24	convind	Convertible debt indicator	Annual
25	currat	Current ratio	Annual
26	depr	Depreciation / $PP\&E$	Annual
27	divi	Dividend initiation	Annual
28	divo	Dividend omission	Annual
29	dolvol	Dollar trading volume	Monthly
30	dy	Dividend to price	Annual

Table A.1: Details of the 92 firm characteristics

Note: 2 characteristics of [Gu et al.](#page-41-0) [\(2020\)](#page-41-0) are not considered; realestate and secured, no. 72, 82 in their paper, respectively. For the authors and journals corresponding to the anomalies, see [Green et al.](#page-41-14) [\(2017\)](#page-41-14).

Table A.2: Grouping of Standard Industry Classification codes

SIC2 digits	Industry
$\mathbf 1$	Agriculture, Forestry, and Fishing
$\overline{2}$	Mining
7	Construction
10	Manufacturing
12 13	Transportation, Communications, Electric, Gas, and Sanitary Services Wholesale Trade
14	Retail Trade
15	Eating and Drinking Places
16	Miscellaneous Retail
17	Finance, Insurance, and Real Estate
20	Services
21 22	Miscellaneous Services Public Administration
23	Non-Classifiable Establishments
24	Educational Services
25	Health Services
26	Legal Services
27	Engineering, Accounting, Research, Management, and Related Services
28	Agricultural Services
29 30	Miscellaneous Services Apparel and Other Finished Products Made From Fabrics and Similar Materials
31	Leather and Leather Products
32	Stone, Clay, Glass, and Concrete Products
33	Primary Metal Industries
34	Fabricated Metal Products, Except Machinery and Transportation Equipment
35	Industrial and Commercial Machinery and Computer Equipment
36 37	Electronic and Other Electrical Equipment and Components, Except Computer Equipment Transportation Equipment
38	Instruments and Related Products
39	Miscellaneous Manufacturing Industries
40	Railroad Transportation
42	Motor Freight Transportation and Warehousing
44	Water Transportation
45	Transportation by Air
46 47	Pipelines, Except Natural Gas Transportation Services
48	Communications
49	Electric, Gas, and Sanitary Services
50	Wholesale Trade-Durable Goods
51	Wholesale Trade-Non-Durable Goods
52	Building Materials, Hardware, Garden Supply, and Mobile Home Dealers
53 54	General Merchandise Stores Food Stores
55	Automotive Dealers and Gasoline Service Stations
56	Apparel and Accessory Stores
57	Home Furniture, Furnishings, and Equipment Stores
58	Eating and Drinking Places
59	Miscellaneous Retail Stores
60 61	Depository Institutions Non-depository Credit Institutions
62	Security and Commodity Brokers, Dealers, Exchanges, and Services
63	Insurance Carriers
64	Insurance Agents, Brokers, and Service
65	Real Estate
67	Holding and Other Investment Offices
70 72	Hotels, Rooming Houses, Camps, and Other Lodging Places Personal Services
73	Business Services
75	Automotive Repair, Services, and Parking
76	Miscellaneous Repair Services
78	Motion Pictures
79	Amusement and Recreation Services
80	Health Services
82 83	Educational Services Social Services
87	Engineering, Accounting, Research, Management, and Related Services
99	Non-Classifiable Establishments

Note: Rows that are marked grey are grouped.

B Details of the Algorithms

Algorithm [1](#page-46-0) shows the early stopping procedure. Early stopping is used by extreme gradient boosting and neural networks.

Algorithm [2](#page-46-1) below shows the Adam optimizer with ω containing both the weights and biases in the neural network.

Algorithm 2 *Adam Optimizer*

In the standard implementation of Optuna, hyperparameters for models like XGBoost and neural networks are typically assigned uniform priors. However, our grid search results indicate that overly aggressive settings for certain hyperparameters, such as a high learning rate and maximum depth for XGBoost, lead to performance degradation. To address this,

we propose using non-uniform priors over the hyperparameter space—specifically, a mixture of two normal distributions, $\mathcal{N}(\mu_1, \Sigma_1)$ and $\mathcal{N}(\mu_2, \Sigma_2)$. Since hyperparameters cannot take negative values, we apply an ad hoc non-negativity constraint during sampling. Figure [B.1](#page-47-0) shows the empirical distributions we sample the initial hyperparameters from. Algorithm [3](#page-48-0) shows this specific sampling procedure. We use this approach for XGBoost and neural networks. For XGBoost we consider a mixture of distributions on the learning rate *η* and the maximum depth *D*, with prior mean and variances

$$
\mu_1 = \begin{pmatrix} 0.1 \\ 4 \end{pmatrix}, \ \mu_2 = \begin{pmatrix} 0.4 \\ 1 \end{pmatrix} \text{ and } \Sigma_1 = \Sigma_2 = \begin{pmatrix} 0.005 & 0 \\ 0 & 1 \end{pmatrix}.
$$
 (B.1)

We then ensure that *D* is an integer by taking the ceiling of a generated variable.

For neural networks we consider mixture of distributions on the adam learning rate *η* and the l_1 -shrinkage α , with prior mean and variances

$$
\mu_1 = \begin{pmatrix} 0.05 \\ 0.2 \end{pmatrix}, \ \mu_2 = \begin{pmatrix} 0.3 \\ 0.001 \end{pmatrix} \text{ and } \Sigma_1 = \Sigma_2 = \begin{pmatrix} 0.003 & 0 \\ 0 & 0.003 \end{pmatrix}. \tag{B.2}
$$

Figure B.1: Empirical Distribution of the Priors used by Optuna

The figure displays the empirical distributions of the hyperparameter combinations Optuna is sampling from. The distributions are mixtures of two, highlighted by the two colors. Panel (a) shows the Extreme Gradient Boosting hyperparameters while Panel (b) shows the Neural Networks' hyperparameters.

Algorithm 3 *Sampling from a Mixture of Distributions with Rejection*

```
Require: Mean vectors \mu_1, \mu_2, covariance matrices \Sigma_1, \Sigma_2 for model m.
Set B = 5,000 as the number of samples to draw.
Initialize empty set S for accepted samples.
while |S| < B do
   Draw v \sim Uniform(0, 1).
   if v < 0.5 then
      Sample x \sim \mathcal{N}(\mu_1, \Sigma_1).
   else
      Sample x \sim \mathcal{N}(\mu_2, \Sigma_2).
   end if
   if x_1, x_2 > 0 then
      if Model m is XGBoost then
         x_2 \leftarrow \text{ceil}(x_2) > Make max. depth D an integer
      end if
      Add x to S ⊳ Accept if both components are non-negative
   else
      Reject x ⊳ Reject the sample if any component is negative
   end if
end while
return S ⊳ Return the set of accepted samples
```
C Additional Empirical Results

C.1 Dynamic Adjustments in the Selected Hyperparameters

To gain insight into how the validation method adapts to the data over time, Figure [C.2](#page-50-0) shows the sequence of hyperparameter values selected over time for the Lasso, Elastic Net, Random Forest, XGBoost, and Neural Networks with 2 and 5 hidden layers. In each figure, the shaded areas represent the full grid available for hyperparameter selection.

For the Lasso approach, panel (a), the hyperparameter α generally falls below 0.01. Approximately 5% of the regression coefficients (β) remain non-zero in most windows, equating to seven distinct features. When $\alpha = 0.012$, the model produces zero predictions. Furthermore, the validated models select a maximum of 18 features, highlighting the amount of shrinkage used.

For the Elastic Net approach, panel (b), the range of validated hyperparameter values is wider with a maximum of $\alpha = 0.015$ while λ fluctuates over the full range between 0.2 and 0.8. Moreover, values for the two hyperparameters are negatively correlated so that when *λ* is high, α tends to be low. When the model selects fewer predictors (high α), it applies less shrinkage of their coefficients while larger models require more shrinkage of the individual coefficients.

Panel (c) shows the sequence of hyperparameter values selected by the validation procedure applied to the Random Forest. The number of trees (B^*) varies, and there is often a trade-off between the depth and number of features, meaning that when *D*[∗] is high, *F* ∗ is often low and vice versa.

For XGBoost, panel (d), the validation procedure tends to favor larger learning rates, leading to overfitting as shown in Table [3.](#page-30-0) However, the validation procedure tends to pick shallow trees with a depth $(D^* = 2)$. Combined with the learning rate η^* , the XGBoost prefers relatively large learning rates with shallow trees to guard against over-fitting.

Panels (e) and (f) show the sequence of the selected hyperparameters for the neural networks. For each architecture, the selected hyperparameters are displayed as the median over the five neural networks with distinct random seeds. A small learning rate, *η*, between 0.0001 and 0.001, is usually chosen. This pattern does not apply uniformly across models validated on the test set, however. The chosen learning rate, η^* , can vary a great deal and sometimes a higher rate of 0.01 is preferred. For the 2-year validation period the network weights require less shrinkage as indicated by a lower α value. Typically, a higher level of shrinkage is associated with a reduced learning rate. This relationship suggests a trade-off between the rate of learning and the degree of regularization applied to the model, with adjustments to one parameter potentially necessitating compensatory changes to another.

Figure C.2: Sequence of hyperparameters selected by the validated models

The Figure displays the sequence of hyperparameters chosen based on a 2-year validation period. The models are refitted every 12 months which explains the steps. Shaded regions in the figure represent the conventional grids for hyperparameter selection.

C.2 Correlations between Predictions across Validated Models

Table [C.1](#page-51-1) shows average stock-level correlation between return predictions from the individual validated model using 6-month, 2-year and 10-year validation sets. In general, correlations tend to be quite low both when comparing return predictions from different models as well as return predictions generated by a particular model but using different validation sets.

Table C.1: Correlations between predictions across validated models

		Lasso			Elastic Net		Random Forest				XGBoost			NN2			NN5		
		6m	2y	10v	6m	2v	10v	6m	2v	10v	6m	2y	10v	6m	2v	10v	6m	2v	10v
Lasso	6m	1.00	0.64	0.50	0.90	0.63	0.49	0.42	0.42	0.42	0.19	0.25	0.19	0.57	0.48	0.31	0.50	0.36	0.30
	2v	0.64	1.00	0.42	0.74	0.95	0.46	0.34	0.33	0.39	0.12	0.17	0.12	0.45	0.64	0.27	0.38	0.39	0.17
	10y	0.50	0.42	1.00	0.55	0.54	0.96	0.35	0.36	0.42	0.22	0.29	0.31	0.30	0.36	0.55	0.24	0.17	0.17
Enet	6m	0.90	0.74	0.55	1.00	0.74	0.58	0.46	0.43	0.45	0.21	0.28	0.18	0.60	0.53	0.34	0.51	0.35	0.28
	2v	0.63	0.95	0.54	0.74	1.00	0.57	0.37	0.38	0.44	0.15	0.21	0.15	0.48	0.66	0.32	0.41	0.38	0.17
	10y	0.49	0.46	0.96	0.58	0.57	1.00	0.39	0.36	0.47	0.26	0.33	0.35	0.30	0.37	0.57	0.24	0.18	0.18
RF	6m	0.42	0.34	0.35	0.46	0.37	0.39	1.00	0.70	0.56	0.48	0.44	0.39	0.38	0.33	0.23	0.35	0.27	0.19
	2v	0.42	0.33	0.36	0.43	0.38	0.36	0.70	1.00	0.53	0.38	0.45	0.43	0.35	0.35	0.16	0.34	0.30	0.17
	10y	0.42	0.39	0.42	0.45	0.44	0.47	0.56	0.53	1.00	0.38	0.41	0.46	0.42	0.40	0.20	0.42	0.37	0.27
XGBR	6m	0.19	0.12	0.22	0.21	0.15	0.26	0.48	0.38	0.38	1.00	0.55	0.29	0.09	0.05	0.17	0.05	-0.03	0.08
	2v	0.25	0.17	0.29	0.28	0.21	0.33	0.44	0.45	0.41	0.55	1.00	0.32	0.09	0.08	0.17	0.06	-0.04	0.11
	10v	0.19	0.12	0.31	0.18	0.15	0.35	0.39	0.43	0.46	0.29	0.32	1.00	0.12	0.18	0.15	0.12	0.14	0.03
NN2	6m	0.57	0.45	0.30	0.60	0.48	0.30	0.38	0.35	0.42	0.09	0.09	0.12	1.00	0.57	0.09	0.96	0.59	0.16
	2v	0.48	0.64	0.36	0.53	0.66	0.37	0.33	0.35	0.40	0.05	0.08	0.18	0.57	1.00	0.22	0.52	0.78	0.37
	10v	0.31	0.27	0.55	0.34	0.32	0.57	0.23	0.16	0.20	0.17	0.17	0.15	0.09	0.22	1.00	0.03	0.06	0.27
NN ₅	6m	0.50	0.38	0.24	0.51	0.41	0.24	0.35	0.34	0.42	0.05	0.06	0.12	0.96	0.52	0.03	1.00	0.64	0.20
	2v	0.36	0.39	0.17	0.35	0.38	0.18	0.27	0.30	0.37	-0.03	-0.04	0.14	0.59	0.78	0.06	0.64	1.00	0.46
	10v	0.30	0.17	0.17	0.28	0.17	0.18	0.19	0.17	0.27	0.08	0.11	0.03	0.16	0.37	0.27	0.20	0.46	1.00

Note: The average over the time series correlations between predictions from different models for each firm with over 60 observations in the test sample.

C.3 Evolution in Forecasting Performance for the Linear Models

Figure [C.3](#page-51-0) shows the cumulative sum of squared error differentials for the linear models across different validation windows. For these linear models, a shorter validation periods helps mitigate downturns during crises.

Figure C.3: Cumulative sum of squared error differentials

This figure displays the Cumulative Sum of Squared Error Differentials (CSSED) for validated linear Lasso and Elastic Net models compared to a zero prediction benchmark. The data covers the sample period from 1997 to 2021. Grey shaded areas correspond to NBER recession periods.

